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Asymptotic analyse of Riemann problem for multiphase compositional flow in porous media with application to subterranean reservoirs

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Laboratoire d'Énergétique et de Mécanique Théorique et Appliquée
École Doctorale EMMA

THÈSE

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DOCTEUR DE L'I.N.P.L.

Spécialité :

Mécanique-Énergétique

Par :

Anahita ABADPOUR

**Analyse asymptotique du problème de Riemann pour les
écoulements compositionnels polyphasiques en milieux poreux et
applications aux réservoirs souterrains**

Soutenue publiquement le 4 Décembre 2008

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Avant Propos

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Résumé

l'écoulement et le transport de deux ou plusieurs phases dans les milieux poreux sont observés dans la récupération assistée du pétrole (EOR : Enhanced Oil Recovery) dont l'objectif est déplacer efficacement les hydrocarbures par l'injection de fluides qui solubilisent et / ou mobilisent la phase oléique, en la poussant vers les puits de production.

Dans la récupération du pétrole, de l'eau ou du gaz sont injectés dans le réservoir en créant les fronts miscibles ou partiellement miscibles entre les fluides.

Au cours de l'injection, les composants du fluide injecté se dissolvent partiellement ou complètement dans la phase initiale. Ce processus, qui détermine un échange de masse entre les phases, conduit à des changements souhaitables dans les propriétés de l'huile telle que la une réduction de sa viscosité et / ou l'évaporation partielle ou complete.

En réalité, la situation est souvent complexée par la présence d'un troisième fluide, autre que le fluide injecté et le fluide déplacé. Il s'agit de l'eau résiduelle au venue de l'aquifère adjacent lors de l'exploitation du réservoir elle joue un rôle important dans le processus de déplacement. En particulier, une partie du gaz injecté dissolvant dans l'eau peut réduire l'efficacité de EOR. Un autre exemple de présence de l'eau est WAG : l'injection artificielle des tranches d'eau alternées avec le gaz. Cette technique permet, d'une part, augmenter l'efficacité de EOR (à cause de l'augmentation moyenne de la viscosité du fluide déplaçant), mais aussi de résoudre le problème de stockage des gaz acides (CO_2) dans les couches géologiques.

Des considérables efforts sont été appliqués pour développer la théorie analytique de l'écoulement simultanée de deux phases partiellement miscibles dans les milieux poreux sont

connues dans la littérature scientifique. La modélisation d'un écoulement unidimensionnel des systèmes tri-phasiques entièrement immiscibles (pétrole/eau/gaz) a été également intensivement développée. En même temps, très peu de résultats sont disponibles sur l'écoulement partiellement miscible en trois phases.

L'hydrodynamique de ces processus est fortement couplée avec la thermodynamique du système multiphasique multicompositionnel, ce qui rend difficile l'analyse mathématique de ces systèmes et leur modélisation numérique.

Dans la pratique, tous les systèmes multiphasiques sont multicomposants et contiennent N composants chimiques tels que les hydrocarbures à partir de CH_4 jusqu'à $C_{10}H_{22}$ et plus lourds même, ainsi que H_2O , CO_2 , N_2 et parfois le sulfure.

Le modèle mathématique complet d'écoulement multiphasique multi-compositionnel consiste aux équations de bilan de la quantité du mouvement pour chaque phase et aux équations de bilan de la masse pour chaque composant chimique présent dans le système. Ce modèle doit être complété aux relations thermodynamiques décrivant l'équilibre et l'état des phases.

L'hypothèse de l'équilibre local est traditionnellement appliquée dans le cadre de cette théorie, étant basée sur le fait que la surface de contact entre les phases en milieux poreux est très grande.

Par conséquent, l'écoulement d'un tel mélange est décrit par N équations différentielles nonlinéaires de conservation de masse pour chaque composant et $N + 2$ relations transcendantales thermodynamiques dans le cas d'écoulement diphasique, et $2N + 3$ relations dans le cas d'écoulement triphasique. L'analyse qualitative efficace d'un tel modèle est pratiquement impossible.

Si on considère que seule la partie thermodynamique, on constate que, la théorie thermodynamique de ces systèmes est bien développée dans les ouvrages fondamentaux. Sa description mathématique, qui est souvent appelée le modèle compositionnel, consiste aux équations d'état des phases, équations d'état rhéologiques des phases et équations d'équilibre reliant les potentiels chimiques de chaque composant dans chaque phase, les pressions et les températures de phases. Habituellement, un tel modèle constitue un ensemble

d'équation non-linéaires transcendantes qui peut être résolu numériquement en utilisant procédures d'itération multiples.

Si les effets de la capillarité, la diffusion, et la dispersion sont négligeables, le transport dans les systèmes dominés par la convection est décrit par un système des équations différentielles non linéaires, hyperboliques, de premier ordre. Lorsque les conditions d'injection et initiale sont constantes et uniformes, le problème de déplacement représente un problème de Riemann.

Problème de Riemann en cas d'un écoulement diphasique : état d'art

La théorie mathématique du problème de Riemann pour les conditions initiales généralisées est bien développée. Dans le cas auto-similaire, le problème de Riemann a des solutions analytiques qui peuvent être construites par la méthode de caractéristique (MC). La structure générale de ces solutions est universelle : elle comprend les chocs alternés avec des zones où la solution reste continue et non-triviale, appelées les ondes simples de rarefaction ou de compression, et des zones de plateau où la solution reste constante.

Techniquement, le problème majeur consiste à déterminer les paramètres et le positionnement des chocs, qui est a priori non unique. ce problème de non unicité a été résolu en appliquant la conservation de la masse à travers un choc (relation de Hugoniot) et condition entropiques.

[Buckley et Leverett 1941] ont développé les premières solutions analytiques pour l'écoulement mono dimensionnel dans en milieux poreux, correspondant au déplacement d'huile par l'eau. Ils ont construit la solution pour le problème de déplacement de deux phases entièrement immiscibles et incompressibles.

[Welge 1952] a simplifié la technique de résolution de le problème de déplacement de l'eau-huile avec une méthode graphique de construction du choc. Il a montré que les conditions au choc ont une interprétation graphique et sont présentées par une ligne droite tangente

à la courbe de fractional flow. Cette tangente est connue dans le théorie mathématique du problème de Riemann comme l'enveloppe d'Oleinick.

Dans [Helfferich 1979] la théorie analytique générale basée sur la méthode des caractéristiques pour les déplacements diphasiques compositionnels a été présenté. Il a étudié l'injection du gaz miscible dans l'huile étant limité aux systèmes ternaires (3 composants chimiques).

Pour les systèmes à trois composantes le modèle constituait deux équations hyperboliques non-linéaires, formulées les concentrations totales de deux composants. La solution était fortement basée sur le fait que les concentrations de phase ne pouvaient changer que la façon discontinue, étant donc constantes par morceaux. Cette propriété de solution a nécessité l'introduction des tie-lignes qui ne sont que des lignes de la concentration de phase constante sur les diagrammes de phase. La construction global de la solution représentait donc des ondes de raréfaction des concentrations totales qui correspondaient aux valeurs constantes de concentration de phase situées sur des tie-lines différentes, et des chocs entre les tie-lines.

La première solutions au système quaternaire a été développés par [Monroe *et al.* 1990]. Avec cette solution, le concept de la tie-line intermédiaire a été introduit, créant les bases pour la résolution des systèmes multi-composants qui représentent mieux les mélanges de gaz et de pétrole.

Dans les solutions développées par Monroe, il était accepté que les concentrations des phases peuvent varier par les chocs.

Une solution unidimensionnelle du problème de Riemann pour deux phases et quatre et plus que quatre composants a été proposé plus tard par [Bedrikonetsky, Chumak 1992]. Ensuite, MC a été utilisée pour trouver des solutions analytiques du problème avec un nombre arbitraire de composants [Johns 1992 ; Dindoruk *et al.* 1992 ; Yuan 2003 ; Wang 1998 ; Jessen *et al.* 1999 ; Pires *et al.* 2004 ; Yuan et Johns 2002].

Le système diphasique à trois composantes détermine les propriétés basiques de la solution du problème de Riemann. Ce système est entièrement caractérisé par deux tie-lignes : une d'elles correspond à la condition du gaz injecté, tandis que la deuxième représente la

condition du fluide initial.

Dans un système à N composants, le changement de la composition de phase entre celle injecté et celle initiale passe à travers $N - 1$ tie-lignes. Deux tie-lignes sont toujours imposées par les conditions de Riemann (elles sont appelées "extérieurs"), tandis que $N - 3$ tie-lignes intérieures sont inconnues.

[*Wang* 1998] a utilisé le fait d'intersection des tie-lignes pour mettre au point un algorithme rapide et efficace permettant d'obtenir des solutions analytiques pour des systèmes multicompositionnels avec un nombre arbitraire de composants. Dans cette analyse, seulement des segments de chocs dans une séquence des tie-lines basiques ont été assumés.

Comme suite du développement de cette théorie, le concept de "trajet" (path) est devenu crucial dans la technique de construction de la solution : toute solution de problème hydrodynamique (de Riemann) a son image bijective sur le diagramme de phase. Il suffit donc construire le trajet thermodynamique pour déterminer toute la solution.

Problème de Riemann en cas d'un écoulement triphasique

Le déplacement totalement immiscible en trois phases a été étudié dans plusieurs publications. La méthode de caractéristique (MC) pour le cas de trois phases est construite de la même manière que pour le problème diphasique. [*Falls et Schulte* 1992 et *Guzman* 1995] illustre des discussions détaillées sur la construction des routes de composition de flux en trois phases non miscibles.

Il y a eu une somme de recherches mathématiques considérable consacrée à la compréhension des solutions non-unique dans MOC de l'écoulement immiscible triphasique [*Azevedo et Marchesin* 1995 ; *Azevedo textit et al* 1996, 1999, et 2002].

Généralement, il est possible d'avoir le flux d'un certain nombre de composants en trois phases qui coule dans les milieux poreux. De cette façon, chaque élément a une certaine miscibilité dans toutes les phases, lorsque les composants sont mélangés chacune des phases contient un certain nombre de chaque élément ; cependant quelques composants peuvent

contribuer vraiment peu à certains phases. Dans les systèmes triphasiques partiellement miscible on trouve l'ensemble des compositions qui ont un, deux ou trois phases. Il y a aussi trois régions diphasiques, un sur chaque frontière de la région triphasique.

Il y a eu relativement peu de travaux de recherche portant sur le déplacement triphasique partiellement miscible. Il y en a également très peu dans la littérature scientifique sur le développement de la méthode de caractéristique (MOC) pour l'écoulement à trois phases partiellement miscibles, [Giordano et Salter 1984].

La première solution pour le problème de Riemann partiellement miscible en trois phases trois composantes a été développé par [Laforce (et al.) 2005] à l'aide de la méthode de caractéristique. La solution unique a été trouvée et se basait sur l'argument de la continuité, des conditions de choc, des contraintes de l'entropie et des contraintes de la vitesse. Plus tard dans [Laforce, Jessen et Orr 2007] la même méthode a été développée pour traiter quatre composants partiellement miscible en déplacement triphasique.

Modèle réduit de mélange idéales

La plupart des résultats analytiques et semi-analytique obtenus dans le domaine de la problèmes multiphasique de Riemann basée sur les hypothèses simplificatrices. Dans les majorités des cas, la solution a été trouvée en acceptant les hypothèses ci-dessous :

- i) La pression est supposée constante. Cette hypothèse est trop forte et ne correspond pas du tout à la réalité. En effet, ayant une pression constante signifie l'absence de la gradient de pression qui conduirait les vitesses d'écoulement à zéro ce qui signifierait arrêter toute circulation.
- ii) La loi de Amagat a été supposé qui dit, le volume occupé par une quantité d'un élément est constant quelle que soit la phase qui composante apparaît dedans. Cette hypothèse de mélange idéal entraînera une densité constante qui pourrait être éliminé de l'équation et de la rendre moins compliquée à résoudre.
- iii) Comme un équilibre de potentiel chimique le cas élémentaire de K-value constante

a été assumé. Cette hypothèse signifie que les ratios de concentration d'équilibre des éléments dans les différentes phases sont constants. Selon le haut de couplage hydrodynamique et thermodynamique du problème, il serait impossible de trouver les résultats analytique ou semi-analytique sans cette hypothèse forte.

Modélisation numérique d'écoulement multiphasique compositionnel

En laissant de côté les hypothèses émises ci-dessus la seule méthode pour analyser ce système est la simulation numérique. Toutefois, même la méthode numérique semble être peu efficace quand on l'applique aux systèmes non linéaires de grande dimension.

Afin d'analyser le comportement dynamique d'un système compositionnel, la thermodynamique du système doit être complétée par les équations de bilan de la masse et la quantité de mouvement.

Ainsi, à chaque itération de solution de sous-système hydrodynamique, le sous-système thermodynamique non linéaire des équations d'équilibre de potentiel chimique et les équations de l'état doivent être résolus à chaque point de l'espace et à chaque moment du temps. De cette façon, l'algorithme global devient si complexe que souvent il ne peut être réalisé dans la pratique, lorsque menant à manque de temps et de mémoire, divergences de l'algorithme, ou des instabilités numériques.

La question est alors de savoir comment séparer la thermodynamique de l'hydrodynamique. Dans le cadre de cette séparation, il est possible de simuler la thermodynamique du système une fois pour tous l'espace et le temps et alors d'appliquer le résultat en vue de résoudre le problème hydrodynamique.

Découpage de l'hydrodynamique et de la thermodynamique

[Entov 1997] a montré que le système d'équations pour le problème de Riemann de déplacement diphasique multi- compositionnel peut être divisés en deux parties physico-

chimiques et hydrodynamiques. [Pires, Bedrikovetsky et Shapiro 2005] ont également développé leur technique de séparation afin de réduire le système d'équation à $N - 1$ équations auxiliaires contenant seulement les variables thermodynamiques et une équation de transport contenant seulement les paramètres hydrodynamiques. Mais, les deux modèles de la division ci-dessus sont fondés sur la supposition présentée plus haut.

Fractionnant sur la ligne de courant entre thermodynamiques et hydrodynamique pour l'écoulement du gaz-liquide en milieux poreux a été proposé dans [Oladyskhin et Panfilov 2006]. Dans ce travail, aucune de ces hypothèses simplificatrices a été utilisée et seulement deux propriétés physiques du système ont été prises en compte :

- i) Tout d'abord ils assument la petite mobilité relative entre les phases gazeuse et oléique.
- ii) Deuxièmement ils considèrent que le temps de stabilisation de la pression imposée soit beaucoup plus court que le temps de déplacement total du liquide dans le réservoir.

De cette manière, les équations de flux compositionnel ont été portées à $N - 2$ équations différentielles de thermodynamique qui pourraient être résolues de façon indépendante à l'aide de les équations de fermeture de thermodynamique, et à seulement 2 équations différentielles de transport.

Toutes ces tentatives performées pour découper les parties thermodynamique et hydrodynamique effectuent pour le cas de déplacement diphasique, et jusqu'à présent, rien a été proposé pour le flux triphasique compositionnel.

La technique asymptotique de HT-splitting est développé à l'aide de la transformation utile du système à une forme asymétrique, qui sera appelé "canonique". Le système sera appelé canonique, si les dérivés principaux de chaque équation différentielle décrivent le comportement d'une variable physique de base de problème de manière à ce que toutes les équations décrivent différentes variables.

La transformation dans la forme canonique peut être effectué tout en transformant de

chaque équation étape par étape, en excluant progressivement les dérivés principaux (ou de leurs parties principales) de la précédente équations. La partie principale d'un dérivé est celui qui ne contient pas les petits facteurs.

Brouillon de cette thèse

L'objectif de cette thèse est de faire progresser la théorie du flux compositionnel en évitant les simplifications fortes mentionnées. Sur la base de la méthode HT-splitting proposée par [Oladyshkin et Panfilov 2006], comme indiqué auparavant cette méthode a dit que la thermodynamique peut être totalement séparée de l'hydrodynamique dans la limite d'un infiniment grand ratio entre les mobilités des phases. Dans la thèse présente nous appliquons ce théorème pour développer la théorie du processus de déplacement (déplacement d'une phase par un autre) décrit par le problème de Riemann.

Le modèle mathématique utilisé a la structure suivante : selon HT-splitting, le modèle compositionnel est réduit au système fermé des deux seules équations différentielles quasi-linéaires qui concernent la pression et la saturation du gaz, indépendamment du nombre de composants chimiques présents dans l'écoulement diphasique et trois équations différentielles quasi-linéaires qui concernent la pression et de deux saturations indépendantes, dans le cas de flux triphasique. Les concentrations de phase sont déterminées à partir de "système thermodynamique différentiel" qui représente un système transcendant de l'équilibre de phase du système accompli avec des équations différentielles ordinaires de la thermodynamique, responsable du caractère ouvert de deux ou trois phases mobiles possédant différentes vitesses de circulation.

Le système analysé peut avoir des solutions discontinues (ondes de choc), de sorte que les chocs ont des origines physiques diverses : transition de phase, variation forte de la composition, les fronts de déplacements. Ces discontinuités sont décrites par des conditions d'équilibre des masses de Hugoniot.

L'analyse présentée dans les chapitres suivants, révèle que le modèle Ht-split ne peut pas être directement appliqués au cas avec les conditions initiales discontinues , car il fournit des nombres insuffisants de condition de Hugoniot à des chocs. Il s'agit d'un nouveau problème qui est résolu dans ce thèse.

Structure de la première partie - Écoulement diphasique compositionnel

Dans la première partie nous traitons l'écoulement isothermique de gaz-liquides dans les milieux poreux, afin que les deux phases se composent de plusieurs composants chimiques pouvant transiter d'une phase à une autre en raison de la miscibilité partielle. Le processus est décrit par le problème de Riemann en deux phases multi-compositionnelles partiellement miscible, avec les fluides compressibles. Donc le déplacement d'une phase par un autre est analysé.

Nous examinons les mélanges non idéaux. La pression est variable dans l'espace et le temps. Les compositions des phases, la densité et la viscosité sont les fonctions variables de la pression.

Nous examinons le modèle asymptotique sur les lignes des courants, puis l'écoulement devient unidimensionnel dans le système de coordonnées correspondantes.

La méthode de simulation des ligne des courants est fondée sur l'hypothèse que l'équation de la pression :

- i)est indépendante de l'équation de la saturation (et de la concentration)
- ii)est stationnaire

Dans ce cas, la solution de cette équation prévoit un système des lignes des courants, qui sont défini que pour un écoulement stationnaire. Les équations de transport de la saturation (et les concentrations), étant puis reformulées sur chaque ligne de courant, deviennent unidimensionnels, qui assure une solution extrêmement rapide de le système compositionnel. Dans certains cas particuliers, ces équations unidimensionnelles peuvent être résolues même de la manière analytique.

nous supposons que le système des lignes de courants sont compacts, c'est-à-dire n'importe quel point du domaine examiné est traversé par une ligne de courante et uniquement défini, donc les lignes des courants ne traversent pas une autre.

Nous examinons le cas lorsque tous les ligne des courants convergent à un puits cylindrique, et le débit total traverse cette surface cylindrique dans le sens de la centre de puits.

Nous supposons que tous les ligne des courants forment un système radial symétrique à proximité du puits. Supposant que les vitesses d'écoulement au puits sont identiques pour chaque ligne de courant, nous somme capables de définir le debit, utilisant la loi de Darcy pour la vitesse d'écoulement et en tenant compte que les lignes des courants sont orientées vers le puits.

Le technique HT-splitting développé donne de bon résultats pour le processus de l'épuisement naturel des réservoirs souterrains, dans lequel les solutions sont très continus, mais il est totalement inapplicable au problème de Riemann qui a des solutions discontinus. L'énorme problème consiste en ce que le modèle HT-split détermine une solution discontinue non-unique. Nous montrerons que le modèle asymptotique analysé a deux types de discontinuités de nature différente :

- i) Les discontinuités dans la structure des coefficients de l'équation différentielle de l'hydrodynamique ; elles déterminent le comportement discontinu de la concentration de phase. Ceci est causé par le problème sur-déterminé de Cauchy obtenu pour le système différentiel de thermodynamique ; physiquement les discontinuités dans les concentrations de phase sont causés par les conditions de Riemann pour les concentrations dans le problème compositionnel complet original (non asymptote).-*sc-choc*
- ii) Les discontinuités dans la structure de la solution au problème hydrodynamique ; elles déterminent le comportement discontinue de la saturation, elles sont causés par le problème de Riemann de saturation qui impose le choc initial qui ne peut pas disparaître avec le temps.-*s-choc*

Le comportement des discontinuités est déterminé par les équations de bilan massique élaboré juste à proximité de chaque choc et appelé la condition de Hugoniot. Ces conditions remplacent les équations différentielles originales qui ne sont pas valides à une discontinuité. Une des façons de construire les conditions de Hugoniot est d'intégrer la forme originale de l'équation différentielle de transport sur une zone infiniment mince près de la discontinuité et sur la infiniment petit intervalle de temps.

Une autre relation pour les chocs est la condition d'entropie qui représente une inégalité, en fournissant des limites strictes pour le paramètre à la variation de choc, afin que le principe de l'entropie augmentant en passant par le choc est satisfait. Ce principe est formulé sous des formes diverses, et en particulier sous la forme d'inégalités de Lax.

Même si nous complétons le modèle HT-split par les conditions de Hugoniot et l'entropie, il est pas capable de nous donne des bons résultats.

En bref, le modèle HT-split fournit un nombre insuffisant de relation Hugoniot à chaque discontinuité, comme nous sommes capable de trouver seulement deux conditions de choc avec notre modèle HT-split, une condition de Hugoniot pour l'équation de la saturation et une condition de entropie.

Ces deux équations sont malheureusement largement insuffisante, comme un choc simultané de la saturation et les concentrations est déterminée par $(N + 1)$ paramètres au chaque côté du choc : la vitesse de choc , et $(N - 1)$ saturation et les concentrations à l'état de choc, où N est le nombre de composants.

Le problème est alors la façon d'obtenir des conditions supplémentaires pour les concentrations de phase ?

Le problème révélé du manque des conditions de Hugoniot est causé par le fait que, dans le modèle HT-split, $(N - 2)$ équations initiales de transport de concentration sont transformées, par la limite de transition de modèle, dans les relations thermodynamique. Le nombre restant d'équations hydrodynamiques est 2 quel que soit le nombre de composants chimiques.

Cela nous donne l'idée que les conditions de Hugoniot nécessaires devraient être obtenus à partir du modèle complet compositionnel avec la limite de transition consécutive aux relations obtenus.

Évidemment, ce processus nous donne N conditions de Hugoniot formelles. Si l'on ajoute une relation d'entropie, nous obtenons alors $N + 1$ relations à un choc, équivalent au nombre des paramètres inconnus de choc. Le choc modèle sera ensuite fermé.

Donc tout d'abord, nous avons développé le système des conditions asymptotiques de Hugoniot et résolu le problème de manque des conditions de Hugoniot dans le modèle HT-split.

Comme nous avons déjà mentionné, un choc simultané de la saturation et la concentration de phase exige N conditions, tandis que deux équations différentielles ne peuvent fournir que deux relations de Hugoniot. Cette contradiction est résolue par le développement des conditions Hugoniot du modèle compositionnel complet, puis par l'obtention de leur comportement à la limite de contraste de mobilité. Nous avons montré que le système limité n'est pas équivalent à celui obtenu directement à partir du modèle HT-split.

Cela nous a donné la possibilité de développer la théorie générale du procédé de déplacement diphasique multi compositionnel décrit par le problème de Riemann dans le cadre de la technique de HT-split. La théorie développée n'a rien de commun avec la technique classique pour un mélange idéal, à l'exception de la notion de tie-lignes qui n'était pas utilisée directement, mais était généralisée et remplacée par la notion de P-surfaces pour les mélanges non-idéaux à pression variable.

Si la pression est invariable (comme supposé dans la théorie du mélange idéal), puis la concentration de phase ne peut être que constant ou constante par morceau, et les chocs entre les morceaux sont les chocs de concentration, donc ils sont les *sc*-chocs, qui détermine aussi la discontinuité de la saturation. Grâce à cette propriété la structure de la solution est caractérisée par les fragments invariables de la concentration de phase (les plateaux) entre les chocs. Un état invariable de phase correspond à ce que l'on appelle la tie-ligne dans le diagramme thermodynamique de phase. Le diagramme de phase représente l'ensemble des états disponibles pour la fluide examiné.

Une tie-ligne est une ligne droite traversant la zone diphasique et marquant des compositions des deux phases. Sur une tie-ligne les compositions des phases sont fixes tandis que la saturation des phases et les compositions totales du système varient.

Une tie-ligne est la représentation graphique de les équations d'équilibre des phases ; ce qui concerne les couples de concentrations en phase liquide et du gaz coexistent. Ces valeurs sont déterminées par les équations d'équilibre. À pression constante, les concentrations des phases peuvent varier seulement par les chocs reliant deux tie-lignes, ce sont les *sc*-chocs. En revanche, une *s*-choc se déplace sur une tie-ligne fixe.

Les tie-lignes jouent un rôle important dans la théorie de déplacement d'un fluide, parce

que le comportement de la concentration de phase est souvent constante par morceau dans l'espace, comme mentionné au-dessus.

En termes de tie-ligne, ce signifie que les compositions des phases sautent d'une tie-ligne à une autre. Ce saut correspond à des chocs de la solution de problème de Riemann. En d'autres termes, un choc de concentration concerne deux tie-lignes afin que avant et après le choc des concentrations correspondent exactement à ces deux tie-lignes.

Si la pression varie, alors le système devrait être caractérisé par l'ensemble des diagrammes de phase qui correspondent à chaque pression. En ajoutant l'axe de pression on obtient alors le diagramme trois dimensionnels de phase.

Ce diagramme en 3D avec toutes les tie-lignes à chaque pression peut être construit à l'aide de les équations d'équilibre seulement : les tie-lignes sont la solution des équations d'équilibre de potentielle chimique pour les compositions totales données, tandis que l'enveloppe diphasique limite le domaine de l'existence de ces solutions. Malgré cela, ce diagramme est insuffisant pour décrire le comportement du système lorsque la pression varie. En d'autres termes, il est impossible, en utilisant uniquement les équations classiques de thermodynamique, de déterminer comment une tie-ligne à la pression P_1 se transforme en une autre tie-ligne à la pression P_2 .

Physiquement cela est lié au fait que, lorsque la pression varie, l'ensemble du système compositionnel change également, alors que la variation de les compositions totales ne dépend pas seulement de la pression, mais aussi de les processus hydrodynamiques. En effet, si nous examinons un représentant élémentaire du volume de milieu poreux, les compositions totales peuvent rester invariables, si les deux phases s'écoulent comme un ensemble indissociable unique, c'est-à-dire à la même vitesses.

Si, toutefois, les vitesses d'écoulement sont différentes, les compositions totales en volume examiné changeront. Ainsi, la variation de la composition totale dépend de la vitesse d'écoulement, c'est-à-dire sur la système hydrodynamique.

Nous avons analysé le comportement thermodynamique d'un système compositionnel di-

phasique à pression variable. Au lieu des tie-lignes (lignes d'une composition de phase invariable) utilisés dans la théorie classique à pression constante, nous avons introduit le nouveau concept de P-surface, qui représente l'emplacement des solutions de modèle différentiel thermodynamique de sorte que chaque section d'une telle surface à une pression fixe représente une tie-ligne. Nous mettons en évidence que la partie continue de la solution du problème de Riemann correspond à une P-surface fixe, tant qu'un choc se produit toujours entre deux P-surfaces.

Dans le modèle asymptotique la thermodynamique est séparée de l'hydrodynamique. Cela signifie en particulier que la transition entre les tie-lignes sur l'axe de pression peut être calculé uniquement par le sous-système thermodynamique. Ces transitions sont déterminés par le nouveau système des équations différentielles de thermodynamique.

Ces équations déterminent la variation de les concentrations des phases par rapport des autres concentrations de phase connus. Ces concentrations connus sont déterminé par le système des équations d'équilibre de potentielle chimique. En réalité des équations différentielles de thermodynamique et des équations d'équilibre de potentielle chimique devraient être résolus simultanément.

Dans le cas general d'écoulement diphasique en N compositions, nous avons N équations d'équilibre de potentielle chimique et $N - 2$ équations différentielles de thermodynamique et aussi 2 équations de normalization des concentrations des phase. Donc nous avons $2N$ équation pour déterminer $2N$ concentrations de phase, ainsi, le système est fermé.

Si nous pouvons calculer les concentrations des phases, alors cela signifie que nous pouvons déterminer la transition de chaque point d'une tie-ligne sur l'axe de pression. Cela signifie donc que nous pouvons déterminer la transition d'un tie-ligne dans un autre l'axe de pression.

Le système consécutives de tie-lignes transit l'un dans l'autre représente une surface 3D. Une telle surface, déterminé par le système des équations différentielles de thermodynamique et des équations d'équilibre de potentielle chimique et une tie-ligne dans chaque section transversale (c'est-à-dire à chaque pression) sera appelé la P-surface.

Le long d'une P-surface, la composition de liquide varie d'un premier point le long de la courbe de changement de pression. Dans la même manière la composition de gaz varie depuis le point initial le long de la courbe. Tout nouveau couple de points des compositions des gaz et liquide à une autre pression est liée par une tie-ligne dans le diagramme de phase correspondant à la pression.

Pour un système contenant N composants chimiques, la P-surface représente une hypersurface en N dimensions. Ainsi, le système des équation d'équilibre de potentielle chimique et les équations différentielle de thermodynamique détermine le diagramme de phase à tout pression, toutes les tie-lignes à tout pression et aussi les P-surfaces.

La notion de P-surface remplace le concept de tie-ligne pour les systèmes avec la pression variable. Dans la structure de la solution du problème de Riemann, les concentration des phases ne sont plus obligé d'être constant entre les chocs, ils peuvent varier de manière continue le long de la P-surfaces et peuvent sauter entre les P-surfaces.

A l'étape suivante nous avons élaboré la procédure de "front-tracker". Il est montré que le système asymptotique des conditions Hugoniot obtenus, complétée par le bloc thermodynamique, peut être réduit à un système fermé d'équations algébriques qui concerne les concentrations des phases à l'avant et en arrière de tous les chocs. Cela nous permet d'obtenir tous les paramètres de chocs et la trace de leur mouvement dans l'espace avant de résoudre les équations différentielles d'écoulement.

Le système des conditions de Hugoniot aux *sc*-chocs, que nous avons trouvé ne contient pas des vitesses, mais seulement des paramètres thermodynamiques et une seul paramètre non-thermodynamique, La saturations de gaz. Cela pose la question de savoir si c'est possible de séparer saturation et d'obtenir un sous-système purement thermodynamiques des conditions de Hugoniot? La réponse à ces questions est affirmative.

En d'autre terme, le principe de HT-splitting peut être développé pas seulement pour les équations différentielles d'écoulement, mais pour les conditions de Hugoniot aussi.

La spécificité des conditions de Hugoniot formulées dans ce modèle consiste à ce système des $N - 3$ équations ne contient que les concentrations des phases. Cela signifie que nous

avons divisé thermodynamique à partir de variables hydrodynamiques dans les condition de Hugoniot.

Ce système des $N - 3$ équations contient $4N - 4$ concentrations inconnus, $2N - 2$ au chaque coté de choc. Ensuite, même étant complété avec les N équations d'équilibre de potentielle chimique de côté en avant de choc, N équations d'équilibre de la partie arrière de choc, et $N - 2$ équations différentielles de thermodynamique, on obtient $4N - 5$ équations, qui ne sont pas suffisants pour obtenir un solution unique.

Par ailleurs, ce n'est pas clair que quelle conditions thermodynamiques de Cauchy devrait être prendre pour chaque choc. En plus, la utilisation des conditions différentielles de thermodynamiques n'est pas approuvé car elles déterminent le comportement de la solution entre deux chocs mais pas sur un choc.

Malgré cela, il est possible de construire un problème fermé pour les concentrations de choc simultanément à tous les chocs. Pour cela, il faut connaître le nombre de chocs apparaissant dans la solution.

Un des résultats qualitatifs importants de la théorie analytique du problème de Riemann pour un mélange idéal annonce que, dans un problème de N composants chimiques en deux phases qui ne change pas le nombre de phases (c'est-à-dire ni l'évaporation totale ni la condensation totale sont observées) les concentrations des phases devraient suivre $N - 3$ tie-lignes "intermédiaire" ou "Crossover" situées entre deux tie-line "externe" qui correspondent aux états initiale et injection. Donc, au total, les concentrations des phases devraient suivre $N - 1$ tie-lignes. Ce résultat n'est pas strictement prouvé en mathématique, il est empirique, mais il est entièrement confirmé par l'ensemble des données numériques. Dans le cas de pression variable, nous supposons que le même résultat soit valide, de sorte que, dans un système de N composants chimiques en deux phases qui ne change pas le nombre de phases les concentrations des phases devrait suivre $N - 1$ différentes P-surfaces dont deux P-surfaces "externes" qui correspondent à deux pressions frontière et $N - 3$ P-surfaces "intermédiaire" ou "Crossover".

Comme un P-surface se situe entre les deux *sc*-chocs voisins, puis les $N - 3$ P-surfaces sont

situées entre $N - 2$ *sc*-chocs. Cela signifie que le nombre total de *sc*-chocs intermédiaire est $N - 2$. Tout cela n'est valable que pour le cas où le système ne change pas sa phase d'état. Sinon, d'autres chocs de la transition de phase peuvent se poser.

Les équations différentielles de thermodynamique déterminent les P-surfaces entre deux chocs voisins. Cela signifie que l'ensemble du système des condition de Hugoniot et les équations différentielles de thermodynamique à tous les chocs représente un système couplé des équations. Il est donc nécessaire de chercher pour les paramètres de tous les chocs simultanément.

Donc nous avons calculé le nombre des variables et les équations. Les concentrations entre le point d'injection et le premier choc interne sont totalement déterminé par le modèle thermodynamique. Les équations différentielles de thermodynamique sont prises avec la condition de Cauchy correspondant à la pression d'injection. La situation similaire concerne les concentrations entre le dernier choc et le point final (les concentrations sont calculées à partir du dernier point d'écoulement). Par conséquent, seulement les concentrations après le premier et avant le derrière choc sont indéterminées. Cela nous donne $2(N - 3)$ côtés des chocs au cours de laquelle nous avons besoin de déterminer les concentrations. Le nombre total des concentrations inconnues à des chocs sera alors $4(N - 1)(N - 3)$.

Aux $N - 2$ chocs nous avons $(N - 3)(N - 2)$ relations de Hugoniot. Chaque côté de choc nous fournit N équations d'équilibre de les phases. Entre deux chocs voisins nous avons $N - 2$ équations différentielles de thermodynamique, de sorte entre tous les chocs, nous aurons $(N - 3)(N - 2)$ relations différentielles de thermodynamique. De ce fait, nous possédons $2(N - 3)(N - 2) + 2N(N - 3) = 2(N - 3)(2N - 2) = 4(N - 3)(N - 1)$ équations qui contient seulement les concentrations des phases comme les variables inconnues.

Par conséquent, le système est fermé et a une solution unique. Il y a de même nombre des variables inconnus et des équations se présente dans le système.

Alors ce système fournit un outil capable de déterminer les concentrations à l'arrière et avant de tous les chocs, avant résoudre les équations différentielles de hydrodynamique.

Une telle procédure de détection des paramètres de choc est appelée front-tracker.

Pour les saturations avant et arrière de chaque choc, il est également possible de mettre au point la procédure analytique explicite de tracker.

Deux conditions supplémentaires qui permettent de déterminer la solution unique est la dernière condition de Hugoniot et la condition d'entropie. Dans la pratique, leur emploi n'est pas techniquement simple. Au lieu de cela, lors de la première étape du développement de cette théorie nous suggérons un rapprochement qui permet de simplifier significativement tous les calculs. Nous allons utiliser le résultat obtenu pour la vitesse totale de l'écoulement lors d'une s -choc. Semblable à cela, nous supposons que la vitesse totale est aussi continue en passant d'un sc -choc. Cette hypothèse est confirmée par le fait que la vitesse totale est une fonction suffisamment conservatrice tels qu'elle est responsable de la continuité des flux, contrairement à la vitesse de phase, qui peut subir les sauts, en passant par une frontière ou d'un front.

Cette hypothèse est strictement satisfaite dans la théorie classique sur la base d'un mélange idéal. En plus, dans la théorie classique la vitesse totale est invariable dans l'espace, donc l'hypothèse de la vitesse continue est évidemment beaucoup plus faible que la vitesse constante.

Ensuite, nous avons développé la solution numérique de l'équation différentielle de transport à prendre en compte du fait que les paramètres de choc sont déjà déterminés. Cela permet l'application des schémas numériques très économique et rapide. Dans certains cas, le problème de Riemann a des solutions analytiques basées sur l'application d'une technique diagrammatique particulière. Les solutions analytiques sont également obtenues.

La procédure de front-tracker développée dans cette thèse établit l'algorithme suivant pour la construction de la solution de problème de déplacement :

Étape 1 Front-tracker pour les concentrations : Utilisant le procédure de front-tracker pour les concentrations, les équations différentielle de thermodynamic et $(N - 3)$ relations de Hugoniot nous pouvons déterminer tous les concentrations en avant et arrière de tous les sc -chocs. En réalité, nous calculons l'ensemble des P-surfaces in-

termédiaires, car elles sont les solutions au système des équations différentielles de thermodynamique.

Étape 2 Front-tracker pour les saturations : cela se fera à l'aide de front-tracker pour les saturations qui représente deux relation de Hugoniot.

Étape 3 Front-tracker pour la vitesse : cela se fait aussi explicitement à l'aide de la dernière relation de Hugoniot.

Étape 4 Simulation des parties continues de la solution entre les chocs : grâce à la simulation numérique des équations différentielles de l'hydrodynamiques nous sommes capables de trouver la saturation et la pression sur les différents le long de la P-surfaces correspondants.

Ainsi, les chocs sont détectés analytiquement, tandis que les ondes de raréfaction sont simulées numériquement.

Le lien entre les solutions numériques et les relations analytiques est réalisée dans le manière suivante : la pression et la saturation sont calculées numériquement de la point de départ $x = 0$. Une fois les valeurs de saturation atteindre l'une des valeurs qui correspond à un choc probable, ce point mobile est considéré comme la mise en place de choc. Après cela, nous commencer à simuler la prochaine onde de raréfaction en prenant en compt la saturation avant le choc comme une valeur initiale, et ainsi de suite.

Comme expliquer avant, la troisième étape de notre algorithme de la solution est la construction des solution des équations de la saturation et de la pression sur chaque P-surface. Afin de résoudre cette équation en même temps, nous utilisons la forme finale de l'équation de transport de saturation et nous essayons de le résoudre avec la méthode des caractéristiques qui est une méthode bien connue dans la résolution de ce type d'équations aux dérivées partielles.

Nous rappelons que, grâce à l'homogénéité des équations la variable dépendante, ici la saturation de gaz, reste constante le long de chaque caractéristique, et les courbes caractéristiques sont tout les lignes droites et parallèles dans le plan de (x, t) . C'est ce fait qui rend

la construction de la solution si simple. De toute évidence, il n'est pas le cas si l'équation est nonhomogeneous. Comme mentionné avant l'apparition d'un terme différent de zéro dans la partie droite de l'équation de transport de saturation, saturation de gaz n'est plus constant sur les caractéristiques et dépend de temps, et les caractéristiques sont non plus les lignes d'équilibre.

Dans cette partie comme nous avons voulu de trouver une solution analytique, les densités et les viscosités des phases sont supposées constantes à l'égard de la pression, donc les conductivités hydrauliques des phases sera constantes et elles sont égales à l'unité. Nous avons également accepté la perméabilité relative de chaque phase d'être le carré de sa saturation.

Ensuite les caractéristiques sont calculées dans le plan de (x, t) , nous avons calculé les caractéristiques associées avec composition initiale, et les caractéristiques associées à composition d'injection. Les courbes de caractéristique associées à la discontinuité à l'entrée sont aussi calculées.

Lorsque les caractéristiques sur le plan (x, t) se croisent, un choc doit apparaître. Mais comme nous avons vu dans la figure obtenue il n'y a pas d'intersections entre les caractéristiques, de sorte que nous n'aurons pas des sauts de saturation dans notre problème.

En fait, dans notre problème comme on peut le voir dans la figure montrant le comportement de la fonction d'écoulement fractionnelle, en raison de la petitesse de la mobilité relative des phases, cette fonction qui détermine la vitesse d'onde n'a pas du tout des points d'inflexions à moins que pour la saturation initiale très petite, et la vitesse d'onde augmente avec la diminution de la saturation. Alors, nous n'aurons pas du tout des non-unicités dans notre solution à remplacer par une discontinuité.

Enfin nous avons simulé un écoulement simultané de gaz et de pétrole dans le cas de trois éléments : dioxyde de carbone, méthane, décane, et de quatre éléments : dioxyde de carbone, méthane, N-butane, décane. Le gaz injecté est en équilibre avec le liquide sur place et se compose de tous les composants dans le réservoir.

Le système des équations différentielles de l'hydrodynamique a été discrétisé par la mé-

thode de différences finies arrière, entièrement explicite dans le temps.

Nous envisageons un processus isotherme ; le sous-système thermodynamique a été simulé sur la base des équations d'états de Peng-Robinson pour les deux phases. Les simulations thermodynamique ont été effectuées de façon indépendante pour une température fixe et les diverses pressions. Les valeurs obtenues de la concentrations des phases ont été estimés par des polynômes de pression et elles ont été utilisés dans la partie hydrodynamique. Nous avons également utilisé ces polynômes pour trouver les densités des phases et les viscosités en fonction de la pression et de la concentration de phase.

Le profil de saturation a été obtenu pour un réservoir mono dimensionnelle pour les différents temps après le début de l'injection.

Afin de vérifier la validité des solutions obtenues, nous avons les comparés à deux types des solutions obtenues par d'autres méthodes : (1) tout d'abord, nous avons comparé avec la solution numérique pour le même problème mais formulées en termes du modèle compositionnel total ; (2) d'autre part, la comparaison a été faite avec la solution analytique obtenue dans le cadre d'un ratio constante entre les paramètres, ce qui conduit au modèle officiellement identique à celui utilisé dans la théorie de mélange idéal. La solution numérique du modèle compositionnel complet a été développée par l'application de la méthode de différences finies. La solution analytique a été obtenue en utilisant la technique classique basée sur la détection analytique des chocs et sur la méthode des caractéristiques entre les chocs.

Structure de la deuxième partie - Transitions de phase

Dans la deuxième partie, nous avons examiné le cas avec les transitions de phase : lors de flux diphasique peut former des zones monophasiques avec un fluide sur- ou sous-saturé de certains composants. Dans le diagramme de phase les fluides sur et sous-saturés sont situés loin de l'enveloppe de deux phases, contrairement aux états monophasiques en équilibre situés juste à l'interface entre les régions diphasique et monophasique.

La zone diphasique est situé à l'intérieur du domaine limité par l'enveloppe et une tie-ligne, qui détermine la composition invariable de phase, est maintenant une ligne horizontale que correspond à une pression constante. Le long de la tie-ligne les compositions monophasiques sont les points d'intersection de tie-ligne et l'enveloppe de deux phases. La phase seul gaz-sur-saturé avec la composante léger se trouve sur la droite du point de composition de gaz, ainsi que la phase seul liquide sous-saturé avec la composant lourde se trouve sur la gauche du point de composition de liquide. Comme le phase sous-saturé de liquide est sur-saturé en gaz, nous allons utiliser le même terme de fluide sur-saturés pour le gaz et liquide non-équilibre.

Il est nécessaire de noter que la valeur de saturation n'est pas suffisante pour distinguer le gaz en équilibre du gaz sursaturé, étant égale à 1 pour les deux (même pour les liquides). Il est significatif que le comportement du fluide monophasique sur- ou sous-saturé et le fluide en équilibre sont qualitativement différente. Contrairement à fluides en équilibre, les compositions de fluide sur et sous-saturé ne sont plus contrôlées par les lois d'équilibre de phase, mais aussi par d'autres mécanismes (comme la diffusion,...). Pour cette raison le contact entre les fluides diphasiques et les fluides sur- ou sous-saturés est caractérisé par un comportement non-équilibré à transition intense de phase dans la zone de contact.

La différence entre les fluides en équilibre et les fluides monophasiques sur- ou sous-saturés est également manifeste dans le modèle mathématique d'écoulement. Le modèle d'un fluide en équilibre est le cas limite du modèle diphasique lorsque la saturation de gaz tend vers zéro ou un, ce qui n'est pas le cas du fluide sur- ou sous-saturé dont le modèle est totalement indépendant du diphasique.

Par conséquent, le flux dans les zones diphasique et dans les zones monophasique sur ou sous-saturées est décrit par deux systèmes d'équations indépendants, qui conduit à des graves problèmes dans la modélisation de ces processus. En particulier, tous les algorithmes de modélisation de ces processus doit prendre en compte quand et où ils doivent procéder à l'échange entre ces deux modèles. Cela signifie que l'emplacement des interfaces entre les zones diphasiques et monophasiques doivent être détectées avant la résolution des équations différentielles de flux. Cependant il n'est pas possible de le faire que dans les quelques cas les plus simples. Dans le cas général, la détection des interfaces mobiles devaient être effectuée en cours de résolution des équations différentielles de flux, ce qui semble être impossible dans ce cas.

Un autre problème est lié au fait que les conditions initial et à la limite, physiquement correcte devraient être formulées en termes de la concentration totale et pas de saturation, tandis que les équations d'écoulement diphasiques sont formulées en termes de saturation. Pour vaincre ces problèmes, nous suggérons d'utiliser le système uniforme des équations classiques de flux diphasique formulées en termes de pression et de saturation à la fois pour les zones diphasiques et les zones monophasiques sur- ou sous-saturées, mais tout en élargissant le concept de saturation de phase afin qu'elle puisse devenir négatif ou supérieur à un. La valeur absolue de la saturation négative représente le degré la distance du système à la zone diphasique.

Dans le cadre de cette partie, le nombre de composant ne joue aucun rôle, donc, par souci de simplicité, nous considérons le cas $N = 2$, qui est plus illustrative pour montrer le but de méthode.

Malgré la diffusion qui est un processus suffisamment non-équilibre, il est possible de accepter l'hypothèse d'équilibre locale des phases dans les zones diphasique, à l'aide du principe de Curie.

Afin d'assurer de l'apparence des zones monophasique sous- et sur-saturée nous les intro-

duisons directement par les conditions d'initiale et d'injection. Nous examinons un domaine fini monodimensionnel dans lequel le premier fluide est un liquide sous-saturé. Nous injectons un fluide sur-saturé à travers le côté gauche de la frontière de domaine $x = 0$.

La partie restante de la frontière sert à évacuer le fluide originale déplacé par le fluide injecté. Le contact entre le gaz sur-saturé et le liquide sous-saturé conduira nécessairement à l'apparition des zone diphsiques en équilibre. Le problème est analysé à la cohérence avec des situations pratiques qui correspondent à l'injection des gaz miscibles comme CO_2 dans les reservoirs de l'huile ou de l'eau.

Selon la description du processus, nous supposons que au minimum trois zones mobile existent dans le domaine : la zone dans laquelle le fluide est un gaz sur-saturé, la zone dans laquelle le fluide est un liquide sous-saturé, et la zone dans laquelle le fluide est un system de gaz-liquid en équilibre.

Les interfaces mobiles de la transitions des phase ne sont pas connus a priori et doit être déterminé comme le résultat de la solution du problème. En réalité, le nombre de zones et leur alternance peut être beaucoup plus compliqué, de sorte que les zones diphasique peut être suivie par la seconde zone d'un gaz sur-saturé, après dont la nouvelle zone diphasique apparaît et ainsi de suite. Il est alors souhaitable que la méthode de solution serait en mesure de détecter automatiquement toutes les zones et leur alternance.

Comme nous avons déjà précisé, dans les modèles classiques de solution de ce type de problème les domaines diphasique, sont formulés par les équations à l'égard de la pression et la saturation et dans les partie monophasique des équations élaborées à l'égard de pression et la concentration totale, sont utilisées.

Le fait que deux systèmes indépendants d'équations formulées par les différentes variables sont utilisés dans les zone diphasiques et les zones monophasiques cause des problèmes graves dans la modélisation des processus. En effet, afin de passer entre les équations et les variables nous avons besoin de précédemment détecter l'emplacement des interfaces mobiles. En même temps, les relation de Hugoniot qui déterminent ces interfaces sont formulées par les variables mixtes (saturation d'un côté, concentration totale de l'autre

côté), ce qui rend impossible de passer entre les variables. En raison de ça, la detection a priori du choc est impossible.

La méthode efficace pour surmonter cette difficulté consiste à introduire des variables uniformes pour toutes les zones. Mais nous suggérons une méthode avancée, par l'introduction des équations uniformes de l'écoulement dans toutes les zones.

Au lieu de remplacer la saturation par la concentration totale, nous proposons une autre méthode qui consiste à utiliser les équations d'écoulement uniformes dans tout les zones diphasique et monophasique, formulées par le concept de la saturation étendue. Formellement ces équations sont équivalentes au modèle classique d'écoulement diphasique.

Le grand avantage de cette méthode consiste à ce que les équations d'écoulement diphasique gardent leur forme originale. Cela signifie tout d'abord, que toutes les méthodes mises au point pour l'écoulement diphasique sans transition de phase devient uniformément valable pour le cas des transitions de phase aussi. Deuxièmement, cela signifie que toutes les simulateurs numériques peuvent être appliqués pour simuler les apparence de la zone sur-saturées, en ajoutant un simple sous-routine.

La méthode de saturation négatif est proposé basée sur le théorème de l'équivalence établie dans la thèse présente, selon laquelle un flux monophasique peut être remplacé par un système hydrodynamiquement et thermodynamiquement équivalent du flux diphasique imaginaire dans lequel les phases sont partiellement miscible, les compositions des phases sont en équilibre, la perméabilité relative, la pression capillaire, la diffusion phasique interne, les densité et viscosité des phases satisfont des conditions spéciales de consistance, et les saturations des phases sont négatives et supérieures à un. Nous avons aussi obtenu la formulation correcte des conditions initiale et à la limite en termes de la saturation étendue.

