



HAL
open science

Innovative process for the dimethyl ether direct synthesis from captured CO₂ and renewable Hydrogen in multifunctional reactors

Chakib R Behloul, Jean-Marc Commenge, Christophe Castel

► To cite this version:

Chakib R Behloul, Jean-Marc Commenge, Christophe Castel. Innovative process for the dimethyl ether direct synthesis from captured CO₂ and renewable Hydrogen in multifunctional reactors. 16th Greenhouse Gas Control Technologies Conference, Oct 2022, Lyon, France. . hal-04661131

HAL Id: hal-04661131

<https://hal.univ-lorraine.fr/hal-04661131>

Submitted on 24 Jul 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



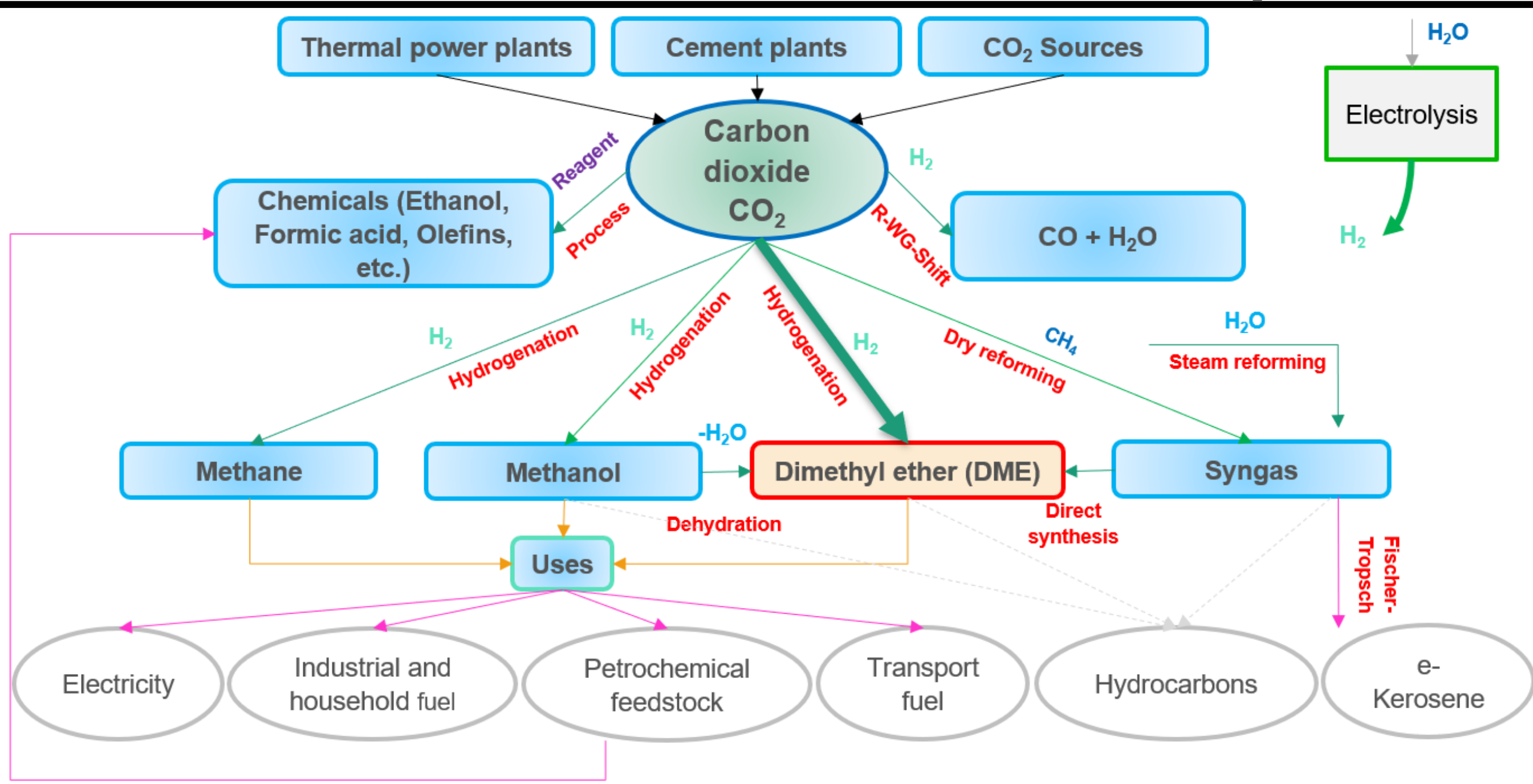
LYON, FRANCE

Innovative process for the dimethyl ether direct synthesis from captured CO₂ and renewable Hydrogen in multifunctional reactors

