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WP 4.3.2

2D DME REACTOR MODELLING

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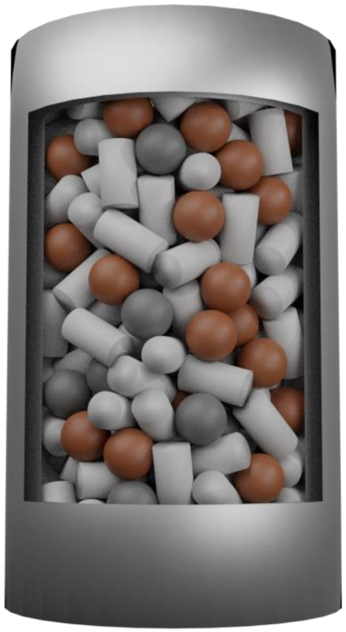
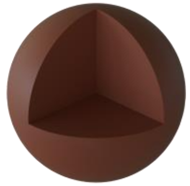
POLITECNICO MILANO 1863

Laboratory of Catalysis and Catalytic Processes LCCP

Introduction



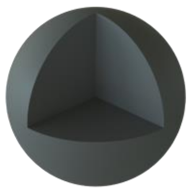


Cu/ZnO/Al$_2$O$_3$

$$CO + 2\ H_2 \leftrightarrow CH_3OH$$

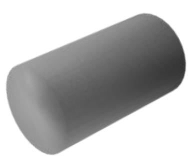
$$CO_2 + H_2 \leftrightarrow CO + H_2O$$

$$CO_2 + 3\ H_2 \leftrightarrow CH_3OH + H_2O$$



γ-Al$_2$O$_3$

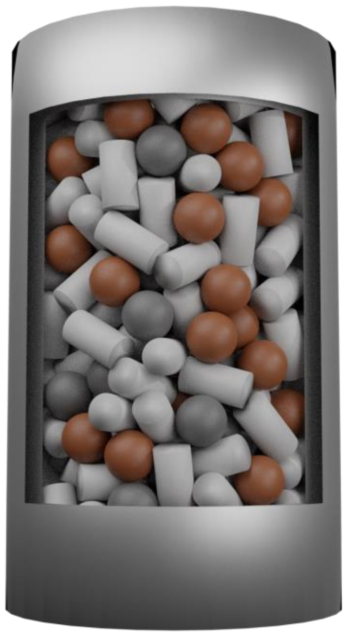
$$2\ CH_3OH \leftrightarrow CH_3OCH_3 + H_2O$$