Nous remplaçons le vrai fluide monophasique par un fluide imaginaire en deux phases avec le phase liquide fictif et le phase gazeuse fictif qui ont des propriétés non-vrai différentes de celles de la fluide vrai, mais ces propriétés sont de sorte que le fluid diphasique

est équivalent à la véritable fluide monophasique.

La possibilité de ce remplacement est justifiée par le théorème fondamental que nous proposons. Nous appellerons ce théorème *le principe d'équivalence*. Le théorème établit les propriétés spéciales et exacts des fluides imaginaires qui assurent la consistance physique entre les deux phases formelles et le véritable fluide monophasique. Ces propriétés sont appelées *les conditions de consistance*.

Dans la zone sur-saturée de gaz le liquide imaginaire doit avoir la même densité et viscosité comme le vrai gaz, les deux phases devraient avoir les perméabilités relatives diagonales, la pression capillaire doit être zéro. Les concentrations de phase pour les deux phases sont calculés par les relations d'équilibres qui déterminent le vrai zone diphasique.

Le plus compliqué est le calcul du coefficient de diffusion de la phase imaginaire, qui dépend du gradients de saturation et de pression. En même temps, la saturation dans les zones sur-saturées est souvent constante ou faiblement variable. Dans ce cas, nous aurons les coefficients de diffusion égaux pour les deux phases.

La preuve de théorème d'équivalence permet d'introduire l'extension du concept de saturation qui peut maintenant être négatif ou supérieur à un. La saturation étendue, sera également appelé la saturation négatif.

Cette méthode nous permet d'utiliser le modèle du flux diphasique pour l'ensemble des domaines monophasiques et diphasiques et d'appliquer la même méthode numérique de simulation de l'ensemble du problème. Et donc toutes les interfaces entre les zones sont déterminés automatiquement.

À l'aide de la méthode proposée, nous avons obtenu des solutions numériques pour plusieurs exemples formulées par des équations différentielles diphasique par tout le problème en utilisant les conditions de consistance.

Tout d'abord nous avons analysé le cas unidimensionnel du mélange idéal à une pression constante. La pression capillaire, la diffusion et la gravité sont négligés. Cet exemple est important comme il a la solution analytique.

La même méthode a été appliquée à un cas plus général d'un mélange non-idéal à la pression variable. Les forces de capillarité, la diffusion et la gravité sont toujours négligés. Le

système est décrite par le même problème que dans le cas précédent dans lequel les concentrations des phases et les densités ne sont plus constants, mais dépendent de la pression. L'équation d'état idéale a été utilisée pour le gaz, et le modèle faiblement compressible pour le liquide. Les viscosités des phases ont été supposé être invariables.

Le troisième exemple nous permet d'analyser l'efficacité de la méthode dans le cas de la diffusion et l'influence de la diffusion sur le comportement de la saturation, ce qui est difficile de prévoir a priori.

En effet, dans le cadre de la zone diphasique la diffusion des influence que les concentrations des phases, mais pas la saturation. De ce point de vue, rien ne l'interdit la saturation d'être discontinue. En revanche, le comportement de la saturation entre les zones diphasique et monophasique n'est pas claire. Nous montrons également que, dans le cas de la diffusion, où les chocs de saturation n'existent pas, la méthode est capable de détecter les interfaces comme les faibles discontinuités.

La méthode de saturation négative développés dans cette partie sera après présenté dans le formalisme asymptotique du modèle compositionnel. Nous analyserons comment le fait de transitions de phase influence les résultats obtenus de modèle asymptotique.

En utilisant la méthode de saturation négative, nous avons examiné les problèmes de Riemann avec les compositions initiale et / ou injection monophasique et nous compléterons notre méthode de fractionnement à couvrir tous les cas qui peuvent se produire dans la réalité.

Structure de la troisième partie - Ecoulement triphasique compositionnel

La dernière partie de cette thèse a consacré ensuite à élargir la méthode HT-split pour le cas d'écoulement triphasique (gaz / eau / huile) compositionnel en milieu poreux, à l'aide de contraste entre les mobilité du gaz et pétrole, et du gaz et de l'eau.

Mathématiquement c'est exprimée sous la forme de l'apparition de deux petites paramètres : le rapport de la mobilité du gaz et de l'huile, et le rapport de la mobilité du gaz et de l'eau. Le modèle asymptotique est obtenu comme la limite du processus quand ces rapports sont très petites. Ce processus asymptotique prend à compte de la présence du troisième petit paramètre qui est le temps adimensionnel de la relaxation du champ de pression qui est toujours aussi faible dans la pratique.

Nous examinons le fluide composé de N composants chimiques que peuvent former trois phases coexistent : gaz, liquide-1 (l'huile), le liquide-2 (l'eau). Il est clair que le cas de coexistent de deux phases gazeuses est impossible (à l'exception de certains cas très particulier, spécialement étudié en physique moléculaire), parce que deux gaz sont totalement miscibles entre eux.

Mathématiquement l'augmentation simple du nombre de phases liquides dans un système semble d'être une généralisation naturelle du cas diphasique qui n'impose pas des problèmes techniques. Toutefois, du point de vue de la physique, la formation de la troisième phase liquide coexistant dans un système de composants n'est pas un phénomène si simple. Il suffit à noter que en principe dans le système à deux composants la troisième phase liquide ne peut pas apparaître.

Selon la définition de deux phases coexistent, elles sont deux fluides qui sont séparés par une interface. L'interface est définie comme la surface de la discontinuité des propriétés physique et chimiques de ces fluides. Par exemple, l'interface entre le gaz et le liquide représente la surface de la discontinuité de la densité de fluide. Dans le cas de deux liquides coexistant, la densité n'est pas la propriété principale qui détermine une interface, les den-

sités des liquides sont souvent identiques. Le facteur principal qui détermine l'apparition de la discontinuités entre les deux liquides est leur composition très différente.

Cette différence apparaît dans les compositions, à son tour, en raison du fait que le mélange contient au moins deux composants chimiques qui ont la nature chimique très différente, de sorte que leur coexistence dans une phase est difficile et ils préfèrent être séparés l'un de l'autre. Cette séparation produit la formation de deux phases. Chaque phase ne contient pas du composant non-cohérent. L'exemple typique est le système coexistant de l'huile et l'eau. Le composant chimique H_2O est très difficile d'être dissous dans l'huile liquide, alors qu'il est largement présent dans la phase liquide aqueux. Dans la même façon, les hydrocarbures lourds qui font la base de la phase huile sont pratiquement insoluble dans la phase aqueuse. En même temps, ces phases peut contenir plusieurs composantes communes, comme CH_4 , CO_2 , O_2 , et d'autres. Tous ces composants peuvent être dissous dans l'huile ainsi que dans l'eau.

Donc, la présence de la deuxième phase liquide dans notre système signifie que la composition de phase doit maintenant être caractérisée par trois groupes de composants :

- I Les composantes qui peuvent être dissout dans toutes les phases ;
- II Les composants qui ne peuvent pas être dissous dans le phase aqueuse ;
- III Les composants qui ne peuvent pas être dissous dans l' la phase l'huile.

(Dans la pratique, la non-dissolution absolue devrait être remplacé par un très faible dissolution.)

Cette propriété n'a pas d'influence sur les équations hydrodynamiques de manière significative, mais simplifie les relations thermodynamique en réduisant son ordre. En effet, plusieurs équations de l'équilibre de phase devient sans signification et disparaissent.

Dans la thèse présente cette propriété sera pas exploité en raison du fait que nous avons seulement analysé les systèmes à faible nombre de composants. Toutefois, dans les futurs développements cette propriété peut jouer un rôle très important.

La première étape dans le développement du modèle asymptotique consiste à l'élabora-

tion du modèle compositionnel, dans la forme "canonique", similaire à celle obtenue pour le cas diphasique.

Comme nous l'avons déjà mentionné la forme de système est appelé canonique, si les dérivés principaux de chaque équation différentielle décrit le comportement physique d'une variable de base, de manière que toutes les équations décrivent les variables différentes. De ce fait, chaque équation de la forme canonique, considéré en ce qui concerne les dérivés principaux, peut être interpréter comme l'équation de transport de la variable correspondante. La forme canonique a donc un sens physique claire.

Dans la forme canonique finale, nous allons trouver la liste ci-dessous des équations : La première équation formulée pour l'ensemble de fluide, peut être examiner que celle décrivant l'écoulement de gaz, car les termes correspondant aux liquides sont de petite taille. La deuxième équation décrit les transports commun de deux saturations de l'huile et de l'eau. La troisième équation décrit le transport de saturation de l'eau, et la dernière série des équations décrivent le transport des concentrations des phases.

En utilisant les règles mnémoniques établies pour l'écoulement diphasique, nous avons facilement obtenu le modèle asymptotique pour l'écoulement triphasique à l'ordre zéro de la forme canonique du modèle compositionnel.

Le modèle limite obtenu constitue le système de trois équations hydrodynamiques pour pression et de deux saturations et le modèle thermodynamique indépendant, qui comprend $N - 3$ nouvelles équations différentielles.

Les dernières $N - 3$ équations pourraient être transformées en système des équations différentielles de thermodynamique si l'on examine le long d'une ligne de courant.

Donc nous avons obtenu le modèle général de thermodynamique divisé, avec $N - 3$ équations différentielles qui pourrait être résolu de façon indépendante à l'aide de la relation fermeture de thermodynamique.

Le modèle divisé de thermodynamique, décrit le comportement d'un système compositionnel du gaz l'huile et l'eau en mouvement le long d'une ligne de courant dans le milieu poreux.

Ce système des équations ajoutées aux relations d'équilibre de potentiel chimique contient $3N - 3$ équations et $3N - 2$ variables inconnues : $N - 1$ variables des concentrations dans la phase de gaz, $N - 1$ variables des concentrations dans la phase de l'huile, $N - 1$ concentrations dans la phase de l'eau, et la pression. Ce système détermine tous les concentrations des phases comme fonction de la pression.

Ce système est totalement indépendant du sous-système hydrodynamique. Comme précédemment, un tel modèle n'est valable que le long d'une ligne de courant.

Les autres relations thermodynamique ne changent pas : trois équations d'états déterminent les densités des phases, et trois équations d'états rhéologiques déterminent les viscosités des phases.

Similaire au modèle diphasique, il est possible de montrer que les sens physiques des équations différentielles de thermodynamique sont le fait que l'échange de débit de la phase totale est égale à celle de chaque composant.

Comme pour le cas diphasique, il est possible d'améliorer le modèle asymptotique de zéro ordre, par l'ajouter de certains termes qui sont formellement petits, mais peut devenir important dans certaines situations ou à l'intérieur de certaines couches limites, comme cela a été fait pour le cas d'écoulement diphasique.

Le modèle asymptotique de l'hydrodynamique est présenté par trois équations. De toute évidence, la première équation perd la condition initiale, donc il est valable uniquement en dehors de la couche limite de temps, formé dans le voisinage du point initial. Afin d'obtenir le modèle uniforme valable pour tous les temps, nous allons introduire le dérivé de temps à partir d'équation originale.

Le deuxième problème est lié à la non-linéarité du modèle compositionnel avec l'égard de deux saturations. En raison de la non-linéarité et la dégénérescence des perméabilités relatives, les deux liquides peuvent être également mobile et par fois plus mobiles que le gaz (à faible saturation en gaz). Afin de prendre en compte cet effet, nous allons conserver le terme responsable de la mobilité en liquide dans l'équation de la pression.

Troisièmement, il est utile de garder parfois les termes non-stationnaires qui dépendent de la dérivée par rapport de la pression dans les deuxième et troisième équations. Ces termes sont perdus dans l'expansion asymptotique car ils sont de l'ordre ω_j ou ε . Toutefois, dans certains cas particuliers, lorsque la motion de deux phases et la variation de la composition de phase sont très faible, alors la variation de la saturation est déterminée essentiellement par $\partial p/\partial t$. Mais en raison de la complexité suffisante du modèle asymptotique, dans le cadre de cette thèse nous allons négliger ces termes partout dans le modèle.

Comme le modèle asymptotique de la thermodynamique est valable seulement le long des lignes des courants, on est alors capable d'analyser la version 1D de tous les modèles. Comme dans le cas diphasique, nous examinons le système des coordonnées cartésiennes, ce qui implique un système des lignes des courants suffisamment droits avec une densité uniforme des lignes dans l'espace.

Comme dans le cas d'écoulement diphasique, le modèle thermodynamique asymptotique montre que les concentrations des phases dépendent de la pression et la pression constante au point de départ ou point d'arrêt de chaque ligne de courant. Ensuite, dans le cas d'une pression invariable, qui est le cas plus facile pour l'analyse, les concentrations de phase ne peut être que constant ou constant par morceaux. Le comportement des concentrations des phases est alors caractérisée par les discontinuités probables et les compositions invariables de la phase entre les chocs.

Les mélanges de trois composants sont représentés de la même diagrammes de phases comme le diagramme diphasique, mais avec l'apparition d'une zone triphasique le long de domaine diphasique. Dans la cas de trois composantes à pression et température fixes, la zone triphasique ne peut pas être présentée que par une courbe, conformément à la règle de phase de Gibbs. Pour les systèmes de quatre composants, le montant total des compositions de trois composants sont donnés sur trois axes, dans le diagramme cartésien de la phase. Une surface curviligne représente l'enveloppe de la zone diphasique qui constitue maintenant un volume. La zone triphasique donc sera présentée par une surface qui peut

être 2D ou 3D.

Le locus de composition invariable de phase est présentée par une surface plane à l'intérieur du domaine diphasique, qui est appelé le tie-plan ou le tie-triangle (parce qu'il devient triangulaire étant continué jusqu'aux côtés de pyramide). Cette trace de l'intersection de ce tie-triangle avec la surface trois-phase correspond à la tie-ligne pour l'état triphasique. Les tie-triangles sont équivalentes à des tie-lignes dans le cas de trois composantes.

Pour le cas de pression variable, les tie-lignes passant la zone de trois phases et quatre composantes seront remplacés par les P-surfaces, comme dans le cas pour deux phases et trois composantes. Les tie-triangles passant la zone diphasique vont former les P-volumes le long de l'axe de la pression.

Tout comme le cas de deux phases, le problème que nous examinons est le processus de variation de pression d'une valeur initiale P_1 dans le mélange triphasique jusqu'à la dernière pression P_2 .

Si le système reste en deux phases entre P_1 et P_2 , il est donc décrit par le P-volume. Si le système reste en trois phases, il est décrit par une P-surface appartenant à ce P-volume. La variation entre le fluide initial et le fluide d'injection va se produire le long d'un P-volume. Selon la construction de cette thèse, chaque intersection de celui-ci à une pression fixe représente un plan qui est un tie-triangle.

Nous examinons le problème de Riemann pour le gaz, l'huile et l'eau formulé en termes de nos équations fractionnées de l'hydrodynamique. Nous supposons la saturation initiale de l'huile et de l'eau et la saturation d'injection au point $x = 0$ pour le problème de Riemann. Le choc initial de saturation sera transporté par le mécanisme de convection et probablement déformé dans le temps par le côté droit de nos équations.

Ce problème devrait également être complété avec une condition au limite pour l'équation de pression qui définit la pression d'injection (la pression au point de départ de ligne de courant).

Les équations différentielles de thermodynamique devraient également satisfaire deux

conditions de Cauchy pour deux pressions au frontières du problème, la pression d'injection, où est la pression de départ, tandis que la pression initiale, est la pression à $x = 1$. La méthode de calcul de pression initiale est la même que dans le cas diphaseique. Ainsi, le modèle asymptotique conduit à un couple des problèmes thermodynamique de Cauchy qui détermine les compositions de deux fluides différents. Cela permet de déterminer au moins deux différents systèmes des relations de fermeture de thermodynamique, ou de la discontinuité dans les coefficients du système. L'emplacement de cette discontinuité n'est pas connu a priori.

Si le système reste en état de trois phase dans tout le domaine, à tout moment, la structure globale de la solution se compose des trois éléments suivants :

- S-choc Double qui est le choc simultanée à la fois de la saturation de l'huile et l'eau déterminé par les conditions de Hugoniot déduites directement des équations différentielles de l'hydrodynamique.
- S-choc Unique qui est le choc d'une seule saturation de l'huile ou de l'eau déterminée par les relations de Hugoniot aussi déduites directement des équations différentielles de l'hydrodynamique.
- SC-choc complet qui est le choc simultanée de les saturations et de toutes les concentrations des phases, qui sont induites par des discontinuités dans les coefficients de système des équations différentielles de l'hydrodynamiques.
- SC-choc Partielle qui est le choc simultanée d'une seule saturation et de toutes les concentrations des phases, qui sont aussi induites par des discontinuités dans les coefficients de système des équations différentielles de l'hydrodynamiques.
- Les ondes de raréfaction qui sont les fragments continues entre les chocs. Elles représentent une solution unique et continue pour les équations différentielles de l'hydrodynamiques.

Notez que les éléments tels que un "plateau" ne peut pas exister dans ce cas que les équations différentielles sont non-homogènes.

Si le système peut modifier son état de phase, la solution aura deux autres éléments :

- 3/2-choc qui est le choc de la transition de phase entre un fluide diphasique et un fluide triphasique.
- 3/1-choc qui est le choc de la transition de phase entre un fluide monophasique et un fluide triphasique.
- 2/1-choc qui est le choc de la transition de phase entre un fluide diphasique et un fluide monophasique.

L'admissibilité de l'ensemble de ces types de chocs et l'inadmissibilité des autres types peuvent être prouvées par des méthodes standard (similaire au cas diphasique), basé sur l'étude des condition de Hugoniot.

Le système complet des conditions de Hugoniot résultant de la modèle compositionnel complet, qui déterminent les chocs de la structure de solution ainsi que les chocs des coefficients du modèle hydrodynamique sont obtenus.

Chaque SC-choc est alors déterminé par les conditions asymptotiques additionnelles de Hugoniot, obtenues à partir du modèle compositionne complet.

l'agrandissant les résultats obtenus dans le cas d'écoulement diphasique, nous avons développé le système des conditions asymptotiques de Hugoniot quand les rapports des mobilités tendent vers zéro.

Le sous-système obtenu de $N - 2$ conditions de Hugoniot ne contient pas de vitesses, mais seulement des paramètres thermodynamiques et de la saturations.

L'un des points faibles de la théorie triphasique consiste à ce fait que le nombre de SC-chocs est inconnu. Nous suggérons la méthode indirecte à le déterminer, en inversant les résultats obtenus pour la cas d'écoulement diphasique. Dans le cas diphasique, nous avons montré que, si on accepte le nombre de choc égal à $N - 2$, qui est la valeur connue de la théorie général diphasique, le système des équations de la thermodynamique, de l'équilibre et de Hugoniot est fermé, en ce qui concerne des paramètres de tous les SC-chocs présentés dans la structure de la solution.

Maintenant, nous supposons que le nombre de chocs, M , est inconnu, mais il peut être détecté à partir de la condition qui dit le système des équation de la thermodynamique, de Hugoniot, et de l'équilibre est fermé en ce qui concerne des paramètres de tous les chocs. Le nombre des concentrations inconnues est $6(M - 1)(N - 1)$, tandis que le nombre des équations est $M(N - 4) + (M - 1)(5N - 3)$. La solution est unique, si ces deux valeurs sont identiques. Donc, le nombre des SC-chocs partielle va être $N - 3$.

Dans la même manière il est possible de montrer que le nombre de SC-chocs est fractionné. Cela signifie qu'il est impossible d'avoir seulement les SC-chocs complets dans le domaine de la circulation. Nous voyons également que pour un système des trois composants en trois phase les SC-chocs complets ou partiels n'existent pas.

Dans la thèse présente, nous avons simulé numériquement que le cas des systèmes de trois composantes en trois phases, profitant du fait que ces systèmes ont la structure de solution suffisamment simple que dans le cas général. En particulier, les systèmes de trois composants en trois phases ne peut pas avoir des SC-chocs, mais seulement le S-chocs et les chocs de transition de la phase.

Si le fluide injecté et initial sont tout les deux dans la zone triphasique, la solution devra avoir que les S-chocs.

Nous avons simulé l'écoulement du gaz, de l'huile et de l'eau dans deux cas différents :

I Mélange ternaire de méthane, décane et de l'eau.

II Mélange ternaires de dioxyde de carbone, décane et de l'eau.

Le système des équations asymptotiques de l'hydrodynamique a été discrétisée par la méthode des différences finies, entièrement explicite dans le temps.

Nous envisageons un processus isotherme.

Les équations d'équilibre ont été acceptés dans la forme de Wilson pour les K-valeurs qui sont les fonctions de la pression.

Si les concentrations totales de chaque composent sont données, alors les deux valeurs de K sont suffisantes pour déterminer des équilibres entre les phases pour l'ensemble de problème. Nous somme capable de trouver la troisième valeur de K (entre les phase aqueux

et phase gazeuse, par exemple) comme le rapport de deux K-values données.

La saturation a été simulée finalement dans un réservoir unidimensionnel à différents temps après le début de l'injection.

Grâce à ces résultats, nous avons résolu le problème de Riemann de transport en trois phases et trois composantes. Nous avons appliqué les solutions obtenues à l'analyser l'efficacité des différents technique de récupération du pétrole. En particulier, nous avons analysé la récupération améliorée du pétrole par l'injection de CO_2 et nous avons prouvé l'efficacité qualitativement différente de cette méthode en fonction de la présence ou de l'absence d'eau. En terme des solutions obtenues, nous sommes également capable d'analyser la technique connue de WAG (l'eau en alternance d'injection de gaz), qui est souvent appliqué pour récupérer l'huile.

Dans la dernière partie de cette thèse nous examinons deux cas différents de problème triphasique de Rimenn.

Premièrement le cas d'injection de l'eau dans un réservoir contenant initialement un mélange de méthane et de décane dans les phases gazeuse et oléique est examiné.

Nous examinons deux cas différents de ce problème. Le premier cas est lorsque la phase oléique est immobile, ce qui implique que sa saturation est inférieure à la saturation résiduelle. Le second cas correspond à l'huile mobile. Comme le SC-chocs n'existe pas dans un système ternaire, puis le comportement des concentrations sera continu et elles dépendent uniquement de la pression.

Dans les résultats obtenus les saturations du gaz et de l'huile dans la plupart de réservoir unidimensionnel est la même que leur saturations initiales. Ainsi, le processus d'injection semble être vraiment non efficace.

Comme le second cas dans le problème d'injection de l'eau, nous avons examiné un réservoir avec la phase oléique mobile. Les salutations obtenues du gaz et de l'huile montrent le déplacement des phases gazeuse et oléique et comme prévu un apex de l'huile produit juste après le choc de la phase aqueux.

Deuxièmement nous examinons le cas d'injection de dioxyde de carbone dans un réservoir contenant initialement des phase oléique et aqueux.

Nous examinons trois cas différents :

- 1) la phase aqueuse n'existe pas
- 2) l'eau initial est immobile
- 3) l'eau initial est mobile

Un déplacement piston-like de pétrole par le gaz se produit dans le premier cas, et près de tout le pétrole est poussé vers le puits de production.

Ce cas correspond au cas d'écoulement diphasique (gaz et pétrole) avec la dissolution complète de CO_2 dans l'huile. Les scénarios d'écoulement correspond à l'évaporation totale de pétrole ; le déplacement est de type piston-like, avec 100% de l'huile récupérée.

Dans le second cas, l'effet principal de l'injection consiste en l'évaporation du pétrole, le déplacement est toujours piston-like. En raison de la diminution de la masse initiale de pétrole, dans ce cas le déplacement est plus rapide. Le fait qu'une partie de CO_2 ne participe pas à la récupération du pétrole, étant dissous et perdus dans l'eau, ne réduit pas l'efficacité du récupération. Cela est dû le fait que la saturation de l'eau initial est faible.

Dans le dernier cas l'efficacité du déplacement est considérablement réduit, comme une partie importante de CO_2 maintenant dissout dans l'eau et ne déplace pas de l'huile. En outre, le volume de l'eau augmente de manière significative a cause de la dissolution de CO_2 .

Deux S-chocs sont observés dans la solution de tous les trois saturations. Le chock avant déplace que le pétrole. Le choc arrière déplace le mélange de pétrole et de l'eau. L'eau aussi forme un banc derrière le choc avant, de sorte que le pétrole est déplacé à la fois par le gaz et l'eau. Derrière le choc de l'arrière tout le pétrole est déplacé.

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Chapitre 1

Introduction

In the present thesis we will analyze the problems of modeling the processes of displacement of one fluid by another in porous medium, while concentrating our efforts on the adequate description of the internal fluid structure that can be very complicated and consist of several thermodynamic phases and a number of chemical components dissolved in these phases. Such fluids are usually called *compositional*. The mathematical models of such processes can be frequently reduced to a so-called Riemann problem, which explains the title of this thesis.

The theory of two- and three-phase compositional flow through porous media was developed basically according to the needs of forecasting the efficiency of enhanced oil recovery (EOR). The EOR methods consist of influencing reservoir process by physical or chemical agents (surfactant, polymers, heat, solvents, ...) with the objective to increase oil mobility and/or the sweep efficiency of the displacement process.

One of the most efficient EOR methods is the injection of miscible gases. The typical example is the injection of CO₂. During such an injection, chemical components of gas partially or completely dissolve in liquids, which can lead to a significant increase in oil mobility due to the reduction of oil viscosity or even to its partial or total evaporation. The miscibility between the injected and initial phases approaches the system to quasi single-phase behavior, so that the relative permeabilities becomes diagonal, the residual saturations tend to zero, the displacement tends to be piston-like. All these tendencies enhance oil recovery [Johns 1992; Bedrikovetsky *et al.* 1996].

From the theoretical point of view, in this case we deal with a two-phase system (gas - liquid) containing several chemical components presented in both the phases. The composition of the phases is variable in space and time due to permanent mass exchanges and is controlled by the individual dissolution laws of each component in each phase. Usually the hypothesis of the local equilibrium is accepted, based on the fact that the interface between the phases is very large in porous medium, so that the time of mass exchanges between phases is much lower than the characteristic macroscopic time of the displacement process. In this case, the dissolution of the components in phases is controlled by the laws of phase equilibrium. Thus, the hydrodynamics of the process is strongly coupled with the

thermodynamics.

In reality, the situation is frequently complicated by the presence of the third phase, other than oil and injected gas. This is the case of the connate water or mobile water coming from the adjacent aquifer. The role of this third phase can be very significant, as a part of the injected gas being dissolved in water can reduce the EOR efficiency. At the same time, the same gas dissolved in water can be considered as the positive effect ensuring the sequestration of CO_2 in geological strata. Another example of a three-phase compositional process is the WAG technique (water alternated gas) : the injection of the slugs of water alternated with gas.

Considerable efforts were spent to develop the theory of such processes. All this theory is based on analyzing the mono-dimensional displacement problem. The major parts of publications are devoted to the two-phase case. Three-phase immiscible flow problems (oil - water - gas) were also intensively studied. At the same time, a very low number of publications are devoted to three-phase compositional flow.

This chapter provides a review of the previous research in the areas of the immiscible and partially miscible two and three-phase flow through porous media. After this the objective of the present thesis will be formulated, and the selected approaches, methods and results obtained will be shortly described.

1.1 Compositional model and structure of solutions

1.1.1 About the mathematical model of compositional flow

First of all, it is necessary to mention that within all the theory which is analyzed below the reservoir temperature is assumed to be constant. This assumption is entirely acceptable if we do not analyze thermal EOR. This means also that the relation $T = const$ represents our trivial energy equation, so only the mass and momentum conservation equations are sufficient to model such systems.

All the multiphase fluids observed in oil engineering are multicomponent and contain N

chemical components like hydrocarbons from CH_4 to $C_{10}H_{22}$ and even heavier, as well as H_2O , CO_2 , N_2 , aromatic and benzoic components and probably sulfur. The full mathematical model of multiphase multicomponent flow consists of the momentum balance equations for each phase and the mass balance equations for each chemical component presented in the mixture. This model should be coupled with thermodynamic relations describing phase equilibrium and phase states. The flow of r -phase N -component mixture is described by $N + r$ nonlinear differential conservation equations for each component and phase, and $(r - 1) * N + r$ transcendental thermodynamic relations. The effective qualitative analysis of such a model is practically impossible. The solution to this system of equations should provide the behavior of the reservoir pressure, the volumetric saturations of each phase and the concentrations of each component in each phase. The total concentration are also of interest, but are not the independent variables being related to the phase concentrations and saturations.

The high order of the system of differential equations which constitute this model, their strongly nonlinear character and coupling with high-order thermodynamic sub-system makes the mathematical analysis and numerical modeling of such processes extremely difficult.

If one considers only the thermodynamic part one can state that the thermodynamic theory of such systems is sufficiently well developed in fundamental works : [Coats 1980], [Firoozabadi 1999], [Danesh 1998]. Its mathematical description, which is frequently called the compositional model, consists of the equations of state for each phase, the rheological equations of state and the equations of equilibrium which assert that the chemical potential of a given component is the same in all the phases and the phase pressure and temperatures are identical. Usually such a model represents a high-order nonlinear transcendent system of equations which may be solved numerically by using various iteration procedures.

Very frequently the dissipative effects of capillarity, diffusion, and dispersion are negligible. In this case the transport is dominated by advection and is then described by a system of nonlinear, hyperbolic, first-order differential equations. The typical displacement problem is described by a couple of conditions that specify the initial state of the fluid and

the properties of the injected fluid through a boundary. As an example, we can specify the initial composition of the fluid in place and its volumetric saturation and the composition and the saturation of the injected fluid. This is formulated in terms of the specific initial conditions containing an initial shock at the domain boundary. Such a mathematical problem is known as the Riemann problem.

1.1.2 Reduced model of ideal mixing

The theoretical analysis of the full compositional model is practically impossible. The analytical qualitative theory was developed only for a reduced model which is based on three simplified laws of component mixing. This model is accepted everywhere, by all research groups working in this field, despite of its very approximative origin.

i) The pressure is assumed to be constant in thermodynamic sub-system. Due to this the thermodynamics is controlled only by component concentrations, moreover the number of these independent concentrations is frequently very low. According to the rule of Gibbs, the number of independent thermodynamic variables (pressure and phase concentrations) which can be varied without changing the phase state of an isothermal system is equal to $N - r + 1$ where N is the number of chemical components and r is the number of phases. If we fix pressure, then the number of independent phase concentrations that determine the phase behavior becomes $N - 2$ for two-phase system and $N - 3$ for three-phase case. So, the three-component system is controlled only by one phase concentration in two-phase case and is totally invariable in three-phase case. In both cases the thermodynamics becomes practically trivial. This is the reasons why it is interesting to introduce the assumption of constant pressure.

Such an assumption, based on the fact that the EOR processes have the objective of maintaining the reservoir pressure, is however too strong and does not correspond to the reality. Indeed, having a constant pressure means the absence of pressure gradients which would lead to the zero flow velocity.

ii) The ideal mixing law is assumed for all the components in all the phases, which says

that the volume occupied by a given mass of a component at fixed P, T is constant whatever contain of the fluid phase. This assumption leads to the fact that the volume of a phase represents the sum of the volumes occupied by the pure components. This assumption means also that the mixing of several components in a phase happens without phase compression or expansion. So the system is incompressible. At the same time, this does not exclude the variation of the phase densities, which happens due to adding or subtracting more or less dense portions of components. Due to this it is possible to change oil properties which is the desired final effect. Due to the incompressibility, it is possible to introduce the volumetric phase concentrations of the components which significantly simplifies the flow model.

In practice the ideal mixing is observed only when the concentration of the solute is very low. In other cases, the true mixing can be very different from the ideal mixing, which leads to the fact that the sum of the volumetric concentrations is no longer equal to one, i.e. they are not the true concentrations. This can produce significant quantitative errors in modeling.

- iii) The dissolution law is accepted (especially in three- and four-component cases and higher) in the form of constant K -values. For a given component its K -value is the ratio between the concentrations of this component in gas and liquid. Thus, a constant K -value (at a constant pressure) corresponds to the Henry law which assumes the linear relation between the concentrations in gas and liquid.

It is however well known that the Henry law can be applied only to describe the weak dissolution of gaseous components in liquid. In addition, this law is valid only for low pressure and temperature.

The assumption about the constant K -values determines the effect of the invariable shock structure in time. This means that the parameters of shocks (forward and backward saturations and concentrations) are sufficient to be determined once. If this assumption is not accepted, the structure of the solution changes qualitatively, the shocks become non-stationary, and the qualitative analysis of the process be-

comes practically impossible, especially in the case of high number of components and phases.

All these assumptions are very strong, which determines the sufficiently weak link of the developed theory with the practice. At the same time, any theoretical developments seem to be impossible for more complicated systems approaching the reality. Moreover, despite of these simplifications, the developed analytical theory predicts qualitatively well the fluid dynamics in reservoirs.

The compositional model of ideal mixing (neglecting the dissipative terms) is reduced to the system of $N - 1$ quasi-linear homogeneous differential equations of first order. The unknown variables of this system are : $N - 1$ phase saturations and $N - r$ independent phase concentrations. The homogeneity of these equations results from the conservation of the total mass of each component, as the chemical reactions are totally ignored.

So the number of phases does not influence the order of the flow model, as the increase of the number of phases provokes simultaneously the reduction of the thermodynamic degree of freedom (i.e. the reduction of the number of the independent phase concentrations).

1.1.3 Shocks in the solution structure and related problems

The initial shock (of concentrations or saturation) introduced in the Riemann problem will be kept in the structure of the solution if the dissipative effects capable to destroy it are ignored. The evolution and motion of this shock can be very complicated with generation of new mobile shocks whose parameters are unknown and should be determined in the course of solving the entire problem. Physically these shocks correspond to various displacement fronts as the mechanical piston-line front, the front of liquid evaporation, or the front of a sharp variation of liquid composition, and so on...

The practically inevitable presence of shocks in the solution structure, which are very strong singularities, play simultaneously positive and negative role. The negative role is proved in numerical modeling of such systems, which determines the necessity to develop very fine methods of shock detection. At the same time, the problem containing disconti-

nities enables frequently to develop fully analytical or semi-analytical solutions, which is practically impossible in the case when the shocks are eliminated by introducing dissipative effects. The existence of the exact analytical solutions (in strongly nonlinear equations) has determined the success of this theory. Even if these solutions are impossible to use in sophisticated practical cases, they play the role of a template to verify the validity of approximate numerical methods.

The presence of a shock provokes two related problems which concern its description.

First of all, in the vicinity of a shock differential equations become invalid. From the fundamental theory of gas dynamics it is known that the mass balance equations in the vicinity of the shock can be reformulated in the form of some algebraic relationships called the Hugoniot conditions. The technique of obtaining these conditions is well known and does not pose any problems. At the same time, we will show that within the framework of the present thesis a new non-trivial problem will arise related to the insufficient number of Hugoniot conditions in several models.

The second fundamental problem in the development of this theory was related to the non-uniqueness of shocks : various discontinuous solutions satisfy the Riemann problem and Hugoniot relations. In order to select the unique physically acceptable solution, the additional conditions should be used at each shock, which compensates for the loss of some physical effects caused by neglecting dissipative phenomena in the flow model. Such a conditions should ensure the stability of shocks, the principles of thermodynamics, and some other fundamental principles. We will call these conditions *structural*. One distinguishes three kinds of structural conditions.

First of all the structural condition should take into account the fact that the shocks are only a mathematical idealization of the true physics which is obtained by eliminating dissipative effects. A dissipative effect represents a non-equilibrium process which should tend, according to the thermodynamics, to an equilibrium state. This means that the entropy increases in any dissipative processes. The additional condition at a shock is then called the entropy condition ; it says that the system entropy should increase while passing through the shock. For the first time the entropy conditions were suggested by [Lax 1957].

This condition was presented finally in the form of some inequality between the number of characteristic lines entering in the shock and leaving the shock. Such a condition can be obtained technically in various ways. The direct way consists of formulating the equation for the entropy production and analyzing its behavior while passing through the shock.

Another structural condition can be obtained by adding the dissipative terms in the model and by analyzing the limit of these equations when the dissipative effect tends to zero. It was shown that this technique leads exactly to the entropy condition. At the same time, in several situations, various dissipative terms added to the flow model can lead to various structural conditions at the shocks [Oleinik 1959].

Another kind of structural conditions is based on the principle of the continuous dependence of the solution on the initial conditions. This condition is obtained by perturbing the initial conditions and by analyzing the limit behavior of the perturbed solution when the perturbation tends to zero. In the major part of cases the obtained result is equivalent to the entropy condition.

It is known that, for the system of high order, all the mentioned conditions become insufficient even if they provide non-identical mathematical relations. This is typical for multicomponent three-phase systems. In this case it is necessary to apply additional reasonable conditions (like continuity of the velocity...) and use the trial-and-error method of constructing the solution, which is however based on the personal experience of researchers rather than on the strict theory.

1.1.4 General structure of solutions

Within the framework of the model of ideal mixing it was shown that the Riemann problem completed with the Hugoniot and entropy conditions has the solution which is stable and unique, under condition that this system is hyperbolic or non-strictly hyperbolic. The conditions of hyperbolicity are usually satisfied in the major part of the practical cases.

If, in addition, the Riemann conditions are constant, then the problem is self-similar and has analytical solution. It can be constructed by using the method of characteristics

(MC).

The general structure of the solutions has been shown to be universal; it contains the alternation between three basic elements :

- *the shocks* or solution discontinuities ;
- *the rarefaction waves* : the zones in which the solution remains continuous and non-trivial ;
- *the plateau* : the zones in which the solution is constant.

In major parts of cases, the parameters of shocks are invariable in time, which significantly simplifies the solving technique.

1.1.5 Piece-wise constant approximation for phase concentrations

The simplifying hypotheses accepted to advance the qualitative theory used in various papers do not concern only the mixing laws, but also various details of the solution structure. The most significant assumption which is very frequently used, especially in the case of three-phase flow with high number of components, consists in the particular behavior of the independent phase concentrations.

The phase concentrations are frequently assumed to be piece-wise constant. The discontinuities in the behavior of phase concentrations, which are authorized by the conservation equations, are mobile.

This hypothesis is based on the fact that the transport of the phase concentrations is almost linear. Indeed, the non-linearity in the concentration transport can be caused by fluid compressibility or by non-linear diffusion. Within the framework of the ideal mixing model, the fluid is globally incompressible and the diffusion is totally neglected. So the transport of phase concentrations is purely convective (advective) and is not explicitly influenced by nonlinear effects. Such a transport is expected to be described by a linear transport convection equation. The Riemann problem with constant initial and boundary conditions for a linear hyperbolic equation has a piece-wise constant solution with the shock propagating at the given velocity.

In reality, the equation of transport of phase concentration is weakly non-linear, as the velocity transport contains a weak nonlinearity with respect to concentrations. Due to this, the behavior of phase concentrations may be non-linear, and thus different than piece-wise constant. The piece-wise behavior of the phase concentrations is proved to be exact in the two-phase three-component case, but is not strictly justified for more complicated fluids. The non piece-wise solutions have been constructed in [Orr 2003] for multicomponent problem. At the same time, the sizes of the zones of non-constant continuous behavior are so small that they can be neglected. Due to this we consider the piece-wise constant approximation as a very good idea for all the cases.

1.2 Ideal mixing theory for two- and three-phase compositional problems : State of the art

1.2.1 Two-phase partially miscible displacement theory

In the case of two-phase compositional system the Riemann problem has analytical solutions that have a sufficiently simple structure.

[Buckley and Leverett 1941] developed the first analytical solutions for one-dimensional immiscible two-phase flow through porous media, as the model of oil displacement by water. The phases were also incompressible. The authors constructed the graphical-analytical solution.

[Welge 1952] simplified the water-oil displacement problem with a graphical method to construct the shock. He has shown that the shock conditions have a graphical interpretation, being presented by a straight line tangent to the fractional flow function ($F(s)$) on the $F - s$ diagram. This tangent line is known in the mathematical theory of quasi-linear differential equations as the Oleinik enveloped.

In [Helfferich 1979] the general analytical theory based on the method of characteristics for two-phase multi-component displacement was presented.

The analysis of the miscible gas and surfactant injection in oil was initially limited

by ternary systems (three chemical components) : [Helfferich 1982 ; Hirasaki 1981 ; Larson 1979 ; Wachman 1964 ; Zanotti *et al.* 1983].

The model with three components, represents two differential equations, hyperbolic and non-linear, formulated for the total concentrations of two components. The solution is strongly based on the fact that the phase concentrations remain pieces-wise constant and can change only in a discontinuous way. Such a property of solution induced the introduction of the concept of tie-lines that are the lines of a constant phase composition on the phase diagram. Each rarefaction wave of the total concentration in the structure of the solution has been shown to correspond to an invariable phase concentration, or two a fixed tie-line. The shocks between the rarefaction waves are then the shocks between two different tie lines.

The two-phase three-component system determines the main properties of the solution of the Riemann problem. It is entirely characterized by two *external tie-lines* : one of them corresponds to the composition of the injected fluid, while the second one represents the composition of the initial fluid in the reservoir. Both the external tie-lines are imposed by the Riemann conditions. The variation of the phase composition happens suddenly, in the form of a shock relating two tie lines. This shocks is double as it determines also the shock of the total composition (and the liquid saturation too). It was also shown that in the zone of invariable phase composition, the total composition (and saturation) can also have shocks, which is however single. These principles of constructing the solution were used further in multicomponent case.

The first solutions to quaternary systems were developed by [Monroe *et al.* 1990]. Through this solution he has shown that in a two-phase system with the number of components higher than three, the *crossover tie-lines* arise, which are intermediate between two external tie-lines and which are unknown. Monroe accepted that the phase concentrations can vary only in a discontinuous way while the passage from a tie-line to another one happened through the shocks (only). This assumption has given him the possibility to develop the technique able to determine the crossover tie-lines.

One-dimensional solution to the Riemann problem for two-phase case with four and

more chemical components was suggested by [Bedrikonetsky, Chumak 1992]. In a fluid consisted of N chemical components, it was accepted that the variation of the phase composition between the injected composition and the initial one happens through $(N - 3)$ crossover tie-lines.

Later the MC has been used to find analytical solutions to two-phase problem with an arbitrary number of components [Johns 1992; Dindoruk *et al.* 1992; Yuan 2003; Wang 1998; Jessen *et al.* 1999; Pires *et al.* 2004; Yuan and Johns 2002]. A lot of papers were focused on the case of the single-phase initial state (a liquid oil). The case of the two-phase initial state was analyzed in [Lake 1989; Jessen and Orr 2003; Bedrikovetsky *et al.* 1996].

[Wang 1998] used the fact that the tie-lines cross one another to develop a fast and efficient algorithm to obtain analytical solutions for multicomponent systems with an arbitrary number of components.

As a consequence of this theory the concept of a *compositional path* became significant in the technique of solution construction. It was shown that a solution to the Riemann problem with the alternation of rarefaction waves, shocks and plateaux, has a bijective image on the phase diagram in the form of a *path* relating the corresponding tie-lines. Such a path is quantitatively informative, as its vertices determine the forward and backward concentrations at the corresponding shocks. It is then sufficient to construct the path to determine the entire solution structure. Mathematically a path on the phase diagram represents practically the entire analogue of the trace or the projection of the Riemann invariant to the space of total concentrations.

1.2.2 Three-phase immiscible displacement theory

The immiscible three-phase displacement was extensively studied in a number of publications. The MC for three-phase case is applied in the similar way as in two-phase case. [Falls and Schulte 1992 and Guzman 1995] suggest the detailed discussion on the construction of some analogues to compositional paths for three-phase immiscible flow. At the same time, the three-phase case described by the system of two coupled nonlinear hyperbolic

equations, has revealed two new research problems which had no analogues in two-phase case.

First of all, there is the problem of non-uniqueness of the entropy conditions. A considerable number of mathematical researches were devoted to this problem. First of all it was shown that the classical Lax and Liu entropy conditions at the shock often fail or are insufficient : [Azevedo and Marchesin 1995 ; Azevedo *et al.* 1996, 1999, and 2002]. Some more general conditions can be obtained by the classical method of including dissipative effects (diffusion-dispersion) in the flow model and by tending next these terms to zero. The resulting conditions determine the unique solution [Isaacson *et al.* 1990 ; Marchesin *et al.* 1997 and 1999]. However it was shown that various dispersion tensors lead to different zero-dispersion limits. In particular, this implies that a numerical solution influenced by the artificial numerical dispersion can converge to a false solution of equation with true physical dispersion [Marchesin *et al.* 1997]. It was also shown that in three-phase case a new kind of transitional shocks arises : [Isaacson *et al.* 1990]. [Schechter *et al.* 1996] discusses the origin and the construction of transitional shocks in detail.

The second new problem was the demonstration of a probable flow instability in three-phase case. It was discovered in [Bell, Trangenstein, and Shubin, 1986] that two quasi-linear equations describing three-phase flow without dissipative terms can lose the hyperbolicity and become elliptic. As the initial problem for an elliptic system is unstable, this means the physical instability arising in the system behavior within a region of saturation variation. [Shearer and Trangenstein 1989] showed that the probable loss of hyperbolicity is influenced by the form of the relative permeability curves and can be reached for many physically meaningful relative permeability models at least at one saturation value. Thus, in contrast to the two-phase flow model, the three-phase flow without dissipative terms may not be necessarily hyperbolic, but also non-strictly hyperbolic, or mixed hyperbolic and even elliptic, depending on the relative permeability model used [Guzman, 1995]. At the next step it was shown that only the relative permeability model in which each phase permeability depends only on its own phase saturation (the model of Stone) are guaranteed to not have elliptic regions [Trangenstein 1989]. Even in models where non strictly

hyperbolic behavior is guaranteed, the hyperbolicity may fail at more than one interior saturation values [Guzman and Fayers 1994].

A detailed discussion on the relative permeability (RP) models is beyond the scope of this work. We suggest only a brief review. Various models of three-phase RP were studied in [Leverett and Lewis 1941]. [Johnson *et al.* 1959] first proposed a method enabling to determine RP from core flood experiments. [Grader and O’Meara 1988] studied the three-liquid RP in packed beads and concluded that RP of each phase was the function of all three saturations. [Siddiqui *et al.* 1996] studied the flow of three immiscible liquids in glass packed beads and also concluded that RP of each phase was the function of all three saturations. In the water/oil/gas system studied in [Leverett and Lewis 1941] the water RP was a function of its own saturation, while the oil and gas RP were dependent on the saturation of all three phases. [DiCarlo *et al.* 2000] studied RP in water-wet, mixed-wet and oil-wet packed sands and found that oil RP was non sensitive to oil saturation, (at sufficiently low oil saturation values), while the gas RP was sensitive to all three saturations. [Corey *et al.* 1956], [Saraf and Fatt 1967], and [Saraf *et al.* 1982] studied flow of water, oil, and gas through sandstones and concluded that only the oil-phase RP was affected by saturation of the other two phases.

1.2.3 Three-phase partially miscible displacement theory

In the case of three phases containing N chemical components each component is assumed to possibly dissolve in any phases. However the contents of several components in several phases may be very low. As a result the three-phase system is thermodynamically not too stable and transits frequently into a two-phase system (or even becomes single phase). Due to this the thermodynamic diagram of a multicomponent system contains large two-phase zones alternated with narrower three-phase zones.

Considerable number of publication devoted to three-phase partially miscible displacement, [Giordano and Salter 1984].

Despite the fact that the number of differential equations in the ideal mixing model

does not depend on the number of phases (see section 1.1.2), the structure of these equations in three-phase case is sufficiently different. For instance, according to 1.1.2, for a two-phase four-component system the flow model consists of three differential equations which determine one saturation and two phase concentrations, while a three-phase four-component model is described also by three equations which contain however other physical variables : two saturations and one phase concentration. The concentrations are transported almost linearly (see section 1.1.5 and the relative discussion on this subject), while the saturation transport is highly nonlinear, as the transport velocity depends on the relative permeabilities (RP) which are non-linear functions of saturations. So the introduction of an additional saturation in three-phase model instead of a concentration increases the degree of nonlinearity of the system.

The increasing complexity of the three-phase compositional system is also determined by the more complicate behavior of RP regarding to the immiscible three-phase flow. The RP in a compositional system should depend on phase concentrations but not only on phase saturations. Indeed, the presence of some components highly soluble in all the phases reduces the difference in phase properties. This means that the system approaches to a quasi single-phase behavior, which is characterized by diagonal RP. So the phase composition can influence RP. The experimental information on such a dependence is practically non-existing. Some very rare experimental measurements of three-phase RP (and two-phase too) in compositional system were undertaken in [Delshad *et al.* 1987]. The authors used a partially miscible brine, n-decane, and IBA alcohol mixture. The three-phase relative permeabilities appear to be the functions of their own phase saturations. The dependence on phase composition was not detected.

The first solutions to the Riemann problem of partially miscible three-phases three-component system were obtained in [Laforce *et al.* 2005] using the MC. As mentioned in section 1.1.2, the three-component three-phase ideal mixing model has a trivial thermodynamics (the zero degrees of freedom). This means an invariable phase composition, which simplifies the solution. However, the problem consists in the inevitable appearance of the zones where the three-phase system transits to two-phase and even to single-phase.

The determination of the placement and the parameters of the shocks between these zones called the shocks of phase transitions represents a true puzzling problem.

The insufficiency of the standard system of Hugoniot and entropy conditions was illustrated. Due to this the unique solution was obtained by using the Hugoniot shock conditions, the entropy constraints, some velocity constraints, and some arguments in favor of the continuity of several functions. The obtained solutions correspond to the physics of the process, but are not justified as the true unique physical solutions.

Later in [Laforce, Jessen and Orr 2007] the same method was developed for the case of four-component partially miscible three- phase displacement. The insufficiency of the structural conditions at the shocks, is typical for this case.

One of the new results of this approach concerned the fact that the phase concentrations can vary in a continuous way, but not only by shocks. This means, in particular, that all the previous techniques of solution were inapplicable in this case. The authors have developed another technique based totally on analyzing the compositional paths in the phase diagrams without using the fractional flow diagrams. At the same time, the construction of several path elements required significant efforts. As in the two-phase case, a path corresponds to a projection of the Riemann invariants on the space of total concentrations. In the four-component case, two qualitatively different Riemann invariants exist which determine two kinds of paths (slow and fast). Both they are determined through a nonlinear implicit system of equations whose graphical interpretation can be obtained only numerically. Due to this, the suggested graphical technique of solution was sufficiently complicated and required to perform a serious volume of numerical simulations in order to construct the paths.