Chakib R. Behloul*, Jean-Marc Commenge, Christophe Castel

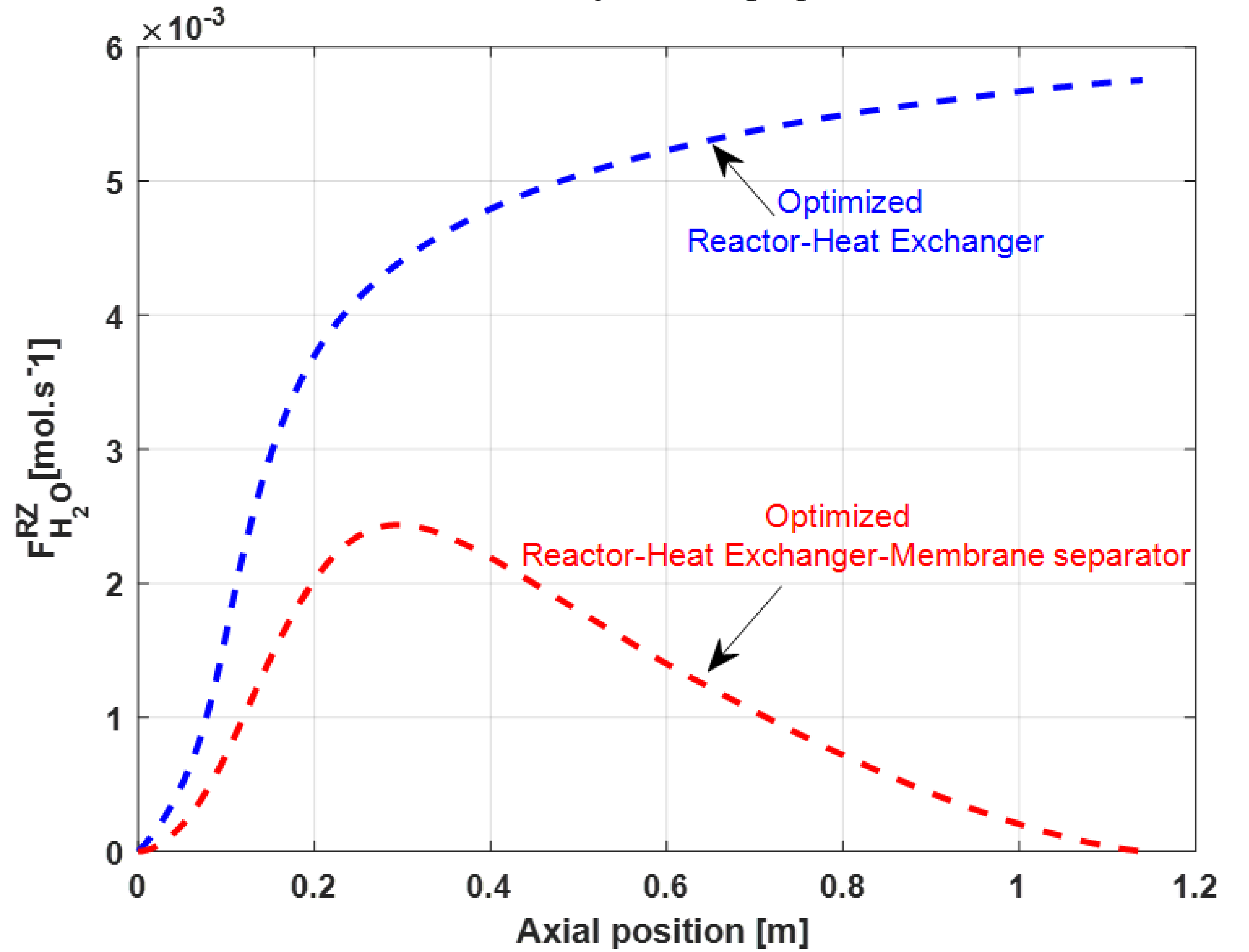
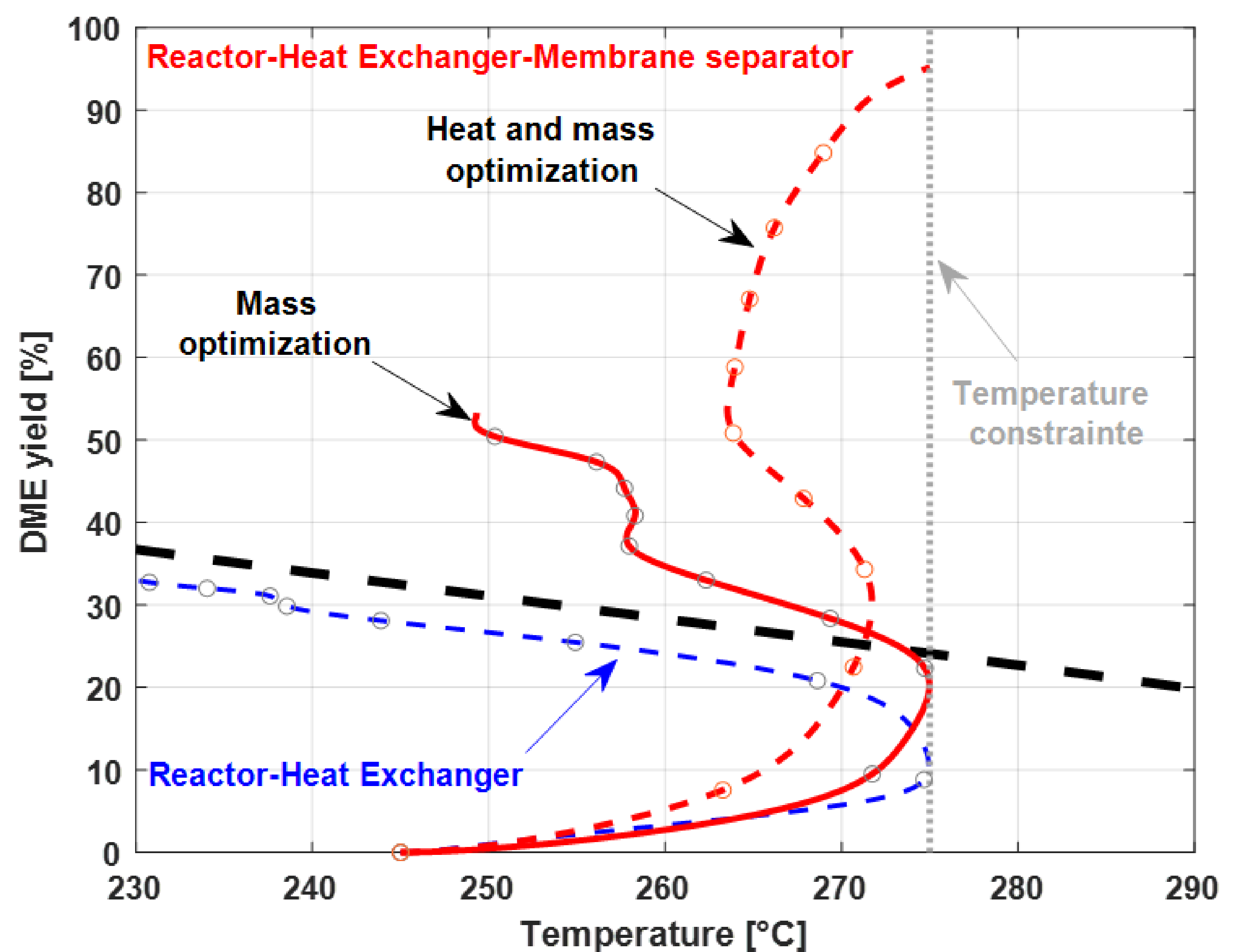
Laboratoire Réactions et Génie des Procédés, Université de Lorraine, CNRS, 1 rue Grandville, F-54000 Nancy, France