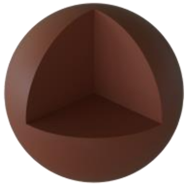


Zeolite 3A

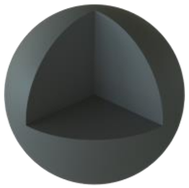
$$H_2O \rightarrow H_2O_{ads}$$

Introduction





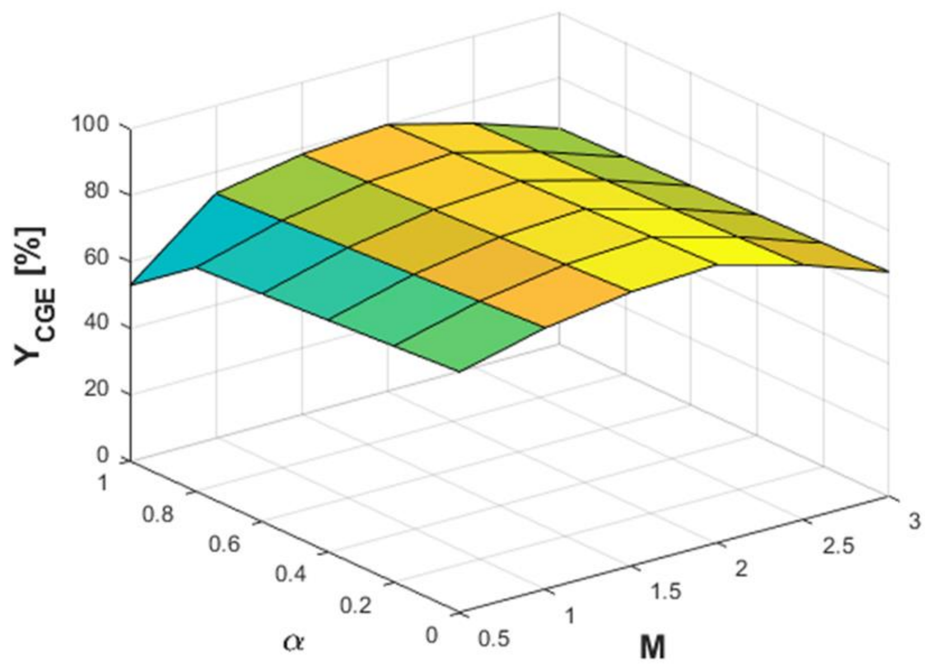
$Cu/ZnO/Al_2O_3$



γ-Al_2O_3

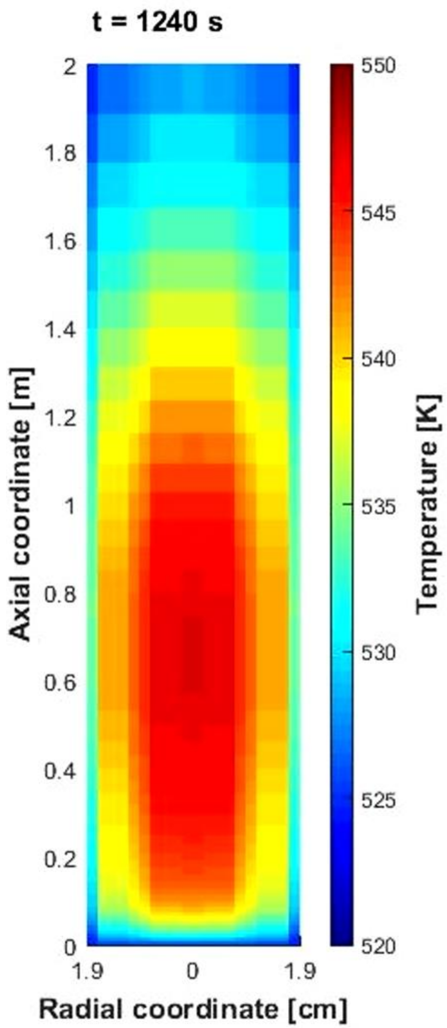
Zeolite 3A

$$Y_{CGE} = \frac{LHV_{DME_{out}}}{LHV_{syngas_{in}}}$$

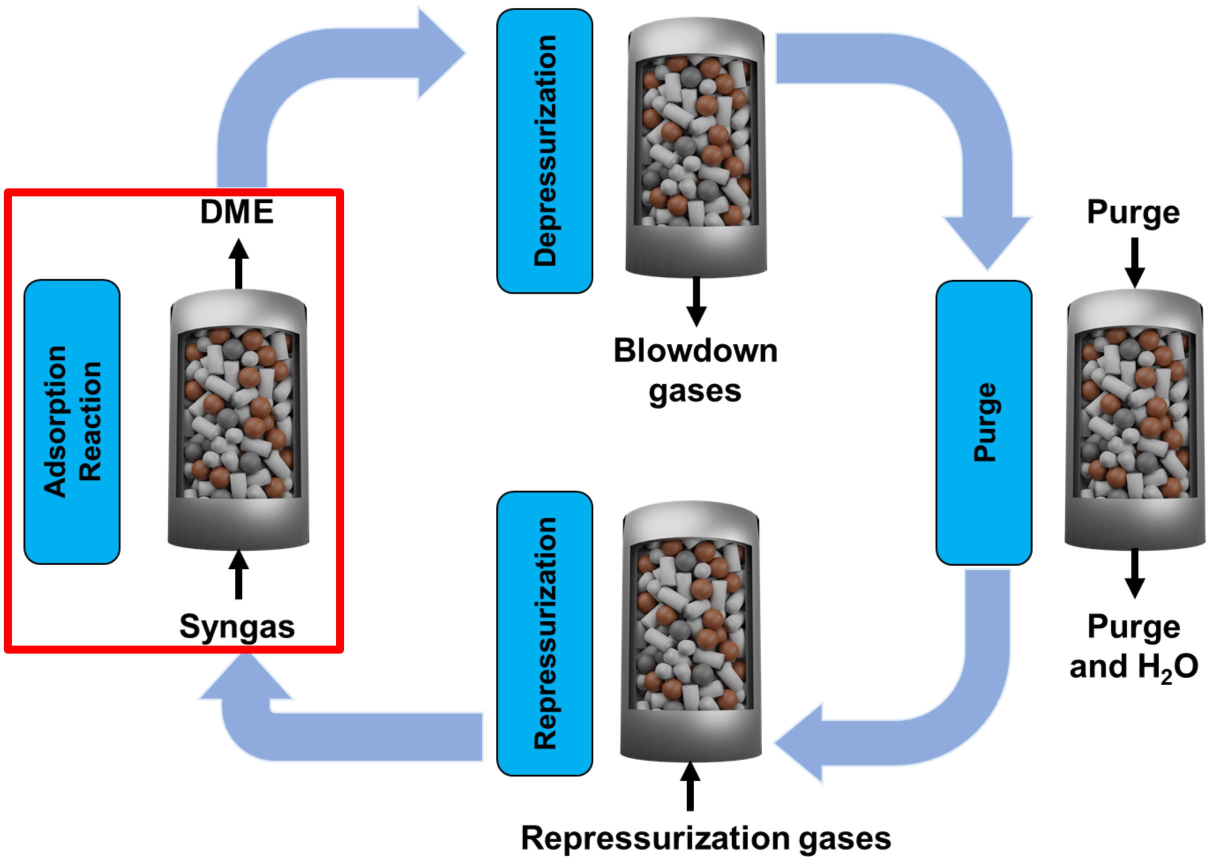


$$\alpha = \frac{CO}{CO + CO_2} \qquad M = \frac{H_2 - CO_2}{CO + CO_2}$$

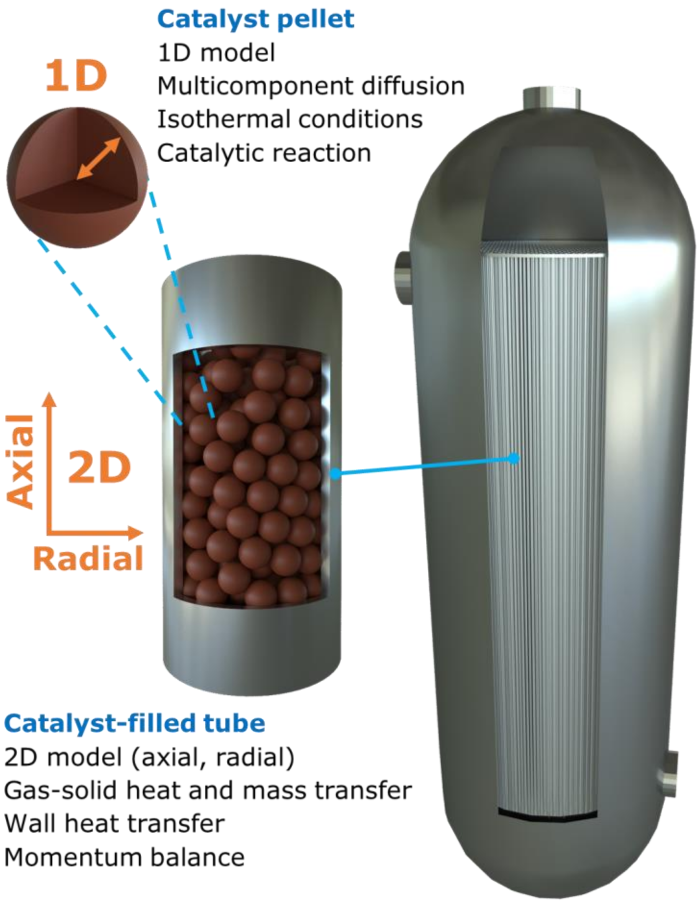
Introduction



Pressure Swing Adsorption (PSA) cycle

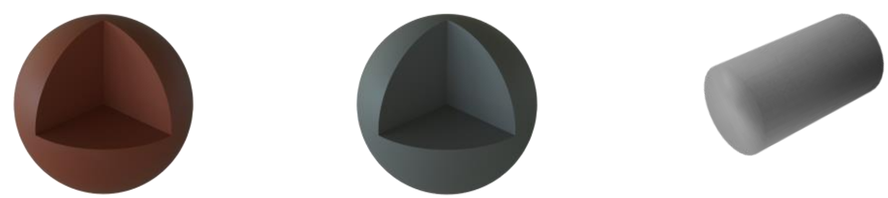


Reactor model