1.2.4 Numerical modeling of multiphase compositional flow

For real systems that are not described by the simplifying mixing assumptions introduced in section 1.1.2, the only method of analyze is the numerical simulation [Eilerts, Sumner and Potts 1965], [Eilerts and Sumner 1967], [Aziz and Settari 1979], [Coats 1980].

However, the numerical method appears to be weakly efficient being applied to nonlinear systems of high dimension possessing several shocks in the solution structure and coupled with high-order system of thermodynamic relationships.

Due to this coupling, at each step of solution the thermodynamic nonlinear high-order sub-system should be solved at each space point and in each time instant. Therefore, the global algorithm becomes so complex that it frequently can not be realized in practice, while leading to the lack of time and CPU memory, algorithm divergences, or numerical instabilities.

1.3 HT-split compositional models

Other attempts were undertaken with the objective to develop the theory of real compositional fluids that are not based on simplifying mixing laws. The most significant attempt consists in separating the thermodynamics from the hydrodynamics (*the HT-splitting*). Within the scope of this separation it is expected to simulate the thermodynamics once for all the space and time points and then to substitute the calculated thermodynamic functions into the hydrodynamic problem.

Only three attempts to split H and T are known in the literature. Two of them concerns however the ideal mixing model.

All the suggested split models concern two-phase flow, and up to now nothing was proposed for three-phase compositional flow.

1.3.1 HT-splitting in the ideal mixing model

First of all, [Entov 1997] showed that the Riemann problem for the ideal mixing model in two-phase multicomponent case can be formally split into a physico-chemical and a hydrodynamic parts, if the piece-wise constant approximation for phase concentrations is assumed (section 1.1.5). Such an approximation really means automatically that the H and T are split, but the introduction of this hypothesis is simply postulated. Moreover, the

splitting is reached within the ideal mixing model, which does not improve the modeling of real systems.

[Pires, Bedrikovetsky and Shapiro 2005] suggested another way to split H and T , by introducing the specific replacement of variables into the two-phase compositional model. They reduced the system of equations to auxiliary system containing only $N - 1$ thermodynamical variables and to one flow equation containing one hydrodynamic parameter (saturation). Unfortunately this method was developed for the ideal mixing model for the cases which can be treated by traditional technique.

1.3.2 Asymptotic HT-split model for real systems

The asymptotic splitting between thermodynamic and hydrodynamics in gas-liquid flow was proposed in [Oladyshkin and Panfilov 2006]. In this work the full compositional model is used and none of the simplifying assumption introduced in the ideal mixing model (section 1.1.2) is used. The true properties of the fluids and the true laws of mixing are considered.

The procedure is based on two physical properties of the natural multiphase system :

- i) the liquid-gas mobility ratio is small; this is typical for any natural gas-liquid systems due to the high difference in phase viscosities. This assumption means that the characteristic parameter responsible for the liquid-gas mobility ratio ω is small.
- i) the time of stabilization of the pressure field is much smaller than the macroscopic time of total displacement in the reservoir. This property is also satisfied for all the natural reservoirs, which was shown in [Panfilov 1986], [Panfilov and Shilovich 2000]. Indeed the time of pressure stabilization is determined by fluid expansion or rock compaction, which is very fast processes having the characteristic time of several minutes, while the total time of displacement has the order of several years. Mathematically this means that the compositional model contains the parameter responsible for this time ratio ε which is also small.

Using these properties and assuming $\varepsilon, \omega \rightarrow 0$ the authors have succeeded in transfor-

ming $N - 2$ mass conservation equations into differential thermodynamic equations that did not include time and space variables. These new thermodynamic equations expressed the variation of composition in gas phase due to its exchange with low mobile liquid in an open thermodynamic system (the system in which gas flows through an immobile liquid is thermodynamically open).

Due to this the compositional model was split into the thermodynamic and hydrodynamic independent systems. Only the two-phase model was analyzed. For the two-phase case, the thermodynamic system includes $2N - 2$ equations : N classic equations of phase equilibrium and $N - 2$ new differential thermodynamic equations. This systems contains $2N - 1$ variables : $2(N - 1)$ phase concentrations and pressure. So this system determines the phase concentrations as the functions of pressure. The remaining hydrodynamic closed sub-system contains only two mass conservation equations with respect to two variables : pressure and saturation. The number of hydrodynamic equations does not depend of the number of chemical components.

The solution to two hydrodynamic equations was obtained for the problems of reservoir depletion characterized by continuous behavior of all the functions. In this case the solution does not impose any technical problems. However for the Riemann problem with discontinuous solutions this model was never applied before.

1.4 Outline of this thesis

The objective of this thesis is to advance the theory of compositional flow by avoiding strong simplifications typical for the ideal mixing model, and/or the a priori assumptions concerning the structure of the solution, as the piece-wise constant approximation for phase concentrations. Due to this, we preferred to base our analysis on the HT-split model developed in [Oladyshkin and Panfilov 2006] which leads to significant advancements by using only two universal properties of all the reservoir systems. In the present thesis we apply this approach to the displacement processes described by the Riemann problem. As this model corresponds to the limit of an asymptotic process, we will also call this model

asymptotic.

The analysis presented in the next chapters reveals that the Ht-split model can not be directly applied to the case of discontinuous initial conditions, as it provides an insufficient number of Hugoniot conditions at the shocks. This a new problem which is solved in this thesis. For the three-phase case, we develop the new HT-split compositional model.

1.4.1 New results obtained

The basic new results we pretend to obtain are the following :

- the derivation of the HT-split model as the limit of the asymptotic process when the liquid-gas mobility ratio and time ratio tend to zero (chapter 2,3);
- detection of the insufficiency of the Hugoniot conditions produced by the HT-split model for shocks (chapter 4);
- development of the full system of Hugoniot condition as an asymptotic process (chapter 4);
- development of the *front tracker* procedure, which yields to an independent closed system of algebraic equations that determines the parameters at all the shocks before solving the entire hydrodynamic problem (chapter 5);
- theorem of equivalence between the over-saturated single-phase fluid and the two-phase fluid (chapter 6);
- method of *negative saturations* which allows using the same system of two-phase compositional equations uniformly for two-phase and single-phase zones, whit an automatic detection of the fronts of phase transition (chapter 6);
- development of the asymptotic HT-split model for three-phase compositional flow (chapter 7);

1.4.2 Structure of the first part-Two phase compositional flow

In the first part we deal with the two-phase isothermal gas-liquid flow in porous media so that both the phases consist of several chemical components which can transit from

one phase to another one due to the partial miscibility. The displacement of one phase by another one is analyzed. The process is described by the Riemann problem for two-phase multicomponent flow of partially miscible, compressible fluids. We examine non ideal mixing. The pressure is variable in space and time. The phase compositions, densities and viscosities are variable functions of pressure.

The asymptotic HT-splitting technique has shown good results for the problems having continuous solutions, but it was totally inapplicable to determine the solution of the Riemann problem having discontinuities. The serious problem consists in that the HT-split model provides the insufficient number of Hugoniot relationships at each discontinuity.

We resolve this problem in chapter 4. The full system of Hugoniot conditions is obtained from the full compositional model by applying its asymptotic behavior in the vicinity of the shocks. We show that the obtained limit system is not equivalent to that obtained directly from the HT-split model.

This gave us the possibility to develop the general theory of displacement for two-phase multicomponent processes described by the Riemann problem within the framework of the HT-splitting technique. This theory has nothing common with the classical technique developed for the ideal mixtures, except the concept of tie-lines which is not however used directly but is generalized and replaced by the concept of P-surfaces for the non-ideal mixtures at a variable pressure.

We then analyzed the thermodynamic behavior of a compositional two-phase system at variable pressure. As mentioned before instead of the tie-lines (lines of an invariable phase composition) used in the classic theory at constant pressure, we introduced the new concept of P-surfaces which represents the location of the solutions of the differential thermodynamic model, so that each cross-section of such a surface at a fixed pressure represents a tie-line. We make in evidence that the continuous part of the solution of the Riemann problem corresponds to a fixed P-surface, while a shock happens always between two different P-surfaces.

In the next step we developed the front-tracker procedure. It is shown that the obtained system of asymptotic Hugoniot conditions, being completed with the thermodynamic block,

can be reduced to a closed system of algebraic equations with respect to forward and backward concentrations of all the shocks. This enables us to obtain all the parameters of the shocks and trace their movement in space before solving the differential flow equations.

Then we developed the numerical solution to the differential flow equations with taking into account the fact that the parameters of shock are already determined. This allows application of very economic and fast numerical schemes. In some cases, the Riemann problem has analytical solutions based on applying a special diagrammatical technique. The analytical solutions are also obtained.

1.4.3 Structure of the second part-Phase transition

In the second part we examined the case with phase transitions, when the two-phase flow can form the zones with single-phase fluid over- or undersaturated by some components. In the phase diagram the over- and undersaturated fluid is situated far from the two-phase envelop, in contrast to the equilibrium single-phase states situated just at the interface between the two-phase and the single-phase regions.

It is necessary to note that the saturation value is not sufficient to distinguish the equilibrium gas and the oversaturated gas, being equal to 1 for both of them (similar for liquid). But it is significant that the behavior of the over- and undersaturated single-phase fluids and the single-phase equilibrium fluids are qualitatively different. In contrast to the equilibrium fluid, the composition of the over- and undersaturated single-phase fluids are no longer controlled by the phase equilibrium laws, but by other mechanisms (as diffusion,...). Due to this the contact between a two-phase fluid and an over- or undersaturated fluid is characterized by significant non-equilibrium behavior leading to intensive phase transitions in the contact zone.

The difference between the equilibrium single-phase fluid and the over- or undersaturated fluid is also manifested in the mathematical flow model. The model of an equilibrium single-phase fluid is the limit case of the two-phase model when the gas saturation tends to zero or one, which is not the case of the over- or undersaturated fluid whose model is

totally independent of the two-phase model.

Therefore, the flow in two-phase zones and in single-phase over- or undersaturated zones is described by two independent systems of equations, which imposes serious problems in modeling such processes.

In particular, any algorithm of modeling such processes should know when and where it has to switch between these two models. This means that the location of the interfaces between the two-phase and the single-phase zones must be detected before solving the differential flow equations. This is however possible to do only in some simple cases. In general case, the detection of the mobile interfaces is performed in course of solving differential flow equations, which appears to be impossible in this case.

Another problem, is related to the fact that the physically correct boundary and initial conditions should be formulated in terms of the total concentration and not saturation, whereas the two-phase flow equations are formulated in terms of the saturation.

To overcome these problems, we suggest to use the uniform system of classic two-phase flow equations formulated in terms of pressure and saturation for both the two-phase and single-phase over or undersaturated zones, but while extending the concept of phase saturation so that it may become negative or higher than one. The absolute value of the negative saturation stands for the degree of distance the system has from the two-phase zone.

Method of negative saturation was suggested based on the theorem of equivalence proved in the present thesis, which says that any single-phase flow can be replaced by a hydrodynamically and thermodynamically equivalent imaginary two-phase system in which the phases are partially miscible, the phase composition is in equilibrium, the relative permeabilities, capillary pressure, interne phase diffusion, phase densities and viscosities satisfies special consistence conditions, and the phase saturations are negative and higher than one.

Using the saturation which is negative or more than one, we have also obtained the physically correct formulation of the boundary and initial conditions in terms of the extended saturation.

So the method enabled us to use the uniform two-phase flow model for all the single-phase and two-phase domains and to apply the numerical method through all over the simulation. Due to this, all the interfaces between zones are determined automatically.

We also showed that in the case of diffusion, where the shocks do not exist, the method is capable to detect the interfaces as weak discontinuities.

Using the method of negative saturation we examined the multicomponent Riemann problems in terms of Ht-split model with single phase initial and/or injection compositions and we completed our splitting method to cover all the cases that may happen in reality.

1.4.4 Structure of the third part-Three phase compositional flow

The last part then is devoted to extend the asymptotic HT-split model to the case of three-phase compositional flow in porous media, by using the fact of different mobility between gas and liquids. We have obtained the general asymptotic model, in which the thermodynamics and hydrodynamics are split. The thermodynamic part contains $N - 3$ differential thermodynamic equations and $2N$ phase equilibrium equations that determine phase concentrations as pressure functions. The asymptotic hydrodynamic model contains three equations independently of the number of chemical components that determine two saturations and pressure.

Using these results we have solved the three-phase three-component Riemann problem. As in the two-phase case, we developed the full system of Hugoniot conditions and the front tracker procedure.

We applied the obtained solutions to analyze the efficiency of various technological systems of oil recovery. In particular we analyzed the enhanced oil recovery by CO_2 injection and we proved the qualitatively different efficiency of this method depending on the presence or absence of water. In terms of the obtained solutions we are also able to analyze the technique known as WAG (water alternated gas injection) which is frequently applied to recover oil.

Chapitre 2

Two-phase compositional model

In this chapter we analyze the two-phase gas-liquid case within the scope of the asymptotic approach. We examine the general case of a non-ideal mixing and variable pressure in space and in time. The dissolution of chemical components in phases is described by the system of equilibrium equations formulated in general form. As the result, the phases are compressible, so that their densities and viscosities are variable and depends on pressure and phase composition.

2.1 Hydrodynamic equations

2.1.1 Mass and momentum conservation

Consider the two-phase gas-liquid system containing N chemical components that can be dissolved in both phases.

The mass conservation of each component yields the following system of equations :

$$\Phi \frac{\partial(\rho C^{(k)})}{\partial t_D} = \text{div} \left(\frac{\rho_g c_g^{(k)} K k_g(s)}{\mu_g} (\text{grad } P + \rho_g \vec{g}) + \rho_g D_g s \Phi \text{grad } c_g^{(k)} \right) + \text{div} \left(\frac{\rho_l c_l^{(k)} K k_l(s)}{\mu_l} (\text{grad } P_l + \rho_l \vec{g}) + \rho_l D_l (1-s) \Phi \text{grad } c_l^{(k)} \right), \quad k = 1, \dots, N \quad (2.1)$$

$$P \equiv P_g, \quad \rho \equiv \rho_g s + \rho_l (1-s), \quad C^{(k)} \equiv \frac{\rho_g c_g^{(k)} s + \rho_l c_l^{(k)} (1-s)}{\rho} \quad (2.2)$$

herein the superscript (k) refers to k^{th} chemical component; indexes g and l refer to gas and liquid phases; $c_l^{(k)}$ and $c_g^{(k)}$ are the mass (or molar) fractions ('concentrations') of k^{th} component in each phase, s is the saturation of the gas phase; P_g and P_l are the phase pressures; ρ_g and ρ_l are the mass phase densities [kg/m^3] or molar phase densities [mol/m^3] respectively to the choice of type of concentrations; μ_g and μ_l are the phase dynamic viscosities; ρ is the total mass or molar density; $C^{(k)}$ is the total molar fraction of component k ; K is the intrinsic permeability; Φ is the porosity; k_g and k_l are the relative permeabilities; $D_i^{(k)}$ is the diffusion coefficient of component k in phase i ; t_D is the time; $\vec{X} = \{X_1, X_2, X_3\}$ are the space variables.

The chemical components are assumed to be ordered decreasingly, so that the first component is the lightest.

The formulation (2.1) means that the transport velocity of the component k in phase

i , $\vec{V}_i^{(k)}$, is governed by the sum of the Darcy law and the Fick diffusion law :

$$\begin{aligned}\vec{V}_l^{(k)} &= -\frac{Kk_l(s)}{\mu_l} (\text{grad } P_l + \rho_l \vec{g}) - \frac{D_l^{(k)}(1-s)\Phi}{c_l^{(k)}} \text{grad } c_l^{(k)}, \\ \vec{V}_g^{(k)} &= -\frac{Kk_g(s)}{\mu_g} (\text{grad } P_g + \rho_g \vec{g}) - \frac{D_g^{(k)}s\Phi}{c_g^{(k)}} \text{grad } c_g^{(k)}\end{aligned}\tag{2.3}$$

In general case the diffusion velocity should be proportional to the gradients of the chemical potentials, but we will take in consideration only the classical molecular diffusion caused by phase concentration gradients, by neglecting the role of the thermo- and baro-diffusion. Within the framework of the present thesis the diffusion plays a secondary role and will be analyzed only in chapter 2. The diffusion coefficients should satisfy some consistence conditions which mean that the sum of all the diffusion fluxes must be zero. In particular in a binary mixture the diffusion coefficients of both components are identical, so that :

$$D_g^{(1)} = D_g^{(2)} \equiv D_g, \quad D_l^{(1)} = D_l^{(2)} \equiv D_l$$

The differential equations (2.1) determine N variables P , s and $N - 2$ basic phase concentrations. Other concentrations and phase densities and viscosities are determined from the thermodynamic system of equations.

To simplify the consecutive asymptotic analysis, we will neglect the capillary, gravity and diffusion effects within the first chapter, which yields the following system :

$$\Phi \frac{\partial(\rho C^{(k)})}{\partial t} = \text{div} \left(\left(\frac{\rho_g c_g^{(k)} K k_g(s)}{\mu_g} + \frac{\rho_l c_l^{(k)} K k_l(s)}{\mu_l} \right) \text{grad } P \right), \quad k = 1, \dots, N \tag{2.4}$$

2.1.2 Dimensionless form of the conservation equations

In the next sections we will analyze the flow problem characterized by some geometry of the domain and some initial and boundary conditions which introduce characteristic scales of all the variables functions : the reservoir size L , the characteristic time of fluid

displacement t_* , the maximal pressure difference over the domain P^0 , the mean permeability and porosity $\langle K \rangle$, $\langle \Phi \rangle$, the initial gas and liquid densities and viscosities ρ_g^0 , ρ_l^0 , μ_l^0 and μ_g^0 . In order to avoid the appearance of non-significant parameters, for phase densities we will use the same characteristic value ρ_g^0 while assuming that the difference in gas and liquid densities is not too high (in contrast to the difference in viscosities). Then we can introduce the dimensionless variables :

$$\varphi_g = \frac{\rho_g}{\rho_g^0}, \quad \varphi_l = \frac{\rho_l}{\rho_g^0}, \quad \psi_g = \frac{\rho_g \mu_g^0 K}{\rho_g^0 \mu_g \langle K \rangle}, \quad \psi_l = \frac{\rho_l \mu_l^0 K}{\rho_l^0 \mu_l \langle K \rangle}$$

$$p = \frac{P}{P^0}, \quad t = \frac{t_D}{t_*}, \quad x_i = \frac{X_i}{L}, \quad \phi = \frac{\Phi}{\langle \Phi \rangle}$$

Then equations of mass conservation of each component (2.4) can be formulated in dimensionless form :

$$\varepsilon \phi \frac{\partial}{\partial t} \left(\varphi_g c_g^{(k)} s + \varphi_l c_l^{(k)} (1 - s) \right) = \text{div} \left((\psi_g c_g^{(k)} k_g + \omega \psi_l c_l^{(k)} k_l) \text{grad} P \right), \quad k = 1, \dots, N \quad (2.5)$$

where the operators div and grad are executed in terms of the dimensionless variables x_i .

We will assume that this system of N equations is formulated with respect to the following N variables :

$$P, \quad s, \quad c_g^{(2)}, \quad c_g^{(3)}, \dots, c_g^{(N-1)} \quad (2.6)$$

All other concentrations, as well as densities and viscosities are determined from the thermodynamic subsystem.

2.1.3 Main parameters

Two dimensionless parameters ε and ω play the significant role in the analysis of the process.

Parameter ω is the liquid-gas mobility ratio defined as the ratio between liquid and gas cinematic viscosities, while ε is the pressure relaxation parameter defined as the ratio

between the pressure stabilization time and the displacement time :

$$\omega = \frac{\rho_l^0 \mu_g^0}{\rho_g^0 \mu_l^0}, \quad \varepsilon = \frac{t^*}{t_*} \quad (2.7)$$

where $t^* \equiv L^2 \langle \phi \rangle \mu_g^0 / (\langle K \rangle P^0)$ is the characteristic time of pressure perturbation propagation throughout the domain.

In real systems, the liquid mobility is much lower than that of gas due to high difference in viscosities. The time of pressure perturbation propagation is of order of several hours or days, which is much lower than the time of fluid displacement between the injection well and a production well (of order of several months or years).

Thus, both the parameters ω and ε are small. In practice they are of the same order 0.01 – 0.05.

2.2 Thermodynamic subsystem

2.2.1 General thermodynamic closure relationships

The thermodynamics closure relationships for system (2.5) contain :

- N equilibrium equations formulated in terms of the chemical potentials :

$$\nu_g^{(k)}(P, c_g^{(1)}, \dots, c_g^{(N)}) = \nu_l^{(k)}(P, c_l^{(1)}, \dots, c_l^{(N)}) \quad , \quad k = 1, \dots, N \quad (2.8)$$

where $\nu_j^{(k)}$ is the chemical potential of k^{th} component in j^{th} phase.

- two equations of the phase state :

$$\rho_j = \rho_j(p, c_j^{(1)}, \dots, c_j^{(N)}) \quad , \quad j = g, l \quad (2.9)$$

- two rheological equations of state that determine the variation of the phase viscosities :

$$\mu_j = \mu_j(p, c_j^{(1)}, \dots, c_j^{(N)}) \quad j = g, l \quad (2.10)$$

- and two normalizing equations :

$$\sum_{k=1}^N c_j^{(k)} = 1, \quad j = g, l \quad (2.11)$$

2.2.2 General relation for chemical potential

Let us consider the fixed phase j which is in contact with a second phase.

The chemical potential of the component k in the examined phase represents the varia-

tion of the Gibbs energy of this phase due to the variation of the amount of this component :

$$\nu_j^{(i)} = \left(\frac{\partial (G_j)}{\partial n_j^{(i)}} \right)_{T,P,n_j^{(k) \neq (i)}} \quad (2.12)$$

where $n_j^{(i)}$ is the number of moles of component i in phase j ; N is the total number of components.

For the sake of simplicity, in the consecutive formula of this section we will omit the index of the phase.

The Gibbs energy of the examined phase is defined from the second thermodynamic law :

$$dG = -SdT + VdP + \sum_{i=1}^N \nu^{(i)} dn^{(i)}$$

where S is the entropy, T is the absolute temperature, V is the volume, P is the pressure.

Using the property of the homogeneity of the Gibbs energy and the volume with respect to the total number of moles n , it is possible to find, by using the properties of homogeneous functions, an explicit relation for the Gibbs energy :

$$G = \sum_{i=1}^N \left\{ n^{(i)} \int v^{(i)} dP + RTn^{(i)} \ln c^{(i)} + n^{(i)} \psi^{(i)}(T) \right\}$$

where $v^{(i)} = (\partial V / \partial n^{(i)})_{P,T,n^{(k) \neq (i)}}$ is the partial molar volume; R is the universal gas constant; $c^{(i)} = n^{(i)} / n$ is the mole fraction; ψ is an arbitrary function of temperature. This relation gives the explicit formula for chemical potential :

$$\nu^{(i)} = \int v^{(i)} dP + RT \ln c^{(i)} + \psi^{(i)}(T)$$

Frequently this relation is presented through the chemical potential of the pure component i . The last is easily derived from the previous relation. Then we obtain :

$$\nu^{(i)} = \int (v^{(i)} - v^{(i),pure}) dP + RT \ln c^{(i)} + \nu^{(i),pure} \quad (2.13)$$

Frequently it is preferable to use the function called the fugacity that is scaled to have units of pressure, instead of the chemical potential that has unit of energy per mole.

As seen, to calculate the integral operator in (2.13) it is necessary to substitute the relation between the molar volume and pressure. Such a relation is provided by the equation of state.

2.2.3 Cubic equations of state

The equation of state describes the behavior of the entire phase and determines the dependence between phase pressure, temperature, and volume for a fixed mass of the considered phase under stable equilibrium conditions.

In practice the most applications are related to the "cubic" equations of state. They has origin in the Van-Der-Waals equation (VDW EOS) which was suggested in 1873 and which is cubic with respect to the volume :

$$P = \frac{RT}{V - b} - \frac{a}{V^2} \quad (2.14)$$

where parameters a and b were introduced in order to take into account the forces of attraction and repulsion between molecules. They are evaluated through the critical parameters of the fluid, by taking into account the fact that the first and the second derivatives of function $P(V)$ are zero at critical point.

The development of VDW determined the appearance of the Peng-Robinson EOS :

$$P = \frac{RT}{v - b} - \frac{a}{v^2 + 2bv - b^2} \quad (2.15)$$

where v is the mole volume of the considered phase (volume divided by the number of moles), while parameters a and b for a pure component k are equal to the individual

parameters of this component, $a^{(k)}$ and $b^{(k)}$ which are defined as :

$$a^{(k)} = 0.4274800232 \frac{R^2 T_{cr}^{(k)2}}{P_{cr}^{(k)}} \left[1 + m^{(k)} \left(1 - \sqrt{\frac{T}{T_{cr}^{(k)}}} \right) \right]^2,$$

$$m^{(k)} = 0.37464 + 1.5422\omega^{(k)} - 0.26992\omega^{(k)2},$$

$$b^{(k)} = 0.086640350 \frac{RT_{cr}^{(k)}}{P_{cr}^{(k)}}$$

where $T_{cr}^{(k)}$ and $P_{cr}^{(k)}$ are the critical temperatures and pressures of component k ; ω^k is the acentric Pitcer factor.

For a single-phase mixture parameters a and b are determined by using some mixing rules :

$$a = \sum_{k=1}^N \sum_{j=1}^N c^{(k)} c^{(j)} a^{(kj)}, \quad a^{(kj)} = \sqrt{a^{(k)} a^{(j)}} (1 - \delta^{(kj)}), \quad b = \sum_{k=1}^N c^{(k)} b^{(k)}$$

where $\delta^{(kj)}$ is the binary interaction parameter [Danesh 1998]; $c^{(k)}$ is the mole fraction of k^{th} component in the considered phase.

Substituting the EOS in (2.13), it is easy to obtain the explicit algebraic relation for chemical potential.

2.2.4 Ideal mixing law

The ideal solution (or the ideal mixture) is an approximation to the true mixing law which determines how the chemical components are mixed within one phase.

Let us consider the given phase at a fixed pressure and temperature. The phase consists of N chemical components. The ideal mixture assumes that the volume of the phase is the sum of the individual volumes of pure components taken at the same P, T . In other words, the volumes are additive.

This property allows obtaining the EOS for a mixture. For a pure component, the EOS relates pressure P , temperature T , volume $V^{(k)}$ and number of moles $n^{(k)}$. As the volume

is an extensive parameter which is additive with respect to the number of moles, then the general form of the individual EOS is : $V^{(k)} = n^{(k)} f^{(k)}(P, T)$, where $f^{(k)}$ are given functions.

The EOS of mixture becomes :

$$V = \sum_{k=1}^N n^{(k)} f^{(k)}(P, T), \quad \text{or} \quad v = \sum_{k=1}^N c^{(k)} f^{(k)}(P, T) \quad (2.16)$$

where $v = V/n$ is the molar volume of the phase.

This EOS is totally defined.

2.3 Approximative dissolution laws

The mixing law (or rule) represents the method of mixing of chemical components within one phase. It determines the structure of the EOS of mixture. In contrast, the dissolution law determines how the chemical components are distributed between two (or more) phases. So this is the same as the phase equilibrium law.

Instead of the very complicated transcendent equilibrium equations in terms of chemical potential, frequently one uses the approximative equilibrium laws which describe the behaviour of some components in some phases under some particular conditions.

2.3.1 Raoult's Law

This law describes the situation when both the liquid and gas phases are composed basically by one (the same) chemical component. Let the second component be present only in liquid. The presence of component 2 leads to the increase of the distance between the molecules of the component 1 in liquid. When these molecules pass to gas, the increased distance between them is keeping, so that the gas pressure reduces. Thus the higher the concentration of component 2 (or lower the concentration of component 1) in liquid, lower the gas pressure.

If the component 2 is presented both in liquid and gas, then its presence in liquid reduces the partial pressure of component 1 in gas, or increases the partial pressure of component 2 in gas.

As a result, for multicomponent systems, the concentration of component k in liquid can be considered as proportional to the partial pressure of the same component in gas :

$$c_l^{(k)} = c_g^{(k)} \frac{P}{P_{sat}^{(k)}} \quad (2.17)$$

where the constant value P_{sat} has the dimension of pressure. We have also used the Dalton law. It is possible to show that the pressure P_{sat} is the pressure of gas-liquid coexistence for the pure component (the saturation pressure). It can be calculated by using the formula of Wilson :

$$P_{sat}^{(k)} = P_{cr}^{(k)} \exp \left\{ 5.373 (1 + \omega^{(k)}) \left(1 - \frac{T_{cr}^{(k)}}{T} \right) \right\} \quad (2.18)$$

The Raoult law (2.17) can be derived from the general equilibrium relation by assuming that pressure is low and the system is dominated by one component.

2.3.2 Henry's Law

Henry's law is formally similar to (2.17), but is purely empirical and can not be deduced from theory. Strictly speaking, it is destined to describe the very weak dissolution of volatile components in liquid. It is based on the evident fact that the concentration of a component in liquid is higher at high pressure and at high presence of this component in gas (otherwise, nothing can be dissolved in liquid). The Henry law assumes that this dependence is linear :

$$c_l^{(k)} = H^{(k)} P_g c_g^{(k)} \quad (2.19)$$

where $H^{(k)}$ is the Henry constant determined experimentally.

2.3.3 Approximation of constant K-values

The K -value, or the equilibrium ratio, is :

$$K^{(k)} \equiv \frac{c_g^{(k)}}{c_l^{(k)}}$$

In particular cases, according to the Henry law :

$$K^{(k)} = \frac{1}{H^{(k)} P}$$

whereas the Raoult law yields :

$$K^{(k)} = \frac{P_{sat}^{(k)}}{P}$$

Thus the K -values decrease with pressure.

Under particular conditions when pressure is constant, it is possible to accept approximately that the K -values are invariable.

Chapitre 3

Asymptotic compositional model

Using the presence of two small parameters in the general compositional model, it is possible to obtain the asymptotic version of this model. This model was obtained first in [Oladyshkin and Panfilov, 2006]. In this section we explain the method of derivation of this model and its structure, as this model will be used in all the consecutive chapters.

3.1 Asymptotic model and HT-splitting

3.1.1 Formulation of the general flow problem

Let us consider Eqs. (2.5) in the domain $x \in \Omega \subset R^2$, $0 < t \leq T_*$, where Ω is bounded and has "holes" or excluded points that represents wells (the sources). The boundary of each source is assumed to be circular. The characteristic distance between the sources L is much larger than the internal radius of a source r_w , so that in several situations it is possible to consider only punctual sources. We will examine R^2 only to simplify the developments.

The system is formulated with respect to N unknown variables (2.6).

We will analyze a sufficiently general boundary-value problem that determines a wide spectrum of practical processes :

- at the external boundary $\partial\Omega$:

$$p = p_* \tag{3.1a}$$

- at the source boundary number m with coordinates (x_1^m, x_2^m) i.e. at $r = r_m$, $r^2 \equiv (x_1 - x_1^m)^2 + (x_2 - x_2^m)^2$:

$$(\psi_g k_g + \omega \psi_l k_l) r \frac{\partial p}{\partial r} = q_m, \tag{3.1b}$$

$$s = s_m^{inj}, \tag{3.1c}$$

$$c_g^{(k)} = c_{g,m}^{(k),inj}, \quad k = 2, 3, \dots, N - 1 \tag{3.1d}$$

- the initial condition :

$$p = p^0, \quad (3.1e)$$

$$s = s^0, \quad (3.1f)$$

$$c_g^{(k)} = c_g^{(k)0}, \quad k = 2, 3, \dots, N - 1 \quad (3.1g)$$

Condition (3.1b) means that the mass flow rate q_m is given at the source number m .

The boundary functions $p_*(x, t)$, $q_m(t)$, $s_m^{inj}(t)$ and $c_{g,m}^{(k),inj}$, and the initial functions $p^0(x)$, $s^0(x)$, $c_g^{(k)0}(x)$ are given.

The consistence condition requires that

$$p_*(x, 0) = p^0|_{\partial\Omega} \quad (3.2)$$

In contrast, functions $s^0(x)$ and $c_g^{(k)0}(x)$ are not consistent with $s_m^{inj}(t)$ and $c_{g,m}^{(k),inj}$. This determines the initial discontinuities of the saturation and concentrations at the boundaries of several sources (the injection wells), which that correspond to the initial fronts of displacement. Physically, $s_m^{inj}(t)$ and $c_{g,m}^{(k),inj}$ mean the injected values of saturation and concentrations.

Model (2.5) contains the second derivatives of pressure, but only the first derivatives of saturation and concentrations. So its behavior is expected to be close to a system of one parabolic equation and a hyperbolic sub-system of the first-order. Due to that only the initial conditions are sufficient for saturation and concentrations.

A couple of relations (3.1c) and (3.1f) represents the typical Riemann conditions for saturation, while (3.1d) and (3.1g) - for concentrations.

We will study the behaviour of this problem at $\omega, \varepsilon \rightarrow 0$.

As seen, the perturbation in the system behaviour is introduced through the sources, the external boundary and the non-uniform initial state. In order to avoid the appearance of excessive number of boundary layers (in the vicinity of the external boundary and in the vicinity if the initial instant), we will assume that the external boundary function p_* ,

and the initial functions p^0 , s^0 , $c_g^{(k)0}$ are constant. In contrast we will keep the probable boundary layers in the vicinity of the sources.

3.1.2 "Canonical form" of the compositional model

Before to get down to the asymptotic analysis, it is useful to transform the system (2.5) to an asymmetric form, which will be called "canonical". The system form will be called canonical, if the leading derivatives of each differential equation describe the behaviour of one physical basic variable from the list (2.6) in such a way that all the equations describe different variables. The canonical form for (2.5) is :

$$\varepsilon\phi\frac{\partial\varphi}{\partial t} = \nabla \cdot \left([\omega\Psi_l + \Psi_g] \nabla p \right), \quad (3.3a)$$

$$\begin{aligned} \varepsilon\phi\Delta c^{(N)}\frac{\partial\varphi_l(1-s)}{\partial t} + \varepsilon\phi\sum_{j=g,l}\varphi_j s_j\frac{\partial c_j^{(N)}}{\partial t} = \\ \omega\Delta c^{(N)}\nabla \cdot \left(\Psi_l\nabla p \right) + \omega\Psi_l\nabla c_l^{(N)}\nabla p + \Psi_g\nabla c_g^{(N)}\nabla p, \end{aligned} \quad (3.3b)$$

$$\begin{aligned} \varepsilon\phi\left[\varphi_l(1-s)\frac{\partial}{\partial t}\left(\zeta_l^{(k)} - \zeta_l^{(N)}\right) + \varphi_g s\frac{\partial}{\partial t}\left(\zeta_g^{(k)} - \zeta_g^{(N)}\right)\right] = \\ \omega\Psi_l\nabla p \cdot \nabla \left(\zeta_l^{(k)} - \zeta_l^{(N)}\right) + \Psi_g\nabla p \cdot \nabla \left(\zeta_g^{(k)} - \zeta_g^{(N)}\right), \quad k = 2, \dots, N-1 \end{aligned} \quad (3.3c)$$

where $\Psi_i = \psi_i k_i(s)$, $\varphi = \varphi_g s + \varphi_l(1-s)$; $\Delta c^{(k)} \equiv c_l^{(k)} - c_g^{(k)}$, $k = 2, \dots, N$; $\nabla() \equiv \text{grad}()$, $\nabla \cdot () \equiv \text{div}()$; $s_l = 1 - s$; the following notation is also introduced

$$\nabla\zeta_l^{(k)} \equiv \frac{1}{\Delta c^{(k)}}\nabla c_l^{(k)}, \quad \nabla\zeta_g^{(k)} \equiv \frac{1}{\Delta c^{(k)}}\nabla c_g^{(k)}$$

The transformation of (2.5) into the canonical form (3.3) is performed while transforming each equation step-by-step, by excluding progressively the leading derivatives (or their main parts) from the preceding equations. The main part of a derivative is the one, which does not contain the small factors.

At the first step, the sum of all the equations provides a total mass balance equation with a leading derivative with respect to pressure (3.3a). This equation will replace the first equation in (2.5).

At the second step, in all the remaining equations (2.5) the main term of the second-order derivative with respect to pressure $\text{div}(\Psi_g \text{grad} P)$ is excluded while using (3.3a) :

$$\varepsilon \phi \left[\frac{\partial \varphi C^{(k)}}{\partial t} - c_g^{(k)} \frac{\partial \varphi}{\partial t} \right] = \omega \Delta c^{(k)} \nabla \cdot (\Psi_l \nabla p) + \omega \Psi_l \nabla c_l^{(k)} \nabla p + \Psi_g \nabla c_g^{(k)} \nabla p \quad (3.4)$$

Differentiating by parts, we easily obtain :

$$\frac{\partial \varphi C^{(k)}}{\partial t} - c_g^{(k)} \frac{\partial \varphi}{\partial t} = \Delta c^{(k)} \frac{\partial \varphi_l (1-s)}{\partial t} + \sum_{j=g,l} \varphi_j s_j \frac{\partial c_j^{(k)}}{\partial t}$$

Taking $k = N$ we obtain (3.3b).

At the third step, the leading derivative $\nabla \cdot (\Psi_l \nabla p)$ is excluded from the first $N - 2$ equations (3.4) by subtracting (3.3b). This yields (3.3c).

3.1.3 Asymptotic expansion of the compositional model

Let us assume that $\varepsilon \sim \omega$. Then the following asymptotic expansion results from (3.3) :

$$\begin{aligned} p &= p_0(x, t) + \omega p_1(x, t) + \varepsilon p_2(x, t) + \dots, \\ s &= s_0(x, t) + \omega s_1(x, t) + \varepsilon s_2(x, t) + \dots, \\ c_g^{(k)} &= c_g^{(k)0} + \omega c_{g1}^{(k)}(x, t) + \varepsilon c_{g2}^{(k)}(x, t) + \dots \end{aligned}$$

so that (3.3) yields :

$$\begin{cases} \nabla \cdot (\Psi_{g0} \nabla p_0) = 0, \\ p_0|_{\partial\Omega} = p_*, \\ \Psi_{g0} c_g^{(k)0} r \frac{\partial p}{\partial r} \Big|_{r=r_m} = q_m \end{cases} \quad (3.5a)$$

$$\begin{cases} -\phi \varphi_{l0} \Delta c^{(N)0} \frac{\partial s_0}{\partial t} = \Delta c^{(N)0} \nabla \cdot (\psi_{l0} k_l(s_0) \nabla p_0) + \Psi_{g0} \nabla c_{g1}^{(N)} \nabla p_0, \\ s_0|_{t=0} = s^0, \\ s_0|_{r=r_m} = s_m^{inj} \end{cases} \quad (3.5b)$$

$$\begin{cases} \nabla p_0 \cdot \nabla \left(\zeta_{g1}^{(k)} - \zeta_{g1}^{(N)} \right) = 0, \quad k = 2, \dots, N-1 \\ c_{g1}^{(k)} \Big|_{r=r_m} = c_{g,m}^{(k),inj} \end{cases} \quad (3.5c)$$

where f_0, f_1, \dots mean the corresponding terms in the expansion for an arbitrary function f .

System (3.5a) is a well posed boundary-value problem for the elliptic equation (with respect to p_0).

System (3.5b) is the Riemann problem for saturation s_0 described by the first-order quasi-linear equation.

System (3.5c) is the well posed Cauchy problem for steady-state first-order equation describing function $c_{g1}^{(k)}$.

As seen, the initial conditions for p_0 and $c_{g1}^{(k)}$ are lost, due to the fact that we ignored the time boundary layer.

3.1.4 Zero-order asymptotic model

Let us introduce the zero-order approximation for pressure, saturation and concentrations :

$$p \sim p_0, \quad s \sim s_0, \quad c_g^{(k)} \sim c_g^{(k)0} + \omega c_{g1}^{(k)}$$

Then the zero-order asymptotic model for them follows from (3.5) :

$$\nabla \cdot (\psi_g k_g(s) \nabla p) = 0, \quad (3.6a)$$

$$-\varepsilon \phi \varphi_l \frac{\partial s}{\partial t} = \omega \nabla \cdot (\psi_l k_l(s) \nabla p) + \frac{\psi_g k_g(s)}{\Delta c^{(N)}} \nabla c_g^{(N)} \nabla p, \quad (3.6b)$$

$$\nabla p \cdot \nabla (\zeta_g^{(k)} - \zeta_g^{(N)}) = 0, \quad k = 2, \dots, N - 1 \quad (3.6c)$$

3.1.5 Mnemonic rule for deriving the asymptotic model

Comparing the model (3.6) with (3.3), it is easy to formulate a formal mnemonic rule that enables to obtain the asymptotic model without performing long asymptotic developments.

Indeed, we see that it is sufficient to do the following :

- 1) To present the full compositional model in the "canonical" form (3.3).
- 2) To remove the terms containing ε and ω in the first equation (3.3a). This provides the first equation of the asymptotic model (3.6a).
- 3) To remove two terms $\varepsilon \phi \sum_{j=g,l} \varphi_j s_j \frac{\partial c_j^{(N)}}{\partial t}$ and $\omega \Psi_l \nabla c_l^{(N)} \nabla p$ in (3.3b), which leads to the second equation in the zero-order asymptotic model (3.6b).
- 4) To remove the terms containing small parameters ε and ω in (3.3c), which yields asymptotic equations (3.6c).

This rule will be used in the case of three-phase flow.

3.1.6 Separation of the thermodynamics

If we examine the asymptotic model along a streamline, then the flow becomes mono-dimensional in the corresponding coordinate system. Let l be the coordinate axe whose ort is tangent to the considered streamline at each point. The value of l is equal to the length of the streamline. The origin of the streamline is placed at the boundary of the source

(injected well). Then equations (3.6c) give :

$$\frac{\partial}{\partial l} (\zeta_g^{(k)} - \zeta_g^{(N)}) \equiv \frac{1}{\Delta c^{(k)}} \frac{\partial c_g^{(k)}}{\partial l} - \frac{1}{\Delta c^{(N)}} \frac{\partial c_g^{(N)}}{\partial l} = 0, \quad k = 2, \dots, N - 1$$

This system of $N-2$ homogeneous and autonomous differential equations contains $N-1$ variables : p and $N-2$ concentrations $c_g^{(k)}$. Coordinate l plays the role of the parameter. This means that all the concentrations $c_g^{(k)}$ are the functions of pressure only. Then we obtain :

$$\frac{1}{\Delta c^{(k)}} \frac{dc_g^{(k)}}{dp} - \frac{1}{\Delta c^{(N)}} \frac{dc_g^{(N)}}{dp} = 0, \quad k = 2, \dots, N - 1 \quad (3.7)$$

So, $N-2$ transport equations of the compositional model are transformed into the differential thermodynamic equations, which do not possess time and space variables.

This system describes phase exchanges between gas and liquid in an open thermodynamic system presented by a very low mobile liquid and a highly mobile gas passing through this liquid.

3.1.7 Asymptotic thermodynamic model

The split thermodynamic model, which describes the behaviour of a compositional gas-liquid mixture moving in porous medium is :

- equilibrium equations :

$$\nu_g^{(k)} \left(p, \{c_g^{(q)}\}_{q=1}^{N-1} \right) = \nu_l^{(k)} \left(p, \{c_l^{(q)}\}_{q=1}^{N-1} \right), \quad k=1, \dots, N \quad (3.8a)$$

- mass exchange between high mobile gas and low mobile liquid :

$$\frac{1}{\Delta c^{(k)}} \frac{dc_g^{(k)}}{dp} = \frac{1}{\Delta c^{(N)}} \frac{dc_g^{(N)}}{dp}, \quad k = 2, \dots, N - 1 \quad (3.8b)$$

This system of $2N-2$ equations contain $2N-1$ variables : $N-1$ concentrations in gas $c_g^{(k)}$, $N-1$ concentrations in liquid $c_l^{(k)}$, and pressure p . This system determines all the phase concentrations as the function of pressure.

This system is totally independent of the hydrodynamic sub-system. At the same time, such a model is valid only along streamlines.

Other thermodynamic relations do not change : two EOS determine phase densities, and two rheological EOS determine phase viscosities.

3.1.8 Physical meaning of the differential thermodynamic equations

The physical meaning of the differential thermodynamic system (3.8b) (DTS) can be easily revealed from the analysis of the equation (3.4) from what the DTS was derived. Equation (3.4) is, in turn, equivalent to (3.3b) written for k instead of N . Let us present (3.3b) in the following form :

$$\Delta c^{(k)} \left[\varepsilon \phi \frac{\partial \varphi_l (1-s)}{\partial t} - \omega \nabla \cdot (\Psi_l \nabla p) \right] = \sum_{j=g,l} \left(\omega_j \Psi_j \nabla c_j^{(k)} \nabla p - \varepsilon \phi \varphi_j s_j \frac{\partial c_j^{(k)}}{\partial t} \right)$$

where $\omega_g \equiv 1$, $\omega_l \equiv \omega$. Dividing by $\Delta c^{(k)}$ we obtain :

$$\left[\varepsilon \phi \frac{\partial \varphi_l (1-s)}{\partial t} - \omega \nabla \cdot (\Psi_l \nabla p) \right] = \frac{1}{\Delta c^{(k)}} \sum_{j=g,l} \left(\omega_j \Psi_j \nabla c_j^{(k)} \nabla p - \varepsilon \phi \varphi_j s_j \frac{\partial c_j^{(k)}}{\partial t} \right) \equiv R^{(k)} \quad (3.9)$$

As the left-hand side of this equation does not depend on k , then we obtain : $R^{(k)} \equiv R$, $\forall k$. What does this mean ?

The left-hand side of this equation represents the variation of the mass of the liquid phase in a mobile elementary element of porous medium strictly connected to the examined liquid particles. Without mass exchange with gas (i.e. the phase transition) this part would be identically equal to zero. Thus, the right-hand side of this equation $R^{(k)}$ is the rate of the variation of the mass of the liquid phase due to phase transition.

Let us examine now the term :

$$q_j^{(k)} \equiv \varepsilon \phi \varphi_j s_j \frac{\partial c_j^{(k)}}{\partial t} - \omega_j \Psi_j \nabla c_j^{(k)} \nabla p$$

It obviously represents the variation of mass of phase j only due to the variation of its own composition. The variation of the phase composition can happen only due to the phase exchange (we have no diffusion). So the values $q_g^{(k)}$ represent clearly the mass flux of the component k coming from gas to liquid in course of the mass exchange, while $q_l^{(k)}$ is the flux from liquid to gas. The resulting flux of the component k in the total mass exchange rate is $q^{(k)} = q_l^{(k)} + q_g^{(k)}$ (one of these values is negative). Then relation (3.9) becomes :

$$\frac{q^{(k)}}{\Delta c^{(k)}} = R^{(k)} \equiv R, \quad \forall k$$

The flux of the component k in course of the exchange is caused by the difference between the concentrations of this component in phases, i.e. $q^{(k)} = R^{(k)} \Delta c^{(k)}$, where $R^{(k)}$ is the rate of mass exchange by component k . Without diffusion the components are inseparable in the total exchange flow, so the rate of mass exchange by an individual component is the same as the total rate : $R^{(k)} \equiv R = const, \quad \forall k$.

Writing this relation for k and N we obtain : $R^{(k)} \equiv R^{(N)}$, or

$$0 = R^{(k)} - R^{(N)} \equiv \frac{1}{\Delta c^{(k)}} \sum_{j=g,l} \left(\omega_j \Psi_j \nabla c_j^{(k)} \nabla p - \varepsilon \phi \varphi_j s_j \frac{\partial c_j^{(k)}}{\partial t} \right) - \frac{1}{\Delta c^{(N)}} \sum_{j=g,l} \left(\omega_j \Psi_j \nabla c_j^{(N)} \nabla p - \varepsilon \phi \varphi_j s_j \frac{\partial c_j^{(N)}}{\partial t} \right)$$

In the limit when $\omega, \varepsilon \rightarrow 0$ this yields :

$$0 = R^{(k)} - R^{(N)} \equiv \Psi_g \left(\frac{1}{\Delta c^{(k)}} \nabla c_g^{(k)} - \frac{1}{\Delta c^{(N)}} \nabla c_g^{(N)} \right) \nabla p$$

After eliminating space variable we obtain (3.8b) :

$$0 = R^{(k)'} - R^{(N)'} \equiv \left(\frac{1}{\Delta c^{(k)}} \frac{dc_g^{(N)}}{dp} - \frac{1}{\Delta c^{(N)}} \frac{dc_g^{(N)}}{dp} \right)$$

where $R^{(k)'}$ is the rescaled exchange mass rate of component k due to the phase transition.

Thus the differential thermodynamic equations (3.8b) mean that the rate of mass exchange in one component (between liquid and gas) is identical to the exchange mass rate of the entire phase. The fact that the exchange flux is independent of x and t takes only place for a high difference mobilities between phase.

3.1.9 Improved asymptotic hydrodynamic compositional model

The asymptotic hydrodynamic model is presented by two remaining equations (3.6a) and (3.6b). This model represent the formal limit when two small parameters tend to zero, but it does not take into account the nonlinear character of the two-phase flow equations and the probable existence of some boundary layers. The improved asymptotic model can be obtained by including some small terms which can be however important sometimes.

As mentioned, the first equation losses the initial condition, therefore it is valid only outside the time boundary layer formed in the vicinity of the initial point. In order to obtain the model uniformly valid for all times, we will introduce the time derivative from the original Eq. (3.3a).

The second problem which was not taken into consideration while developing the asymptotic expansion in section 3.1.3 is related to the nonlinearity of the compositional model with respect to saturation. Due to the nonlinearity and degeneration of the relative permeabilities, the liquid can become equally mobile and event more mobile than gas (at low gas saturations). In order to take into account this effect, we will keep the term responsible for the liquid mobility in (3.3a).