Introduction



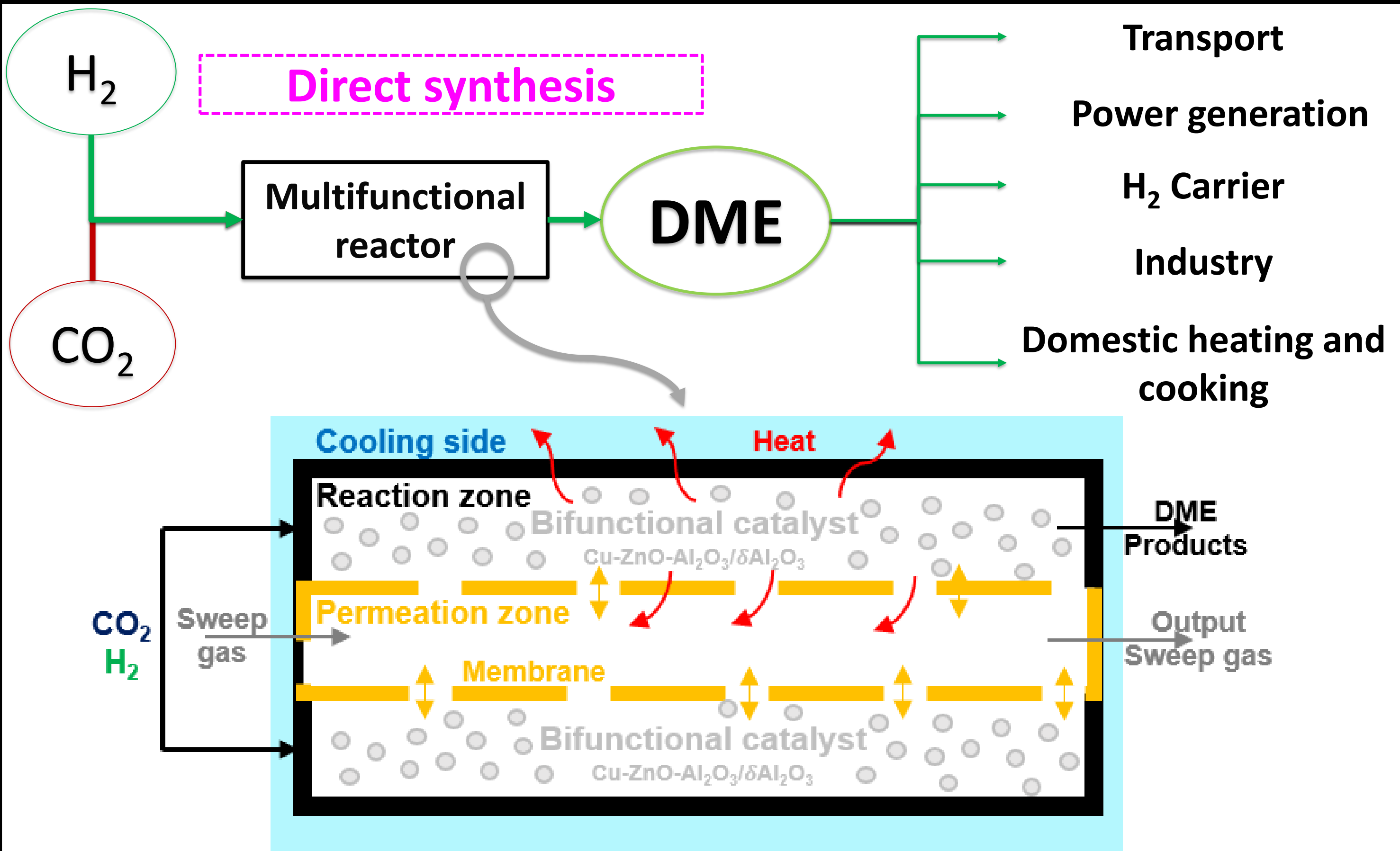
- ❖ Carbon capture and storage technologies must be supported by its conversion into high value-added products to meet environmental and economic requirements
- ❖ Excess electricity production → H₂ production from intermittent carbon-free sources (renewable energies / water electrolysis)
- ❖ The Power-to-X concept enables the synthesis of useful products through the CO₂ hydrogenation reaction
- ❖ Synthesis of e-fuels (dimethyl ether (DME), methane (SNG), methanol, e-Kerosene and olefins from DME, etc.) is a promising way to decarbonize the economy

Results and Discussions



- FRZ_{H_2O} : water molar flow rate in the reaction zone
- ❖ The appropriate optimization of the multifunctional reactor enables to overcome the limitations and improve the reactor performances
 - ❖ Up to **98% of CO₂ conversion** and **95% of DME yield per pass** are achievable
 - ❖ Possibility to **remove a distillation column** (water/methanol) : dry mixture at the reactor outlet

Objectives / Modeling



- ❖ The reactor consists of coaxial tubes
- ❖ How does this **tri-functional** coupling improve the process performances?

Optimization problem

$$\begin{aligned} & \text{Min}_u J(u) \\ & \dot{x} = f(x, u) \\ & \text{s.t.} \\ & g_p(u) \leq 0 \quad p = 1 \dots P \\ & h_q(u) = 0 \quad q = 1 \dots Q \\ & u_k^{lw} \leq u_k \leq u_k^{up} \quad k = 1 \dots K \end{aligned}$$

J: vector of objective functions
f: dynamic model
u: vector of decision variables
g: vector of inequality constraints
h: vector of equality constraints

$$\text{Min}_{(J_{Heat}(S_w)\{1 \leq w \leq 10\}, J_{Mass}(S_w)\{1 \leq w \leq 10\})} \left\{ OF = -Y_{DME} + P_p \sum_{i'} G_{i'}^2 \right\}$$

J_{Heat} : heat flux ; J_{Mass} : mass flux ; Y_{DME} : DME yield



Conclusions

- The **High synergy** between elementary functions should be optimally exploited
- **Comparison between optimized multifunctional device and optimized innovative architectures is carried out : the different designs offer high performances**
- The analysis of the synergy between the elementary functions of mass and energy transfer allows the design of more compact equipment adapted to delocalized production

References

Behloul, C. R.; Commenge, J.-M.; Castel, C., Chem. Eng. Process. Process Intensification 167 (2021) 108513
 Behloul, C. R.; Commenge, J.-M.; Castel, C., Chem. Eng. Sci. 260 (2022) 117850
 Behloul, C. R.; Commenge, J.-M.; Castel, C., Ind. Eng. Chem. Res. (2022)