It is also useful to keep sometimes the non-stationary terms which depend on $\partial p/\partial t$ in the second equation, (3.3b). These terms are lost in the asymptotic expansion as they are of order $\omega \cdot \varepsilon$. However in particular cases, when the motion of both the phases and the variation of the phase composition $\frac{dc_g^{(N)}}{dp}$ are very low, then the variation of saturation is determined basically by $\partial p/\partial t$.

The definite form of the hydrodynamic asymptotic model is :

$$\varepsilon\phi\frac{\partial\varphi(p,s)}{\partial t} = \operatorname{div}\left(\left(\psi_g(p)k_g(s) + \omega\psi_l(p)k_l(s)\right)\operatorname{grad}p\right), \quad (3.10a)$$

$$-\varepsilon\phi\varphi_l(p)\frac{\partial s}{\partial t} + \varepsilon\phi\eta(p,s)\frac{\partial p}{\partial t} = \omega\operatorname{div}\left(\psi_l(p)k_l(s)\operatorname{grad}p\right) + \psi_g(p)k_g(s)\lambda_g(p)\left(\operatorname{grad}p\right)^2 \quad (3.10b)$$

where

$$\eta(s,p) = \varphi_l(1-s)\lambda_l + \varphi_g s\lambda_g, \quad \lambda_i \equiv \frac{1}{\Delta c^{(N)}} \frac{dc_i^{(N)}}{dp}, \quad i = g, l$$

We will however frequently omit the term with $\partial p/\partial t$ in (3.10b).

3.2 1D asymptotic compositional model

As the asymptotic model is valid only along streamlines, it is necessary to analyze the 1D version of this model. This allows in principle to develop the effective streamline approach in modeling compositional flow.

The method of streamline simulation is based on the assumption that the pressure equation is : i) independent of the saturation (and concentration) equation, ii) is steady-state. In this case the solution to this equation provides a system of streamlines, which are defined only for a steady-state flow. The transport equations for saturation (and concentrations), being then reformulated along each streamline, become one-dimensional, which ensures an extremely fast solution of the compositional system. In some particular cases, these one-dimensional equations can be even solved analytically.

3.2.1 Streamline technique of flow modelling

Let us assume the system of streamlines is compact, i.e. any point of the examined domain is crossed by a streamline, and uniquely defined, i.e. the streamlines do not cross one another.

Let us introduce the following assumptions :

- the *pressure field is steady-state or quasi steady-state* ;
- the *total velocity depends weakly* on the saturation (and concentration) at least during sufficient periods of time ;
- the *capillary pressure is negligible* ;
- the *permeability is isotropic*, so the pressure gradient and the flow velocity are collinear ;

The neglected capillary pressure implies that the velocities of both phases are collinear

being proportional to the same pressure gradient. This means that the system of streamlines is common for gas and liquid (even if the absolute values of flow velocities are different).

The assumption concerning the medium isotropy means that the flow velocities for both phases are collinear to the pressure gradient. In an anisotropic medium, the components of the pressure gradient orthogonal to the streamline are non zero. This is why the implementation of the streamline approach becomes much more complicated.

Let \mathcal{S} be an arbitrary streamline and Y an orthogonal curvilinear coordinate system $Y = (y^1, y^2, y^3)$ with unit vectors $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ in such a way that the vector \mathbf{e}_1 is tangent to the streamline \mathcal{S} at each point, then : $\mathbf{e}_1 = \mathbf{v}_t / \|\mathbf{v}_t\|$, where \mathbf{v}_t is the total Darcy velocity. The two other coordinate vectors, \mathbf{e}_2 and \mathbf{e}_3 , are located on the curvilinear iso-pressure surface orthogonal to all the streamlines, as shown in Figure 3.1.

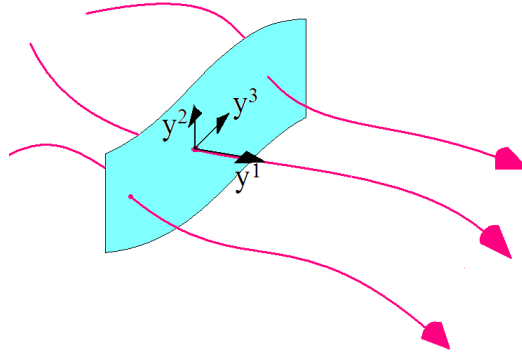


FIG. 3.1 – Curvilinear frame (y^1, y^2, y^3) associated to the streamlines

The Riemann metrics in the introduced curvilinear space is defined by the metric tensor $\mathbf{g} = [g_{ij}]$ whose components are defined as the scalar products of the base vectors $g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$. It determines the metric properties of the space such as length, angles, areas and volumes in the vicinity of any space point. In an orthogonal frame, only the diagonal elements of this tensor are non nil.

Instead of y^1 , let us introduce l : the curvilinear abscise (length) measured along the current streamline. It is easy to show that [Korn and Korn 1968] :

$$dl = \sqrt{g_{11}} dy^1$$

3.2.2 1D asymptotic model along streamlines

To reformulate the saturation equation (3.10b) along a streamline, we need to use the general relationship for the gradient operator of any arbitrary function Φ in an orthogonal curvilinear coordinate system, [Korn and Korn 1968] :

$$\begin{aligned}\text{grad}\Phi &= \frac{1}{\sqrt{g_{11}}} \frac{\partial\Phi}{\partial y^1} \mathbf{e}_1 + \frac{1}{\sqrt{g_{22}}} \frac{\partial\Phi}{\partial y^2} \mathbf{e}_2 + \frac{1}{\sqrt{g_{33}}} \frac{\partial\Phi}{\partial y^3} \mathbf{e}_3 \\ \text{div}(\mathbf{v}) &= \frac{1}{\sqrt{g}} \left[\frac{\partial}{\partial y^1} \left(\sqrt{\frac{g}{g_{11}}} v^1 \right) + \frac{\partial}{\partial y^2} \left(\sqrt{\frac{g}{g_{22}}} v^2 \right) + \frac{\partial}{\partial y^3} \left(\sqrt{\frac{g}{g_{33}}} v^3 \right) \right]\end{aligned}$$

for an arbitrary scalar function Φ and vector \mathbf{v} . Parameter g is $g = g_{11}g_{22}g_{33}$.

In the frame Y associated to the streamline the total velocity vector and pressure gradient become mono-dimensional, so :

$$\begin{aligned}\text{grad}p &= \frac{1}{\sqrt{g_{11}}} \frac{\partial p}{\partial y^1} \mathbf{e}_1 = \frac{\partial p}{\partial l} \mathbf{e}_1 \\ \text{div}(\text{grad}p) &= \frac{1}{\sqrt{g}} \frac{\partial}{\partial y^1} \left(\frac{\sqrt{g}}{g_{11}} \frac{\partial p}{\partial y^1} \right) = \sqrt{\frac{g_{11}}{g}} \frac{\partial}{\partial l} \left(\sqrt{\frac{g}{g_{11}}} \frac{\partial p}{\partial l} \right)\end{aligned}\quad (3.11)$$

Due to this, system (3.10) being formulated along a streamline, becomes :

$$\varepsilon\phi \frac{\partial\varphi(p, s)}{\partial t} = \sqrt{\frac{g_{11}}{g}} \frac{\partial}{\partial l} \left(\left(\psi_g(p)k_g(s) + \omega\psi_l(p)k_l(s) \right) \sqrt{\frac{g}{g_{11}}} \frac{\partial p}{\partial l} \right), \quad (3.12a)$$

$$-\varepsilon\phi\varphi_l \frac{\partial s}{\partial t} + \varepsilon\phi\eta(p, s) \frac{\partial p}{\partial t} = \omega \sqrt{\frac{g_{11}}{g}} \frac{\partial}{\partial l} \left(\psi_l k_l \sqrt{\frac{g}{g_{11}}} \frac{\partial p}{\partial l} \right) + \psi_g k_g \lambda_g \left(\frac{\partial p}{\partial l} \right)^2 \quad (3.12b)$$

3.2.3 First integral. Advanced equation for saturation

If we neglect again the small time derivative in Eq. (3.12a), then this equation has the first integral :

$$\left(\psi_g k_g + \omega\psi_l k_l \right) \sqrt{\frac{g}{g_{11}}} \frac{\partial p}{\partial l} = -q(t)$$

where parameter $q(t)$ has the meaning of the dimensionless mass flow rate which is individual for each streamline. It is defined from the boundary-value conditions at the bore of the wells, (3.1b).

Due to this, Eq. (3.12a) becomes :

$$-\varepsilon\phi\varphi_l \frac{\partial s}{\partial t} + \varepsilon\phi\eta(p, s) \frac{\partial p}{\partial t} = -q\sqrt{\frac{g_{11}}{g}} \frac{\partial F_l}{\partial l} + \frac{q^2\lambda_g(1 - F_l)}{(\psi_g k_g + \omega\psi_l k_l)} \frac{g_{11}}{g}$$

where

$$F_l(s, p) \equiv \frac{\omega\psi_l k_l}{\psi_g k_g + \omega\psi_l k_l}$$

is the mass fractional flow of liquid in the total mass flow rate.

Let us introduce the mass fractional flow for gas :

$$F(s, p) \equiv \frac{\psi_g k_g}{\psi_g k_g + \omega\psi_l k_l} = 1 - F_l \quad (3.13)$$

then the equation for saturation becomes :

$$-\varepsilon\phi\varphi_l \frac{\partial s}{\partial t} + \varepsilon\phi\eta(p, s) \frac{\partial p}{\partial t} = q\sqrt{\frac{g_{11}}{g}} \frac{\partial F(s, p)}{\partial l} + \frac{q^2\lambda_g F(s, p)}{(\psi_g k_g + \omega\psi_l k_l)} \frac{g_{11}}{g} \quad (3.14)$$

3.2.4 1D asymptotic model in cartesian frame

For sufficiently straight streamlines of an almost uniform density of lines in space, the metric tensor is cartesian. In this case the asymptotic compositional model may be formulated in two equivalent forms :

- either in the form of the second-order differential equation for pressure :

$$\varepsilon\phi \frac{\partial \varphi(p, s)}{\partial t} = \frac{\partial}{\partial x} \left(\left(\psi_g(p) k_g(s) + \omega\psi_l(p) k_l(s) \right) \frac{\partial p}{\partial x} \right), \quad (3.15a)$$

$$-\varepsilon\phi\varphi_l(p) \frac{\partial s}{\partial t} + \varepsilon\phi\eta(p, s) \frac{\partial p}{\partial t} = \omega \frac{\partial}{\partial x} \left(\psi_l(p) k_l(s) \frac{\partial p}{\partial x} \right) + \psi_g(p) k_g(s) \lambda_g(p) \left(\frac{\partial p}{\partial x} \right)^2 \quad (3.15b)$$

- or in the form of the semi-integrated first-order steady-state equation for pressure :

$$\frac{\partial p}{\partial x} = -\frac{q(t)}{\psi_g k_g + \omega \psi_l k_l}, \quad (3.16a)$$

$$\varepsilon \phi \varphi_l \frac{\partial s}{\partial t} + q \frac{\partial F(s, p)}{\partial x} = -\frac{q^2 \lambda_g F(s, p)}{\psi_g k_g + \omega \psi_l k_l} - \varepsilon \phi \eta(p, s) \frac{\partial p}{\partial t} \quad (3.16b)$$

3.2.5 Relation for q

Parameter q is not always independent and in some situations can be related to parameter ε .

Let us examine the case when all the streamlines converge to a cylindrical well of radius R_w and height H_w . The total flow rate crossing this cylindrical surface in the direction of the well center is q [m³/s]. Let all the streamlines form a symmetrical radial system just in the vicinity of the wellbore. Assume that the flow velocities at the wellbore are identical for each streamline. Then using the Darcy law for flow velocity and taking into account that the streamlines are oriented towards the well, also returning back to the variables with dimension in (3.16) or (3.1b), it is easy to obtain that :

$$q = \frac{G \mu_g^0 L}{P^0 \rho_g^0 \langle K \rangle A}$$

where G is the mass flow rate through the cross-section A .

The pressure relaxation time t^* is defined as :

$$t^* = \frac{L^2 \mu_g^0 \langle \Phi \rangle}{P^0 \langle K \rangle}$$

Then we obtain for q :

$$q = \frac{G t^*}{\rho_g^0 \langle \Phi \rangle A L} = \frac{G t^*}{M_g^0}$$

where M_g^0 is the characteristic mass of gas which will be injected into all the reservoir. So

the ratio M_g^0/G is the characteristic time of oil displacement by gas (t_*). Then we obtain :

$$q = \frac{t^*}{t_*} = \varepsilon \tilde{q}(t) \quad (3.17)$$

where $\tilde{q}(t)$ is the dimensionless flow rate (at the well) which is equal to 1 when the flow rate is constant in time.

Chapitre 4

Riemann problem for two-phase case

4.1 Formulation of the problem in terms of the asymptotic model

We will analyze the 1D compositional flow problem which describes the displacement of one phase by another one in porous medium. The results of this analysis can be used next within the technique of streamline simulations.

We will analyze only the cartesian coordinate system. The difference of using any other curvilinear frame consists in the appearance of some coefficients in the hydrodynamic model which depends on space coordinate. This does not change qualitatively any result obtained in the present chapter.

4.1.1 Hydrodynamic equations

As shown in the previous chapter, the asymptotic compositional model contains only two hydrodynamic differential equations independently of the number of components. We will take them in the form (3.16) while neglecting the small term with $\partial p/\partial t$ in the second equation and while taking into account (3.17) :

$$\frac{\partial p}{\partial x} = -\frac{\varepsilon}{\psi_g k_g + \omega \psi_l k_l}, \quad (4.1a)$$

$$\phi \varphi_l \frac{\partial s}{\partial t} + \frac{\partial F(s, p)}{\partial x} = -\frac{\varepsilon \lambda_g F(s, p)}{\psi_g k_g + \omega \psi_l k_l} \quad (4.1b)$$

This model is formulated with respect to pressure p and gas saturation s .

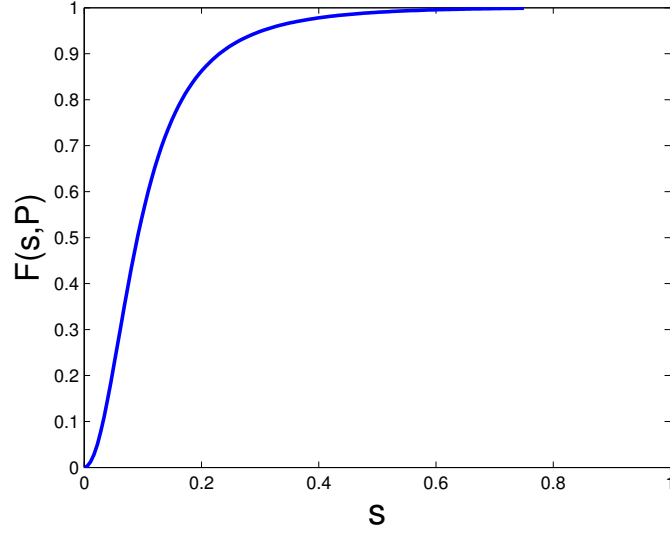


FIG. 4.1 – Fractional mass flow function for gas at a fixed pressure

Function $F(s, p)$ is the fractional mass flow for gas :

$$F(s, p) \equiv \frac{\psi_g(p)k_g(s)}{\psi_g(p)k_g(s) + \omega\psi_l(p)k_l(s)} \quad (4.2)$$

The typical behaviour of this function for a fixed pressure is shown in Fig. 4.1.

This shape clearly shows that gas dominates in the total mass flow rate at any saturation except the small values, due to the low relative mobility of liquid.

The relative permeabilities $k_l(s)$ and $k_g(s)$ will be considered in general form, as some monotonic smooth functions of saturation.

4.1.2 Closure thermodynamic equations

The model contains several coefficients which depend on the pressure :

$$\left\{ \begin{array}{l} c_g^{(k)} = c_g^{(k)}(p), \quad c_l^{(k)} = c_l^{(k)}(p), \quad k = 1, \dots, N \\ \lambda_g(p) = \frac{1}{\Delta c^{(N)}} \frac{dc_g^{(N)}}{dp}, \quad \Delta c^{(N)} = c_l^{(N)} - c_g^{(N)} \\ \psi_g(p) = \frac{\rho_g(p)\mu_g^0}{\rho_g^0\mu_g(p)}, \quad \psi_l(p) = \frac{\rho_l(p)\mu_l^0}{\rho_l^0\mu_l(p)}, \quad \varphi_l(p) = \frac{\rho_l(p)}{\rho_g^0} \end{array} \right. \quad (4.3)$$

The densities $\rho_i(p)$ are calculated by using the EOS of gas and liquid, while the viscosities are calculated through rheological EOS. Both these operations are possible once the phase composition ($c_g^{(k)}$ and $c_l^{(k)}$) is already calculated.

All other parameter also depend on phase concentrations.

The phase concentrations are the solutions to the thermodynamic problem (3.8) which represents a coupled system of transcendent and differential thermodynamic equations :

$$\nu_g^{(k)} \left(p, \{c_g^{(q)}\}_{q=1}^{N-1} \right) = \nu_l^{(k)} \left(p, \{c_l^{(q)}\}_{q=1}^{N-1} \right), \quad k=1, \dots, N \quad (4.4a)$$

$$\frac{1}{\Delta c^{(k)}} \frac{dc_g^{(k)}}{dp} = \frac{1}{\Delta c^{(N)}} \frac{dc_g^{(N)}}{dp}, \quad k = 2, \dots, N - 1 \quad (4.4b)$$

4.1.3 Displacement problem

The flow problem represents the 1D version of the general flow problem formulated as (3.1). At the same time, the asymptotic model introduces some modifications related essentially to the fact that a part of partial differential equations are transformed into the thermodynamic equations. This means that the new thermodynamic equations no longer can satisfy the initial and boundary conditions.

We examine the problem of displacement of liquid by gas formulated as the Riemann problem for equation (4.1b) resulting from (3.1c) and (3.1f). Assuming that the gas is injected at point $x = 0$, the injection saturation is $s^{inj}(t)$, and at the initial state of the

gas saturation is $s^0(x)$:

$$\begin{aligned} s|_{t=0} &= s^0(x) \\ s|_{x=0} &= s^{inj}(t) \end{aligned} \tag{4.5}$$

The problem should be also complemented with one boundary condition for Equation (4.1a) :

$$p|_{x=0} = p^{inj}(t) \tag{4.6}$$

which defines the *starting pressure*, i.e. the pressure at the starting point of the considered streamline (the injection pressure).

This condition causes however a contradiction from the fact that we have already used another boundary condition for the flow rate (3.1b) at the well to derive (4.1), and we have not used the boundary condition at the external boundary (3.1a). Strictly speaking, the well-bore pressure (4.6) is not independent and should be calculated iteratively as the result of solving the overall problem. In practice however the use of the Dirichlet condition (4.6) for 1D problem is much more comfortable than for the flow rate. Due to this, we will assume that the flow rate $q = \varepsilon$ in (4.1a) is unknown a priori ($\tilde{q}(t)$ is assumed to be constant and equal to 1), and should be calculated through the well-bore pressure. This is possible to do in the approximate way, by accepting the logarithmic law of pressure variation in the vicinity of well : $p = a \ln r + p_*$. Then (4.1a) reformulated in radial coordinate system, gives :

$$\frac{(p^{inj} - p_*)}{r_w \ln r_w} = - \frac{\varepsilon}{\psi_g(p^{inj})k_g(s^{inj}) + \omega\psi_l(p^{inj})k_l(s^{inj})}$$

where the well-bore saturation s^{inj} is imposed by Riemann conditions, r_w is the well radius, p_* is the pressure at the external boundary.

This yields for the flow rate $q = \varepsilon$ the explicit equation :

$$\varepsilon = \frac{(p_* - p^{inj})}{r_w \ln r_w} \left(\psi_g(p^{inj})k_g(s^{inj}) + \omega\psi_l(p^{inj})k_l(s^{inj}) \right)$$

The initial condition for pressure (3.1e) is now lost, as the time derivative of pressure

in the asymptotic model was neglected. At the same time, "the traces" of this conditions are kept due to the consistence condition between the initial and the boundary conditions (3.2) :

$$p|_{x=1,t=0} \equiv p_*|_{t=0} = p^0|_{x=1}$$

In the particular cases where these values are constant, the pressure is quasi-stationary, then the consistence condition strictly defines the pressure at the external boundary as that equivalent to the initial pressure :

$$p|_{x=1} \equiv p_* = p^0 \tag{4.7}$$

4.1.4 Twice Cauchy problem for the thermodynamic differential subsystem

The differential thermodynamic subsystem (4.4b) should be completed with some initial conditions. According to the method of derivation of these equations, they represent the result of the explicit integration of the concentration transport equations along streamlines. Moreover, these transport equations were supposed to verify the Riemann conditions for concentrations : the boundary condition at the injected wells (3.1c) which specifies the composition of the injected fluid, and the initial condition (3.1g) which specifies the composition of the fluid initially in place.

These conditions should be now transformed into the equivalent boundary conditions in terms of pressure, as the phase concentrations depend on pressure only. Evidently the boundary condition (3.1c) transforms into the Cauchy condition at the starting pressure p^{inj} . The initial condition (3.1g) corresponds to the initial pressure, that is the same as the external boundary pressure according to the consistence condition (4.7).

So we obtain two Cauchy problems for the differential thermodynamic subsystem (4.4b),

for $k = 2, 3, \dots, N - 1$ for points of pressure :

$$c_g^{(k)} \Big|_{p=p^{inj}} = c_g^{(k),inj}, \quad (4.8a)$$

$$c_g^{(k)} \Big|_{p=p_* = p^0} = c_g^{(k)0} \quad (4.8b)$$

where p^{inj} is the starting pressure, while p^0 is the initial pressure, p_* is the pressure at $x = 1$.

So the asymptotic model leads to a couple of thermodynamic Cauchy problems which determines two different fluid compositions.

We will call (4.8a) the injection Cauchy problem, while (4.8b) will be the initial Cauchy problem.

4.2 Discontinuities in the asymptotic model

We will show that the analyzed asymptotic model has two types of discontinuities of different nature :

- the discontinuities in the structure of the coefficients of the hydrodynamic differential equations ; they determine the discontinuous behaviour of the phase concentrations ; formally this is caused by the over-determined Cauchy problem obtained for the differential thermodynamic system ; physically the discontinuities in phase concentrations are caused by the Riemann conditions for the concentrations in the original full (non asymptotic) compositional problem ;

- the discontinuities in the structure of the solution to the hydrodynamic problems ; they determine the discontinuous behaviour of saturation ; they are caused by the Riemann problem for saturation which imposes the initial shock which cannot disappear with time.

4.2.1 Coefficient discontinuity of the hydrodynamic equations

Let us remind that the thermodynamic problem (4.4) determines the variation of the fluid composition for all the pressure values starting from the pressure imposed as the boundary value. So problem (4.8a) determines the variation of the phase composition of the injected fluid as the function of pressure, while problem (4.8b) describes the variation of the composition of the initial fluid with pressure. We obtain thus two families of thermodynamic parameters (4.3) as the functions of p . Physically, this determines two different flow problems described by the same differential equations (4.1), but having different coefficients.

At the same time, both the families of the Cauchy conditions (4.8a) and (4.8b) must be satisfied simultaneously. This is impossible for a continuous variation of the phase

concentrations, as the concentrations calculated from the injection Cauchy problem will be certainly different at point p^0 than the concentrations imposed by the initial Cauchy conditions, and vice versa.

This means that the hydrodynamic model (4.1) is the system of two differential equations with discontinuous coefficients (4.3) and with unknown placement of the coefficient discontinuity.

Such a strange mathematical object is not very frequently observed in the scientific literature (we do not know any example).

The existence of the undefined discontinuities coefficient means that the problem is not well posed. To determine these discontinuities it is necessary to complete the model by some additional equations. Such additional equations are the degenerated Hugoniot conditions which were lost under the asymptotic transition.

Thus, the phase concentrations have to be discontinuous functions. The number of discontinuities and their parameters will be determined in the next sections.

4.2.2 Discontinuities in the solution structure

Along with the coefficient discontinuities, the problem contain other discontinuities caused by the Riemann conditions. Indeed, the Riemann conditions (4.5) determine the initial shock of saturation which will be transported by the convection term and deformed in time by the right-hand side of equation (4.1b). Due to the absence of diffusion and dissipation terms, the initial shock can be modified, decomposed into several shocks, but it cannot be dissipated totally in general case.

Therefore the solution to this problem is characterized by the saturation discontinuities.

The behavior of this discontinuity is determined by the classic Hugoniot conditions derived from (4.1b) and completed with the entropy conditions.

The presence of two types of discontinuities determines two kinds of admissible shocks :

- the S -shocks : they correspond to the shock of saturation only ; the proof to this affirmation will be shown later ;

- the *SC*-chocs : they are simultaneous shocks of saturation and phase concentrations.
This will be proved later.

4.2.3 Hugoniot conditions at *S*-chocs

The behavior of discontinuities is determined by the mass balance equations formulated just in the vicinity of each shock and called the Hugoniot conditions. They replace the original differential equation which is not valid at a discontinuity.

One way to construct Hugoniot conditions is to integrate the original transport differential equation over the infinitely thin zone near the discontinuity and over the infinitely small interval of time- see appendix A for more details.

The Hugoniot condition provided by the saturation transport equation (4.1b) will have the same form as for the homogenous hyperbolic equations (see appendix A for more details), as the right-hand side of Eq. (4.1b) does not contain space and time derivatives. The resulting Hugoniot condition is :

$$\varphi_l [s] V_f = [F(s, p)] \quad (4.9)$$

where V_f is the shock velocity ; and $[A] = A^+ - A^-$. Symbols A^+ and A^- means the forward and the backward values of A at the shock.

4.2.4 Entropy condition

Another relation at the shock is the entropy condition which represents an inequality, by providing strict bounds for parameter variation at the shock so that the principle of entropy increasing when passing through the shock is satisfied. This principle is formulated in various forms, in particular in the form of the Lax inequalities (see Appendix B for more details) :

$$\sigma(s^-) \leq \sigma(s^-, s^+) \leq \sigma(s^+) \quad (4.10)$$

where $\sigma(s^-)$ and $\sigma(s^+)$ are the wave velocity before and after the shock and $\sigma(s^-, s^+)$ is the shock velocity. As we can see above, the form of the entropy condition and Lax inequalities is the same for the homogeneous and inhomogeneous parabolic differential equations, as in the case of Hugoniot condition- see appendix B for more details.

Rewriting the saturation transport equation (4.1b) in the following form :

$$\frac{\partial s}{\partial t} + \frac{1}{\varphi_l} \frac{\partial F(s, P)}{\partial s} \frac{\partial s}{\partial x} = \frac{1}{\varphi_l} G(s) \quad (4.11)$$

we can find the wave velocities :

$$\sigma(s) = \frac{1}{\varphi_l} \frac{\partial F(s, P)}{\partial s} \quad (4.12)$$

So the Lax inequalities become :

$$\frac{\partial F(s, P)}{\partial s} \Big|_{s=s^-} \leq \frac{[F]}{[s]} \leq \frac{\partial F(s, P)}{\partial s} \Big|_{s=s^+} \quad (4.13)$$

where $[F]/[s]$ is the shock velocity which can be extracted from Hugoniot condition (4.9) :

$$\frac{[F]}{[s]} = \frac{F^+ - F^-}{s^+ - s^-}$$

.

4.2.5 Admissible discontinuities

The presence of two types of discontinuities determines two kinds of admissible shocks :

- the s-shock : this corresponds to the shock of saturation only ; the proof to this affirmation will be shown later ;

- the sc-shock : this is a simultaneous shock of saturation and phase concentrations.

While analyzing the admissible shocks, we can forget the presence of pressure in the structure of the coefficients, as the pressure p remains always a continuous function.

Let us examine the probable pure S -shock. This is certainly possible when the coeffi-

coefficients of the equations are continuous. So in (4.9) both $[s]$ and $[F(s, p)]$ are nonzero. So the shock velocity V_f can be properly defined as a bounded nonzero value. So the *s-shock* is admissible.

The admissibility of a *SC*-shock can be detected from the analysis of the Hugoniot condition (4.9) as this condition is relative to saturation, but not to phase concentrations which are determined from the thermodynamic model. The admissibility of *SC*-shocks results immediately from the fact that the concentration discontinuities are caused by the coefficient discontinuities. Indeed, a discontinuity of the coefficients of Eq. (4.1b) for saturation necessarily determines the discontinuity in the solution.

Due to this the existence of the shocks of the phase concentrations only is impossible.

4.2.6 Lack of Hugoniot conditions

As mentioned before, we are able to find only two jump conditions from our HT-split model; one Hugoniot condition from the equation of saturation and one entropy condition. These two equations are unfortunately largely insufficient, as a simultaneous shock of saturation and concentrations is determined by $(N + 1)$ parameters on each side of the shock : the shock velocity, $(N - 1)$ concentrations and saturation at the shock, where N is the number of components. The problem results from the fact, already discussed, that the asymptotic model (4.1) does not determine the coefficient discontinuities.

The problem is then how to obtain additional conditions for phase concentrations ?

4.2.7 Additional Hugoniot conditions for coefficient discontinuities

The revealed problem of lack of Hugoniot conditions is caused by the fact that in the HT-split model $(N - 2)$ original concentration transport equations are transformed, by the limit transition $\omega, \varepsilon \rightarrow 0$, into the thermodynamic relations (4.4b). The number of remaining hydrodynamic differential equations is 2 whatever the number of chemical components. This gives us the idea that the needed Hugoniot conditions should be obtained from the

full compositional model with the consecutive limit transition in the obtained relationships $\omega, \varepsilon \rightarrow 0$.

Evidently, the system of equations (2.5) gives N formal Hugoniot conditions. If we add one entropy condition, then we obtain $N + 1$ relations at a shock, which is equivalent to the number of unknown shock parameters. The shock model will then be closed.

Let us rewrite system (2.5) in the compact form :

$$\varepsilon \frac{\partial \varphi^{(k)}}{\partial t} + \frac{\partial}{\partial x} \left(W_g c_g^{(k)} + \omega W_l c_l^{(k)} \right) = 0, \quad k = 1, \dots, N \quad (4.14)$$

in which :

$$\varphi^{(k)} = \varphi_g c_g^{(k)} s + \varphi_l c_l^{(k)} (1 - s), \quad W_j = -\psi_j k_j \frac{\partial p}{\partial x}, \quad j = g, l \quad (4.15)$$

The intrinsic permeability and porosity are assumed to be constant and homogeneous.

It is preferable to use $(N - 1)$ equations in the form of (4.14) and one overall equation describing the total mass conservation. Then for a given shock, from (4.14) we will obtain the following relation (the procedure is described in Appendix A) :

$$\varepsilon [\varphi] V_f = [W_g] + \omega [W_l] \quad (4.16)$$

$$\varepsilon [\varphi^{(k)}] V_f = [W_g c_g^{(k)}] + \omega [W_l c_l^{(k)}], \quad k = 2, \dots, N \quad (4.17)$$

herein V_f is the shock velocity, $\varphi = \varphi_g s + \varphi_l (1 - s)$ and $[A] = A^+ - A^-$, as mentioned before is the variation of the value of A before and after the shocks.

Note that the terms containing small factors ω and ε cannot be eliminated for the moment as this will give an invalid result : continuous gas velocity and concentrations in gas phase, which is impossible for the concentration shocks.

We will find the limit of this system at $\omega, \varepsilon \rightarrow 0$ in the following sections.

These relations determine both the SC -shocks and the S -shocks. It is however possible to show that for a S -shock the obtained system transforms into (4.9).

4.2.8 Asymptotic form of the Hugoniot conditions at SC -shocks

The Hugoniot conditions (4.16) and (4.17) can be significantly simplified if we examine their limit behavior when $\omega, \varepsilon \rightarrow 0$. Note that if we neglect the term of order ε in the left-hand side, we will have $[c_g^{(k)}] = 0$ which contradicts to the concentration jump. Due to this the system should be transformed before considering its limit behavior.

Let us multiply equation (4.16) by $c_g^{(k)+}$ and subtract it from (4.17) :

$$\varepsilon V_f ([\varphi^{(k)}] - c_g^{(k)+} [\varphi]) = W_g^- [c_g^{(k)}] + \omega [W_l c_l^{(k)}] - \omega c_g^{(k)+} [W_l], \quad k = 2, \dots, N \quad (4.18)$$

It is possible to eliminate the shock velocity from $N - 2$ equations :

$$\frac{W_g^- [c_g^{(k)}] + \omega [W_l c_l^{(k)}] - \omega c_g^{(k)+} [W_l]}{[\varphi^{(k)}] - c_g^{(k)+} [\varphi]} = \frac{W_g^- [c_g^{(N)}] + \omega [W_l c_l^{(N)}] - \omega c_g^{(N)+} [W_l]}{[\varphi^{(N)}] - c_g^{(N)+} [\varphi]}, \quad k = 2, \dots, N-1$$

Now we take the limit when $\omega \rightarrow 0$:

$$\frac{([\varphi^{(k)}] - c_g^{(k)+} [\varphi])}{[c_g^{(k)}]} = \frac{([\varphi^{(N)}] - c_g^{(N)+} [\varphi])}{[c_g^{(N)}]}, \quad k = 2, \dots, N-1 \quad (4.19)$$

So, equations (4.16), (4.18) for $k = N$, and (4.19) gives the following system of relations :

$$\left\{ \begin{array}{l} \varepsilon V_f [\varphi] = [W_g + \omega W_l], \\ \varepsilon V_f ([\varphi^{(N)}] - c_g^{(N)+} [\varphi]) = W_g^- [c_g^{(N)}] + \omega [W_l c_l^{(N)}] - \omega c_g^{(N)+} [W_l], \\ \frac{([\varphi^{(k)}] - c_g^{(k)+} [\varphi])}{[c_g^{(k)}]} = \frac{([\varphi^{(N)}] - c_g^{(N)+} [\varphi])}{[c_g^{(N)}]}, \quad k = 2, \dots, N-1 \end{array} \right. \quad (4.20)$$

It is useful to replace the mass velocities W_i by the standard velocities V_i (dimensionless)

and, at the next step, by the total velocity V and gas fractional flow \widehat{F} defined as :

$$V_g = -\frac{Kk_g \mu_g^0}{\langle K \rangle \mu_g} \frac{\partial p}{\partial x}, \quad V_l = -\frac{Kk_l \mu_g^0}{\langle K \rangle \mu_l} \frac{\partial p}{\partial x}; \quad V = V_g + V_l; \quad \widehat{F}(s) = \frac{V_g}{V} = \frac{k_g/\mu_g}{k_g/\mu_g + k_l/\mu_l} \quad (4.21)$$

(note that the factor μ_g^0 is identical for both the cases, which is not a typos).

Then the relation between W_i and V_i is :

$$W_g = \varphi_g V_g, \quad \omega W_l = \varphi_l V_l \quad (4.22)$$

After the replacement $W_i \rightarrow V_i \rightarrow (V, \widehat{F})$ system (4.20) takes the following form :

$$\varepsilon V_f = \frac{\left[V \left(\varphi_g \widehat{F} + \varphi_l (1 - \widehat{F}) \right) \right]}{[\varphi]}; \quad (4.23a)$$

$$\frac{V^- \widehat{F}^- \varphi_g^- \left[c_g^{(N)} \right] + \left[V(1 - \widehat{F}) \varphi_l c_l^{(N)} \right] - c_g^{(N)+} \left[V(1 - \widehat{F}) \varphi_l \right]}{[\varphi^{(N)}] - c_g^{(N)+} [\varphi]} = \frac{\left[V \left(\varphi_g \widehat{F} + \varphi_l (1 - \widehat{F}) \right) \right]}{[\varphi]}; \quad (4.23b)$$

$$\frac{\left([\varphi^{(k)}] - c_g^{(k)+} [\varphi] \right)}{[c_g^{(k)}]} = \frac{\left([\varphi^{(N)}] - c_g^{(N)+} [\varphi] \right)}{[c_g^{(N)}]}, \quad k = 2, \dots, N - 1 \quad (4.23c)$$

where we have removed the shock velocity from the second equation in (4.20) by means of the first equation.

The most significant results consists in that the subsystem of $N - 2$ conditions (4.23c) contains only the thermodynamic parameters (phase concentrations and pressure) and saturations, while the velocities are removed.

4.2.9 S -shock : Continuity of the total velocity

For a S -shock, the useful result can be obtained concerning the behavior of the total flow velocity. At a S -shock the phase compositions are continuous, so we are able to rewrite

equations (4.16) and (4.17) as :

$$\begin{aligned}\varepsilon [\varphi] V_f &= [W_g] + \omega [W_l], \\ \varepsilon [\varphi^{(k)}] V_f &= c_g^{(k)} [W_g] + \omega c_l^{(k)} [W_l], \quad k = 2, \dots, N\end{aligned}$$

or :

$$\varepsilon(\varphi_g - \varphi_l) [s] V_f = [W_g] + \omega [W_l], \quad (4.24)$$

$$\varepsilon(\varphi_g c_g^{(k)} - \varphi_l c_l^{(k)}) [s] V_f = c_g^{(k)} [W_g] + \omega c_l^{(k)} [W_l], \quad k = 2, \dots, N \quad (4.25)$$

In order to eliminate the liquid velocity term $[W_l]$, let us multiply equation (4.24) by c_l^k and subtract it from equations (4.25) :

$$\varepsilon(\varphi_g c_g^{(k)} - \varphi_g c_l^{(k)}) [s] V_f = c_g^{(k)} [W_g] - c_l^{(k)} [W_g] \quad \rightarrow \quad \varepsilon V_f = \frac{[W_g]}{[s] \varphi_g} \quad (4.26)$$

Repeating the same procedure to eliminate the gas velocity term $[W_g]$, we multiply equation (4.24) by c_g^k and subtract it from equations (4.25) :

$$\varepsilon(-\varphi_l c_l^{(k)} + \varphi_l c_g^{(k)}) [s] V_f = \omega c_l^{(k)} [W_l] + \omega c_g^{(k)} [W_l] \quad \rightarrow \quad -\varepsilon V_f = \frac{[\omega W_l]}{[s] \varphi_l} \quad (4.27)$$

Summing equations (4.26) and (4.27) we obtain :

$$0 = \frac{[W_g]}{[s] \varphi_g} + \frac{[\omega W_l]}{[s] \varphi_l} \quad \rightarrow \quad \left[\frac{W_g}{\varphi_g} + \frac{\omega W_l}{\varphi_l} \right] = 0$$

Using the expression of W_i we have :

$$0 = \left[\frac{K}{\langle K \rangle} \frac{\partial p}{\partial x} \left(k_g \frac{\rho_g \mu_g^0}{\rho_g^0 \mu_g} \cdot \frac{\rho_g^0}{\rho_g} + k_l \frac{\rho_l \mu_l^0}{\rho_l^0 \mu_l} \cdot \frac{\rho_l^0 \mu_g^0}{\rho_g^0 \mu_l^0} \cdot \frac{\rho_g^0}{\rho_l} \right) \right] = \left[\frac{K \mu_g^0}{\langle K \rangle} \frac{\partial p}{\partial x} \left(\frac{k_g}{\mu_g} + \frac{k_l}{\mu_l} \right) \right]$$

or

$$0 = \left[\frac{\partial P}{\partial X} \left(\frac{K k_g}{\mu_g} + \frac{K k_l}{\mu_l} \right) \right] = [V_g + V_l] = [V]$$

This means that the total velocity is continuous through a S -shock.

Chapitre 5

Solution to the Riemann problem :
semi-analytical method

The basic technical difficulty in solving any problem with discontinuous solution consists in detecting the number, placement and forward and backward parameters of the shocks. This is usually done numerically, by introducing some special sophisticated numerical procedures which try to detect, in the course of solving, a possible shock. Such a numerical procedures, called front tracking algorithms, based on the analysis of Hugoniot and entropy conditions, significantly complicate the numerical method and increase the simulation time. In the case of a large number of existing shocks, which is typical for compositional two-phase problems, detection of all the shocks and their adequate parameters represents a true challenge and remains an open problem. In any case, a priori detection of shocks is impossible and they are being discovered in course of solving the entire hydrodynamic problem.

The suggested asymptotic compositional model allows to develop a very efficient analytical procedure of front tracking, which detects all the parameters of the *SC*-shocks through an auxiliary thermodynamic problem. This is done before solving the hydrodynamic problem, which represents a huge advantage of the method.

This is due to the fact that asymptotic model, which leads to split the thermodynamics and hydrodynamics, allows to split them in Hugoniot conditions too.

5.1 Diagrammatical representation of the thermodynamic part

5.1.1 Phase diagrams and tie lines

The reduction of the concentration transport equations to the differential thermodynamic equations (4.4) (differentiation is performed with respect to p) in the asymptotic thermodynamic model means that the phase concentrations depend on pressure p and constant parameters imposed by Cauchy conditions (4.8). This means the following.

If the pressure is invariable (as it is assumed in ideal mixing theory), then the phase concentrations can be only constant or piece-wise constant. The shocks between them are the shocks of concentration, so they are the *SC*-shocks, which determines the discontinuities of the saturation too. Due to this the solution structure is characterized by invariable fragments of phase concentrations (the plateaux) between the shocks.

An invariable phase state corresponds to the so-called tie-line in the thermodynamic phase diagram. The phase diagram represents the ensemble of states available for the examined fluid. For three-component two-phase case, which represents the basic example of a compositional system, at constant pressure the phase diagram is shown in Fig. 5.1.

The axes represent the total concentrations of light (1) and heavy (3) components. The concentration of the intermediate component is calculated on the bisector of the right-angle. The two-phase zone is encircled by an envelop. A tie-line is a straight line crossing the two-phase zone and marking a constant composition of both the phases. These compositions are presented by the coordinates of points A and B . Along a tie-line the phase compositions are fixed while the saturation of the phases and the total composition of the system vary.

A tie-line is the graphical representation of the phase equilibrium equations (4.4a)

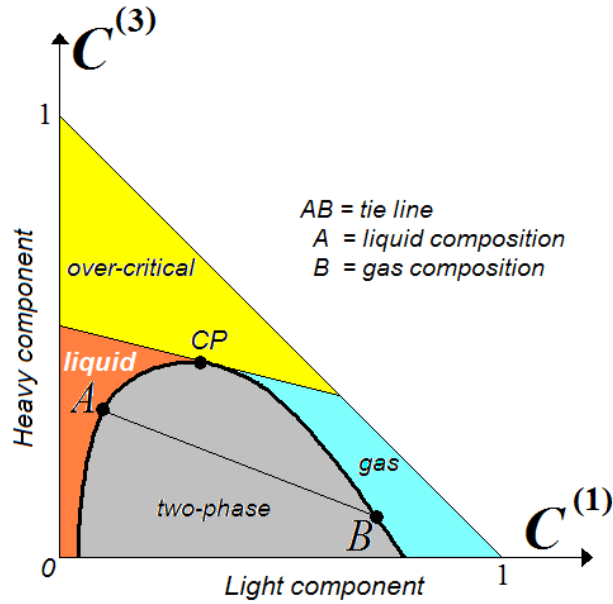


FIG. 5.1 – Ternary phase diagram for three-component system : CP is the critical point, AB is a tie-line

(only); it relates the couples of phase concentrations in coexisting liquid and gas. These values are just determined by the equilibrium equations.

At constant pressure, the phase concentrations can vary only by the shocks relating two tie-lines; these are the SC -shocks. In contrast, a S -shock moves along a tie-line.

The tie-lines play a significant role in the theory of fluid displacement, because the behavior of phase concentrations is frequently piece-wise constant in space, as mentioned above. In terms of tie-lines, this means that the phase composition jumps from one tie-line to another one. Such a jump corresponds to the shocks of the solution to the Riemann problem. In other words, a concentration shock relates two tie-lines so that the forward and the backward concentrations at the shock correspond exactly to these two tie-lines.

In the case of four components and more, the tie lines has the same meaning but the phase diagrams are more complicated to be presented (even impossible), although the principle concepts do not change. Due to this, within the qualitative analysis of this section we will consider three-component system.

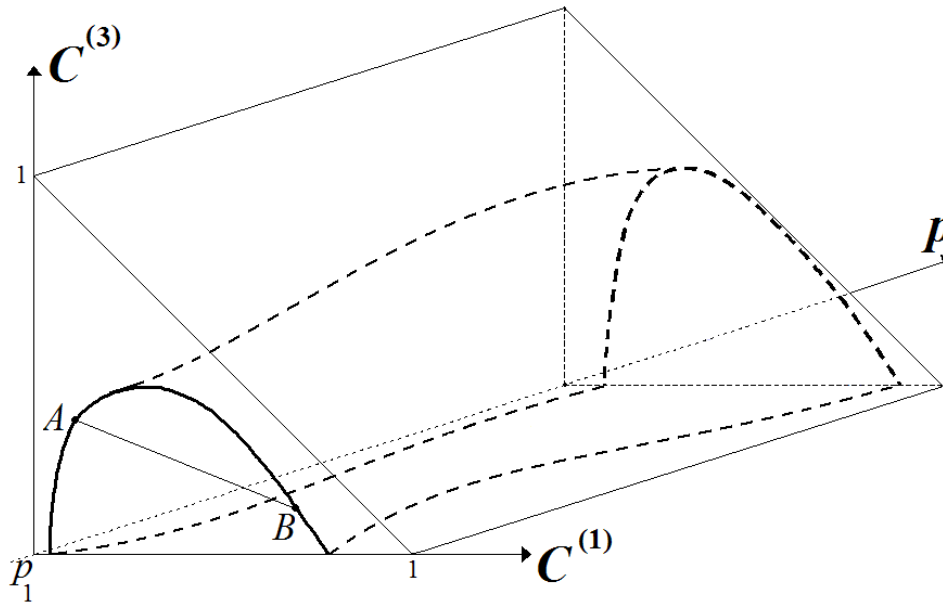


FIG. 5.2 – Ternary phase diagram for three-component system at variable pressure

5.1.2 Phase diagram for variable pressure

If pressure varies, then the system should be characterized by the set of phase diagrams which correspond to each pressure. By adding the axe p we obtain then the 3D phase diagram, as shown in Fig. 5.2.

Such a 3D diagram with all the tie-lines at each p can be constructed by using the equilibrium equations only : the tie-lines are the solution of the equilibrium equations at a given total composition, while the two-phase envelop limits the domain of existence of these solutions. Despite of this, this diagram is insufficient to describe the system behavior when pressure varies. In other words, it is impossible, by using only the classical thermodynamic equations, to determine how a tie-line at pressure p_1 will transform into another tie-line at pressure p_2 .

Physically this is related to the fact that when pressure changes, the total composition system is also changes, while the variation of the total composition depends not only on pressure but also on the hydrodynamic process. Indeed, if we examine an elementary representative volume of porous medium, the total composition can remain invariable, if

two phases flow as a unique inseparable ensemble, i.e. at the same velocities. If however the flow velocities are different, then the total composition in the examined volume will change. So the variation of the total composition depends on flow velocity, i.e. on the system hydrodynamics.

5.1.3 Concept of a P-Surface

In the asymptotic model the thermodynamic is separated from the hydrodynamics. This means in particular, that the transition between tie-lines along the axe p can be calculated only by the thermodynamic sub-system. These transitions are determined by the new differential thermodynamic equations (4.4b).

Indeed, for a ternary mixture, this system contains only one equation for the intermediary component 2 :

$$\frac{1}{\Delta c^{(2)}} \frac{dc_g^{(2)}}{dp} = \frac{1}{\Delta c^{(3)}} \frac{dc_g^{(3)}}{dp} \quad (5.1)$$

with one of the Cauchy conditions.

This equation determine the variation of the phase concentration $c_g^{(2)}(p)$ if other phase concentrations, $c_g^{(3)}$, $c_l^{(2)}$ and $c_l^{(3)}$ are known. These three concentrations are determined by the system of three equilibrium equations (4.4a). So the system is closed. (in reality three thermodynamic and one differential equations should be solved simultaneously).

If we can calculate $c_g^{(2)}(p)$, then we can determine the transition of point B along axe p . So this means that we can determine the transition of one tie-line into another one along axis p .

The consecutive system of tie-lines transiting into one another represents a 3D surface shown in Fig. 5.3.

Such a surface, determined by the thermodynamic system of equilibrium equations (4.4a) and differential thermodynamic equations (4.4b) and representing a tie-line in each cross-section (i.e. at each p) will be called a *P-surface*.

Along a *P-surface*, the liquid composition varies from the initial point A along the curve AA' . In the similar way the gas composition varies from the initial point B along the curve

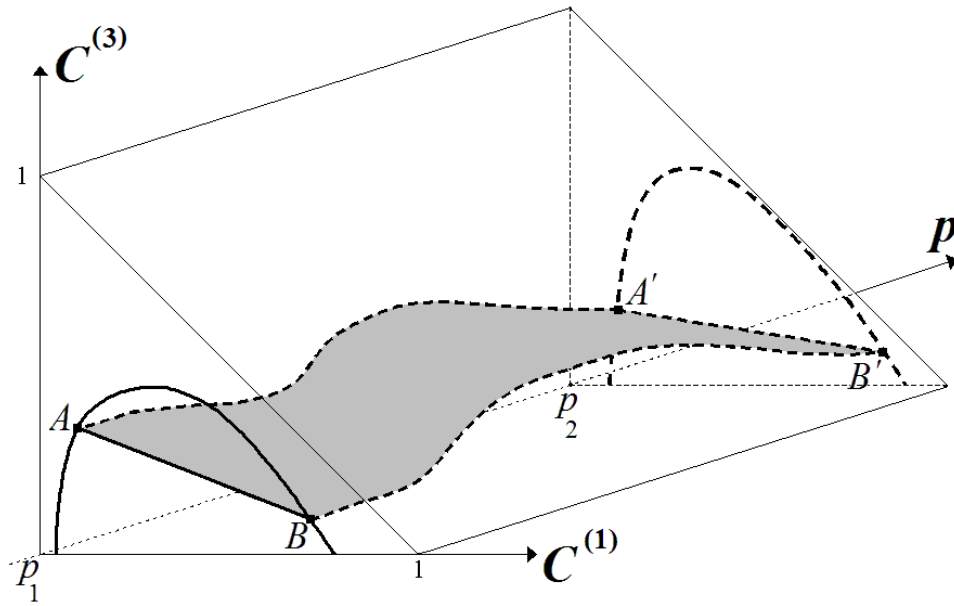


FIG. 5.3 – P-surface for a ternary two-phase system

BB' . Any new couple of points $A'B'$ at another pressure p_2 is related by a tie-line in the corresponding phase diagram which corresponds to p_2 .

For a system containing N chemical components, the P -surface represents a hypersurface in N -dimensional space.

Thus, the system (4.4) determines the phase diagram at any p , all the tie-lines at any p and the P -surfaces.

The concept of P -surface replaces the concept of tie-line for systems with variable pressure.

In the structure of the solution of the Riemann problem, the phase concentrations are no longer forced to be constant between shocks, they can now vary in a continuous way along the P -surfaces and can jump between the P -surfaces.

5.2 Development of the analytical front tracker

5.2.1 HT-splitting in Hugoniot conditions

The system of $N - 2$ Hugoniot conditions at the SC -shocks (4.23c) does not contain velocities, but only thermodynamic parameters and two non-thermodynamic parameters - the backward and forward gas saturations s^- and s^+ . This poses the question whether this is possible to separate saturation and to obtain a purely thermodynamic subsystem of Hugoniot conditions? The answer to this questions is affirmative.

In other words, the principle of HT-splitting can be developed not only for differential flow equations, but for Hugoniot conditions too.

Let us consider $N - 2$ asymptotic Hugoniot conditions (4.23c), which do not contain flow velocity :

$$\frac{c_g^{(k)+} \varphi_g^+ s^+ + c_l^{(k)+} \varphi_l^+ s_l^+ - c_g^{(k)-} \varphi_g^- s^- - c_l^{(k)-} \varphi_l^- s_l^- - c_g^{(k)+} (\varphi_g^+ s^+ + \varphi_l^+ s_l^+ - \varphi_g^- s^- - \varphi_l^- s_l^-)}{c_g^{(k)+} - c_g^{(k)-}} = \frac{c_g^{(N)+} \varphi_g^+ s^+ + c_l^{(N)+} \varphi_l^+ s_l^+ - c_g^{(N)-} \varphi_g^- s^- - c_l^{(N)-} \varphi_l^- s_l^- - c_g^{(N)+} (\varphi_g^+ s^+ + \varphi_l^+ s_l^+ - \varphi_g^- s^- - \varphi_l^- s_l^-)}{c_g^{(N)+} - c_g^{(N)-}} \quad k = 2, \dots, N - 1 \quad (5.2)$$

where $s_l = 1 - s$ is the liquid saturation. Arithmetic transformations lead to :

$$\varphi_l^+ (1 - s^+) \left(c_g^{N-} c_g^{k+} - c_g^{N+} c_g^{k-} - c_l^{N+} c_g^{k+} + c_l^{N+} c_g^{k-} - c_l^{k+} c_g^{N-} + c_l^{k+} c_g^{N+} \right) = \varphi_l^- (1 - s^-) \left(c_l^{k-} c_g^{N+} - c_l^{k-} c_g^{N-} - c_g^{N+} c_g^{k-} + c_g^{N-} c_g^{k+} - c_l^{N-} c_g^{k+} + c_l^{N-} c_g^{k-} \right), \quad k = 2, \dots, N - 1 \quad (5.3)$$

Both the saturations and densities enter in a unique parameter $\varphi_l^+(1 - s^+)/(\varphi_l^-(1 - s^-))$. Therefore, using one of this equation, it is possible to eliminate saturations and densities from $N - 3$ equations :

$$\frac{c_g^{N-}c_g^{2+} - c_g^{N+}c_g^{2-} - c_l^{N+}c_g^{2+} + c_l^{N+}c_g^{2-} - c_l^{2+}c_g^{N-} + c_l^{2+}c_g^{N+}}{c_l^{2-}c_g^{N+} - c_l^{2-}c_g^{N-} - c_g^{N+}c_g^{2-} + c_g^{N-}c_g^{2+} - c_l^{N-}c_g^{2+} + c_l^{N-}c_g^{2-}} = \frac{c_g^{N-}c_g^{k+} - c_g^{N+}c_g^{k-} - c_l^{N+}c_g^{k+} + c_l^{N+}c_g^{k-} - c_l^{k+}c_g^{N-} + c_l^{k+}c_g^{N+}}{c_l^{k-}c_g^{N+} - c_l^{k-}c_g^{N-} - c_g^{N+}c_g^{k-} + c_g^{N-}c_g^{k+} - c_l^{N-}c_g^{k+} + c_l^{N-}c_g^{k-}}, \quad k = 2, \dots, N - 2 \quad (5.4)$$

The specificity of the Hugoniot conditions formulated above consists in that this system of $N - 3$ equations contains only phase concentrations. This means that we have split thermodynamic variables from hydrodynamic in Hugoniot conditions.

This system of $N - 3$ equations contains $4N - 4$ unknown concentrations $c_g^{(k)+}$, $c_g^{(k)-}$, $c_l^{(k)+}$ and $c_l^{(k)-}$. Then even being completed with N equilibrium equations from the forward side of the shock, N equilibrium equations from the backward side, and $N - 2$ differential thermodynamic equations, we obtain $4N - 5$ equations, which is not sufficient to obtain a unique solution. In addition, it is not clear what thermodynamic Cauchy conditions should we take for each shock. Moreover, the use of differential thermodynamic conditions is not approved as they determine the behavior of solution between two shocks but not at a shock.

Despite this it is possible to construct a closed problem for shock concentrations simultaneously for all the shocks. For this, it is necessary to know the number of shocks appearing in the solution.

5.2.2 Number of *SC*-chocks and crossover *P*-surfaces

One of the significant qualitative results of the analytical theory of the Riemann problem based on the ideal mixing announces that in a N -component two-phase system which does not change the number of phases (i.e. neither the total evaporation nor the total condensation are observed) the phase concentrations should follow $N - 3$ different "*intermediate*" or "*crossover*" tile-lines located between two "*external*" tie-lines which correspond to the initial and the injection states [Orr 2002]. So in total, phase concentrations should follow

$N - 1$ tie-lines. This result is not strictly proved mathematically and it is empirical, but is entirely confirmed by all the numerical data.

In the case of variable pressure we will assume the same result to be valid, so that in a N -component two-phase system which does not change the number of phases the phase concentrations should follow $N - 1$ different P-surfaces including two "*external*" P-surfaces that correspond to two boundary pressures and $N - 3$ "*intermediate*" or "*crossover*" P-surfaces.

As one P-surface is situated between two neighboring *SC*-shocks, then the $N - 3$ crossover P-surfaces are situated between $N - 2$ *SC*-shocks. This means that the total number of the intermediate *SC*-shocks is $N - 2$.

All this is valid only for the case where the system does not change its phase state. Otherwise, additional shocks *of phase transition* can arise.

5.2.3 Front tracker for concentrations

The differential thermodynamic equations determine P-surfaces between two neighboring shocks. This means that the total system of Hugoniot conditions and thermodynamic equations for all the shocks represents a coupled system of equations. So it is necessary to search for the parameters of all the shocks simultaneously.

Fig. 5.4 helps to calculate the number of variables and equations.

The concentrations between the injection point and the first internal shock are totally determined by the thermodynamic model. The differential thermodynamic equations are taken with the Cauchy condition corresponding to the injection pressure. The similar situation concerns the concentrations between the last shock and the final point (the concentrations are calculated from the final point counter flow). Thus, only the concentrations before the first and behind the last shock are undetermined. This gives us $2(N - 3)$ sides of shocks at which we need to determine concentrations. The total number of the unknown concentrations at the shocks is then $4(N - 1)(N - 3)$.

At $N - 2$ shocks we have $(N - 3)(N - 2)$ relations (5.4). Each side of shock provides

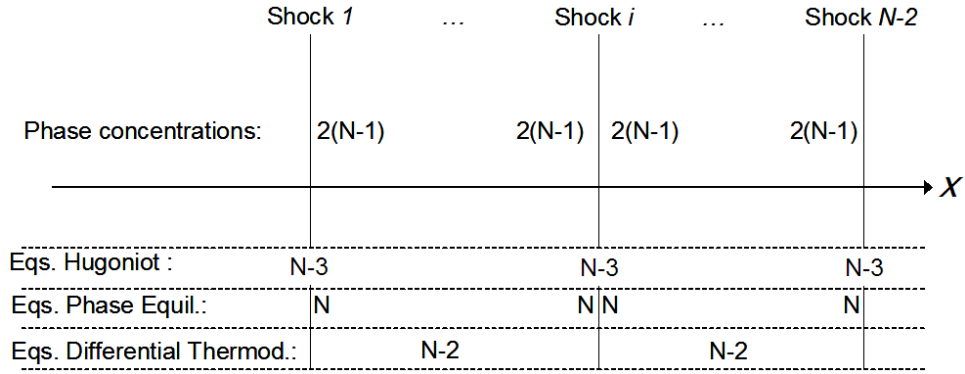


FIG. 5.4 – Schematic illustration of the number of unknown phase concentrations and the number of thermodynamic equations at each side of each shock

TAB. 5.1 – Total Number of unknown concentrations at all the *SC*-shocks

Unknown variables		
Shock type	Number of shocks	Number of concentrations at one shock
First after the injection point	1	2(N-1)
Intermediate	N-4	4(N-1)
Last before the exit point	1	2(N-1)
Total	N-2	4(N-1)(N-3)

us N equations of phase equilibrium (4.4a). Between two neighboring shocks we have $N - 2$ differential thermodynamic equations (4.4b), so between all the shocks we will have $(N - 3)(N - 2)$ differential thermodynamic relations. As a result, we possess $2(N - 3)(N - 2) + 2N(N - 3) = 2(N - 3)(2N - 2) = 4(N - 3)(N - 1)$ equations which contains only phase concentrations as the unknown variables.

Therefore, the system is closed and has unique solution.

The same count of the number of variables and equations is presented in the form of two tables (5.1) and (5.2).

So system (4.4) and (5.4) provides the necessary tool to determine all the backward and forward concentrations at all the shocks before solving the hydrodynamic differential equations.

TAB. 5.2 – Total Number of thermodynamic equations

Equation type	Number of			Total number of equations
	shocks	shock sides	crossover P-surfaces	
Hugoniot (N-3)	N-2			(N-3)*(N-2)
Equilibrium (N)		2(N-3)		2N(N-3)
DTE (N-2)			N-3	(N-2)(N-3)
Total				4(N-1)(N-3)
⁽¹⁾ DTE = differential thermodynamic equations				

Such a procedure for shock parameters detection is called *front tracker*.

5.2.4 Front tracker for saturations

For the backward and forward saturations at each shock it is also possible to develop the explicit analytical procedure of tracking.

The remaining system of Hugoniot conditions, which are not used for concentration tracker, is : (4.23a), (4.23b) and (5.3) :

$$\varepsilon V_f = \frac{\left[V \left(\varphi_g \widehat{F} + \varphi_l (1 - \widehat{F}) \right) \right]}{[\varphi]}; \quad (5.5a)$$

$$\frac{V^- \widehat{F}^- \varphi_g^- \left[c_g^{(N)} \right] + \left[V (1 - \widehat{F}) \varphi_l c_l^{(N)} \right] - c_g^{(N)+} \left[V (1 - \widehat{F}) \varphi_l \right]}{[\varphi^{(N)}] - c_g^{(N)+} [\varphi]} = \frac{\left[V \left(\varphi_g \widehat{F} + \varphi_l (1 - \widehat{F}) \right) \right]}{[\varphi]}; \quad (5.5b)$$

$$\frac{\varphi_l^+ (1 - s^+)}{\varphi_l^- (1 - s^-)} = \frac{c_g^{(N-1)+} (c_g^{N-} - c_l^{N+}) + c_g^{(N-1)-} (c_l^{N+} - c_g^{N+}) + c_l^{(N-1)+} (c_g^{N+} - c_g^{N-})}{c_l^{(N-1)-} (c_g^{N+} - c_g^{N-}) + c_g^{(N-1)+} (c_g^{N-} - c_l^{N-}) + c_g^{(N-1)-} (c_g^{N+} - c_l^{N-})} \quad (5.5c)$$

Herein V is the total flow velocity ($V = V_g + V_l$), while $\widehat{F}(s)$ is the classic (volumetric) fractional flow function of gas phase, (4.21).

Three equations (5.5) contains five unknown parameters : s^+ , s^- , V^+ , V^- and V_f . The additional conditions which allow to determine the unique solution are the entropy

conditions. In practice their use is not technically simple.

Instead of this, at the first step of development of this theory we suggest the approximation which permits significant simplification in all the calculations. We will use the result obtained for the total velocity at a S -shock (section 4.2.9). Similar to this, we will assume that the total velocity is continuous while passing through an SC -shock too. This assumption is confirmed by the fact that the total velocity is a sufficiently conservative function as it is responsible for the flow continuity, in contrast to the phase velocity, which can easily undergo jumps while passing through a boundary or a front.

This assumption is much weaker than that used in the classic theory based on the ideal mixing where the total velocity is not only continuous but also invariable in space.

Using this assumption, we can eliminate both the velocities V^+ and V^- from equation (5.5b). Then equations (5.5b) and (5.5c) becomes :

$$\left\{ \begin{array}{l} \frac{\widehat{F}^- \varphi_g^- [c_g^{(N)}] + [(1 - \widehat{F}) \varphi_l c_l^{(N)}] - c_g^{(N)+} [(1 - \widehat{F}) \varphi_l]}{[\varphi^{(N)}] - c_g^{(N)+} [\varphi]} = \frac{[\varphi_g \widehat{F} + \varphi_l (1 - \widehat{F})]}{[\varphi]}, \\ \frac{\varphi_l^+ (1 - s^+)}{\varphi_l^- (1 - s^-)} = \frac{c_g^{(N-1)+} (c_g^{N-} - c_l^{N+}) + c_g^{(N-1)-} (c_l^{N+} - c_g^{N+}) + c_l^{(N-1)+} (c_g^{N+} - c_g^{N-})}{c_l^{(N-1)-} (c_g^{N+} - c_g^{N-}) + c_g^{(N-1)+} (c_g^{N-} - c_l^{N-}) + c_g^{(N-1)-} (c_g^{N+} - c_l^{N-})} \end{array} \right. \quad (5.6)$$

This is the system of two equations with respect to two saturations s^- and s^+ , as all the phase concentrations are already determined from the concentration tracker (5.4).

The first equation of the system (5.5), which is not used yet, becomes :

$$\varepsilon \frac{V_f}{V} = \frac{[\varphi_g \widehat{F} + \varphi_l (1 - \widehat{F})]}{[\varphi]} \quad (5.7)$$

which determine the relative velocity of the shock.

It is necessary to mention that all the system of relations at a shock is capable to determine only the relative shock velocity. The total flow velocity V is not the proper shock parameter and should be determined from the differential flow equations.

System (5.6) represents the tracker of saturation at both the SC -shocks and S -shocks.

5.2.5 Algorithm of solution of the Riemann problem

The developed procedure of front tracking establishes the following algorithm for constructing the solution to the displacement problem.

Step 1 - tracking the front concentrations : Using the concentration front tracker which consists of system (4.4) and $(N - 3)$ Hugoniot relations (5.4), we determine all the backward and forward phase concentrations at all the *SC*-shocks. In reality we calculate the entire intermediate P-surfaces, as they are the solutions to the differential thermodynamic system.

Step 2 - tracking the front saturations : this is done by using saturation front tracker which represent two Hugoniot relations (5.6).

Step 3 - tracking the front velocity : this is done also explicitly by using the last Hugoniot condition (5.7).

Step 4 - simulation of the continuous parts of the solution between the shocks : by simulating numerically the hydrodynamic equations for saturation and pressure (4.1) along the corresponding P-surface.

So the shocks are detected analytically, while the rarefaction waves are simulated numerically.

The link between the numerical solution and analytical relations is performed in the following way : the pressure and saturation are computed numerically forward from the starting point $x = 0$. Once the values of saturation reach one of the values which corresponds to a probable shock, this mobile point is considered as the shock placing. After this we begin to simulate the next rarefaction wave while taking the forward saturation at the shock as the initial value, and so on.

5.3 Continuous solutions of the flow equations

5.3.1 Method of characteristics

The third step in our algorithm is the construction of the continuous parts of solution to the equations (3.16b) and (3.16a) along each P-surface. The solution to the transport equation (3.16b) is obtained by the method of characteristics.

Let us analyze equation (3.16b) :

$$\frac{\partial s}{\partial t} + \frac{1}{\varphi_l} \frac{\partial F(s, p)}{\partial s} \frac{\partial s}{\partial x} = - \frac{\varepsilon F(s, p)}{\varphi_l \Delta c^{(N)} (\psi_g k_g + \omega \psi_l k_l)} \frac{dc_g^{(N)}}{dp}, \quad F \equiv \frac{\psi_g k_g}{\psi_g k_g + \omega \psi_l k_l} \quad (5.8)$$

The initial condition which corresponds to the Riemann problem may be presented in the form :

$$s(x, 0) = s^{inj} - (s^{inj} - s^0) H(x) \quad (5.9)$$

where $H(x)$ is the Heaviside function.

Let us introduce characteristic directions $x(t)$ and the full time-derivative along $x(t)$:

$$\frac{dx}{dt} = \frac{1}{\varphi_l} \frac{\partial F(s, p)}{\partial s}, \quad \frac{ds}{dt} \equiv \frac{\partial s}{\partial t} + \frac{dx}{dt} \frac{\partial s}{\partial x} \quad (5.10)$$

Then equation (5.8) becomes :

$$\frac{ds}{dt} = - \frac{\varepsilon F(s, p)}{\varphi_l \Delta c^{(N)} (\psi_g k_g + \omega \psi_l k_l)} \frac{dc_g^{(N)}}{dp} \quad (5.11)$$

It is impossible to neglect small terms $\sim \omega$ in the left-hand side of the equation (5.8) and, consequently, in the equation of the characteristic lines (5.10), as equation (5.8) will be degenerating. Nevertheless it is possible to neglect small terms $\sim \omega$ in the right-hand

side of (5.8). Then equation (5.11) takes the form :

$$\frac{ds}{dt} = \frac{C_1}{k_g(s)}, \quad C_1(p) \equiv -\frac{\varepsilon}{\varphi_l \psi_g \Delta c^{(N)}} \frac{dc_g^{(N)}}{dp} \quad (5.12)$$

In which C_1 does not depend on saturation. As pressure is quasi-stationary, then C_1 does not depend on time as well.

Two equations (5.8) and (5.12) completed with the initial condition (5.9) represent the solution to the problem. It can be solved numerically, which will give us the evolution of the function $s = s(t)$ along the family of curve $x(t)$ and the location of the curves $x(t)$ in the plane (x, t) .

As the equation (5.10) or (5.12) are non-homogeneous then the saturation is not constant along the characteristic line. Due to this the characteristic lines (5.8) are non straight. So these two equations are inseparable from one another and should be solved simultaneously.

5.3.2 Example of solution

Let us consider a simplified case in order to illustrate the technique of solution. Assume the phase densities and viscosities, as well as the coefficient C_1 to be constant. Then ψ_g and ψ_l are equal to 1 according to their definition. The relative permeability of each phase are quadratic functions of the proper saturation : $k_g = s^2$, $k_l = (1 - s)^2$.

The solution (5.8) and (5.12) becomes :

$$\frac{ds}{dt} = \frac{C_1}{s^2}, \quad \frac{dx}{dt} = \frac{C_2 (s - s^2)}{(s^2 + \omega(1 - s)^2)^2}; \quad C_2 \equiv \frac{2\omega}{\varphi_l} \quad (5.13)$$

It is better to transform this system by taking the "phase variables" for the second equation :

$$\frac{ds}{dt} = \frac{C_1}{s^2}, \quad \frac{dx}{ds} = \frac{C_2}{C_1} \frac{s^3(1 - s)}{(s^2 + \omega(1 - s)^2)^2} \quad (5.14)$$

For the characteristics emanating from each point ξ at the x -axis (i.e. at $t = 0$) the

initial conditions for this system are :

$$x|_{t=0} = \xi, \quad s|_{t=0} = s^0$$

The solution of this initial problem for the system of ordinary differential equations (5.14) is :

$$\begin{cases} s^3 = 3C_1t + (s^0)^3 \\ x(t) = \xi + \frac{C_2}{C_1} \int_{s^0}^{(3C_1t+(s^0)^3)^{1/3}} \frac{u^3(1-u)}{(u^2 + \omega(1-u)^2)^2} du \end{cases}$$

where ξ is the parameter.

For the characteristics coming from each point τ at the t -axis (i.e. at $x = 0$) the initial conditions are :

$$x|_{t=\tau} = 0, \quad s|_{t=\tau} = s^{inj}$$

The solution to this problem is :

$$\begin{cases} s^3 = 3C_1(t - \tau) + (s^{inj})^3 \\ x(t) = \frac{C_2}{C_1} \int_{s^{inj}}^{(3C_1(t-\tau)+(s^{inj})^3)^{1/3}} \frac{u^3(1-u)}{(u^2 + \omega(1-u)^2)^2} du \end{cases}$$

where τ is the parameter.

The saturation s_* ($s_0 \leq s_* \leq s^0$) associated with the discontinuity at the origin (i.e. at $x = 0$ and $t = 0$) will propagate according to the similar relations :

$$\begin{cases} s^3 = 3C_1t + s_*^3 \\ x(t) = \frac{C_2}{C_1} \int_{s_*}^{(3C_1t+s_*^3)^{1/3}} \frac{u^3(1-u)}{(u^2 + \omega(1-u)^2)^2} du \end{cases}$$

Varying the value s_* we obtain a fan of different characteristics issuing from the origin.

Three kinds of characteristics, coming from the axis x (the red lines), from the axis t (the black lines) and the fan issuing from the origin (the blue lines) are presented in Fig.5.5.

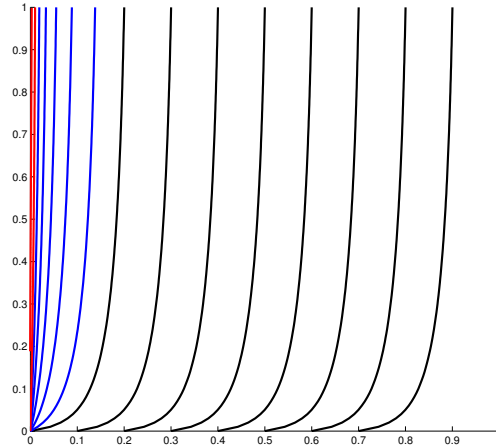


FIG. 5.5 – Characteristic lines transporting the initial composition (black lines), the injection composition (red lines) and the initial shock at the origin (blue curves)

If the characteristics intersect one another, this means that at least two independent values of saturation can meet one another at the same point (x,t) . This can be realized in the form of shock. In the analyzed example, obviously, the solution to the problem is continuous.

5.4 Results of solution for three- and four- components problem

5.4.1 Description of the analyzed examples

We simulated flow of a gas-oil system in the case of three components : carbon dioxide, methane, decane, and four components : carbon dioxide, methane, N-butane, decane. The injection of gas in equilibrium with the liquid consists of all the components into the reservoir containing the oleic phase was particularly of interest.

The system of split hydrodynamics equations (3.16a) and (3.16b) was discretized using backward finite difference method, fully explicit in time.

We consider an isothermal process, as the overall mass of earth rocks surrounding the examined reservoir plays the role of a huge calorimeter possessing a huge integral calorific capacity which maintains a constant temperature inside the reservoir in a natural way. The thermodynamic subsystem then was simulated on the basis of the Peng-Robinson equation of state for both the phases. The thermodynamic simulations were performed independently for a fixed temperature and various pressures. The obtained values of the phase concentrations have been approximated by third order polynomial functions of pressure which were used in the hydrodynamic part. We also used this polynomials to find the phase densities and viscosities as a function of pressure and phase concentrations.

The saturation profile was obtained all over the one dimensional reservoir at various time instants after starting the injection.

5.4.2 Calculation of densities and viscosities

The phase densities and viscosities depend explicitly on pressure and implicitly through the phase composition.

In the calculated examples we used the approximate EOR. In particular, we taken into consideration the variation of the gas density and liquid viscosity only, assuming that the variation of liquid density and gas viscosity are much lower.

To find the viscosity of the oil phase we assumed that only the concentration of the lightest component would have the essential effect :

$$\mu = \mu_{od} - a * c_l \quad (5.15)$$

where μ_{od} is the dead-oil viscosity and c_l is the concentration of the lightest component in the liquid phase, and $a = (\mu_{od} - \mu_0)/c_l^0$.

For the gas density we used the EOS for true gases :

$$\rho_g = \gamma \frac{P}{Z(P, T)} \quad , \quad \gamma = \frac{\rho_0}{P_0 Z_0} \quad (5.16)$$

in which $Z(P, T)$ is the z-factor or the coefficient of gas compressibility which is defined according to the empirical equations of Gurevich-Latonov :

$$Z = (0.4 \log(\tau(T)) + 0.37)^{\pi(P)} + 0.1\pi(P) \quad (5.17)$$

$$\tau(T) = \frac{T}{125(1 + \bar{\rho})} \quad , \quad \pi(P) = \frac{P}{50 - 5\bar{\rho}} \quad , \quad \bar{\rho} = \frac{\sum_{i=1}^N (c_g^i M^i)}{28.96} \quad (5.18)$$

where N is the number of chemical components in gas phase, c_g^i is their molar concentrations and M^i is their molar weights.

5.4.3 Three-components two-phase problem

As an example of ternary problem we examined a mixture of carbon dioxide, methane, decane with the injection composition of :

$$CO_2 = 0.6110$$

$$CH_4 = 0.3447$$

$$C_{10} = 0.0443$$

and the initial composition of :

$$CO_2 = 0.2259$$

$$CH_4 = 0.0710$$

$$C_{10} = 0.7031$$

The phase equilibrium of this system was simulated using the equilibrium equations with Peng-Robinson equation of state for a fixed reservoir temperature (T=300 K) and various pressures between P=150 bar and P=90 bar.

The simulator has been developed in the laboratory. The simulator solves the system of nonlinear equilibrium equations using the Newton iteration method. The initial approximation for the iterations was obtained by using Wilson correlations for the K-values at low pressures.

The results of these simulations were then treated statistically using MATLAB in order to obtain analytical correlations for all the thermodynamic functions.

For all the concentrations on each phase we have obtained ([P]=bar) :

Injection compositions

CO_2 :

$$c_l^{(1)}(P) = 0.2143 * 10^{-6} P^3 - 0.8454 * 10^{-4} P^2 + 0.1220 * 10^{-1} P + 0.3023$$

$$c_g^{(1)}(P) = 0.2994 * 10^{-7} P^3 + 0.1731 * 10^{-4} P^2 - 0.1569 * 10^{-2} P + 0.6855$$

CH_4 :

$$c_l^{(2)}(P) = 0.2994 * 10^{-7} P^3 - 0.9954 * 10^{-5} P^2 + 0.2250 * 10^{-2} P - 0.7686$$

$$c_g^{(2)}(P) = 0.1057 * 10^{-5} P^3 - 0.4820 * 10^{-3} P^2 + 0.6855 * 10^{-1} P - 2.7457$$

C_{10} :

$$c_l^{(3)}(P) = -0.2479 * 10^{-6}P^3 - 0.9586 * 10^{-4}P^2 - 0.1462 * 10^{-1}P + 1.3860$$

$$c_g^{(3)}(P) = 0.8871 * 10^{-7}P^3 - 0.1571 * 10^{-4}P^2 + 0.8230 * 10^{-3}P - 0.8030 * 10^{-2}$$

Initial compositions

CO_2 :

$$c_l^{(1)}(P) = 0.4036 * 10^{-7}P^3 - 0.1576 * 10^{-4}P^2 + 0.2052 * 10^{-2}P + 0.9261 * 10^{-1}$$

$$c_g^{(1)}(P) = -0.1859 * 10^{-6}P^3 + 0.6489 * 10^{-4}P^2 - 0.6394 * 10^{-2}P + 0.8124$$

CH_4 :

$$c_l^{(2)}(P) = -0.2214 * 10^{-8}P^3 + 0.7411 * 10^{-6}P^2 - 0.5208 * 10^{-4}P + 0.3853$$

$$c_g^{(2)}(P) = 0.1971 * 10^{-6}P^3 - 0.6886 * 10^{-4}P^2 + 0.6812 * 10^{-2}P + 0.1728$$

C_{10} :

$$c_l^{(3)}(P) = -0.4428 * 10^{-7}P^3 + 0.1735 * 10^{-4}P^2 - 0.2293 * 10^{-2}P + 0.8810$$

$$c_g^{(3)}(P) = -0.1640 * 10^{-7}P^3 + 0.5893 * 10^{-5}P^2 - 0.6481 * 10^{-3}P + 0.2393 * 10^{-1}$$

In Fig. 5.6 the gas saturation profile has been shown for four different time steps. The pure S -shocks do not exist in this case, only SC -shocks relate the injection and initial P -surfaces.

5.4.4 Four-components two-phase problem

As an example of four-components displacement we examined the mixture of carbon dioxide, methane, propane and decane with the following injection composition :

$$CO_2 = 0.2906$$

$$CH_4 = 0.5909$$

$$C_4 = 0.1000$$

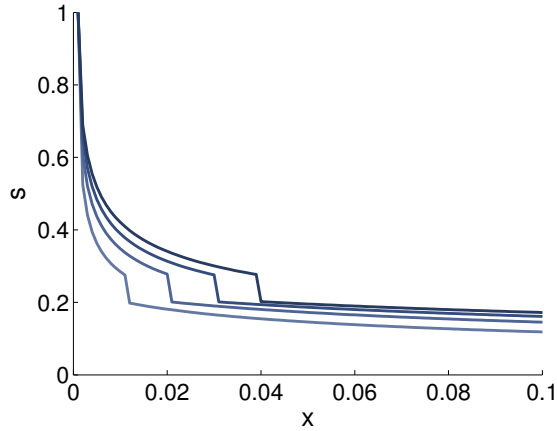


FIG. 5.6 – Three component problem - Gas saturation profile at $t = 0.05$ (lower curve) and $t = 0.1$ (upper curve)

$$C_{10} = 0.0185$$

and the initial composition :

$$CO_2 = 0.1619$$

$$CH_4 = 0.0487$$

$$C_4 = 0.2649$$

$$C_{10} = 0.5244$$

Again we found the phase behavior of the system by using our phase equilibrium simulator linked with the Peng-Robinson EOS. The simulation was performed for a fixed reservoir temperature $T = 300$ K and various pressures between $P = 150$ bar and $P = 90$ bar. The results of multi-variant simulations were treated statistically by MATLAB in order to obtain an analytical form for the correlations of all the thermodynamic functions.

For phase concentrations we have obtained ($[P]=\text{bar}$) :

Injection compositions

CO_2 :

$$c_l^{(1)}(P) = 0.6434 * 10^{-7} P^3 - 0.2629 * 10^{-4} P^2 + 0.3965 * 10^{-2} P - 0.7231 * 10^{-1}$$

$$c_g^{(1)}(P) = -0.1197 * 10^{-7} P^3 + 0.3492 * 10^{-5} P^2 - 0.5608 * 10^{-3} P + 0.3338$$

CH_4 :

$$c_l^{(2)}(P) = 0.4025 * 10^{-7} P^3 - 0.1529 * 10^{-4} P^2 + 0.3149 * 10^{-2} P - 0.8244 * 10^{-1}$$

$$c_g^{(2)}(P) = 0.1741 * 10^{-7} P^3 - 0.1123 * 10^{-4} P^2 + 0.1266 * 10^{-2} P + 0.5869$$

C_4 :

$$c_l^{(3)}(P) = 0.7195 * 10^{-7} P^3 - 0.2021 * 10^{-4} P^2 + 0.3234 * 10^{-3} P + 0.3420$$

$$c_g^{(3)}(P) = -0.4367 * 10^{-7} P^3 + 0.1450 * 10^{-4} P^2 - 0.1039 * 10^{-2} P + 0.8060 * 10^{-1}$$

C_{10} :

$$c_l^{(4)}(P) = -0.1714 * 10^{-6} P^3 + 0.5980 * 10^{-4} P^2 - 0.7182 * 10^{-2} P + 0.8020$$

$$c_g^{(4)}(P) = 0.4849 * 10^{-7} P^3 - 0.1041 * 10^{-4} P^2 + 0.7604 * 10^{-3} P - 0.1781 * 10^{-1}$$

Initial compositions

CO_2 :

$$c_l^{(1)}(P) = 0.3248 * 10^{-7} P^3 - 0.1148 * 10^{-4} P^2 + 0.1320 * 10^{-2} P + 0.1123$$

$$c_g^{(1)}(P) = -0.1159 * 10^{-6} P^3 - 0.4167 * 10^{-4} P^2 - 0.4816 * 10^{-2} P + 0.6545$$

CH_4 :

$$c_l^{(2)}(P) = 0.1554 * 10^{-7} P^3 - 0.6406 * 10^{-5} P^2 + 0.9139 * 10^{-3} P + 0.5994 * 10^{-2}$$

$$c_g^{(2)}(P) = 0.4926 * 10^{-6} P^3 - 0.1603 * 10^{-3} P^2 + 0.1534 * 10^{-1} P + 0.6254 * 10^{-4}$$

C_4 :

$$c_l^{(3)}(P) = -0.7148 * 10^{-8} P^3 + 0.3705 * 10^{-5} P^2 - 0.6641 * 10^{-3} P + 0.3011$$

$$c_g^{(3)}(P) = -0.3699 * 10^{-6} P^3 + 0.1163 * 10^{-3} P^2 - 0.1027 * 10^{-1} P + 0.3364$$

C_{10} :

$$c_l^{(4)}(P) = -0.2518 * 10^{-7} P^3 + 0.8525 * 10^{-5} P^2 - 0.8928 * 10^{-3} P + 0.5537$$

$$c_g^{(4)}(P) = -0.4351 * 10^{-8} P^3 - 0.1452 * 10^{-5} P^2 - 0.1407 * 10^{-3} P + 0.4540 * 10^{-2}$$

5.4.5 Determination of an intermediate P-surface

In two-phase four-component problem we have $N - 3 = 1$ intermediate P-surface and two intermediate shocks. One shock is placed between the injection P-surface and the unknown intermediate P-surface, while the second shock connects the mentioned intermediate P-surface to the initial one.

Thus system (5.4) provides us one equation which will be applied for two shocks.

For the shock between the injection and the intermediate P-surfaces we will have :

$$\frac{c_g^{(4),inj} c_g^{(2),int} - c_g^{(4),int} c_g^{(2),inj} - c_l^{(4),int} c_g^{(2),int} + c_l^{(4),inj} c_g^{(2),int} - c_l^{(2),int} c_g^{(4),inj} + c_l^{(2),int} c_g^{(4),int}}{c_l^{(2),inj} c_g^{(4),int} - c_l^{(2),inj} c_g^{(4),inj} - c_g^{(4),int} c_g^{(2),inj} + c_g^{(4),inj} c_g^{(2),int} - c_l^{(4),inj} c_g^{(2),int} + c_l^{(4),inj} c_g^{(2),inj}} =$$

$$\frac{c_g^{(4),inj} c_g^{(3),int} - c_g^{(4),int} c_g^{(3),inj} - c_l^{(4),int} c_g^{(3),int} + c_l^{(4),inj} c_g^{(3),inj} - c_l^{(3),int} c_g^{(4),inj} + c_l^{(3),int} c_g^{(4),int}}{c_l^{(3),inj} c_g^{(4),int} - c_l^{(3),inj} c_g^{(4),inj} - c_g^{(4),int} c_g^{(3),inj} + c_g^{(4),inj} c_g^{(3),int} - c_l^{(4),inj} c_g^{(3),int} + c_l^{(4),inj} c_g^{(3),inj}} \quad (5.19)$$

where the subscript *inj* refers to the injection P-surface and *int* to the intermediate one.

For the jump between the intermediate and initial P-surfaces we will find :

$$\frac{c_g^{(4),int} c_g^{(2)0} - c_g^{(4),0} c_g^{(2),int} - c_l^{(4)0} c_g^{(2)0} + c_l^{(4)0} c_g^{(2),int} - c_l^{(2)0} c_g^{(4),int} + c_l^{(2)0} c_g^{(4)0}}{c_l^{(2),int} c_g^{(4)0} - c_l^{(2),int} c_g^{(4),int} - c_g^{(4)0} c_g^{(2),int} + c_g^{(4),int} c_g^{(2)0} - c_l^{(4),int} c_g^{(2)0} + c_l^{(4),int} c_g^{(2),int}} =$$

$$\frac{c_g^{(4),int} c_g^{(3)0} - c_g^{(4)0} c_g^{(3),int} - c_l^{(4)0} c_g^{(3)0} + c_l^{(4),int} c_g^{(3),int} - c_l^{(3)0} c_g^{(4),int} + c_l^{(3)0} c_g^{(4)0}}{c_l^{(3),int} c_g^{(4)0} - c_l^{(3),int} c_g^{(4),int} - c_g^{(4)0} c_g^{(3),int} + c_g^{(4),int} c_g^{(3)0} - c_l^{(4),int} c_g^{(3)0} + c_l^{(4),int} c_g^{(3),int}} \quad (5.20)$$

The subscript 0 refers to the initial P-surface.

Taking the equations of the normalization into account we would have six unknown concentration on the intermediate P-surface to find, the rest of equations will be found from the equilibrium relations.

In order to obtain the parameters of shocks analytically, we used the simplified Wilson

relations for K-values :

$$K_i = \frac{c_g^i}{c_l^i} = \frac{P_{ci}}{P} \exp \left[5.37(1 + \omega_i) \left(1 - \frac{T - T_{ci}}{T} \right) \right] \quad (5.21)$$

Relations for gas and liquid concentrations as the functions of pressure for each component were obtained. We used the data prepared in [Orr, 2002] for our calculation in this part. Using the Symbolic Toolbox of MATLAB, a code was generated to find the solution of above six equations for 10 different pressures value between 150 and 90 bar. Then the results were treated statistically in order to obtain analytical relations for all the intermediate concentrations :

Intermediate compositions

CO_2 :

$$c_l^{(1)}(P) = -0.1784 * 10^{-6}P^3 + 0.5415 * 10^{-4}P^2 - 0.2379 * 10^{-2}P + 0.3631 * 10^{-1}$$

$$c_g^{(1)}(P) = -0.2400 * 10^{-7}P^3 - 0.1487 * 10^{-4}P^2 + 0.5925 * 10^{-2}P - 0.1776$$

CH_4 :

$$c_l^{(2)}(P) = 0.6072 * 10^{-7}P^3 - 0.1665 * 10^{-4}P^2 + 0.5072 * 10^{-2}P - 0.2293$$

$$c_g^{(2)}(P) = 0.2812 * 10^{-6} - 0.1204 * 10^{-3}P^2 + 0.2022 * 10^{-1}P - 0.6683$$

C_4 :

$$c_l^{(3)}(P) = 0.2443 * 10^{-6}P^3 - 0.8384 * 10^{-4}P^2 + 0.2275 * 10^{-2}P + 1.020$$

$$c_g^{(3)}(P) = -0.2528 * 10^{-6}P^3 + 0.1338 * 10^{-3}P^2 - 0.2500 * 10^{-1}P + 1.8413$$

C_{10} :

$$c_l^{(4)}(P) = -0.1266 * 10^{-6}P^3 + 0.4634 * 10^{-4}P^2 - 0.4968 * 10^{-2}P + 0.1728$$

$$c_g^{(4)}(P) = -0.4351 * 10^{-8}P^3 + 0.1452 * 10^{-5}P^2 - 0.1407 * 10^{-3} + 0.4540 * 10^{-2}$$

In Fig. 5.7 the gas saturation profile has been shown for four different time steps. According to the theoretical results, two SC -shocks relate the injection P-surface to the

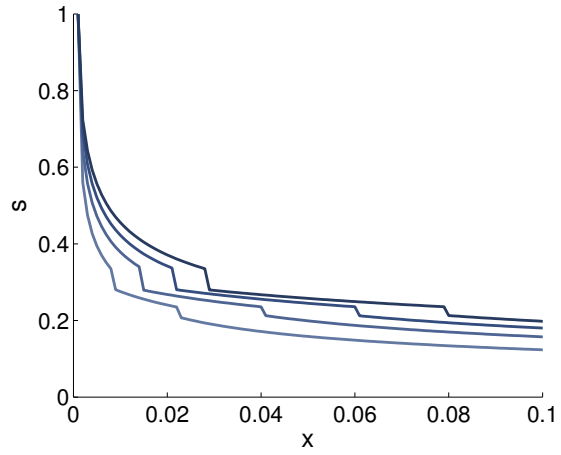


FIG. 5.7 – Four-component displacement of oil by gas : gas saturation at $t = 0.05$ (lower curve) and $t = 0.1$ (upper curve).

intermediate one and then to the initial P-surfaces.

5.5 Comparison with numerical and analytical solutions

In order to check the validity of obtained solutions, we compared it with two kinds of solutions obtained by other methods : (1) first of all, we compared with the numerical solution of the same problem but formulated in terms of the full compositional model ; (2) secondly, the comparison was done with the analytical solution obtained within the framework of a particular ratio between parameters, which leads to the model formally identical to that used in the ideal mixing theory.

The numerical solution to the full compositional model was developed by applying the finite difference method. The analytical solution was obtained by using classical technique based on the analytical detection of the shocks and on the method of characteristics between shocks.

5.5.1 Construction of the numerical solution

In order to find the system of equations which should be solved numerically we write the mass conservation equations in their conservative form :

$$\frac{\partial \varphi^{(k)}}{\partial \tau} + \frac{\partial}{\partial x} \left(\Psi^{(k)} \frac{\partial p}{\partial x} \right) = 0, \quad k = 1, \dots, N; \quad \tau \equiv \frac{t}{\varepsilon} \quad (5.22)$$

where $\Psi_i \equiv \psi_i k_i(s)$, $\varphi^{(k)} \equiv \left(\varphi_g c_g^{(k)} s + \varphi_l c_l^{(k)} (1 - s) \right)$, $\Psi^{(k)} \equiv c_g^{(k)} \Psi_g + \omega c_l^{(k)} \Psi_l$.

Assuming the quasi-stationary behavior for the pressure we will obtain the following system of equations :

$$\frac{\partial \varphi^{(k)}}{\partial \tau} + \frac{\partial F^{(k)}}{\partial x} = 0, \quad k = 1, \dots, N - 1; \quad F^{(k)} \equiv \frac{\Psi^{(k)}}{\psi_g k_g + \omega \psi_l k_l} \quad (5.23)$$

This equation can be solved while applying the scheme fully explicit in time and backward in space :

$$(\varphi^{(k)})_i^{n+1} = (\varphi^{(k)})_i^n - \frac{\Delta\tau}{\Delta x} \left((F^{(k)})_i^n - (F^{(k)})_{i-1}^n \right), \quad k = 1, \dots, N - 1 \quad (5.24)$$

where i indicates the grid block and n the time step.

Thus, we calculate explicitly parameters $\varphi^{(k)}$ which represent $\varphi^{(k)} = C^{(k)}\varphi$, $C^{(k)}$ being the total composition, while φ the total density of fluid. Assuming that $(C^{(k)})_i^n = (\varphi^{(k)})_i^n / (\varphi)_i^{n-1}$ we obtain the total composition at step n . This gives us the possibility to determine the phase composition at the step n by using standard thermodynamics flash calculation. After this we calculate phase densities. Using the relation between the total concentrations and phase concentrations, we obtain gas saturation at the step n .

5.5.2 Comparison with numerical solution

The fluid consisted of three components : carbon dioxide, methane and decane. The initial mass concentrations were :

$$\begin{aligned} CO_2 & : 0.0 \\ CH_4 & : 0.4 \\ C_{10}H_{22} & : 0.6 \end{aligned}$$

The injection compositions were :

$$\begin{aligned} CO_2 & : 0.8 \\ CH_4 & : 0.1 \\ C_{10}H_{22} & : 0.1 \end{aligned}$$

The saturation profile for an arbitrarily selected intermediate time instant calculated by both methods is shown in Fig. 5.8. The equivalence between the asymptotic model and

the full compositional models was satisfactory in all the cases of simulation.

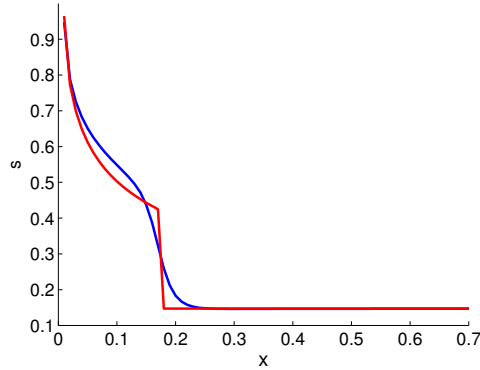


FIG. 5.8 – Gas saturation for a ternary system : the asymptotic model (red) and the numerical solution to the total compositional model (blue)

5.5.3 Construction of a particular analytical solution

Another type of verification for the validity of the proposed asymptotic model is based on comparing it with the analytical results obtained for a particular selection of the parameters of the model. Let the phase densities be identical and invariable.

Let us assume also that the pressure field is quasi-stationary. This is conform to the basic assumptions of the asymptotic model.

Then the full compositional model becomes :

$$\frac{\partial C^k}{\partial t} + \frac{\partial \widehat{F}^k}{\partial x} = 0, \quad k = 1, \dots, N - 1 \quad (5.25)$$

$$C^k = c_g^{(k)} s + c_l^{(k)} (1 - s), \quad \widehat{F}_k = c_g^{(k)} f(s) + c_l^{(k)} (1 - f), \quad f(s) = \frac{k_g(s)}{k_g(s) + \omega k_l(s)}$$

System (5.25) is formally equivalent to the fundamental model used in the ideal mixing theory (it is however useful to note that (5.25) is formulated through mass concentrations, while in the ideal mixing theory one uses the volume concentrations).

The Riemann problem for (5.25) has analytical solution if the number of components is

two or three. It is constructed by using classical technique based on the analytical detection of the shocks and on the method of characteristics between shocks.

5.5.4 Comparison with the analytical solution

The fluid consisted of three components : carbon dioxide, methane and decane. The initial mass concentrations were :

$$\begin{aligned} CO_2 & : 0.0 \\ CH_4 & : 0.475 \\ C_{10}H_{22} & : 0.525 \end{aligned}$$

The injection compositions were :

$$\begin{aligned} CO_2 & : 0.4 \\ CH_4 & : 0.6 \\ C_{10}H_{22} & : 0.0 \end{aligned}$$

For the ternary mixture, only two tie-lines can exist : the initial and the injection ones. So only one *SC*-shock can exist.

In order to solve the problem system of Hugoniot and entropy conditions in analytical approach were solved to determine the saturation before and after the only *SC*-shock. for the above initial and injection compositions the discontinuity saturations were find as : $s^- = 0.20$ and $s^+ = 0.38$.

We also solved the system of asymptotic Hugoniot condition and entropy relation in the solution with the asymptotic HT-splitting method then the saturations before and after the *SC*-shock were founded as : $s^- = 0.21$ and $s^+ = 0.35$.

These system of nonlinear equations were solved analytically using the symbolic math toolbox of MATLAB.

The solutions obtained by two methods are presented in Fig. 5.9 and 5.10 for different time instants.

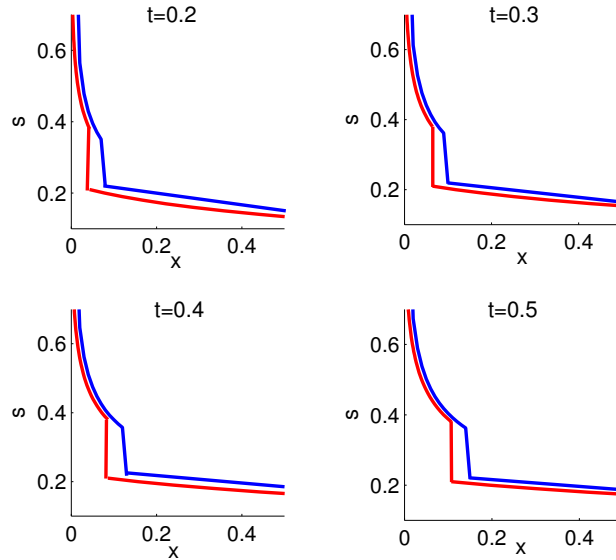


FIG. 5.9 – Gas saturation for three-component problem at different time instants : the asymptotic model (blue) and the analytical solution (red).

The qualitative form of the solution obtained within the asymptotic model is absolutely identical to the true form. At the beginning stage of displacement, the velocity of shock is a little bit higher than the true velocity. The difference reaches 5% and is caused by the approximation accepted in the asymptotic model that concerns the continuity of the total velocity through the shocks. For large times the asymptotic model provides very satisfactory results.

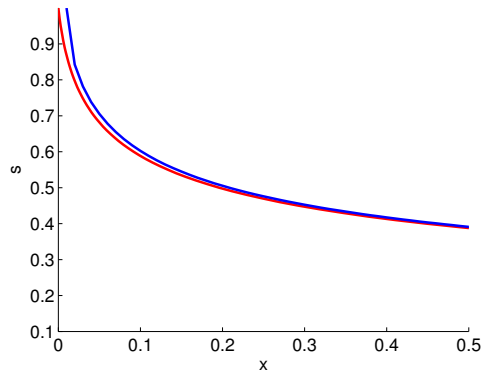


FIG. 5.10 – Gas saturation for three-component problem at $t=2.5$: the asymptotic model (blue) and the analytical solution (red).

Chapitre 6

Modeling two-phase compositional flow
with over/under-saturated single-phase
zones

In this chapter we examine the cases of flow with phase transitions, when the two-phase flow can form the zones with single-phase fluid over- or under-saturated by some components, as in many cases the initial and/or injection composition in the displacement problem are single-phase fluids. One of the basic problem in modeling such a systems is that the fluids in single-phase zones are significantly remote from the equilibrium two-phase region. In over- and undersaturated zones the two-phase flow equations degenerate and cannot be used any longer, which provokes serious numerical problems.

In particular, the detection of the shocks in the Riemann problem with phase transitions becomes a much more complicated problem.

In this chapter we propose the new method of modeling such processes, which allows to describe the ensemble of two-phase and over- and under-saturated single-phase zones by a uniform system of classic equilibrium two-phase equations while extending the concept of the phase saturation so that it may be negative and higher than one. This is based on the theorem of equivalence that we have proved and that permits to replace a single-phase non-equilibrium fluid by an imaginary two-phase fluid having artificial properties which are determined from the principle of equivalence with the true single-phase fluid. Such a result enables us to apply the same two-phase asymptotic model and the same semi-analytical method of solving the Riemann problem developed in previous chapters to the case of flow with phase transitions.

6.1 Description of the problematic

6.1.1 Phase transitions and over/under-saturated zones

We focus now our attention on the more complicated cases where the fluid can change the number of phases due to phase transitions. This means that within a two-phase fluid single-phase zones can appear in which the fluid is significantly remote from the equilibrium two-phase region. If such a single-phase fluid is gaseous, this means that it contains an excessive mass of light components, i.e. it is over-saturated with light components. If, in contrast, this fluid is a single-phase liquid, this means that it is under-saturated with light components. This situation is different from the equilibrium single-phase states situated just at the interface between the two-phase and the single-phase regions.

In Fig. 6.1 the typical phase diagram is presented in coordinates pressure in gas P versus total concentration of the lightest component C , so that the system is gaseous at high C .

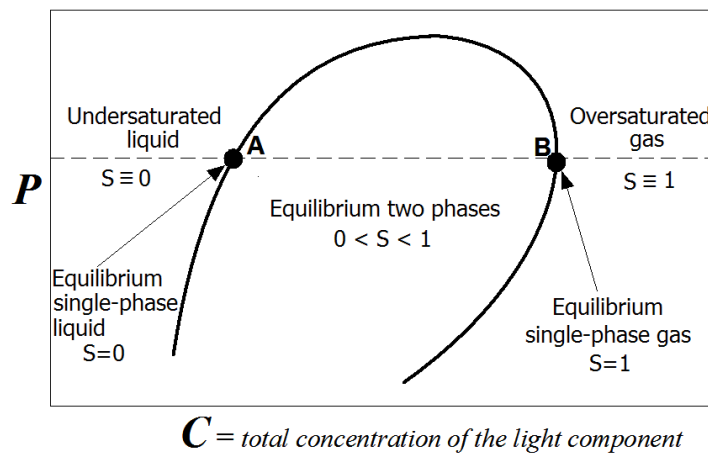


FIG. 6.1 – Phase diagram for a two-component system

The two-phase states are situated inside the domain limited by the two-phase envelop.

A tie-line, which determines an invariable phase composition, is now a horizontal line that corresponds to a constant pressure. Along the tie-line the equilibrium single-phase states are presented by points A and B . The single-phase gas over-saturated with the light component is located on the right of point B , as well as the single-phase liquid under-saturated with the light component is located on the left of point A . As the under-saturated fluid is over-saturated with the heavy component, we will use the same term *over-saturated fluid* for both the non-equilibrium liquid and gas.

Symbol s represents the gas saturation defined as the volume fraction of the gas phase in the total fluid. It is necessary to note that the saturation value is not sufficient to distinguish the equilibrium gas and the over-saturated gas, being equal to one for both of them and equal to zero for both equilibrium and under-saturated liquids.

The composition of the over-saturated single-phase fluid is no longer controlled by the phase equilibrium laws, but by other mechanisms (as diffusion,...). Due to this the contact between a two-phase fluid and an over-saturated fluid is characterized by significant non-equilibrium behavior leading to intensive phase transitions in the contact zone. This causes the formation of non-trivial shocks in the solution of the Riemann problem which are called the shocks of phase transition.

As a result, the flow in two-phase zones and in single-phase over-saturated zones is described by two independent systems of equations, having even different basic unknown variables, which imposes serious problems in modelling such processes. The main difficulty is related with the a priori detection of these shocks, which is still a more complicated problem than the two-phase shocks described in the previous sections. The particular role of the shocks of phase transition consists in that they detect the point of switching between two-phase and single-phase flow equations. However the detection of these shocks is only possible in course of the solution of the coupled two-phase and single-phase problem. The explicit determination of the shocks of phase transition before solving the differential flow equations is only possible in some simple cases.

Another problem, as will be shown in the following, is related to the fact that the physically correct boundary and initial conditions should be formulated, in the case of

phase transitions, in terms of the total concentration and not saturation, whereas all our hydrodynamics equations in previous sections are formulated in terms of the saturation.

All these problems are solved in the present chapter, by introducing the extended concept of saturations.

6.1.2 Compositional model for a binary mixture

Within the scope of this chapter the number of components does not play any role, so, for the sake of simplicity, we consider the case $N = 2$, which is more illustrative to the method aim.

We examine the same system as (2.1) while keeping now all the effects of phase diffusion, capillary and gravity effects :

$$\Phi \frac{\partial(\rho C^{(k)})}{\partial t} = \text{div} \left(\frac{\rho_g c_g^{(k)} K k_g(s)}{\mu_g} (\text{grad } P + \rho_g \vec{g}) + \rho_g D_g s \Phi \text{grad } c_g^{(k)} \right) + \text{div} \left(\frac{\rho_l c_l^{(k)} K k_l(s)}{\mu_l} (\text{grad } P_l + \rho_l \vec{g}) + \rho_l D_l (1-s) \Phi \text{grad } c_l^{(k)} \right), \quad k = 1, 2 \quad (6.1)$$

$$P \equiv P_g, \quad \rho \equiv \rho_g s + \rho_l (1-s), \quad C^{(k)} \equiv \frac{\rho_g c_g^{(k)} s + \rho_l c_l^{(k)} (1-s)}{\rho} \quad (6.2)$$

These two differential equations (6.1) determine two variables P and s

The first component is the lightest.

We can use only one concentration in each phase :

$$c_g \equiv c_g^{(1)}, \quad c_l \equiv c_l^{(1)} \quad (6.3)$$

as the second one is $c_j^{(2)} = 1 - c_j$.

For a binary mixture the diffusion coefficients of both the components are identical, so that :

$$D_g^{(1)} = D_g^{(2)} \equiv D_g, \quad D_l^{(1)} = D_l^{(2)} \equiv D_l \quad (6.4)$$

6.1.3 Local phase equilibrium and diffusion. Curie principle

Despite of the diffusion that is a sufficiently non-equilibrium process, it is possible to accept the hypothesis of the local phase equilibrium in two-phase zones, by using the Curie principle. In the non-equilibrium thermodynamics that considers the small deviations from the equilibrium state, a non-equilibrium process is an internal process of the system which causes the entropy growth in time. Such a process is also called the relaxation, which tends to transform the system into an equilibrium one. A non-equilibrium process is characterized by *generalized fluxes*. The typical examples of the non-equilibrium processes proper to the considered system are :

- Diffusion caused by the concentration gradients ;
- Masse exchange between the phases caused by the difference in the specific free energy of phases (chemical potentials) ;
- Capillary redistribution of the phases within porous space caused by an exceeding difference in phase pressures.

The most significant difference between these fluxes consists in that they have different tensorial dimension.

Indeed, the diffusion flux, being determined by the concentration gradients, is a sufficiently vectorial flux oriented in space. This is not however the case of the mass exchange flux and the capillary redistribution flux which are both scalar. Indeed under the assumption of the coexisting continua, when both the phases coexist at each space point, the mass exchange flux at an arbitrary point has no orientation in space. Similar concerns can be drawn for the capillary flux, as for a given point the exceeding pressure difference has no orientation.

The Curie principle of the non-equilibrium thermodynamics announces that the fluxes of different tensorial dimension should be considered as independent of one another. Therefore, the mass exchange between phases and the capillary redistribution can be considered as independent of the diffusion. (At the same time, the mass exchange and capillary redistribution depend on one another).

We can even consider the extreme case of this independency, when the mass exchange between phases can be considered as an equilibrium process. Physically this is based on the fact that the characteristic time of mass exchange is usually very low in porous media due to a huge surface of contact between phases. The similar hypothesis of the local equilibrium can be also applied to the capillary redistribution process, which is usually accepted by everyone, despite the lack of physical reasons.

As a result, we assume the local equilibrium for the mass exchange between the phases and for the capillary redistribution of phases.

The mass exchange is described by two phase equilibrium equations in which $\nu_j^{(k)}$ is the chemical potential of k^{th} component in j^{th} phase :

$$\nu_g^{(k)}(P_g, c_g) = \nu_l^{(k)}(P_l, c_l) \quad , \quad k = 1, 2 \quad (6.5)$$

The local capillary equilibrium equation implies the thermodynamic relation between two phase pressures through a given function of the capillary pressure $P_c(s)$:

$$P_g - P_l = P_c(s) \quad (6.6)$$

This system of three equations relates two concentrations c_g and c_l , two pressures P_g and P_l and saturation s . This means that only two variables are independent, while all other variables depend on them. We will use the pressure in gas phase P_g and gas saturation s as the basic independent thermodynamic variables, so equations (6.5) and (6.6) can be reformulated in the form :

$$c_g = c_g(P, s), \quad c_l = c_l(P, s), \quad P_l = P_l(P, s); \quad P \equiv P_g \quad (6.7)$$

In the case when the capillary pressure is neglecting, the phase concentrations depend on pressure only :

$$c_g = c_g(P), \quad c_l = c_l(P), \quad P_l = P_g \equiv P, \quad (\text{if } P_c \rightarrow 0) \quad (6.8)$$

Note that this means, under the accepted assumptions, that the diffusion flux within phase j is proportional to the pressure gradient :

$$\vec{q}_j^D \sim D_j \text{grad } c_j = D_j \frac{dc_j}{dP} \text{grad } P$$

To close the model we will use two equations of phase state (2.9) and two rheological equations of state (2.10).

Taking into account (6.7) we conclude that these functions depend on pressure and saturation only. If the capillary pressure is neglected, then they depend on pressure only.

The relative permeabilities are assumed to be the functions of saturation only :

$$k_g = k_g(s), \quad k_l = k_l(s) \quad (6.9)$$

6.1.4 Equations of single-phase compositional flow in over-saturated zones

The single-phase two-component flow is described by the mass balance equations :

$$\phi \frac{\partial(\rho_j C^{(k)})}{\partial t} = \text{div} \left(\frac{\rho_j C^{(k)} K}{\mu_j} (\text{grad } P_j + \rho_j \vec{g}) + \rho_j D_j \phi \text{grad } C^{(k)} \right), \quad k = 1, 2 \quad (6.10)$$

where $j = g$, or $j = l$.

Note that relation (2.2) for the total concentration is no longer valid in over-saturated states.

Equations (6.10) represent the exact limit of equations (6.1) when $s \rightarrow 0$ or $s \rightarrow 1$ only for the equilibrium single-phase fluid belonging to the two-phase envelop on phase diagram.

For the over-saturated fluid, equations (6.10) are totally independent of (6.1), as the total concentrations $C^{(k)}$ in (6.10) are not related to the phase concentrations $c_j^{(k)}$ calculated by using equilibrium relationships (6.7) or (6.8). This means that the total concentra-

tions $C^{(k)}$ in (6.10) are the independent variables, while in (6.1) the total and the phase concentrations are the given functions of pressure and saturation.

Therefore, the independent variables in (6.10) are P and $C \equiv C^{(1)}$ (the second concentration is $C^{(2)} = 1 - C$).

6.2 Formulation of the problem of two-phase flow with over-saturated zones

6.2.1 Physical formulation

In order to ensure the appearance of single-phase over-saturated states we introduce them directly through the boundary and initial conditions. Let us examine the one-dimensional bounded domain $\Omega = \{0 < x < L\}$ in which the initial fluid is an under-saturated single-phase liquid. Let an over-saturated single-phase fluid be injected into this domain through the left-hand side of the domain's boundary $x = 0$. The remaining part of the boundary serves to evacuate the original fluid displaced by the injected one. The contact between the over-saturated gas and the under-saturated liquid will necessarily lead to the appearance of the equilibrium two-phase zone.

The analyzed problem is consistent to the practical situations that correspond to the injection of miscible gases like CO_2 in an oil or water reservoir.

In the phase diagram the initial and injection states are presented by two points shown in Fig. 6.2. According to the description of the process, we assume that in minimum three mobile zones exist in the domain Ω : zone $\Omega_g = 0 < x < x_1(t)$ in which the fluid is the over-saturated gas, zone $\Omega_l = x_2(t) < x < L$ in which the fluid is the under-saturated liquid, and zone $\Omega_{gl} = x_1(t) < x < x_2(t)$ in which the fluid is the equilibrium gas-liquid system. The mobile interfaces of phase transition $x_1(t)$ and $x_2(t)$ are unknown a priori and should be determined as a result of the solution of the problem.

In reality the number of zones and their alternation could be much more complicated, so that the two-phase zone may be followed by the second zone of an over-saturated gas, after which the new two-phase zone appears and so on. It is then desirable that the method of

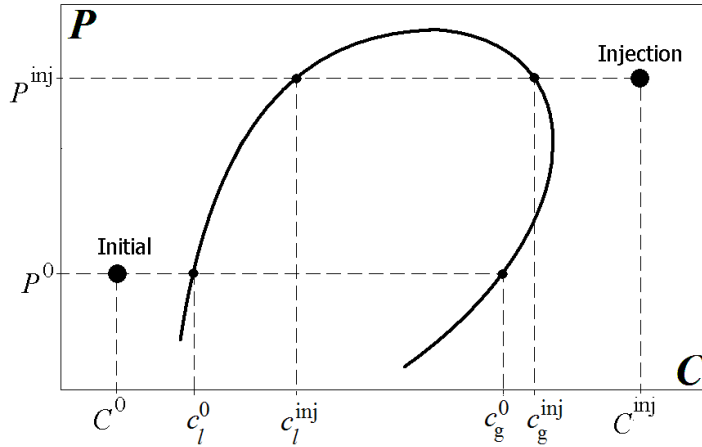


FIG. 6.2 – Initial and injection states on the phase diagram

solution would be able to detect automatically all the zones and their alternation.

In the two-phase domain we have equations (6.1) formulated with respect to pressure P and saturation s . In the single-phase zones we use two equations (6.10) formulated with respect to P and total concentration C .

The respective boundary and initial conditions can be formulated in two different ways with respect to different variables. These two formulations seem to be formally similar to one another, but in reality, they are not identical.

6.2.2 Boundary and initial conditions in terms of the saturation

As the two-phase equations (6.1) are formulated with respect to pressure and saturation, it is natural to write the boundary and initial conditions formulated verbally above in terms of the same variables :

$$s|_{t=0} = s^0 = 0, \quad P|_{t=0} = P^0, \quad (6.11a)$$

$$s|_{x=0} = s^{inj} = 1, \quad P|_{x=0} = P^{inj}, \quad (6.11b)$$

$$s|_{x=L} = S^0, \quad P|_{x=L} = P^0 \quad (6.11c)$$

In order to avoid the appearance of the third characteristic value of pressure and saturation, we will assume that the end of the porous medium ($x = L$) remains unperturbed during all the examined process. This problem, being mathematically correct, is however invalid from the physical point of view.

As mentioned above the saturation is not sensitive to the difference between an equilibrium single-phase state and an over-saturated single-phase state- see Fig. 6.1. Indeed, the saturation $s^{inj} = 1$ is incapable to reflect the fact that the injection point is over-saturated and not equilibrium gas. In the similar way, the initial saturation $s^0 = 0$ is incapable to distinguish what initial liquid is present in the domain, the under-saturated or the equilibrium liquid.

So, problem (6.11) with $s^{inj} = 1$ and $s^0 = 0$ formulated for the equilibrium two-phase equations can only determine the equilibrium single-phase states situated at the two-phase envelop of the phase diagram.

6.2.3 Boundary and initial conditions in terms of the total concentration

The physically correct way to formulate the boundary and initial conditions consists in using the pressure and the total concentration $C \equiv C^{(1)}$:

$$C|_{t=0} = C^0, \quad P|_{t=0} = P^0, \quad (6.12a)$$

$$C|_{x=0} = C^{inj}, \quad P|_{x=0} = P^{inj}, \quad (6.12b)$$

$$C|_{x=L} = C^0, \quad P|_{x=L} = P^0 \quad (6.12c)$$

In the two-phase domain and in the equilibrium single-phase states problems (6.11) and (6.12) are equivalent. However problem (6.12) is also valid in the over-saturated single-phase states, which is not the case of problem (6.11).

6.2.4 Conditions at the interfaces of phase transition

Conditions at the interfaces of phase transition $x_1(t)$ and $x_2(t)$ should describe the contact between a single-phase and a two-phase fluid. Such conditions depend on the behavior of the single-phase fluid. If this fluid is in equilibrium with the two-phase zone, then the saturation and pressure (as well as all the other functions) will be continuous through this interface.

If however the single-phase fluid contacting the two-phase zone is over-saturated, then the total concentration at this interface undergoes a discontinuity (shock). At the shock surfaces the differential equations should be replaced by the Hugoniot relations which represent the mass balance of each chemical component through a shock. For the considered process, the form of the Hugoniot conditions depends on the type of shock. For instance, for the interface $x_1(t)$ it takes the form :

$$U_s = \frac{\rho_g^+ c_g^{(k)+} s^+ U_g^{(k)+} + \rho_l^+ c_l^{(k)+} (1 - s^+) U_l^{(k)+} - \rho_g^- C^{(k)-} U_g^-}{\rho_g^+ c_g^{(k)+} s^+ + \rho_l^+ c_l^{(k)+} (1 - s^+) - \rho_g^- C^{(k)-}}, \quad k = 1, 2 \quad (6.13)$$

while for the surface $x_2(t)$ the Hugoniot conditions have another form :

$$U_s = \frac{\rho_g^- c_g^{(k)-} s^- U_g^{(k)-} + \rho_l^- c_l^{(k)-} (1 - s^-) U_l^{(k)-} - \rho_g^+ C^{(k)+} U_g^+}{\rho_g^- c_g^{(k)-} s^- + \rho_l^- c_l^{(k)-} (1 - s^-) - \rho_g^+ C^{(k)+}}, \quad k = 1, 2 \quad (6.14)$$

Herein superscripts + and - refer to the forward and backward values at the shock, U_s is the shock velocity, $U_j^{(k)}$ is the true transport velocity of the component k in phase j calculated as $U_j^{(k)} = V_j^{(k)} / (\phi s_j)$, where $V_j^{(k)}$ are given by relations (2.3).

6.3 Problems in modeling

6.3.1 Inconsistence of the equations and variables in various zones

The fact that two independent systems of equations formulated through different variables are used within two-phase and single-phase zones causes serious problems in modeling such processes. Indeed, in order to switch between equations and variables we need to detect previously the location of the mobile interfaces $x_1(t)$ and $x_2(t)$ (and other probable interfaces). At the same time the Hugoniot conditions which determine these interfaces are not formulated in a uniform way for any shocks and require possessing a priori information about the relative location of the two-phase and single-phase zones in space. Moreover, the Hugoniot conditions are formulated through the mixed variables (saturation on one side, total concentration on the other side), which prohibits the switch between variables. Thus, a priori detection of the shock locations by using (6.13) and (6.14) is impossible.

The effective method to overcome this difficulty consists in introducing uniform variables in all the zones. We suggest a more advanced way, by introducing the uniform flow equations in all the zones.

6.3.2 Classic method : replacement of saturation by total concentration

As the total concentration is a more informative variable than the saturation, it is possible to use C as the uniform variable in all the zones. In the two-phase zone the saturation s in (6.1) will be then replaced by C by using equations (6.2).

In the case where the capillary pressure is taken into account, we obtain, by taking into

account the equilibrium relations (6.7) :

$$C = \frac{\rho_g(P, s)c_g(P, s)s + \rho_l(P, s)c_l(P, s)(1 - s)}{\rho_g(P, s)s + \rho_l(P, s)(1 - s)}, \quad \text{when } P_c \neq 0 \quad (6.15)$$

which is an implicit equation with respect to the function $s(C)$.

If the capillary pressure is neglected, the equilibrium relations are independent of saturation, so that (6.15) gives the explicit relation for function $s(C)$:

$$s = \frac{\rho_l(P)(c_l(P) - C)}{\rho_l(P)(c_l(P) - C) + \rho_g(P)(C - c_g(P))}, \quad \text{when } P_c \equiv 0 \quad (6.16)$$

Using these replacement of s by C , we obtain the system of flow equations (6.1) and (6.10) formulated through the uniform couple of independent variables : P and C .

The initial and boundary conditions (6.11), as well as the Hugoniot conditions at the interfaces between the over- and under-saturated single-phase and two-phase states can be also formulated in terms of the uniform variables P and C .

Such a method is widely used in the analytical theory of miscible methods of enhanced oil recovery [Bedrikovetsky 1993], [Entov 1997], [Orr 2002], which is based on the very strong assumptions : the component dissolution in phases is governed by the law of ideal mixtures, the pressure and temperature are constant, the capillary pressure is neglected. In this case the molar phase concentrations are preferable to be replaced by the volume phase concentrations equal to the volume of component k in phase j divided by the volume of this component in the pure state :

$$\widehat{c}_j^{(k)} = \frac{\rho_j c_j^{(k)}}{\rho^{(k)}} \quad (6.17)$$

where $\rho^{(k)}$ is the molar density of the pure component k (constant value). For a binary system at $P, T = \text{const}$ the phase concentrations $\widehat{c}_j^{(k)}$ are constant values.

It is easy to show that for the total volume concentrations it holds :

$$\widehat{C} = \widehat{c}_g^{(1)}s + \widehat{c}_l^{(1)}(1 - s)$$

which is the simple linear function of saturation with constant coefficients $\widehat{c}_g^{(1)}$ and $\widehat{c}_l^{(1)}$.

Due to this, the replacement of variables $s \rightarrow \widehat{C}$ in two-phase equations (6.1) is very simple to do and does not produce huge transformations of the differential equations.

As a result, the consecutive formulation of the problem in terms of the total volume concentration occurs to be extremely effective. It allows analytical detection of all the shocks and their parameters as well as the continuous parts of the solution.

In the general case, when the pressure is not constant and the mixing is not ideal, the replacement of variables $P, s \rightarrow P, C$ in (6.1) is a nonlinear operation even in the simplest case of zero capillary pressure (6.16), without even considering alone the nonlinear and implicit replacement in (6.15). Such a replacement of variables will significantly transform all the differential equations (6.1) and will require a new mathematical formulation as well as a new numerical code based on the two-phase P, s formulation.

6.4 Method of negative (extended) saturations

Instead of replacing the saturation by the total concentration, we suggest another method which consists in using the uniform flow equations both in two-phase and single-phase zones, formulated through the extended concept of saturation. Formally these equations are equivalent to the classic two-phase flow model (6.1).

The significant advantage of this method consists in that the two-phase flow equations keep their original form. This means first of all, that all the methods developed for two-phase flow without phase transition becomes uniformly valid for the case of phase transitions too. Secondly, this means that all the numerical simulators can be applied to simulate the appearance of the over-saturated zones by adding a simple subroutine.

6.4.1 Equivalence principle and consistence conditions

Let us replace the true single-phase fluid by an imaginary two-phase fluid with fictive liquid and fictive gas phases with non-true properties different from those of the true fluid, chosen such that but these properties are so that the two-phase fluid is equivalent to the true single-phase one. Is it possible to perform such a formal mathematical replacement without any contradiction to the physical principles? The answer is "yes, this is possible". This possibility is justified by the fundamental theorem that we suggest. We will call this theorem *the principle of equivalence*. The theorem establishes the exact special properties of the imaginary fluids which ensure the physical consistence between the formal two-phase and the real single-phase fluids. These properties are called *the consistence conditions*.

The properties of the imaginary phases will be marked by a tilde, so that \tilde{s} is the saturation of the imaginary gas phase, $\tilde{\rho}_j$ is the density of the imaginary phase j , $\tilde{\mu}_j$ is the dynamic viscosity of the imaginary phase j , \tilde{c}_j is the concentration of the light component

in the imaginary phase j , and so on...

Theorem "Principle of equivalence"

Let us consider a fluid \mathcal{F}_{real} consisting of N chemical components. Let Ω be the domain of the ensemble of two-phase equilibrium states admissible for this fluid. Let the total composition $C^{(k)}$ of the examined fluid and pressure chosen so that it is located outside Ω (i.e. is over- or under-saturated). The flow of this single-phase fluid is described by the equations (6.10).

Then the flow of the single-phase fluid \mathcal{F}_{real} outside Ω is equivalent to the flow of the imaginary two-phase fluid \mathcal{F}_{imag} which has the same total composition as fluid \mathcal{F}_{real} : $\tilde{C}^{(k)} = C^{(k)}$, whose phase composition belongs to Ω (i.e. is in equilibrium), whose flow is described by (6.1), and which has the physical properties defined by the following consistence conditions :

case 1 - fluid \mathcal{F}_{real} is situated in single-phase gaseous zone :

$$\text{The imaginary gas saturation is higher than 1 : } \tilde{s} > 1; \quad (6.18a)$$

$$\tilde{\rho}_l = \tilde{\rho}_g = \rho_g, \quad \tilde{\mu}_l = \tilde{\mu}_g = \mu_g, \quad (6.18b)$$

$$\tilde{k}_l(\tilde{s}) = 1 - \tilde{s}, \quad \tilde{k}_g(\tilde{s}) = \tilde{s}, \quad (6.18c)$$

$$\tilde{P}_c(\tilde{s}) \equiv 0, \quad (6.18d)$$

$$\tilde{D}_g = D_g, \quad \tilde{D}_l = D_g \left(1 + \left(\frac{c_g - c_l}{1 - \tilde{s}} \right) \text{grad } \tilde{s} \cdot \text{grad}^{-1} c_l \right) \quad (6.18e)$$

$$\tilde{c}_l = c_l(P); \quad \tilde{c}_g = c_g(P) = \text{Eq. (6.8)} \quad (6.18f)$$

case 2 - fluid \mathcal{F}_{real} is situated in single-phase liquid zone :

$$\text{The imaginary gas saturation is lower than 0 : } \tilde{s} < 0; \quad (6.19a)$$

$$\tilde{\rho}_l = \tilde{\rho}_g = \rho_l, \quad \tilde{\mu}_l = \tilde{\mu}_g = \mu_l, \quad (6.19b)$$

$$\tilde{k}_l(\tilde{s}) = 1 - \tilde{s}, \quad \tilde{k}_g(\tilde{s}) = \tilde{s}, \quad (6.19c)$$

$$\tilde{P}_c(\tilde{s}) \equiv 0, \quad (6.19d)$$

$$\tilde{D}_l = D_l, \quad \tilde{D}_g = D_l \left(1 + \left(\frac{c_g - c_l}{1 - \tilde{s}} \right) \text{grad } \tilde{s} \cdot \text{grad}^{-1} c_l \right) \quad (6.19e)$$

$$\tilde{c}_l = c_l(P); \quad \tilde{c}_g = c_g(P) = \text{Eq. (6.8)} \quad (6.19f)$$

Under these conditions the relation between the imaginary saturation and total and phase concentrations (6.2) in the single-phase zone becomes :

$$\tilde{s} = \frac{C - c_l}{c_g - c_l}, \quad \text{or} \quad C^{(k)} = c_g^{(k)} \tilde{s} + c_l^{(k)} (1 - \tilde{s}) \quad (6.20)$$

Therefore, in the zone of an over-saturated gas the imaginary liquid and gas should have the same density and viscosity as the true gas, both the imaginary phases should have diagonal relative permeabilities, the capillary pressure for the imaginary fluid has to be zero. The phase concentrations \tilde{c}_g and \tilde{c}_l for both the imaginary phases are calculated by the equilibrium relations which determine the true two-phase zone Ω .

The most complicated is the calculation of the diffusion coefficient of the imaginary phase, which depends on gradients of saturation and pressure. (Note that under all the consistence conditions the gradient of the phase concentration in the definition of D_g and D_l in the single phase zones (6.18) and (6.19) reduces to the pressure gradient). At the same time, as it will be shown in the next section, the saturation in the over-saturated zones is frequently constant or weakly variable. In this case we would have :

$$\tilde{D}_l \approx \tilde{D}_g \quad (6.21)$$

when $\tilde{s} < 0$, or $\tilde{s} > 1$.

The consistence conditions are non contradictory physically and mathematically.

6.4.2 Proof to the equivalence principle

To prove the equivalence principle, let us consider the case when the fluid \mathcal{F}_{real} belongs to single-phase gas. In the phase diagram presented in Fig. 6.2 its state corresponds to point "injection".

1) To prove equations (6.18) and (6.19), it is sufficient to substitute them into (6.1). For the examined case we obtain form (6.1) :

$$\begin{aligned} \phi \frac{\partial}{\partial t} \left(\rho_g \left[c_g^{(k)} \tilde{s} + c_l^{(k)} (1 - \tilde{s}) \right] \right) - \operatorname{div} \left(\frac{\rho_g K}{\mu_g} \left(c_g^{(k)} \tilde{s} + c_l^{(k)} (1 - \tilde{s}) \right) (\operatorname{grad} P + \rho_g \vec{g}) \right) - \\ \operatorname{div} \left(\rho_g D_g \phi \left[\tilde{s} \operatorname{grad} c_g^{(k)} + (1 - \tilde{s}) \operatorname{grad} c_l^{(k)} + (c_g - c_l) \operatorname{grad} \tilde{s} \right] \right) = 0 \quad (6.22) \end{aligned}$$

Using (6.20) we obtain finally :

$$\phi \frac{\partial}{\partial t} (\rho_g C^{(k)}) = \operatorname{div} \left(\frac{\rho_g K C^{(k)}}{\mu_g} (\operatorname{grad} P + \rho_g \vec{g}) \right) + \operatorname{div} (\rho_g D_g \phi \operatorname{grad} C^{(k)}) \quad (6.23)$$

which is equivalent to the single-phase equations (6.10).

2) According to Fig. 6.2, for all the over-saturated single-phase gaseous states the following is true :

$$C > c_g > c_l$$

Then we obtain from (6.20) :

$$\tilde{s} > 1$$

which satisfies (6.18a).

3) In a similar way conditions (6.19) are justified.

6.4.3 Extended concept of saturation

The proved theorem allows to introduce the extended concept of saturation which can be now negative or higher than 1. The extended saturation \tilde{s} , which will be also called *the negative saturation*, is determined in such a way that :

$$\begin{aligned}\tilde{s} &\equiv s, & (0 \leq s \leq 1) & \text{ in two-phase region} \\ \tilde{s} &> 1, & & \text{ in over-saturated gas} \\ \tilde{s} &< 0, & & \text{ in under-saturated liquid}\end{aligned}$$

In particular, the extended saturations satisfy the same relation (6.15) which is valid in true two-phase zones. The extended values of saturation are beyond the two-phase region.

So the negative saturation, being proportional to the total concentration C , determines the degree of distancing of the over-saturated fluid from the equilibrium two-phase zone. The higher the absolute value of \tilde{s} , the higher the degree of fluid's over-saturation.

Inversely, the true saturation is related with the extended saturation in the following way :

$$s = \begin{cases} 0 & \text{when } \tilde{s} < 0 \\ \tilde{s} & \text{when } 0 \leq \tilde{s} \leq 1 \\ 1 & \text{when } \tilde{s} > 1 \end{cases} \quad (6.24)$$

Such a mathematical abstraction gives the possibility to use the same system of two-phase equations uniformly for all the two-phase and single-phase zones.

6.4.4 Boundary, initial and Hugoniot conditions in terms of negative saturation

For the flow model (6.1) uniformly valid in all the domain, we can now formulate conditions (6.11) in the equivalent form by replacing the total concentration C by the

extended (negative) saturation \tilde{s} according to (6.20) :

$$s|_{t=0} = s^0 = 0, \quad P|_{t=0} = P^0, \quad (6.25a)$$

$$s|_{x=0} = s^{inj} = 1, \quad P|_{x=0} = P^{inj}, \quad (6.25b)$$

$$s|_{x=L} = s^0, \quad P|_{x=L} = P^0 \quad (6.25c)$$

where c_j^{inj} ($j = g, l$) are the equilibrium phase concentrations situated on the injection tie-line that corresponds to the injection pressure; c_j^0 are the equilibrium phase concentrations situated on the initial tie-line that corresponds to the initial pressure. These values are shown in Fig. 6.2. They are calculated by using the equilibrium equations (6.5) and $P_c = 0$ (if the injection and initial states are single-phase). For given values of injected and initial total concentration, the initial and injection saturations can be easily calculated.

The Hugoniot conditions at a shock are also formulated in an uniform way for any shocks :

$$U_s = \frac{\left[\tilde{\rho}_g c_g^{(k)} \tilde{s} U_g^{(k)} + \tilde{\rho}_l c_l^{(k)} (1 - \tilde{s}) U_l^{(k)} \right]}{\left[\tilde{\rho}_g c_g^{(k)} \tilde{s} + \tilde{\rho}_l c_l^{(k)} (1 - \tilde{s}) \right]}, \quad k = 1, 2 \quad (6.26)$$

where $[f] \equiv f^+ - f^-$.

As a result, the suggested method allows a throughout penetrating simulation of the uniform flow equations (6.1) with a simultaneous detection of all the shocks of phase transition.

6.5 Application of the method to solve compositional flow problems

Using the suggested method, we have obtained the numerical solutions to several examples formulated by differential equations (6.1), consistence conditions (6.18) and (6.19), the boundary and initial conditions (6.25) and the Hugoniot conditions (6.26).

6.5.1 Example 1 : ideal mixing. Comparison to the analytical solution

In the consecutive examples, we will omit the symbol tilde over the extended saturation.

First of all we analyzed the one-dimensional case of the ideal mixing at a constant pressure. The capillary pressure, diffusion and gravity are neglected. This case is significant as it admits an analytical solution. The uniform flow model has the from :

$$\phi \frac{\partial}{\partial t} \left(\rho_g c_g^{(k)} s + \rho_l c_l^{(k)} (1 - s) \right) = \frac{\partial}{\partial x} \left(\left(\frac{\rho_g c_g^{(k)} K k_g(s)}{\mu_g} + \frac{\rho_l c_l^{(k)} K k_l(s)}{\mu_l} \right) \frac{\partial P}{\partial x} \right), \quad k = 1, 2 \quad (6.27)$$

For the binary system at a constant pressure the values ρ_j , μ_j and c_j ($j = g, l$) are constant. The reservoir is homogeneous : $K, \phi = const.$

The analytical solution is constructed according to the classical scheme. First of all we introduce the volume concentrations \hat{c} (6.17) by dividing equations (6.27) by the density of the pure component. We obtain :

$$\phi \frac{\partial}{\partial t} \left(\hat{c}_g^{(k)} s + \hat{c}_l^{(k)} (1 - s) \right) = \frac{\partial}{\partial x} \left(\left(\frac{\hat{c}_g^{(k)} K k_g(s)}{\mu_g} + \frac{\hat{c}_l^{(k)} K k_l(s)}{\mu_l} \right) \frac{\partial P}{\partial x} \right), \quad k = 1, 2 \quad (6.28)$$

For the ideal mixing the sum of volume concentrations is equal to one. So the sum of two equations (6.28) yields :

$$\frac{\partial}{\partial x} \left(\left(\frac{Kk_g(s)}{\mu_g} + \frac{Kk_l(s)}{\mu_l} \right) \frac{\partial P}{\partial x} \right) = 0$$

which has the first integral :

$$\frac{\partial P}{\partial x} = -\frac{V}{Kk_g(s)/\mu_g + Kk_l(s)/\mu_l}, \quad V = V(t)$$

This enables us to exclude pressure from the second equation (6.28) :

$$\frac{\partial \widehat{C}}{\partial t} + \frac{\partial \widehat{F}(\widehat{C})}{\partial x} = 0 \tag{6.29}$$

$$\widehat{C} \equiv c_g^{(1)}s + c_l^{(1)}(1-s), \quad \widehat{F} \equiv c_g^{(1)}f(s) + c_l^{(1)}(1-f(s)), \quad f(s) = \frac{k_g(s)/\mu_g}{k_g(s)/\mu_g + k_l(s)/\mu_l}$$

The solution to this equations with Riemann conditions is performed by applying classical graphical-analytical technique [Bedricovetsky 1993].

We have also performed direct numerical simulations of compositional flow equations (6.27) in the overall domain, by using the method of negative saturations. We have used the explicit discretization in time and the backward discretization in space. Once the saturation became higher than 1 or lower than 0 the consistence conditions (6.18) and (6.19) were applied.

For simulations, we assumed that two components are CH₄ and C₁₀H₂₂. The properties of the system are as follows : $k_g(s) = s^2$, $k_l(s) = (1-s)^2$, $\mu_l/\mu_g = 5$, $C^0 = 0$, $C^{inj} = 1$, $c_g = 0.97$, $c_l = 0.39$.

The injection and initial extended saturations are : $s^0 = -0.67 < 0$ and $s^{inj} = 1.05 > 1$, which is calculated using (6.20).

Results of numerical simulations and analytical solution are shown in Fig. 6.3.

The solution is characterized by two shocks of phase transition. The backward shock

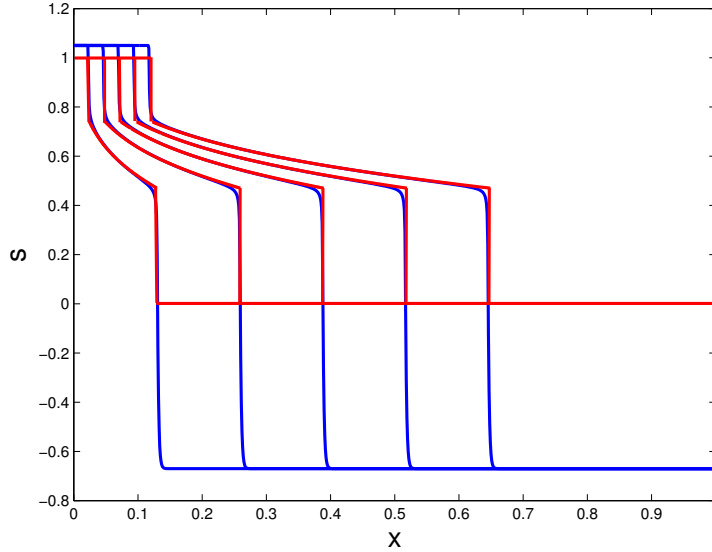


FIG. 6.3 – Solution to the problem of liquid displacement by miscible gas : case of the ideal mixing at a constant pressure. Red curves : exact analytical solution ; blue curves : numerical solution by the method of negative saturations

corresponds to the contact between the over-saturated injected gas and the two-phase fluid, while the rapid forward shock marks the contact between the two-phase fluid and the initial under-saturated liquid.

Both phase transitions shocks are detected automatically in numerical simulation, in course of solving the problem.

As seen, the method of negative saturations gives very satisfactory results.

6.5.2 Example 2 : non-ideal mixing, variable pressure

The same method was applied to a more general case of non-ideal mixtures at variable pressure. The capillary forces, diffusion and gravity were still neglected. The system is described by the same problem as in the previous case in which the phase concentration and densities are no longer constant but depend on pressure. The ideal equation of state was used for gas, and the weakly compressible model for liquid. The phase viscosities were assumed to be invariable.

As previously we examined the binary system $CH_4 - C_{10}H_{22}$. The phase equilibrium was simulated by using the Peng-Robinson EOS for a fixed reservoir temperature ($T = 300K$) and various pressures between 150 bar and 90 bar. This simulation was then approximated by statistical correlations for all the thermodynamics functions.

The following properties were assumed :

$$k_g(s) = s^2, \quad k_l(s) = (1 - s)^2, \quad K = 10^{-14} \text{ m}^2$$

$$c_g = -0.2164 * 10^{-7} P^3 + 0.4638 * 10^{-5} P^2 + 0.3964 * 10^{-3} P + 1.013, \quad [P] = \text{bar}$$

$$c_l = 0.1162 * 10^{-7} P^3 - 0.49571 * 10^{-5} P^2 + 0.1593 * 10^{-2} P - 0.2778 * 10^{-1}$$

$$\rho_g^0 = 10 \text{ Kg/m}^3, \quad \rho_l^0 = 850 \text{ Kg/m}^3, \quad \mu_l = 0.001 \text{ Pa} \cdot \text{s}, \quad \mu_g = 0.00002 \text{ Pa} \cdot \text{s}$$

The injection and initial parameters were : $C^0 = 0$, $C^{inj} = 1$, $P^0 = 90 \text{ bar}$, $P^{inj} = 150 \text{ bar}$. This corresponds to the under-saturated initial liquid and the over-saturated injected gas, so that the corresponding extended saturations are : $S^0 = -0.68$ and $S^{inj} = 1.06$.

The results of simulations are shown in Fig. 6.4.

The red curve is the solution of the problem formulated in terms of the classic saturation : (6.1), (6.11). Comparing this curve with the behavior of the extended saturation, we note that the formulation of the boundary and initial conditions in terms of the classic saturation (6.11) leads not only to the impossibility to detect the over-saturated zones, but to the invalid results with respect to the velocity of all the shocks. Moreover, the backward shock of contact between the injected over-saturated gas and the two-phase zone is not detected at all.

6.5.3 Example 3 : non-ideal solution, variable pressure, diffusion

The third example enables us to analyze the efficiency of the method in the case of diffusion and the influence of the diffusion on the behavior of saturation, which is difficult to predict a priori. The most non trivial question is whether the saturation can be

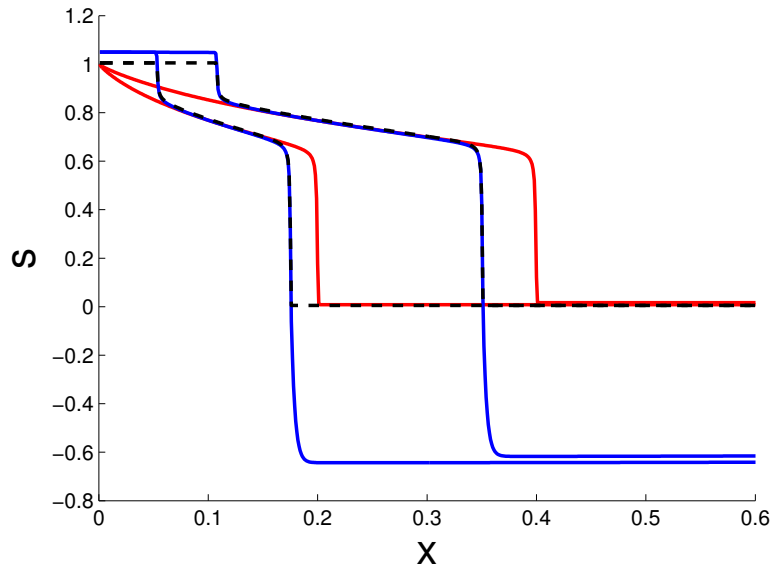


FIG. 6.4 – Solution to the problem of liquid displacement by miscible gas : no-ideal mixing at variable pressure : the extended saturation (the blue curve) and the true saturation (the black curve)

discontinuous or not in the examined case?

Indeed, within the two-phase zone the diffusion influences only the phase concentrations, but not the saturation. From this point of view, nothing prohibits the saturation to be discontinuous there. In contrast, the behavior of the saturation between the single phase zones and the two-phase zone is not clear. For instance, in the zone of the under-saturated initial liquid the total concentration varies between the initial value arbitrarily imposed at the right-hand boundary and the value which corresponds to the gas-liquid equilibrium on the left-hand limit of this zone. Such a shock of concentration within the single-phase zone must be immediately destroyed by diffusion, so that the total concentration is expected to be continuous in the single-phase zone and between the single-phase and two-phase zone too.

The saturation is related to the total concentration by a linear relation, so the saturation is also expected to be continuous at the interface between the single-phase and the two-phase zones.

This expectation based on the physical analysis of the process, is confirmed by formal

mathematics. In particular, the consistence conditions (6.19e) and (6.18e) show that the diffusion coefficient is proportional to the gradient of saturation. Therefore the uniform flow model in single phase zones contains the diffusion term with respect to the extended saturation. This determines a rather continuous behavior of the extended saturation at the interface with the single-phase zone.

We used the uniform equations (6.1), the boundary and initial conditions (6.25) and the consistence conditions (6.18) and (6.19).

We considered the same parameters as in the previous case. The diffusion coefficient was selected in such a way that the Peclet number Pe would be sufficiently low, in order to make evident the diffusion effect. We consider $Pe = 0.03$, where Pe was calculated as $Pe = K\Delta P/(\mu_g D_g L)$. The diffusion in liquid was much lower than in gas : $D_l = D_g * 10^{-4}$. Results of simulations are shown in Fig. 6.5.

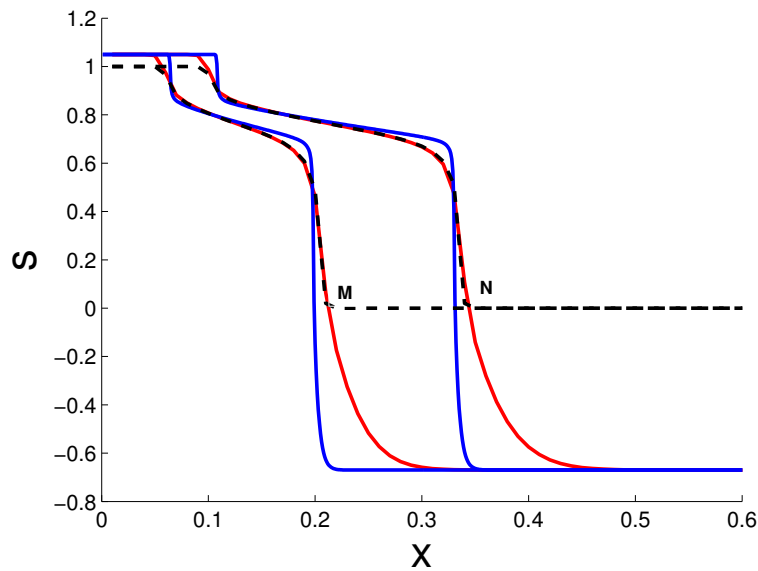


FIG. 6.5 – Solution to the problem of liquid displacement by miscible gas under non-ideal mixing and variable pressure in the case with diffusion (the red curve) and without diffusion (the blue curve)

The black curve represents the behavior of the true saturation.

The spatial step of simulation was very small in order to reduce the role of the numerical diffusion.

6.5.4 On the continuity of the fronts of phase transition induced by diffusion

As seen, the saturation is continuous everywhere, so that the internal phase diffusion suppresses the shocks of saturation. At the same time, the derivative of the saturation is discontinuous (points M, N and so on). These points of a weak discontinuity marks the interfaces between the single-phase and the two-phase zones.

It is significant that the suggested method is very sensitive to detect these weak discontinuities, as seen in the figure, they correspond to the intersection of the horizontal lines $s = 0$ and $s = 1$ by the curve of the extended saturation which usually has high inclination. The behavior of the total concentration of the light component C is shown in Fig. 6.6.

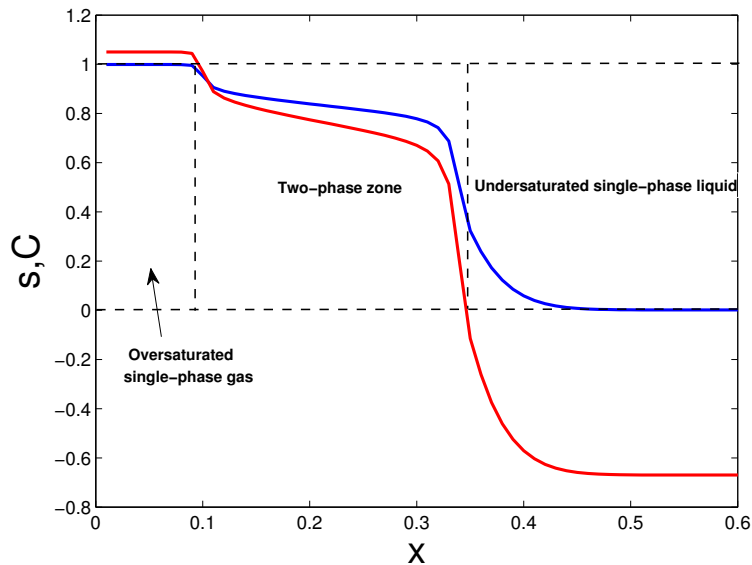


FIG. 6.6 – Total concentration of the light component (C) and extended gas saturation (s) for the case of non-ideal mixing, variable pressure and diffusion

The red curve which corresponds to the extended saturation allows to determine the interfaces between the single-phase zone and the two-phase zone. This enable us to see

the behavior of the total concentration in single-phase zones, which varies between the equilibrium concentration in the two-phase zone and the initial or injected concentrations in a very continuous and smooth way, as expected a priori.

6.6 Method of negative saturation in the asymptotic compositional model

The developed method of negative saturations will be now introduced in the formalism of the asymptotic compositional model. We will analyze how phase transitions influence the results obtained in chapter 5.

6.6.1 Three-components two-phase problem

We analyzed the ternary mixture of carbon dioxide, methane and decane having the same properties as in section (5.4.3). The injected fluid was single phase gaseous with the following composition :

$$CO_2 = 0.6381$$

$$CH_4 = 0.3619$$

$$C_{10} = 0$$

The initial fluid was single-phase liquid with the composition :

$$CO_2 = 0$$

$$CH_4 = 0$$

$$C_{10} = 1$$

The system is expected to consists of (at least) three zones : single phase over-saturated gas, two-phase equilibrium fluid, and single-phase under-saturated liquid. The flow of the overall fluid in all the zones was described by the uniform two-phase equations of the asymptotic compositional model (4.1), while applying the consistence conditions for the imaginary two-phase fluid in over/under-saturated zones within the framework of the me-

thod of negative saturations. Calculations were performed progressively from the injection point into the reservoir center. The extended saturation at the injection point was known a priori. Due to this the calculations started by applying the properties of an imaginary two-phase fluid. Once the saturation became lower than 1 and higher than 0 the properties of two-phase are changed by the real fluid. Once the saturation left the normal interval $(0, 1)$, the imaginary properties were applied again.

In the two-phase zone only one sc -shock is authorized. Along with this, several s -shocks (of saturation only) are possible.

The general algorithm of analytical front tracker described in chapters 4 and 5 was applied to determine the sc -shock.

The results of simulations are presented in Fig. 6.7.

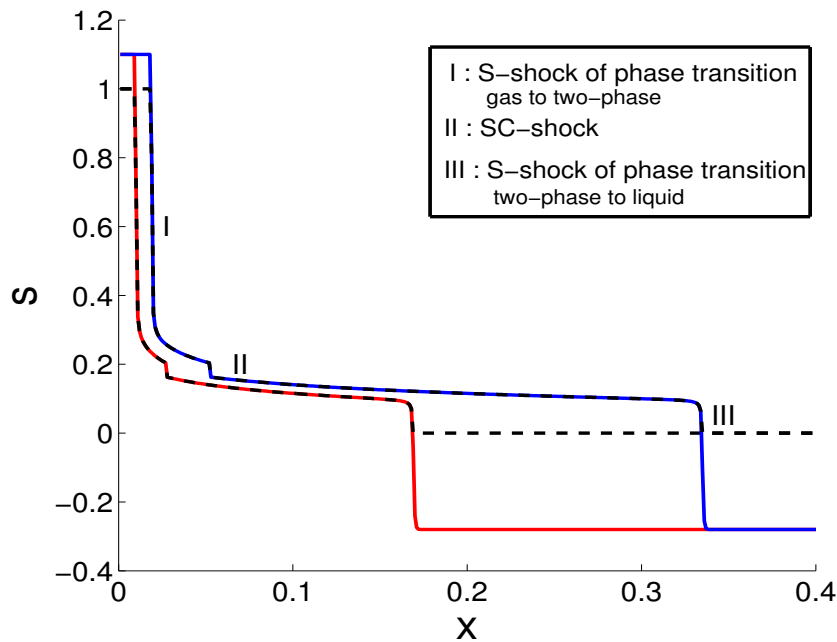


FIG. 6.7 – Gas saturation versus x for two time instants : three-components two-phase flow with single-phase initial and injection compositions. Solution by the analytical front tracker and the negative saturation methods

As expected, the saturation contains three shocks : one s -shock of phase transition between the injected single-phase gas and two-phase fluid, the second s -shock in the forward

part which corresponds to the phase transition between the two-phase fluid and the initial liquid, and one *sc*-shock inside the two-phase zone, which marks one non-trivial P-surfaces other than the injection and initial one.

6.6.2 Four-components two-phase problem

We analyze now the mixture already used in section 5.4.4. It consists of methane, carbon dioxide, propane and decane.

The injection composition (single-phase gas) is :

$$CO_2 = 0.3258$$

$$CH_4 = 0.6742$$

$$C_4 = 0$$

$$C_{10} = 0$$

The initial composition (single-phase liquid) :

$$CO_2 = 0$$

$$CH_4 = 0$$

$$C_4 = 0.2137$$

$$C_{10} = 0.7836$$

The flow of the overall fluid in all the zones was described by the uniform two-phase equations of the asymptotic compositional model (4.1).

In the two-phase zone 2 *SC*-shocks is authorized. Along with this, several *S*-shocks (of saturation only) are possible. We expect to have two shocks of phase transition that will be two *S*-shocks.

The general algorithm of analytical front tracker was applied to determine the *SC*-shocks. It was combined with the technique of negative saturations.

The results of simulations are shown in Fig. 6.8.

The saturation profile in figure (6.8) contains four shocks. Two *S*-shocks entering into

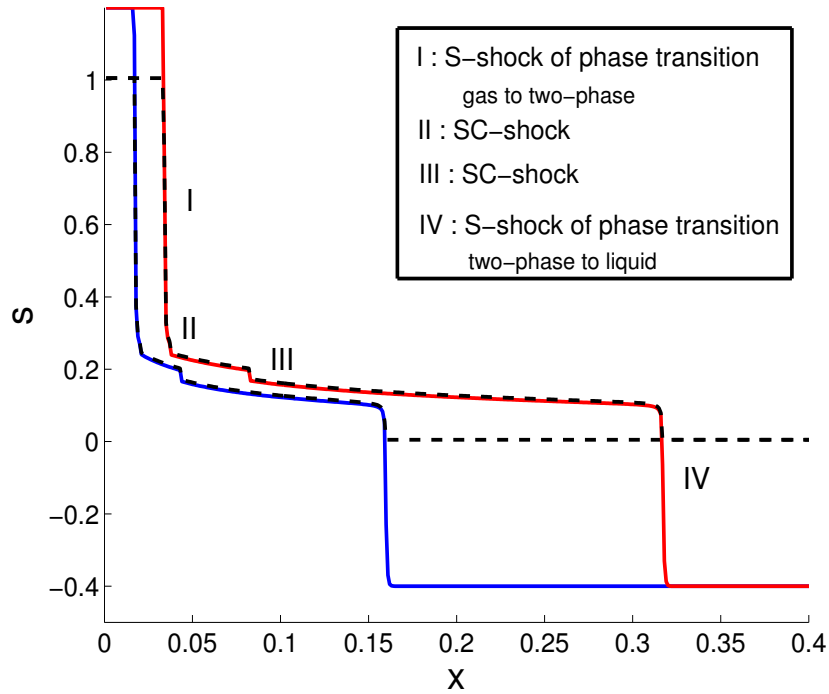


FIG. 6.8 – Gas saturation versus x for two time instants : four-components two-phase flow with single-phase initial and injection compositions. Solution by the analytical front tracker and the negative saturation methods

the phase zone (I) and leaving it (IV). They are both automatically discovered using the method of negative saturations. Two SC -shock (II and III) inside the two-phase domains are determined by the analytical front tracker method.

In the examined examples, the practical role of intermediate shock is sufficiently low (the shock II is even practically invisible), but this is only particular case. In other situations, the intermediate SC -shocks can be sufficiently more important.

Chapitre 7

Asymptotic HT-split model for three-phase compositional flow

In this chapter we develop the asymptotic form of gas-oil-water flow model which results from the full compositional model when oil and water mobilities become contrasting to those of gas due to the high difference in phase viscosities. Mathematically this is expressed in the form of the appearance of two small parameters : ω_o which is the oil-gas mobility ratio, and ω_w which is the water-gas mobility ratio. The asymptotic model is obtained as the limit of the process $\omega_o, \omega_w \rightarrow 0$. This asymptotic process takes into account the presence of the third parameter ε which is the dimensionless time of relaxation of the pressure field which is also always small in practice.

The obtained limit model constitutes the system of three hydrodynamic equations for pressure and two saturations and the independent, split thermodynamic model which include several new differential equations.

7.1 Mathematical model of three-phase multicomponent flow

7.1.1 Hydrodynamics equations

Let us consider the fluid consisted of three phases : gas, oil and water, and N chemical components that can be separated into three groups as shown in Fig. 7.1.

The compositional model consisting of N mass conservation equations of each component has the form similar to (2.1) :

$$\Phi \frac{\partial}{\partial t_D} \left(\rho_o c_o^{(k)} s_o + \rho_w c_w^{(k)} s_w + \rho_g c_g^{(k)} (1 - s_o - s_w) \right) + \operatorname{div} \left(\rho_o c_o^{(k)} \vec{V}_o^{(k)} + \rho_w c_w^{(k)} \vec{V}_w^{(k)} + \rho_g c_g^{(k)} \vec{V}_g^{(k)} \right) = 0, \quad k = 1, \dots, N \quad (7.1)$$

where Φ is the porosity ; $c_o^{(k)}$, $c_w^{(k)}$ and $c_g^{(k)}$ are the mass or molar fractions ("concentrations") of the k^{th} chemical component in oil, water and gas ; ρ is the phase density (mass or molar, according to the type of concentrations) ; s is the volume saturation of the phase ; $\vec{V}_j^{(k)}$ is the Darcy velocity of the component k in phase j ; t_D is the time with dimension. The indexes : o , w and g refer to oil, water and gas respectively.

According to the classification of the components, several concentrations are identically equal to zero :

$$\begin{aligned} c_w^{(k)} &\equiv 0, & k = N^I + 1, \dots, N^{II} \\ c_o^{(k)} &\equiv 0, & k = N^{II} + 1, \dots, N \end{aligned} \quad (7.2)$$

The Darcy velocities are determined through (2.3) in general case. In the present chapter

we will determine the Darcy velocities by neglecting the gravity and capillarity :

$$\vec{V}_j^{(k)} = \vec{V}_j = -\frac{Kk_j(s_o, s_w)}{\mu_j} \text{grad}P, \quad j = o, w, g, \quad \forall k$$

where K is the intrinsic permeability, k_j is the relative permeability, μ_j is the dynamic viscosity of the considered phase. P is the pressure identical in all the phases.

Then velocities may be eliminated from (7.1) :

$$\phi \frac{\partial \rho^{(k)}}{\partial t_D} = \text{div} \left(\left(\frac{\rho_g K k_g c_g^{(k)}}{\mu_g} + \frac{\rho_o K k_o c_o^{(k)}}{\mu_o} + \frac{\rho_w K k_w c_w^{(k)}}{\mu_w} \right) \text{grad}P \right), \quad k = 1, \dots, N \quad (7.3)$$

$$\rho^{(k)} \equiv \rho_o c_o^{(k)} s_o + \rho_w c_w^{(k)} s_w + \rho_g c_g^{(k)} (1 - s_o - s_w)$$

The differential equations (7.3) determine N independent variables :

$$P, \quad s_o, \quad s_w, \quad c_g^{(k)}, \quad k = 1, \dots, N - 3 \quad (7.4)$$

Other concentrations and phase densities and viscosities are determined from the thermodynamic system of equations.

7.1.2 Thermodynamic closure relations

The thermodynamics closure relationships for our hydrodynamics system contain $2N$ equilibrium equations responsible for the equilibrium between oil and gas, and water and gas :

$$\begin{aligned} \nu_g^{(k)} \left(P, c_g^{(1)}, \dots, c_g^{(N)} \right) &= \nu_o^{(k)} \left(P, c_o^{(1)}, \dots, c_o^{(N)} \right), \quad k = 1, \dots, N \\ \nu_g^{(k)} \left(P, c_g^{(1)}, \dots, c_w^{(N)} \right) &= \nu_l^{(k)} \left(P, c_w^{(1)}, \dots, c_w^{(N)} \right), \quad k = 1, \dots, N \end{aligned} \quad (7.5)$$

where $\nu_j^{(k)}$ is the chemical potential of k^{th} component in j^{th} phase.

Phase densities are determined by the equations of state of each phase :

$$\rho_j = \rho_j \left(P, c_j^{(1)}, \dots, c_j^{(N)} \right), \quad j = o, w, g \quad (7.6)$$

while the three rheological equations of state determine phase viscosities :

$$\mu_j = \mu_j \left(P, c_j^{(1)}, \dots, c_j^{(N)} \right), \quad j = o, w, g \quad (7.7)$$

According to the definition of the saturations and concentrations their sum equals to one :

$$\sum_{k=1}^N c_j^{(k)} = 1, \quad j = o, w, g; \quad s_o + s_w + s_g = 1 \quad (7.8)$$

7.1.3 Particularity of a three-phase system

Let us consider the fluid consisted of N chemical components that can form three coexisting phases : gas, liquid-1 (oil), and liquid-2 (water). It is clear that the case of two coexisting gaseous phases is impossible (except some very particular case specially studied in molecular physics) because two gases are absolutely miscible between them.

Mathematically the simple increase in the number of liquids phases in a system seems to be a natural generalization of the two-phase case which does not impose any technical problems. However from the point of view of physics, the formation of the third coexisting fluid phase in a compositional system is not a simple phenomenon. It is sufficient to note that in a two-component system the third fluid phase cannot appear in principle.

According to the definition of two coexisting phases, they are two fluids which are separated by an interface. The interface is defined as the surface of discontinuity of physical or chemical properties of these fluids. For instance, the interface between gas and liquid represents the surface of discontinuity of the fluid density. In the case of two coexisting liquids the density is not the main property which determines an interface ; the density of liquids are frequently identical. The main factor which determines the appearance of the discontinuities between two liquids is their very different composition.

Such a difference in compositions appears, in turn, due to the fact that the mixture contains at least two chemical components which have very different chemical nature, so that their coexistence within one phase is difficult and they prefer to be separated from one another. This separation produces the formation of two phases. Each phase will not contain the in-consistent component. The typical example represents the coexisting system of oil and water. The chemical component H_2O is very difficult to be dissolved in liquid oil, whereas it is largely present in the aqueous liquid phase. In a similar way, the heavy hydrocarbons which make the basis of the 'oil' phase are practically insoluble in the aqueous phase. At the same time, these phases can contain several common components, like CH_4 , CO_2 , O_2 , and other. All these components can both be dissolved in oil and water.

Thus, the presence of the second liquid phase in our system immediately means that the phase composition should be now characterized by three groups of components, as shown in Fig. 7.1 :

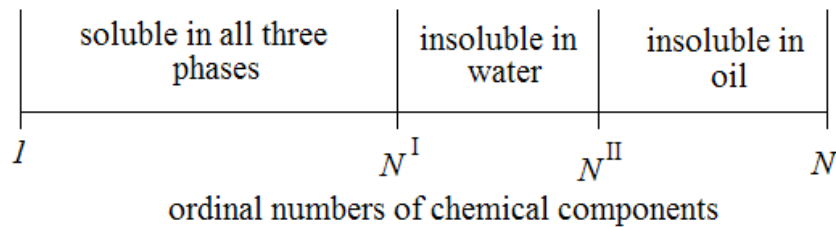


FIG. 7.1 – Three groups of chemical components in three-phase system

- I : "universal" :** components $1, 2, \dots, N^I$ that can be dissolved in all the phases ;
- II : "oil-forming" :** components $N^I + 1, N^I + 2, \dots, N^{II}$ that cannot be dissolved in the aqueous phase ;
- III : "water-forming" :** components $N^{II} + 1, N^{II} + 2, \dots, N$ that cannot be dissolved in the 'oil' phase.

(In practice the absolute non-dissolution should be replaced by a very low dissolution.)

This property does not influence significantly hydrodynamic equations, but simplifies thermodynamic relations by reducing its order. Indeed, several equations of phase equili-

brium becomes meaningless and disappear due to (7.2).

In the present thesis this property will not be exploited due to the fact that we have analyzed only systems with low number of components. However in future developments this property can play a very significant role.

7.1.4 Dimensionless form of the conservation equations

As in section 2.1.2, we introduce characteristic scales of parameter variation, determined by the domain geometry and by initial and boundary conditions : the reservoir size L , the characteristic time of fluid displacement t_* , the maximal pressure difference over the domain P^0 , the mean permeability and porosity $\langle K \rangle$, $\langle \Phi \rangle$, the initial gas and liquid densities and viscosities ρ_o^0 , ρ_w^0 , ρ_g^0 , μ_o^0 , μ_w^0 , μ_g^0 . In order to avoid the appearance of non-significant parameters, for phase densities we will use the same characteristic value ρ_g^0 while assuming that the difference in gas and liquid densities is not too high (in contrast to the difference in viscosities). Then we can introduce the dimensionless variables :

$$\varphi_g = \frac{\rho_g}{\rho_g^0}, \quad \varphi_o = \frac{\rho_o}{\rho_g^0}, \quad \varphi_w = \frac{\rho_w}{\rho_g^0}, \quad \psi_g = \frac{\rho_g \mu_g^0 K}{\rho_g^0 \mu_g \langle K \rangle}, \quad \psi_o = \frac{\rho_o \mu_o^0 K}{\rho_o^0 \mu_o \langle K \rangle}, \quad \psi_w = \frac{\rho_w \mu_w^0 K}{\rho_w^0 \mu_w \langle K \rangle}$$

$$p = \frac{P}{P^0}, \quad t = \frac{t_D}{t_*}, \quad x_i = \frac{X_i}{L}, \quad \phi = \frac{\Phi}{\langle \Phi \rangle}$$

Then equations of mass conservation of each component (7.3) can be formulated in dimensionless form :

$$\varepsilon \phi \frac{\partial}{\partial t} \left(\varphi_g c_g^{(k)} (1 - s_o - s_w) + \varphi_o c_o^{(k)} s_o + \varphi_w c_w^{(k)} s_w \right) =$$

$$\text{div} \left((\psi_g c_g^{(k)} k_g + \omega_o \psi_o c_o^{(k)} k_o + \omega_w \psi_w c_w^{(k)} k_w) \text{grad} p \right), \quad k = 1, \dots, N \quad (7.9)$$

where the operators div and grad are executed in terms of the dimensionless variables x_i .

This system of N equations is formulated with respect to N variables :

$$P, \quad s_o, \quad s_w, \quad c_g^{(k)}, \quad k = 2, \dots, N - 2 \quad (7.10)$$

All other concentrations, as well as densities and viscosities are determined from the thermodynamic subsystem.

Three dimensionless parameters ε , ω_o and ω_w play the fundamental role in the analysis of the process. Parameters ω_j are the liquid-gas mobility ratios defined as the ratio between liquid and gas cinematic viscosities, while ε is the pressure relaxation parameter defined as the ratio between the pressure stabilization time and the displacement time :

$$\omega_o = \frac{\rho_o^0 \mu_g^0}{\rho_g^0 \mu_o^0}, \quad \omega_w = \frac{\rho_w^0 \mu_g^0}{\rho_g^0 \mu_w^0}, \quad \varepsilon = \frac{t^*}{t_*} \quad (7.11)$$

where $t^* \equiv L^2 \langle \phi \rangle \mu_g^0 / (\langle K \rangle P^0)$ is the characteristic time of pressure perturbation propagation throughout the domain.

In real systems, the liquid mobility is much lower than the gas one, due to high difference in viscosities. As mentioned in section 2.1.3, the time of pressure perturbation propagation is of order of several hours or days, which is much lower that the time of fluid displacement between the injection well and a production well (of order of several months or years).

Thus, all these parameters ω_o , ω_w and ε are small. In practice they are of the order 0.01 – 0.05.

7.2 Asymptotic three-phase model and HT-splitting

Using the presence of three small parameters in the general compositional model, it is possible to obtain the asymptotic version of this model. The same method of asymptotic expansion may be applied as in sections 3.1.2 and 3.1.3. This is however equivalent to applying the mnemonic rules described in section 3.1.5.

7.2.1 "Canonical" form of the compositional model

The first step in developing the asymptotic model consists in formulating the compositional model (7.9) in the "canonical" form, similar to that obtained in section 3.1.2. As previously the system form is called canonical, if the leading derivatives of each differential equation describe the behavior of one physical basic variable from the list (7.10), in such a way that each equation describes different variable. As a result, each equation of the canonical form, considered with respect to the leading derivatives, can be interpreted as the equation of transport of the corresponding variable of the list (7.10). The canonical form has thus a clear physical meaning.

The canonical form for (7.9) is :

$$\varepsilon\phi\frac{\partial\varphi}{\partial t} = \nabla \cdot \left([\Psi_g + \omega_o\Psi_o + \omega_w\Psi_w] \nabla p \right), \quad (7.12a)$$

$$\begin{aligned} \varepsilon\phi\frac{\partial\varphi_o s_o}{\partial t} + \varepsilon\phi\eta_o^{(N-1)} \sum_{j=g,o,w} \varphi_j s_j \left(\frac{\partial\zeta_{jo}^{(N-1)}}{\partial t} - \frac{\partial\zeta_{jo}^{(N)}}{\partial t} \right) = \\ \omega_o \nabla \cdot \left(\Psi_o \nabla p \right) + \eta_o^{(N-1)} \nabla p \sum_{j=g,o,w} \omega_j \Psi_j \left(\nabla\zeta_{jo}^{(N-1)} - \nabla\zeta_{jo}^{(N)} \right), \end{aligned} \quad (7.12b)$$

$$\begin{aligned} \varepsilon\phi\frac{\partial\varphi_w s_w}{\partial t} + \varepsilon\phi\eta_w^{(N-1)} \sum_{j=g,o,w} \varphi_j s_j \left(\frac{\partial\zeta_{jw}^{(N-1)}}{\partial t} - \frac{\partial\zeta_{jw}^{(N)}}{\partial t} \right) = \\ \omega_w \nabla \cdot \left(\Psi_w \nabla p \right) + \eta_w^{(N-1)} \nabla p \sum_{j=g,o,w} \omega_j \Psi_j \left(\nabla\zeta_{jw}^{(N-1)} - \nabla\zeta_{jw}^{(N)} \right), \end{aligned} \quad (7.12c)$$

$$\begin{aligned} \Delta_o c^{(k)} \eta_o^{(N-1)} \sum_{j=g,o,w} \left[\omega_j \Psi_j \nabla p \left(\nabla\zeta_{jo}^{(N-1)} - \nabla\zeta_{jo}^{(N)} \right) - \varepsilon\phi\varphi_j s_j \left(\frac{\partial\zeta_{jo}^{(N-1)}}{\partial t} - \frac{\partial\zeta_{jo}^{(N)}}{\partial t} \right) \right] + \\ \Delta_w c^{(k)} \eta_w^{(N-1)} \sum_{j=g,o,w} \left[\omega_j \Psi_j \nabla p \left(\nabla\zeta_{jw}^{(N-1)} - \nabla\zeta_{jw}^{(N)} \right) - \varepsilon\phi\varphi_j s_j \left(\frac{\partial\zeta_{jw}^{(N-1)}}{\partial t} - \frac{\partial\zeta_{jw}^{(N)}}{\partial t} \right) \right] = \\ \sum_{j=g,o,w} \left[\omega_j \Psi_j \nabla p \nabla c_j^{(k)} - \varepsilon\phi\varphi_j s_j \left(\frac{\partial c_j^{(k)}}{\partial t} \right) \right], \quad k = 2, \dots, N-2 \end{aligned} \quad (7.12d)$$

where

$$\Psi_j \equiv \psi_j k_j (s_o, s_w), \quad \varphi \equiv \sum_{j=g,o,w} \varphi_j s_j, \quad s_g = 1 - s_o - s_w, \quad \nabla() \equiv \text{grad}(), \quad \nabla \cdot () \equiv \text{div}()$$

$$\frac{\partial\zeta_{jo}^{(k)}}{\partial t} \equiv \frac{1}{\Delta_o c^{(k)}} \frac{\partial c_j^{(k)}}{\partial t}, \quad \nabla\zeta_{jo}^{(k)} \equiv \frac{1}{\Delta_o c^{(k)}} \nabla c_j^{(k)}; \quad \frac{\partial\zeta_{jw}^{(k)}}{\partial t} \equiv \frac{1}{\Delta_w c^{(k)}} \frac{\partial c_j^{(k)}}{\partial t}, \quad \nabla\zeta_{jw}^{(k)} \equiv \frac{1}{\Delta_w c^{(k)}} \nabla c_j^{(k)}$$

$$\frac{\partial\zeta_{jw}^{(k)}}{\partial t} = \frac{\Delta_w c^{(k)}}{\Delta_o c^{(k)}} \frac{\partial\zeta_{jo}^{(k)}}{\partial t}, \quad \nabla\zeta_{jw}^{(k)} = \frac{\Delta_w c^{(k)}}{\Delta_o c^{(k)}} \nabla\zeta_{jo}^{(k)}$$

$$\Delta_o c^{(k)} \equiv c_o^{(k)} - c_g^{(k)}, \quad \Delta_w c^{(k)} \equiv c_w^{(k)} - c_g^{(k)}; \quad \omega_g \equiv 1$$

$$\eta_o^{(k)} \equiv \frac{1}{\frac{\Delta_o c^{(k)}}{\Delta_w c^{(k)}} - \frac{\Delta_o c^{(N)}}{\Delta_w c^{(N)}}}, \quad \eta_w^{(k)} \equiv \frac{1}{\frac{\Delta_w c^{(k)}}{\Delta_o c^{(k)}} - \frac{\Delta_w c^{(N)}}{\Delta_o c^{(N)}}}$$

Equation (7.12a) formulated for the total fluid may be examined as one describing the flow of gas, as the terms corresponding to liquids are small.

Equation (7.12b) describes the common transport of two saturations : s_o and s_w .

Equation (7.12c) describes the transport of water saturations s_w .

Equations (7.12d) describes the transport of phase concentrations.

7.2.2 Derivation of the canonical form

1) At the first step we obtain Eq.(7.12a) by summing all the equations (7.9). As mentioned, this equation describes basically the gas flow, as the terms responsible for flow of liquids contain small factors. This equations will be used instead of the first equation of the compositional model (7.9).

2) Secondly we subtract this equation multiplied by $c_g^{(k)}$ from all the remaining equations (7.9). The objective of this procedure is to eliminate the main terms responsible for the gas flow. This give us, after some arithmetic transformations :

$$\varepsilon\phi \left[\frac{\partial\varphi^k}{\partial t} - c_g^{(k)} \frac{\partial\varphi}{\partial t} \right] = \sum_{j=o,w} \omega_j \Delta_j c^{(k)} \operatorname{div} \left(\Psi_j \operatorname{grad} p \right) + \sum_{j=g,o,w} \omega_j \Psi_j \operatorname{grad} c_j^{(k)} \cdot \operatorname{grad} p, \quad k = 2, \dots, N \quad (7.13)$$

Differentiating by parts, we easily obtain :

$$\frac{\partial\varphi^{(k)}}{\partial t} - c_g^{(k)} \frac{\partial\varphi}{\partial t} = \Delta_o c^{(k)} \frac{\partial\varphi_o s_o}{\partial t} + \Delta_w c^{(k)} \frac{\partial\varphi_w s_w}{\partial t} + \sum_{j=g,o,w} \varphi_j s_j \frac{\partial c_j^{(k)}}{\partial t}$$

Taking $k = N - 1$ and $k = N$ we obtain the system of two equations :

$$\varepsilon\phi \left[\Delta_o c^{(N-1)} \frac{\partial \varphi_o s_o}{\partial t} + \Delta_w c^{(N-1)} \frac{\partial \varphi_w s_w}{\partial t} + \sum_{j=g,o,w} \varphi_j s_j \frac{\partial c_j^{(N-1)}}{\partial t} \right] =$$

$$\sum_{j=o,w} \omega_j \Delta_j c^{(N-1)} \operatorname{div} \left(\Psi_j \operatorname{grad} p \right) + \sum_{j=g,o,w} \omega_j \Psi_j \operatorname{grad} c_j^{(N-1)} \operatorname{grad} p;$$

$$\varepsilon\phi \left[\Delta_o c^{(N)} \frac{\partial \varphi_o s_o}{\partial t} + \Delta_w c^{(N)} \frac{\partial \varphi_w s_w}{\partial t} + \sum_{j=g,o,w} \varphi_j s_j \frac{\partial c_j^{(N)}}{\partial t} \right] =$$

$$\sum_{j=o,w} \omega_j \Delta_j c^{(N)} \operatorname{div} \left(\Psi_j \operatorname{grad} p \right) + \sum_{j=g,o,w} \omega_j \Psi_j \operatorname{grad} c_j^{(N)} \operatorname{grad} p$$

They can be presented in the form :

$$\begin{cases} \Delta_o c^{(N-1)} \cdot X + \Delta_w c^{(N-1)} \cdot Y = B^{(N-1)}, \\ \Delta_o c^{(N)} \cdot X + \Delta_w c^{(N)} \cdot Y = B^{(N)} \end{cases}$$

$$X \equiv \left[\varepsilon\phi \frac{\partial \varphi_o s_o}{\partial t} - \omega_o \operatorname{div} \left(\Psi_o \operatorname{grad} p \right) \right], \quad Y \equiv \left[\varepsilon\phi \frac{\partial \varphi_w s_w}{\partial t} - \omega_w \operatorname{div} \left(\Psi_w \operatorname{grad} p \right) \right];$$

$$B^{(k)} \equiv \sum_{j=g,o,w} \left(\omega_j \Psi_j \operatorname{grad} c_j^{(k)} \operatorname{grad} p - \varepsilon\phi \varphi_j s_j \frac{\partial c_j^{(k)}}{\partial t} \right) \quad (7.14)$$

Being considered as the linear system of two equations with respect to X and Y , it has the solution in the form of :

$$\left(\frac{\Delta_o c^{(N-1)}}{\Delta_w c^{(N-1)}} - \frac{\Delta_o c^{(N)}}{\Delta_w c^{(N)}} \right) \cdot X = B^{(N-1)} \frac{1}{\Delta_w c^{(N-1)}} - B^{(N)} \frac{1}{\Delta_w c^{(N)}},$$

$$\left(\frac{\Delta_w c^{(N-1)}}{\Delta_o c^{(N-1)}} - \frac{\Delta_w c^{(N)}}{\Delta_o c^{(N)}} \right) \cdot Y = B^{(N-1)} \frac{1}{\Delta_o c^{(N-1)}} - B^{(N)} \frac{1}{\Delta_o c^{(N)}}$$

which gives (7.12b) and (7.12c).

These equations describes flow of oil and water.

3) At the last step we will use equations (7.12b) and (7.12c) in order to simplify all the remaining equations (7.13). They can be presented in the form :

$$\Delta_o c^{(k)} \cdot X + \Delta_w c^{(k)} \cdot Y = B^{(k)}, \quad k = 2, \dots, N - 2$$

Subtracting X and Y from this equations we obtain (7.12d).

7.2.3 Zero-order asymptotic model

using the mnemonic rules established in section 3.1.5 for two-phase flow, we easily obtain the following zero-order asymptotic three-phase model from the canonical form of the compositional model (7.12) :

$$0 = \nabla \cdot (\Psi_g \nabla p), \quad (7.15a)$$

$$\varepsilon \phi \frac{\partial \varphi_o s_o}{\partial t} = \omega_o \nabla \cdot (\Psi_o \nabla p) + \eta_o^{(N-1)} \Psi_g \nabla p \left(\nabla \zeta_{go}^{(N-1)} - \nabla \zeta_{go}^{(N)} \right), \quad (7.15b)$$

$$\varepsilon \phi \frac{\partial \varphi_w s_w}{\partial t} = \omega_w \nabla \cdot (\Psi_w \nabla p) + \eta_w^{(N-1)} \Psi_g \nabla p \left(\nabla \zeta_{gw}^{(N-1)} - \nabla \zeta_{gw}^{(N)} \right), \quad (7.15c)$$

$$0 = \Psi_g \nabla p \left\{ \sum_{j=o,w} \Delta_j c^{(k)} \eta_j^{(N-1)} \left(\nabla \zeta_{gj}^{(N-1)} - \nabla \zeta_{gj}^{(N)} \right) - \nabla c_g^{(k)} \right\}, \quad k = 2, \dots, N - 2 \quad (7.15d)$$

7.2.4 Separation of the thermodynamics

The last $N - 3$ equations (7.15d) may be transformed into the following system of differential thermodynamic equations if we examine them along streamlines :

$$\sum_{j=o,w} \Delta_j c^{(k)} \eta_j^{(N-1)} \left(\frac{d\zeta_{gj}^{(N-1)}}{dp} - \frac{d\zeta_{gj}^{(N)}}{dp} \right) - \frac{dc_g^{(k)}}{dp} = 0, \quad k = 2, \dots, N - 2 \quad (7.16)$$

here we have introduced the full "thermodynamic" derivative with respect to pressure for a "thermodynamic" function $f(p, c_g^{(2)}, \dots, c_g^{(N-2)})$:

$$\frac{df}{dp} \equiv \frac{df}{dp} + \sum_{k=2}^{N-2} \frac{\partial f}{\partial c_g^{(k)}} \frac{dc_g^{(k)}}{dp}$$

In the context of this chapter we call a function "thermodynamic" if it does not depend of space and time variables.

Proof.

Along a streamline the flow becomes mono-dimensional in the corresponding coordinate system. Let l be the coordinate axe whose ort is tangent to the considered streamline at each point. The value of l is equal to the length of the streamline. The origin of the streamline is placed at the boundary of the source (injected well). Then equations (7.15d) becomes :

$$\sum_{j=o,w} \Delta_j c^{(k)} \eta_j^{(N-1)} \left(\frac{\partial \zeta_{gj}^{(N-1)}}{\partial l} - \frac{\partial \zeta_{gj}^{(N)}}{\partial l} \right) - \frac{\partial c_g^{(k)}}{\partial l} = 0, \quad k = 2, \dots, N - 2$$

because the pressure gradient along a streamline $\partial p / \partial l$ is non-zero (except probably at some singular points).

This system of $N - 3$ homogeneous and autonomous differential equations contains $N - 2$ variables : p and $N - 3$ concentrations $c_g^{(k)}$. Coordinate l plays the role of a parameter. All these variables depend on the space coordinate l only, and not on time, as the streamlines are definite only in stationary case.

If $\xi(l)$ is a monotonic function of l , then the last system is invariable with respect to the variable replacement : $l \rightarrow \xi$:

$$0 = \left\{ \sum_{j=o,w} \Delta_j c^{(k)} \eta_j^{(N-1)} \left(\frac{\partial \zeta_{gj}^{(N-1)}}{\partial \xi} - \frac{\partial \zeta_{gj}^{(N)}}{\partial \xi} \right) - \frac{\partial c_g^{(k)}}{\partial \xi} \right\} \frac{\partial \xi}{\partial l}$$

Let us select $\xi(l) = p(l)$ as pressure is monotonic along a streamline. Then we obtain :

$$0 = \sum_{j=o,w} \Delta_j c^{(k)} \eta_j^{(N-1)} \left(\frac{d\zeta_{gj}^{(N-1)}}{dp} - \frac{d\zeta_{gj}^{(N)}}{dp} \right) - \frac{\partial c_g^{(k)}}{\partial \xi}, \quad k = 2, \dots, N-2$$

This system of $N-3$ differential equations contains $N-2$ variables : p and $N-3$ concentrations $c_g^{(k)}$. So the concentrations $c_g^{(k)}$ depend only on pressure p and some parameters, introduced by Cauchy conditions imposed at one point of the streamline (for instance, at the starting point).

So we obtain (7.16).

As seen, the obtained differential thermodynamic model is qualitatively different from the one developed for two-phase flow, (3.8b).

7.2.5 Asymptotic thermodynamic model

The split thermodynamic model, which describes the behavior of a compositional gas-oil-water system moving in porous medium along streamlines :

- equilibrium equations :

$$\nu_g^{(k)} \left(p, \{c_g^{(q)}\}_{q=1}^{N-1} \right) = \nu_o^{(k)} \left(p, \{c_o^{(q)}\}_{q=1}^{N-1} \right) = \nu_w^{(k)} \left(p, \{c_w^{(q)}\}_{q=1}^{N-1} \right), \quad k=1, \dots, N \quad (7.17a)$$

- mass exchange between highly mobile gas and low mobile liquids :

$$\frac{1}{\left[\frac{\Delta_w c^{(k)}}{\Delta_o c^{(k)}} - \frac{\Delta_w c^{(N)}}{\Delta_o c^{(N)}} \right]} \left(\frac{1}{\Delta_o c^{(k)}} \frac{dc_g^{(k)}}{dp} - \frac{1}{\Delta_o c^{(N)}} \frac{dc_g^{(N)}}{dp} \right) =$$

$$\frac{1}{\left[\frac{\Delta_w c^{(N-1)}}{\Delta_o c^{(N-1)}} - \frac{\Delta_w c^{(N)}}{\Delta_o c^{(N)}} \right]} \left(\frac{1}{\Delta_o c^{(N-1)}} \frac{dc_g^{(N-1)}}{dp} - \frac{1}{\Delta_o c^{(N)}} \frac{dc_g^{(N)}}{dp} \right), \quad k = 2, \dots, N-2 \quad (7.17b)$$

which is the developed form of (7.16) after some arithmetic transformations.

This system of $3N-3$ equations contain $3N-2$ variables : $N-1$ concentrations in gas $c_g^{(k)}$, $N-1$ concentrations in oil phase $c_o^{(k)}$, $N-1$ concentrations in water phase $c_w^{(k)}$, and pressure p . This system determines all the phase concentrations as a function of pressure.

This system is totally independent of the hydrodynamic sub-system. As previously, such a model is valid only along streamlines.

Other thermodynamic relations do not change : three EOS determine phase densities, and three rheological EOS determine phase viscosities.

Similar to section 3.1.8, it is possible to show that the physical meaning of the differential thermodynamic equations (7.17b) is the fact that the exchange flow rate of the total phase is equal to that of each component.

7.2.6 Improved asymptotic hydrodynamic model

As for two-phase flow, it is possible to improve the zero-order asymptotic model by adding some terms that are formally small, but can become important in some situations or within some boundary layers, as this was done in section 3.1.9.

The asymptotic hydrodynamic model is presented by three remaining equations (7.15a), (7.15b) and (7.15c). Obviously, the first equation losses the initial condition, therefore it is valid only outside the time boundary layer formed in the vicinity of the initial point. In order to obtain the model uniformly valid for all the times, we will introduce the time derivative from the original Eq. (7.12a).

The second problem is related to the nonlinearity of the compositional model with respect to two saturations. Due to the nonlinearity and degeneration of the relative permeabilities, both liquids can become equally mobile and event more mobile than gas (at low gas saturations). In order to take into account this effect, we will keep the term responsible for the liquid mobility in (7.12a).

Thirdly, it is useful to keep sometimes the non-stationary terms which depend on $\partial p/\partial t$ in the second and third equations, (7.12b) and (7.12c). These terms are lost in the asymp-

otic expansion as they are of order $\omega_j \cdot \varepsilon$. However in particular cases, when the motion of both the phases and the variation of the phase composition $\frac{dc_g^{(N)}}{dp}$ are very low, then the variation of saturation is determined basically by $\partial p / \partial t$. But due to the sufficient complexity of the asymptotic model, within this thesis we will neglect these terms everywhere.

The definite form of the hydrodynamic asymptotic model is :

$$\varepsilon \phi \frac{\partial \varphi}{\partial t} = \nabla \cdot \left((\Psi_g + \omega_o \Psi_o + \omega_w \Psi_w) \nabla p \right), \quad (7.18a)$$

$$\varepsilon \phi \frac{\partial \varphi_o s_o}{\partial t} + \varepsilon \phi H_o \frac{\partial p}{\partial t} = \omega_o \nabla \cdot \left(\Psi_o \nabla p \right) + \eta_o^{(N-1)} \Psi_g \nabla p \left(\frac{1}{\Delta_o c^{(N-1)}} \nabla c_g^{(N-1)} - \frac{1}{\Delta_o c^{(N)}} \nabla c_g^{(N)} \right), \quad (7.18b)$$

$$\varepsilon \phi \frac{\partial \varphi_w s_w}{\partial t} + \varepsilon \phi H_w \frac{\partial p}{\partial t} = \omega_w \nabla \cdot \left(\Psi_w \nabla p \right) + \eta_w^{(N-1)} \Psi_g \nabla p \left(\frac{1}{\Delta_w c^{(N-1)}} \nabla c_g^{(N-1)} - \frac{1}{\Delta_w c^{(N)}} \nabla c_g^{(N)} \right) \quad (7.18c)$$

where

$$H_i(p, s_o, s_w) \equiv \eta_i^{(N-1)} \sum_{j=g,o,w} \varphi_j s_j \left(\frac{d\zeta_{ji}^{(N-1)}}{dp} - \frac{d\zeta_{ji}^{(N)}}{dp} \right), \quad i = o, w$$

7.2.7 1D asymptotic three-phase model

As the asymptotic thermodynamic model is valid only along streamlines, we shall then analyze the 1D version of all the model. As in section 3.2, we examine the cartesian coordinate system, which implies a system of sufficiently straight streamlines of an almost uniform density of lines in space. In this case the asymptotic compositional model may be formulated in two equivalent forms, similar to (3.15) and (3.16) :

- either in the form of the second-order non-steady differential equation for pressure :

$$\varepsilon\phi\frac{\partial\varphi(p, s_o, s_w)}{\partial t} = \frac{\partial}{\partial x} \left(\left(\psi_g(p)k_g + \omega_o\psi_o(p)k_o + \omega_w\psi_w(p)k_w \right) \frac{\partial p}{\partial x} \right), \quad (7.19a)$$

$$\varepsilon\phi\frac{\partial\varphi_o s_o}{\partial t} + \varepsilon\phi H_o \frac{\partial p}{\partial t} = \omega_o \frac{\partial}{\partial x} \left(\psi_o k_o \frac{\partial p}{\partial x} \right) + \psi_g k_g \lambda_{go}(p) \left(\frac{\partial p}{\partial x} \right)^2 \quad (7.19b)$$

$$\varepsilon\phi\frac{\partial\varphi_w s_w}{\partial t} + \varepsilon\phi H_w \frac{\partial p}{\partial t} = \omega_w \frac{\partial}{\partial x} \left(\psi_w k_w \frac{\partial p}{\partial x} \right) + \psi_g k_g \lambda_{gw}(p) \left(\frac{\partial p}{\partial x} \right)^2 \quad (7.19c)$$

- or in the form of the semi-integrated first-order steady-state equation for pressure :

$$\frac{\partial p}{\partial x} = - \frac{\varepsilon q(t)}{\psi_g k_g + \omega_o \psi_o k_o + \omega_w \psi_w k_w}, \quad (7.20a)$$

$$\phi \frac{\partial\varphi_o s_o}{\partial t} = \omega_o q(t) \frac{\partial \widehat{F}_o}{\partial x} + \frac{\varepsilon q^2 \widehat{F}_g \lambda_{go}}{\psi_g k_g + \omega_o \psi_o k_o + \omega_w \psi_w k_w}, \quad (7.20b)$$

$$\phi \frac{\partial\varphi_w s_w}{\partial t} = \omega_w q(t) \frac{\partial \widehat{F}_w}{\partial x} + \frac{\varepsilon q^2 \widehat{F}_g \lambda_{gw}}{\psi_g k_g + \omega_o \psi_o k_o + \omega_w \psi_w k_w}, \quad (7.20c)$$

where :

$$\lambda_{gi}(p) \equiv \eta_i^{(N-1)} \left(\frac{1}{\Delta_i c^{(N-1)}} \frac{dc_g^{(N-1)}}{dp} - \frac{1}{\Delta_i c^{(N)}} \frac{dc_g^{(N)}}{dp} \right); \quad i = o, w$$

$$H_i(p, s_o, s_w) \equiv \eta_i^{(N-1)} \sum_{j=g,o,w} \varphi_j s_j \left(\frac{1}{\Delta_i c^{(N-1)}} \frac{dc_g^{(N-1)}}{dp} - \frac{1}{\Delta_i c^{(N)}} \frac{dc_g^{(N)}}{dp} \right),$$

$$\widehat{F}_i \equiv \frac{\psi_i k_i}{\psi_g k_g + \omega_o \psi_o k_o + \omega_w \psi_w k_w}, \quad i = g, o, w$$

q is the dimensionless flow rate (at the well) equal to 1 when the flow rate is constant in time. Function \widehat{F}_i is the fractional mass flow function for the phase i .

7.3 Diagrammatical representation of the split thermodynamics

7.3.1 Phase diagrams, tie-surfaces, and triangles

As in the case of two-phase flow, the asymptotic thermodynamic model shows that the phase concentrations depend on pressure as well as the imposed pressure at the starting or ending point of each streamline. Then in the case of an invariable pressure, which is the easiest case for the analysis, the phase concentrations can be only constant or piece-wise constant. The behavior of the phase concentrations is then characterized by the probable discontinuities and the invariable phase composition between the shocks.

The three-component mixtures are represented by the same phase diagrams as in Fig. 5.1, but with the appearance of a three-phase zone along with the two-phase domain. In three-component case at fixed P,T, the three-phase zone can be only represented by a curve, according to the Gibbs rule of phases. For four-component systems, the cartesian phase diagram is presented in Fig. 7.2. The total compositions of three components are given on three axes, while the fourth component corresponds to the bisector of the right angle. The curvilinear surface represents the envelop of the two-phase zone which now constitutes a volume. The three-phase zone will be presented by a surface which can either be 3D or 2D (it is not shown in this figure).

The locus of invariable phase composition is presented by a plan surface inside the two-phase domain, which is called the tie-plan or *the tie-triangle* ABD (because it becomes triangular being continued up to pyramid sides). This trace of the intersection of this tie-triangle with the three-phase surface corresponds to the tie-line for three-phase state. The tie-triangles are equivalent to tie-lines in three-component case.

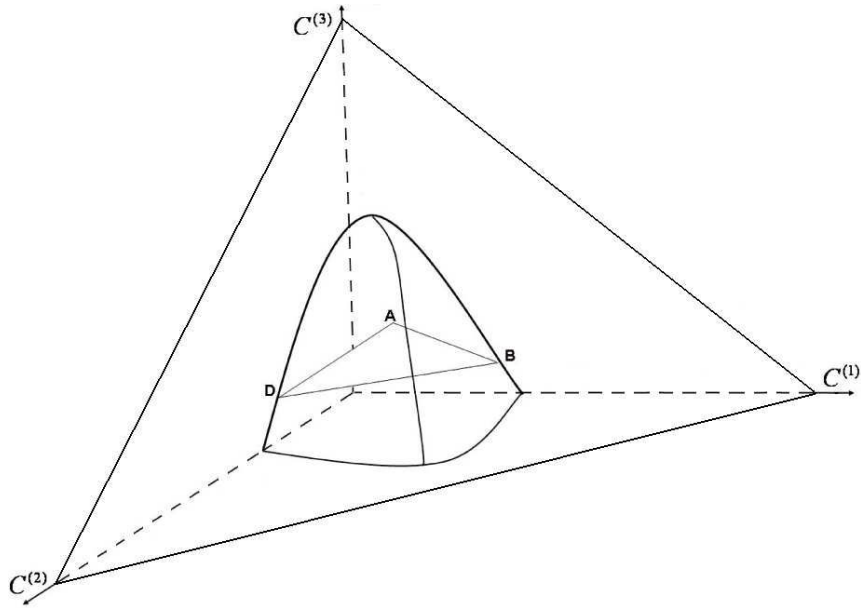


FIG. 7.2 – Two-phase zone and tie-triangle (ABD) in the phase diagram for four-component system

7.3.2 P -surfaces and P -volumes

For the case of variable pressure, the tie-lines crossing three-phase four-component zones will be replaced by P -surfaces, as in section 5.1.3 for two-phase three-component case. The tie-triangles crossing the two-phase zone will form the P -volumes along the axis of pressure, Fig. 7.3.

Just like the case of two-phase problem we examine the process of pressure variation from an initial value p_1 in the three-phase mixture up to the final one p_2 .

If the system remains two-phase between p_1 and p_2 then it is described by the P -volume. If the system remains three-phase, then it is described by a P -surface belonging to this P -volume.

The variation between the initial fluid and the injected fluid will happen along a P -volume. According to the construction of this volume, each cross-section of it at a fixed pressure represents a plan which is a tie-triangle.

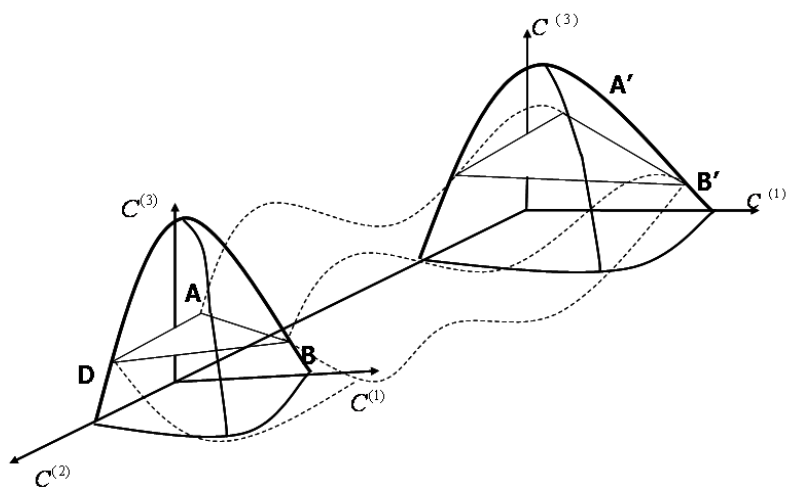


FIG. 7.3 – P-volumes for a four-component system

7.4 Riemann problem in terms of the asymptotic model

7.4.1 Problem formulation

Let us examine the Riemann problem of gas-oil-water flow formulated in terms of the equations (7.20b) and (7.20c). Let the initial saturation of oil and water be s_o^0 and s_w^0 , while the injected saturations (at $x = 0$) are s_o^{inj} and s_w^{inj} respectively :

$$\begin{aligned} s_o|_{t=0} &= s_o^0(x) \quad , & s_w|_{t=0} &= s_w^0(x) \\ s_o|_{x=0} &= s_o^{inj}(t) \quad , & s_w|_{x=0} &= s_w^{inj}(t) \end{aligned} \quad (7.21)$$

The initial shock of saturation will be transported by the convection mechanism and probably deformed in time by the right-hand side of equations (7.20b) and (7.20c).

This problem should be also completed with one boundary condition for equation (7.20a) :

$$p|_{x=0} = p^{inj}(t) \quad (7.22)$$

which defines the injection pressure (the pressure at the streamlines starting points).

The differential thermodynamic equations (7.17b) should satisfy two Cauchy conditions for two boundary points of pressure :

$$\begin{aligned} c_g^{(k)}|_{p=p^{ini}} &= c_g^{(k),ini}, & k &= 2, \dots, N-2 \\ c_g^{(k)}|_{p=p^{inj}} &= c_g^{(k),inj}, & k &= 2, \dots, N-2 \end{aligned} \quad (7.23)$$

where p^{inj} is the starting pressure, while p^0 is the initial pressure, p_* is the pressure at $x = 1$. The method of calculating p^0 is the same as in section 4.1.3.

So the asymptotic model leads to a couple of thermodynamic Cauchy problems which

determines two different fluid compositions. This determines at least two distinct systems of thermodynamic closure relations, or discontinuity in the system coefficients (7.19). The location of this discontinuity is a priori unknown.

7.4.2 Structure of the solution

If the system remains in three-phase state in all the domain at any time instant, then the global structure of the solution will consists of the following three elements :

- double S -shock which is the simultaneous shock of both saturations s_o and s_w determined by the Hugoniot conditions deduced directly from the differential equations (7.19b) and (7.19c);

- single S -shock which is the shock of only one saturation s_o or s_w determined by the Hugoniot conditions also deduced directly from the differential equations (7.19b) and (7.19c);

- full SC -shock which is the simultaneous shock of both the saturations and all the phase concentrations $c_i^{(k)}$, which are induced by the discontinuities in coefficients of system (7.19);

- partial SC -shock which is the simultaneous shock of only one saturation and all the phase concentrations $c_i^{(k)}$, which are induced by the discontinuities in coefficients of system (7.19);

- rarefaction waves which are the continuous fragments between shocks; they represent the unique continuous solutions to (7.19).

Note that the "plateau" elements cannot exist in this case as the differential equations (7.19b) and (7.19c) are non-homogeneous.

If the system can change its phase state, then the solution will have two additional elements :

- 3/2-shock of phase transition between a three-phase and a two-phase fluids;
- 3/1-shock of phase transition between a three-phase and a single-phase fluids;
- 2/1-shock of phase transition between a two-phase and a single-phase fluids.

The admissibility of all these types of shocks and the inadmissibility of other types can be proved by standard methods (similar to the two-phase case) based on the analysis of the Hugoniot conditions.

The full system of the Hugoniot conditions resulting from the full compositional model, which determine both the shocks of the solution structure and the shocks of the coefficients of hydrodynamic model are :

$$\varepsilon [\varphi] V_f = [W_g] + \omega_o [W_o] + \omega_w [W_w], \quad (7.24)$$

$$\varepsilon [\varphi^{(k)}] V_f = [W_g c_g^{(k)}] + \omega_o [W_o c_o^{(k)}] + \omega_w [W_w c_w^{(k)}], \quad k = 2, \dots, N \quad (7.25)$$

herein V_f is the shock velocity, $\varphi = \varphi_g(1 - s_o - s_w) + \varphi_o s_o + \varphi_w s_w$ and $[A] = A^+ - A^-$ is the variation of the value of A before and behind the shocks; $\varphi^{(k)} = \varphi_g c_g^{(k)}(1 - s) + \varphi_o c_o^{(k)} s_o + \varphi_w c_w^{(k)} s_w$, $W_j = -\psi_j k_j \frac{\partial p}{\partial x}$, $j = g, o, w$.

7.4.3 SC-shocks

Any *SC*-shock is determined by the additional asymptotic Hugoniot conditions (7.25) obtained from the full compositional model.

Extending the results obtained in section 4.2.8 (Eq. (4.16)), we will develop the following system of the asymptotic Hugoniot conditions $\omega_o, \omega_w \rightarrow 0$:

$$\varepsilon [\varphi] V_f = [W_g] + \omega_o [W_o] + \omega_w [W_w], \quad (7.26a)$$

$$\varepsilon V_f = \frac{W_g^- [c_g^{(N)}] + \omega_o [W_o c_o^{(N)}] - \omega_o c_g^{(N)+} [W_o] + \omega_w [W_w c_w^{(N)}] - \omega_w c_g^{(N)+} [W_w]}{[\varphi^{(N)}] - c_g^{(N)+} [\varphi]}, \quad (7.26b)$$

$$\frac{([\varphi^{(k)}] - c_g^{(k)+} [\varphi])}{[c_g^{(k)}]} = \frac{([\varphi^{(N)}] - c_g^{(N)+} [\varphi])}{[c_g^{(N)}]}, \quad k = 2, \dots, N - 1 \quad (7.26c)$$

The last subsystem of $N - 2$ conditions does not contain velocities, but only thermodynamic parameters and saturations.

7.5 Solution to the asymptotic three-phase Riemann problem

7.5.1 HT-splitting in Hugoniot conditions

Due to a high variance of different shocks in three-phase case, within this thesis we will only examine one type of partial SC -shocks assuming that saturation s_w remains continuous.

The last $N-2$ equations (7.26c) contains thermodynamic parameters : phase concentrations, and non-thermodynamic ones : saturations s_o^+ , s_o^- , s_w^+ and s_w^- . For partial SC -shocks, it is possible to eliminate all the four saturations. Indeed, it is possible to present (7.26c) in the following form after algebraic transformations :

$$\sum_{i=o,w} \left(\varphi_i^+ s_i^+ \lambda_{i1}^{(k)} + \varphi_i^- s_i^- \lambda_{i2}^{(k)} \right) = 0; \quad k = 2, \dots, N-1 \quad (7.27)$$

$$\begin{aligned} \lambda_{i1}^{(k)} &\equiv c_g^{(N)+} c_i^{(k)+} + c_g^{(N)-} c_g^{(k)+} + c_i^{(N)+} c_g^{(k)-} - c_g^{(N)-} c_i^{(k)+} - c_i^{(N)+} c_g^{(k)+} - c_g^{(N)+} c_g^{(k)-}; \\ \lambda_{i2}^{(k)} &\equiv c_g^{(N)+} c_g^{(k)-} + c_g^{(N)-} c_i^{(k)-} + c_i^{(N)-} c_g^{(k)+} - c_g^{(N)-} c_g^{(k)+} - c_i^{(N)-} c_g^{(k)-} - c_g^{(N)+} c_i^{(k)-} \end{aligned}$$

Assuming that water saturation is continuous, leads to : $[s_w] = 0$. So we have only three saturations.

To remove all the three saturations from this homogeneous system, it is sufficient to consider two equations. We will select the last two equations. Then two variables which include saturations are determined as :

$$X \equiv \frac{\varphi_o^+ s_o^+}{\varphi_w^- s_w^-} = \frac{\Delta_1}{\Delta}, \quad Y \equiv \frac{\varphi_o^- s_o^-}{\varphi_w^- s_w^-} = \frac{\Delta_2}{\Delta}$$

where $\Delta, \Delta_1, \Delta_2$ are the determinants of the system :

$$\begin{pmatrix} \lambda_{o1}^{(N-1)} & \lambda_{o2}^{(N-1)} \\ \lambda_{o1}^{(N-2)} & \lambda_{o2}^{(N-2)} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} \lambda_{w1}^{(N-1)} \varphi_w^+ / \varphi_w^- + \lambda_{w2}^{(N-1)} \\ \lambda_{w1}^{(N-2)} \varphi_w^+ / \varphi_w^- + \lambda_{w2}^{(N-2)} \end{pmatrix} \quad (7.28)$$

After this the saturations may be removed from all the remaining equations of the system (7.27), which yields the following system :

$$\frac{\Delta_1}{\Delta} \lambda_{o1}^{(k)} + \frac{\Delta_2}{\Delta} \lambda_{o2}^{(k)} + \frac{\varphi_w^+}{\varphi_w^-} \lambda_{w1}^{(k)} + \lambda_{w2}^{(k)} = 0, \quad k = 2, \dots, N - 3 \quad (7.29)$$

This system contains only thermodynamic variables : phase concentrations. We will call this subsystem "the thermodynamic Hugoniot conditions".

7.5.2 Concentration tracker. Number of *SC*-shocks

One weakness of three-phase theory is that the number of *SC*-shocks is unknown. We suggest an indirect method to determine it, by reversing the results obtained for two-phase flow. In the two-phase case we have shown that, if we accept the number of shock to be equal to $N - 2$, which is the known value from general two-phase theory, then the system of thermodynamic Hugoniot and equilibrium equations will be closed with respect to the parameters of all the *SC*-shocks presented in the structure of the solution.

Now we assume that the number of shocks M is unknown, but it can be detected from the condition that the system of thermodynamic Hugoniot and equilibrium equations is closed with respect to the parameters of all the shocks.

Let us construct the table similar to 5.1 which counts the number of the shock concentrations and equations used :

The number of unknown concentrations is $6(M - 1)(N - 1)$, while the number of equations is $M(N - 4) + (M - 1)(5N - 3)$. The solution is unique if these two values be

TAB. 7.1 – Total Number of unknown concentrations at all the *SC*-shocks : three-phase case

Unknown variables		
Shock type	Number of shocks	Number of concentrations at one shock
First after the injection point	1	3(N-1)
Intermediate	M-2	6(N-1)
Last before the exit point	1	3(N-1)
Total	M	6(N-1)(M-1)

TAB. 7.2 – Total Number of thermodynamic equations : three-phase case

Equation type	Number of			Total number of equations
	shocks	shock sides	crossover P-surfaces	
Hugoniot (N-4)	M			(N-4)*M
Equilibrium (2N)		2(M-1)		4N(M-1)
DTE (N-3)			M-1	(N-3)(M-1)
Total				M(N-4)+(M-1)(5N-3)
⁽¹⁾ DTE = differential thermodynamic equations				

identical :

$$M(N - 4) + (M - 1)(5N - 3) = 6(M - 1)(N - 1) \quad \rightarrow \quad M = N - 3 \quad (7.30)$$

So the number of partial *SC*-shocks is $N - 3$.

In a similar way it is possible to show that the number of full *SC*-shocks is fractional. This means that it is impossible to have only the full *SC*-shocks in the domain of flow.

We also see that for a three-component system, the tree-phase full and partial *SC*-shocks do not exist.

7.6 Results for three-component problem

7.6.1 Description of the cases

In the present thesis, we have simulated numerically only the three-component systems in three-phase case, profiting of the fact that these systems have sufficiently simpler structure of the solution than the general case. In particular, as it follows from (7.30), three-component three-phase systems cannot have SC -shocks, but only the S shocks and the shocks of phase transition.

If the injected fluid and the initial one are both three-phase, then the solution will only have S shocks.

We simulated flow of a gas, oil and water systems in two different cases :

- Ternary mixture of methane, decane and water.
- Ternary mixture of carbon dioxide, decane and water.

The system of asymptotic hydrodynamics equations (7.20) was discretized by the backward finite difference method, fully explicit in time.

We consider an isothermal process.

The equilibrium equations were accepted in the form of the Wilson equations for K – values as the functions of pressure :

$$K_i = \frac{P_{ci}}{P} \exp \left[5.37(1 + \omega_i) \left(1 - \frac{T - T_{ci}}{T} \right) \right] \quad (7.31)$$

The initial K -values for the partitioning of components in different phases at $p = 70$ bar and $T = 345^\circ K$ are shown in table (7.3); [Laforce *et al.* 2007].

TAB. 7.3 – Initial K -values for water, carbon dioxide, methane and decane

Component	K_1	K_2
CH_4	10	0.05
CO_2	1.5	0.1
H_2O	2	50
C_{10}	0.005	0.001

Herein :

$$\begin{aligned}
 K_1^i &= \frac{c_g^{(i)}}{c_o^{(i)}} \\
 K_2^i &= \frac{c_w^{(i)}}{c_o^{(i)}}
 \end{aligned}
 \tag{7.32}$$

where $c_g^{(i)}$, $c_o^{(i)}$ and $c_w^{(i)}$ are the phase concentrations in gaseous, oleic and aqueous phase respectively.

If the total concentrations are given, then the two K -values are sufficient to determine the phase equilibria all over the problem. The third K – value (between the aqueous and gaseous phase) is given by the relation :

$$K_3^i = \frac{c_w^i}{c_g^i} = \frac{K_2^i}{K_1^i}$$

The saturations was simulated all over the one-dimensional reservoir at various time instants after starting the injection.

7.6.2 Water injection in immobile oil

In this part we examine the case of water injection into the reservoir containing initially a mixture of methane and decane in gaseous and oleic phases. We will consider two different cases of this problem. The first case is when the oleic phase is immobile; which implies that its saturation is lower than the residual saturation. The second case corresponds to

the mobile oil.

As the *SC*-shocks does not exit for a ternary system, then the behaviour of concentrations will be continuous. They depend on pressure only for the examined systems. So for both initial and injection states the phase compositions are :

$$\begin{aligned}
c_g^{(1)} &= (0.9607 * P - 0.3422)/P \\
c_g^{(2)} &= (0.0398 * P - 0.0027)/P \\
c_g^{(3)} &= (-0.0006 * P + 0.3449)/P \\
c_w^{(1)} &= (0.0048 * P - 0.0017)/P \\
c_w^{(2)} &= (0.9953 * P - 0.06727)/P \\
c_w^{(3)} &= (-0.0001 * P + 0.0690)/P \\
c_o^{(1)} &= -0.0005 + 0.0014 * P \\
c_o^{(2)} &= 0.0003 * P - 0.00002 \\
c_o^{(3)} &= -0.0017 * P + 1.0005
\end{aligned} \tag{7.33}$$

The saturation of the oleic phase is assumed to be equal or lower than the residual saturation of this phase which is $s_{res} = 0.2$, so the oleic phase is initially immobile :

Injection composition :

$$CH_4 = 0.0048$$

$$H_2O = 0.9948$$

$$C_{10} = 0.00037674$$

Initial composition :

$$CH_4 = 0.7639$$

$$H_2O = 0.0376$$

$$C_{10} = 0.1688$$

As we are able to see in Fig. 7.4 the gas and oil saturations are approximately in most of the one dimensional reservoir, the same as their initial saturations. So the injection process

seems to be really non efficient.

The results of simulation by using the developed model are presented in Fig. 7.4.

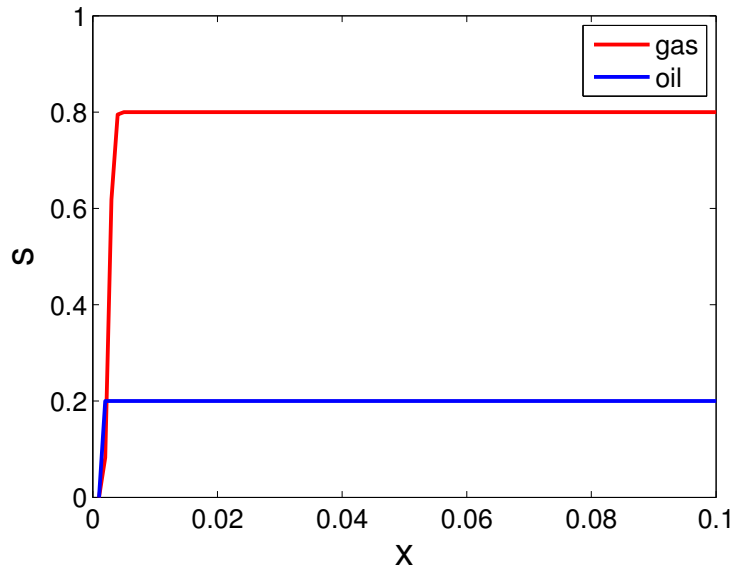


FIG. 7.4 – Gas and oil saturations in space : water injection in immobile oil

7.6.3 Water injection in mobile oil

For the case of a reservoir with mobil oil phase, we examined the Riemann problem with the same injection compositions as previously, but the initial oil composition is now different :

Initial composition :

$$CH_4 = 0.7118$$

$$H_2O = 0.0365$$

$$C_{10} = 0.2517$$

In Fig. 7.5 the gas and oil saturation profiles show the displacement of both the gaseous and oleic phases and as expected an apex of oil produced just after the water phase shock.

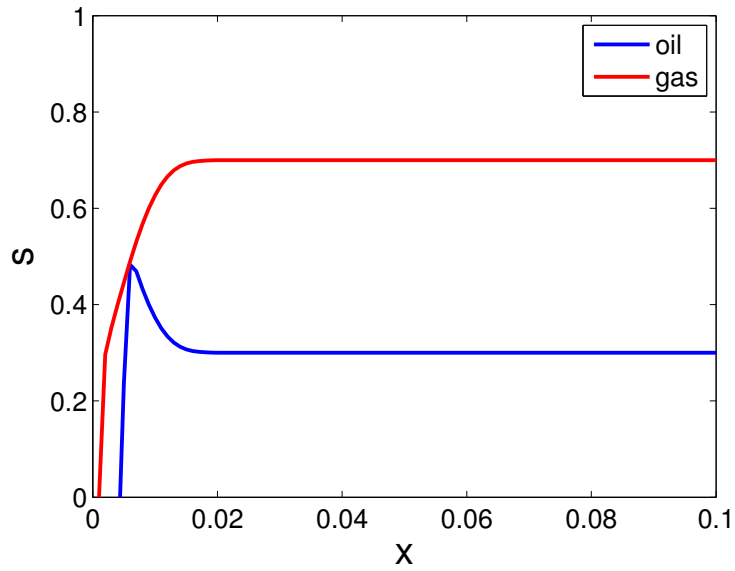


FIG. 7.5 – Gas and oil saturations in space : water injection into mobile oil

7.6.4 Carbon dioxide injection : water is absent

We will examine three different cases :

- 1) the aqueous phase does not exist ;
- 2) the initial water is immobile ;
- 3) the initial water is mobile.

Both initial and injection compositions depend just on pressure and are as follow :

$$\begin{aligned}
c_g^{(1)} &= (0.9659 * P - 0.3440)/P \\
c_g^{(2)} &= (0.0375 * P - 0.0018)/P \\
c_g^{(3)} &= (-0.0033 * P + 0.3458)/P \\
c_w^{(1)} &= (0.0644 * P - 0.0229)/P \\
c_w^{(2)} &= (0.9363 * P - 0.0462)/P \\
c_w^{(3)} &= (-0.0007 * P + 0.0692)/P \\
c_o^{(1)} &= -0.0033 + 0.0093 * P \\
c_o^{(2)} &= 0.0003 * P - 0.00001 \\
c_o^{(3)} &= -0.0096 * P + 1.0033
\end{aligned} \tag{7.34}$$

Saturation of aqueous phase assumed to be zero, and the injection and initial compositions in this case are chosen respectively as below :

Injection composition :

$$CO_2 = 0.9624$$

$$H_2O = 0.0374$$

$$C_{10} = 0.00014565$$

Initial composition :

$$CO_2 = 0.5611$$

$$H_2O = 0.0165$$

$$C_{10} = 0.4224$$

As we see in Fig. 7.6 a piston-like displacement of oil by gas takes place, approximately all the oil is pushed toward the production well.

This case corresponds to the two-phase flow (gas and oil) with an entire dissolution of CO_2 in oil. The scenarios of flow corresponds to the total evaporation of oil; The

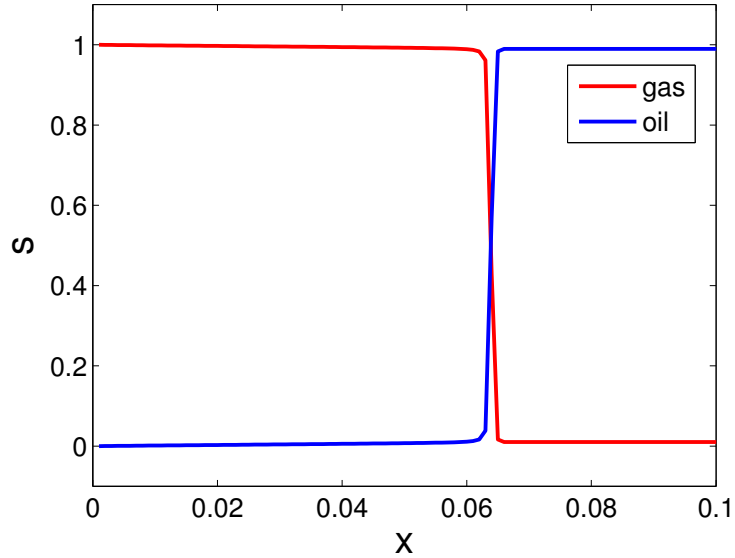


FIG. 7.6 – Gas and oil saturation : CO_2 injection ; the initial water does not exist

displacement is piston-like, with 100% of the recovered oil.

7.6.5 Carbon dioxide injection : immobile water

The saturation of the aqueous phase is assumed to be equal or lower than the residual saturation, which is accepted as $s_{res} = 0.2$. The injection composition is the same as in the previous case. The initial composition is the following :

Initial composition :

$$CO_2 = 0.4625$$

$$H_2O = 0.2003$$

$$C_{10} = 0.3372$$

The main effect of injection consists in evaporating oil ; the displacement is still piston-like. Due to the lower initial mass of oil, the displacement is faster in this case. The fact that part of CO_2 does not participate in oil recovery, being dissolved and lost in water, does not reduce the efficiency of recovery. This is due to the fact that the initial water saturation is low.

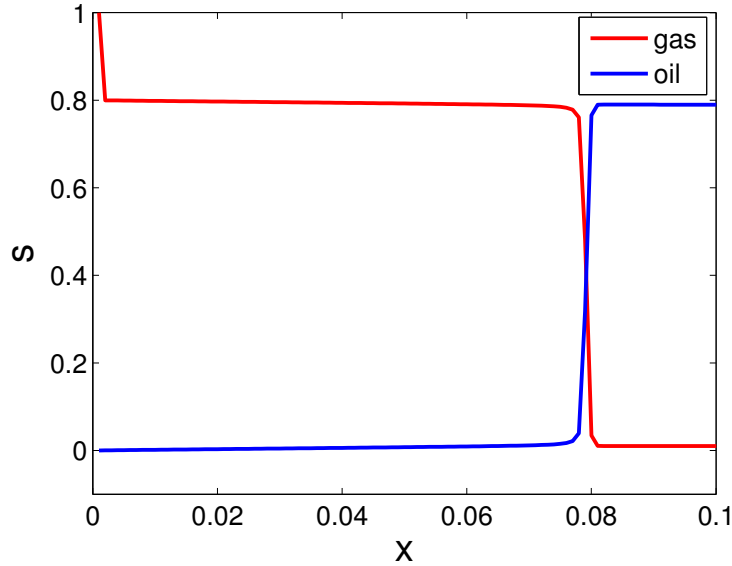


FIG. 7.7 – Gas and oil saturations : CO_2 injection, water is immobile

7.6.6 Carbon dioxide injection : mobile water

The initial water saturation is higher than the percolation threshold. The injection composition is the same. The initial compositions are :

Initial composition :

$$CO_2 = 0.4132$$

$$H_2O = 0.2923$$

$$C_{10} = 0.2946$$

Fig. 7.8 shows the gas and oil saturations.

The efficiency of displacement is significantly reduced, as a significant part of CO_2 dissolves now in water and does not displace oil. Moreover, the volume of water significantly increases due to CO_2 dissolution. Two observed shocks are the S -shocks of all the three saturations. The forward front displaces only oil. The backward front displaces the mixture of oil and water. Water forms a bank behind the forward front, so the forward oil is displaced both by gas and water. Behind the backward front all the oil is displaced.

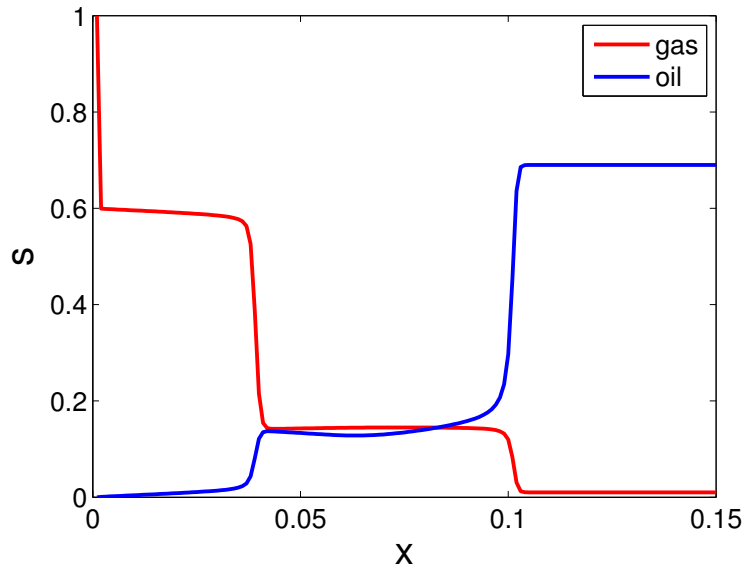


FIG. 7.8 – Gas and oil saturations : CO_2 injection ; water is mobile

Conclusions

Conclusion for chapters 2,3,4,5 : Two phase flow

In these chapters we develop the asymptotic model of compositional two-phase flow in porous media for systems characterized by two fundamental properties : (i) contrasted gas and liquid mobilities, associated with a small liquid-gas mobility ratio ω ; (ii) fast stabilization of the pressure field, which is described by a dimensionless pressure relaxation time ε also considered small. Such a model was first suggested in [Oladyshkin Panfilov 2006] for boundary problems characterized by continuous solutions, which corresponds to the process of natural reservoir depletion.

The advantage of the asymptotic model is determined by two properties : (i) the thermodynamic part is separated from the hydrodynamic part ("HT-splitting"); due to this the asymptotic model is also frequently called the "HT-split model"; (ii) the hydrodynamic part consists of two differential equations independently of the number of chemical components in the fluid. The coefficients of these hydrodynamic equations are determined by the split thermodynamic system, which represents the classic subsystem of equilibrium equations which is now completed with the new differential thermodynamic equations (derivatives with respect to pressure). In the case of continuous behavior of the solution the split thermodynamics entirely determines the coefficients of the hydrodynamic model.

Unfortunately the obvious advantages of such a model give efficient results in the case of continuous solutions, but imposes serious problems when discontinuities appear.

The objective of this part was to extend the asymptotic compositional model to the case

of discontinuous solutions which are proper to problems of enhanced oil recovery when one fluid (miscible gas) displaces the initial oil while changing oil properties and evaporating it. The model of such a displacement process is presented by the Riemann problem which determines an initial shock of fluid composition. This initial shock is then transported by the fluid and undergoes various transformation (into several shocks,...). In the general case the solution to the Riemann problem is characterized by a finite number of mobile discontinuities.

For the case of discontinuous solutions, the asymptotic hydrodynamic model represents the same couple of differential transport equations, but the coefficients of these equations become discontinuous. Moreover the discontinuities in coefficients are mobile and are not defined a priori. The split thermodynamic subsystem is no longer sufficient to determine the coefficient discontinuities.

So the discontinuities in the solution structure are produced by two sources :

1-Discontinuities in the coefficients of the hydrodynamic differential equations caused by the discontinuous behavior of the phase concentrations ;

2-Discontinuities in the structure of the solution to the hydrodynamic problems ; they are caused by the Riemann problem for saturation which imposes the initial shock of phase and total composition. Such a property of the system is non-trivial and is not studied in fluid mechanics.

The primary conclusion of our development are :

1) The asymptotic model can be transformed into the HT-split model only along streamlines. For sufficiently straight streamlines with an almost uniform density of lines in space, we have obtained the formulation of the one-dimensional asymptotic hydrodynamic model in cartesian frame in two different cases : (i) either in the form of the second-order non-stationary differential equation for pressure, or (ii) in the form of the semi-integrated first-order quasi-stationary equation for pressure.

2) We have shown that the asymptotic hydrodynamic model, formulated with respect to saturation and pressure, and the asymptotic thermodynamic model are insufficient to

determine the discontinuities in coefficients of flow equations.

3) The additional conditions for the discontinuities of coefficients were obtained from the full compositional model with the consecutive limit transition in the obtained relationships $\varepsilon, \omega \rightarrow 0$. These relations represent the full system of Hugoniot conditions formulated for an arbitrary shock. Due to this, we have shown that the coefficients discontinuities may be treated as the classic shocks in the solution structure.

4) The general structure of the solution to the Riemann problem is determined as an alternation of the mobile shocks and rarefaction waves (continuous segments). Two admissible types of shocks are detected : the shock of the saturation (*S*-shock) and the simultaneous shock of saturation and phase composition (*SC*-shock). It was shown that the *SC*-shock is exactly the discontinuity of the coefficients to flow equations.

5) The thermodynamic model describes the behavior of the phase concentrations along the rarefaction waves between shocks. The differential thermodynamic equations have the geometrical image in the form of a *P*-surface in ternary phase diagrams, which is the extension of the concept of a tie-lines. Each cross-section of a *P*-surface at fixed pressure represents a tie-line. So the behavior of the phase composition between two shocks is not constant when pressure varies, but is however limited and follows strictly a fixed *P*-surface.

6) One of the fundamental assumptions of the classical analytical theory of the Riemann problem developed within the framework of the ideal mixing propounds that the number of *SC*-shocks in the two-phase domain is $N - 2$, which also means the existence of $N - 3$ intermediate tie-lines. For the non-ideal mixing, we have shown that this hypothesis ensures the existence of a unique solution. (This demonstration was done in a constructive way).

7) The asymptotic Hugoniot conditions also allow the HT-splitting, which means that in the limit, $N - 3$ Hugoniot equations purely represent the thermodynamic formula which only contain the phase concentrations. So the system of Hugoniot conditions is split onto $N - 3$ thermodynamic relations and 3 "hydrodynamic" ones.

8) The overall system of thermodynamic relations which consists in the equilibrium equations, differential thermodynamic equations along *P*-surfaces, and split "thermodynamic" Hugoniot conditions is closed with respect to all the backward and forward concen-

trations at all the SC -shocks presented in the structure of the solution. This system of thermodynamic equations called "*the analytical concentration front tracker*" permits to determine all the phase concentrations at the shocks before solving the hydrodynamic problem.

9) Two "hydrodynamic" Hugoniot equations are able to determine analytically the backward and forward saturations at any SC -shock. This system is called "*the analytical saturation front tracker*". The system of two analytical front trackers enables us to determine all the parameters of shocks before solving the hydrodynamic problem.

10) The saturation front tracker include however an additional approximation. To obtain the explicit system of two equations with respect to two saturations we assumed the simplifying hypothesis that says the total flow velocity is continuous through a SC -shock. This assumption is based on the physical reasons which say that the total velocity is a very conservative function being responsible for the conservation of the total mass.

This assumption was strictly proved only for two cases : (i) for S -shocks it is valid in all the situations ; (ii) for SC shocks in the case of ideal mixing. Such an assumption is however much weaker than the previous assumption of constant total velocity, used in the ideal-mixing model.

11) The numerical solution for the hydrodynamic problem was constructed. The numerical method may be very flexible and not constrained, because all the shocks are a priori determined. This means that the solution of the differential hydrodynamic equations has the objective to construct only the continuous fragments between the shocks. In particular, we have demonstrated the examples, using the method of characteristics, and finite difference method.

12) The solution obtained within the scope of the asymptotic model was compared with the numerical solution of the same problem but formulated within the framework of the classic full compositional model. The consistence of the results obtained is satisfactory.

13) The solution obtained was also compared with the analytical exact solution of the full compositional model obtained in a particular case. Indeed, if the densities of phases are identical, and the pressure in the thermodynamic relations is assumed to be constant,

the number of components is three, then the full compositional model can be formally reduced to the same system of two hyperbolic equations which is used in the ideal-mixing theory. Such a model has exact analytical solutions. The comparison to this solution was satisfactory. It is shown that the asymptotic solution has the same form as the exact solution. At the same time, a small difference in shock velocities was observed (about 5%). This difference is certainly related to the asymptotic character of the suggested model and can be improved in future developments.

Conclusion for chapter 6 : Flow with phase transition

In chapter 6 we examined the flow with phase transitions, when the domain of flow contains a sub-domain occupied by two-phase fluid and other sub-domains occupied by a single-phase fluid. The single-phase fluid can have a composition which is significantly different from the equilibrium composition, i.e. it can be over- or undersaturated with several components. This determines intensive phase transitions at the contact between the single-phase and two-phase fluid. The detection of these mobile contact surfaces is a very difficult scientific problem which is not solved in general case.

The developed method of front tracking described above is devoted to find only the *SC* shock and *S*-shocks within the two-phase domain, but not the shocks of contact between the oversaturated single-phase zone and two-phase zone.

To solve this new problem we have developed a new method which is based on the principle of equivalence between a single-phase fluid and a two-phase fluid that we have proved in the present thesis.

1) The principle of equivalence represents a formal theorem which says that a single-phase oversaturated fluid can be replaced by an imaginary two-phase fluid which is in equilibrium and possesses some specific properties of phases that ensure the equivalence. These properties called the consistence conditions are obtained in this thesis.

2) One of the properties says that the saturation of one of the imaginary fluids should be negative or higher than 1. We have shown that such a non-physical property does not

contradict the mathematical existence of such a formal two-phase system.

3) This principle enabled us to develop the numerical "method of negative saturations" which consists in using the uniform system of two-phase equations for the overall flow domain. The difference between the zones consists only in the structure of the closure relations for the coefficients of this system. Once the saturation becomes negative or higher than 1, we switch the coefficients. This instant marks the appearance of the front of phase transitions. So the fluid may be simulated progressively by using the uniform standard system of equations which gives the possibility to automatically detect the shocks.

4) The evaluation of the method was performed by comparing it to the analytical solutions corresponding to the particular case of ideal mixing at constant pressure. After this we compared it with numerical solutions in the case of non-ideal mixing, and also with the presence of diffusion within each phase. The results obtained are more than satisfactory.

5) The case of presence of diffusion within each phase has a particular research interest. A principal problem whether the diffusion within each phase can diffuse the interface of phase transition, is non-trivial and is yet unsolved. If Diffusion concerns the phase concentrations only, and not the phase saturation. Due to this the diffusion influence certainly the behavior of *SC*-fronts (they are no longer shocks when diffusion exists) but it does not influence *S*-shocks. At the front of phase transition the saturation is discontinuous, but not the phase composition. However the behavior of the phase composition is non-trivial, as they become meaningless for one of the phases in single-phase zone. Due to this the influence of the diffusion on the phase transition shock is still unclear.

We have revealed by numerical experiments within the framework of the developed method that the diffusion influence the fronts of phase transitions. A shock of phase transition, which is the strong shock of saturation without diffusion) transforms into a weak saturation shock due to the diffusion. So the diffusion within each phase cannot destroy totally the shock of phase transition, but changes its type.

6) We have shown that the method of negative saturations is very sensitive with respect to weak shocks.

7) The developed method of negative saturations was introduced in the formalism of

the asymptotic compositional model, which give us the possibility to cover all the spectrum of the two-phase displacement problems by our theory. Within this formalism, the shocks of phase transition are presented as the *SC*-shocks satisfying an additional condition : the backward or the forward saturation is necessarily equal to 1 or 0.

Conclusion for chapter 7 : Three-phase flow

In the last chapter we have extended the developed asymptotic approach to three-phase case (gas-oil-water), taking into consideration that the mobilities of two liquids are very different than that of gas. The asymptotic transition thus corresponds to the limit behavior of $\omega_o, \omega_w \rightarrow 0$ where ω_o is the oil-gas mobility ratio and ω_w is the water-gas mobility ratio.

1) We have obtained the three-phase asymptotic model.

2) This model was shown to allow HT-splitting along streamlines. The HT-split model is obtained. Despite of the formally similar procedures of the model derivation, the resulting model is non-trivial and cannot be obtained as a trivial extension of the two-phase asymptotic model on three-phase case.

The hydrodynamic part is presented by three equations with respect to pressure and two saturations. The coefficients of this system depend on pressure and are calculated through the independent thermodynamic system.

3) The thermodynamic system presents the system of equilibrium equations which describe the variation of phase composition in statics, and new differential subsystem (differentiation with respect to pressure) which describes the exchange rate between the phases. More strictly, this equations means that the rate of mass exchange in the phase, as a whole, is identical to the rate of mass exchange in any individual components.

4) Obtained differential thermodynamic model is qualitatively different from that developed for two-phase flow.

5) One dimensional asymptotic model in cartesian frame was obtained and subjected to a qualitative analysis.

6) As previously, the asymptotic model is characterized by the shocks generated by

the Riemann conditions, or the shocks entering in the coefficients of the differential flow equations.

7) The class of admissible shocks is much larger than in two-phase case. In particular, nothing prohibits the appearance of partial *SC*-shocks which correspond to the shock of all the phase concentrations but only one saturation. The full *SC* shocks are also possible.

8) For partial *SC*-shocks, we suggested a method allowing to determine the number of *SC*-shock should arise in the structure of the solution. We used the inverse logic that used in proving the existence of the concentration tracker. Now let us assume that the concentration front tracker exists, expecting that the number of all the phase concentrations at all the partial *SC*-shocks is equivalent to the number of the thermodynamic relations applied to all the elements of the solution. We have then shown that the number of shocks is $N - 3$. This is consistent to some rare numerical data obtained by other authors.

9) Several three-phase displacement problems are solved : injection of water in oil/gas reservoir ; injection of CO_2 into an oil reservoir. Various versions were examined : a mobile or immobile water, etc.

The future development of this theory will concern :

- (i) attempt to extend the method of negative saturations to three-phase case ;
- (ii) to develop the concentration tracker for all types of shocks ;
- (iii) to develop the saturation front tracker ;
- (iv) to improve the calculation of the shock velocity by adding the first term in asymptotic expansions.

Annexe A

Hugoniot conditions for inhomogeneous differential equations

At the location of the discontinuity, the partial differential equation is no longer valid, and the conservation law must be formulated in the light of the fact that the discontinuity moves with such a speed that there is no accumulation of material at the discontinuity, which will give us the Hugoniot condition.

In order to find the Hugoniot condition for inhomogeneous partial differential equations we start with the general form of the equation in which the right-hand side is non zero and depends on the principal variable :

$$\frac{\partial s}{\partial t} + \frac{\partial f(s)}{\partial x} = g(s) \quad (\text{A.1})$$

The initial condition is :

$$s(x, 0) = \Gamma(x) \quad (\text{A.2})$$

We will introduce the class of smooth test functions $w(x, t)$ that possess continuous first partial derivatives and vanish as $t + |x|$ becomes sufficiently large, i.e. has a *compact support*). Then according to [Lax 1954], $s(x, t)$ is called a weak solution of equation (A.1), with the initial value $\Gamma(x)$, if s , $f(s)$ and $g(s)$ are integrable over every bounded set of

the half-plan $t \geq 0$, and for all such test function $w(s, t)$ the following integral relation is satisfied :

$$\int_0^\infty dt \int_{-\infty}^\infty \left(\frac{\partial w}{\partial t} s + \frac{\partial w}{\partial x} f(s) + wg(s) \right) dx + \int_{-\infty}^\infty w(x, 0)\Gamma(x)dx = 0 \quad (\text{A.3})$$

To see that this ties back into our understanding of the solution of the partial differential equations, we will show, first, that wherever a weak solution is smooth, it satisfies the differential equation (A.1) and, second we will find the relation in the vicinity of the discontinuity of the weak solution (Hugoniot condition).

If $s(x, t)$ has continuous first derivative in any region of the (x, t) -plan and satisfies the partial differential equation (A.1), then we may integrate (A.3) by parts :

$$\begin{aligned} & \left[\int_{-\infty}^\infty w s dx \right]_{t=0}^{t=\infty} - \int_0^\infty dt \int_{-\infty}^\infty dx w \frac{\partial s}{\partial t} + \left[\int_0^\infty w f(s) dt \right]_{x=-\infty}^{x=\infty} - \int_0^\infty dt \int_{-\infty}^\infty dx w \frac{\partial}{\partial x} f(s) \\ & + \int_0^\infty dt \int_{-\infty}^\infty dx wg(s) + \int_{-\infty}^\infty w(x, 0)\Gamma(x)dx = 0 \end{aligned} \quad (\text{A.4})$$

In this equation the integrated parts for $t = \infty$ and $x = \pm\infty$ vanish due to the vanishing of w . The terms at $t = 0$ cancels due to the boundary condition (the last term). Thus we have :

$$\int_0^\infty dt \int_{-\infty}^\infty dx w \left[\frac{\partial s}{\partial t} + \frac{\partial}{\partial x} f(s) - g(s) \right] = 0 \quad (\text{A.5})$$

Since this is true for any smooth function $w(x, t)$, the factor inside the bracket of the integrand must be vanish, so $s(x, t)$ satisfies equation (A.1). If the solution $s(x, t)$ is continuous and piecewise smooth, it satisfies the differential equation in each subregion where it is smooth. However, when $s(x, t)$ is discontinuous, then we must be able to find the appropriate condition.

Without loss of generality we can suppose that there is a single curve of discontinuity, S , that crosses the half-plan $t \geq 0$. If there is more than one curve, we have to repeat the argument ; if it does not cross the whole region, we have only to put the jumps in s , f and

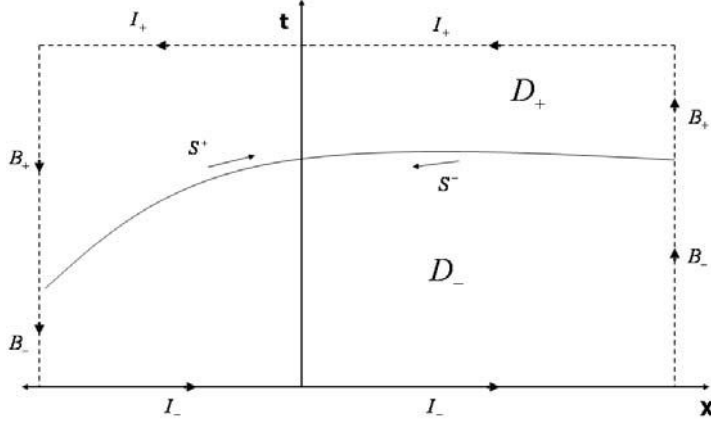


FIG. A.1 – Discontinuity curve S crossing the half-plane $t \geq 0$

g equal to zero. Let S_+ and S_- denote the upper and lower sides of S ; D_+ and D_- are the domains above and below S ; let $(B_+ + I_+ + S_+)$ be the boundaries of D_+ and D_- , as shown in figure (A.1). From the Green's theorem, the double integral :

$$\int \int \left[\frac{\partial}{\partial t}(ws) + \frac{\partial}{\partial x}(wf(s)) \right] dxdt = \oint w(sdx - f(s)dt) \quad (\text{A.6})$$

where the single integral is taken around the boundary of the region.

Applying this to the domain $D_+ + D_-$ we will have :

$$\begin{aligned} & \int \int_{D_+ + D_-} w \left[\frac{\partial s}{\partial t} + \frac{\partial f(s)}{\partial x} - g(s) \right] dxdt + \int \int_{D_+ + D_-} \left[\frac{\partial w}{\partial t} s + \frac{\partial w}{\partial x} f(s) + wg(s) \right] dxdt \\ &= \int_{S_+ + S_-} w(s\sigma - f(s))dt + \int_{I_+ + I_-} w(sdx - f(s)dt) + \int_{B_+ + B_-} w(sdx - f(s)dt) \end{aligned} \quad (\text{A.7})$$

in which we put $\sigma = dx/dt$ along the curve of discontinuity, S .

Now let us make the domain $D_+ + D_-$ large enough, in order to occupy the whole of the half-plane $t \geq 0$. In the integral shown above, the term $\int \int_{D_+ + D_-} wg(s)dxdt$ has been subtracted and added again. On the left-hand side, the first integral vanishes because equation (A.1) holds in each of D_+ and D_- . Since $s(x, t)$ is a weak solution, it satisfies

equation (A.3) and so the second integral in the left is equal to :

$$- \int_{-\infty}^{\infty} w(x, 0) \Gamma(x) dx \quad (\text{A.8})$$

The integral over $I_+ + I_-$ is also equal to :

$$- \int_{-\infty}^{\infty} w(x, 0) \Gamma(x) dx \quad (\text{A.9})$$

because $dt = 0$ over on this path, which is traversed in the negative direction, and $s(x, 0) = \Gamma(x)$.

The integral over $B_+ + B_-$ also vanishes by the vanishing of w , and we obtain :

$$\int_{S_+} w(s\sigma - f(s)) dt + \int_{S_-} w(s\sigma - f(s)) dt = 0 \quad (\text{A.10})$$

Since S_- is traversed in the opposite direction to S_+ , this gives :

$$\int_S w(\sigma[s] - [f(s)]) dt = 0 \quad (\text{A.11})$$

where $[s] = s^+ - s^-$ and $[f(s)] = f(s^+) - f(s^-)$.

Arguing again from the arbitrariness of w , we can see that :

$$\sigma = \frac{dx}{dt} = \frac{[f(s)]}{[s]} = \frac{f(s^+) - f(s^-)}{s^+ - s^-} \quad (\text{A.12})$$

on any line of discontinuity, which is the jump condition that has to be satisfied by the discontinuity (s^+, s^-) and it is totaly the same as the condition for the homogeneous differential equations. The fact that the source term $g(s)$ does not play any role in equation (A.12) is not surprising, since from the physical point of view no action can take place at a sharp discontinuity.

Annexe B

Entropy condition for inhomogeneous differential equations

To obtain the entropy condition in general context, we will consider the same equation as in the previous appendix :

$$\frac{\partial s}{\partial t} + \frac{\partial f(s)}{\partial x} = g(s) \quad (\text{B.1})$$

where the characteristic velocity is given by :

$$\frac{dx}{dt} = f'(s) \equiv \sigma(s) \quad (\text{B.2})$$

Giving the state at one side of the discontinuity, say s^- , and its propagation speed σ , we may determine the state s^+ on the other side by using the Hugoniot condition. However, we immediately find that an ambiguity still exists regarding the direction of jump in s . So the Hugoniot condition is not sufficient to give a unique state for s^+ , which is required for a physically relevant equation.

More generally, the solution of a quasi-linear equation is defined in the sense of weak solution, and this solution is not uniquely defined until we introduce an additional condition to regulate the direction of jumps across a discontinuity. Such a condition is usually referred as the *entropy condition*. This term was used first by [Courant and Friedrichs, 1948] in

their pioneering work on supersonic flow and shock waves.

In fact, [Oleinik 1959] was the first to formulated the generalized entropy condition, which she called the "Condition E" and thus to establish the uniqueness theorem. In our notation the condition reads :

$$\sigma(s^-, s^+) \geq \sigma(s^-, s) \tag{B.3}$$

for every s between s^- and s^+ .

When we compare the slopes among the two tangents to the equilibrium curve $f(s)$ and the chord connecting two points $-$ and $+$, we find the inequality :

$$f'(s^-) < \frac{[f]}{[s]} < f'(s^+) \tag{B.4}$$

or

$$\sigma(s^-) < \sigma(s^-, s^+) < \sigma(s^+) \tag{B.5}$$

According to [Lax 1957], a discontinuity that satisfies this inequality condition is called a *shock*. For this reason, (B.5) is referred to as the *shock condition*. This implies that all the discontinuities encountered in strictly nonlinear problems are the shocks.

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AUTORISATION DE SOUTENANCE DE THESE
DU DOCTORAT DE L'INSTITUT NATIONAL
POLYTECHNIQUE DE LORRAINE

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VU LES RAPPORTS ETABLIS PAR :

Monsieur Franck PLOURABOUE, Directeur de Recherche, IMFT, Toulouse

Monsieur Stéphane ZALESKI, Professeur, Institut d'Alembert, Paris

Le Président de l'Institut National Polytechnique de Lorraine, autorise :

Monsieur ABADPOUR Anahita

à soutenir devant un jury de l'INSTITUT NATIONAL POLYTECHNIQUE DE LORRAINE,
une thèse intitulée :

**"Analyse asymptotique du problème de Riemann pour les écoulements compositionnels
polyphasiques en milieux poreux et applications aux réservoirs souterrains"**

en vue de l'obtention du titre de :

DOCTEUR DE L'INSTITUT NATIONAL POLYTECHNIQUE DE LORRAINE

Spécialité : « **Mécanique et Energétique** »

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Analyse asymptotique du problème de Riemann pour les écoulements compositionnels polyphasique en milieux poreux et application aux réservoirs souterrains

Dans la première partie de cette thèse nous traitons l'écoulement diphasique compositionnel, partiellement miscible et compressible en milieux poreux. Déplacement d'une phase par un autre est analysé. Nous examinons les mélanges non idéals, la pression est variable, et les concentrations de phase, la densité et la viscosité sont les fonctions de la pression. Le processus est décrit par le problème de Riemann qui admet des solutions discontinues. Nous avons développé une méthode numérique-analytique de solution pour déterminer les paramètres à tous les chocs avant résoudre les équations de flux. Cette méthode est basée sur la séparation de thermodynamique et hydrodynamique, proposée dans [Oladyshkin, Panfilov 2006] et qui était inapplicable à problème de Riemann, en raison de manque des conditions d'Hugoniot. Dans cette thèse, nous avons construit les conditions supplémentaires d'Hugoniot. Dans la deuxième partie, nous examinons l'écoulement diphasique lors que les zones monophasique apparaissent, dans cette zone, le fluide est sur/sous-saturés et les équations diphasique dégénèrent. Nous avons proposé de décrire les zones diphasique et sur/sous-saturés avec un système uniforme des équations diphasique classique en étendant le concept de saturation d'être négatif et supérieur à un. Physiquement, cela signifie que les états monophasiques sont considérés comme des états diphasiques consistant une phase imaginaire avec la saturation négative. Une telle extension de la saturation exige développement des conditions de consistance qui sont fait dans cette thèse. La dernière partie est consacrée ensuite à étendre le modèle HT-split pour le cas d'écoulement triphasique compositionnel. Nous avons obtenu le modèle asymptotique, dans lequel la thermodynamique et l'hydrodynamique sont séparées.

Mots clés: Milieux poreux, Ecoulement polyphasique compositionnel, Problème de Riemann, Transition de phase, Dissolution, Récupération assistée de pétrole.

Asymptotic analysis of Riemann problem for multiphase compositional flow in porous media with application to subterranean reservoirs

In the first part of thesis we deal with two-phase multicomponent, partially miscible, compressible flow in porous media. Displacement of one phase by another is analyzed. We examine non ideal solutions, pressure is variable, and phase compositions, densities and viscosities are variable functions of pressure. The process is described by Riemann problem which admits discontinuous solutions. We developed a numerical-analytical method of solution to explicitly determine all shock parameters before solving the flow equations. This method is based on splitting thermodynamics and hydrodynamics, suggested in [Oladyshkin, Panfilov 2006]. Earlier this method was inapplicable to Riemann problem, due to the lack of Hugoniot conditions. In this thesis we have constructed additional Hugoniot conditions. In the second part we examine two-phase flow when the single-phase zones appear, in this zone the fluid is over/under-saturated and two-phase flow equations degenerate and they cannot be used. We proposed to describe two-phase and over/under-saturated single-phase zones by uniform system of classic two-phase equations while extending the concept of phase saturation to be negative and higher than one. Physically it means that the oversaturated single-phase states are considered as pseudo two-phase states consisting an imaginary phase with negative saturation. Such an extension of saturation requires developing some consistency conditions which have developed in this thesis. The last part then is devoted to extend the HT-split model to the case of three-phase compositional flow. We have obtained the general asymptotic model, in which the thermodynamics and hydrodynamics are split.

Key words: Porous media, Multiphase compositional flow; Riemann problem, Phase transition, Dissolution, Enhanced oil recovery.