SEDMES reactor:

- Multitubular fixed bed reactor externally cooled
- Dynamic conditions
- 2D single tube heterogeneous model
- 1D catalyst pellet model
- Linear Driving Force for adsorbent pellet



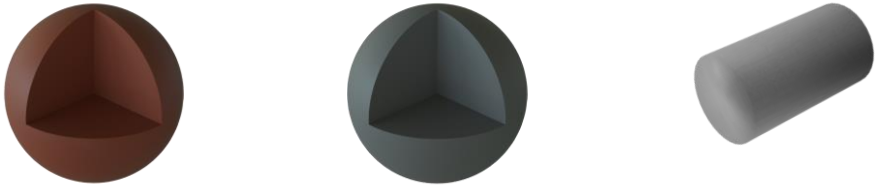
$Cu/ZnO/Al_2O_3$ | γ-Al_2O_3 | Zeolite 3A

Model validation: experimental set up

Input parameters

T_{inlet}	525 K
T_{cool}	525 K
P_{inlet}	25 bar
GHSV	100 h^{-1}
Ads:Cat.	4 : 1 w/w
CZA:γ-Al_2O_3	1 : 1 w/w
L_t	2 m
D_t	38.0 mm

innovation for life



$Cu/ZnO/Al_2O_3$ | γ-Al_2O_3 | Zeolite 3A

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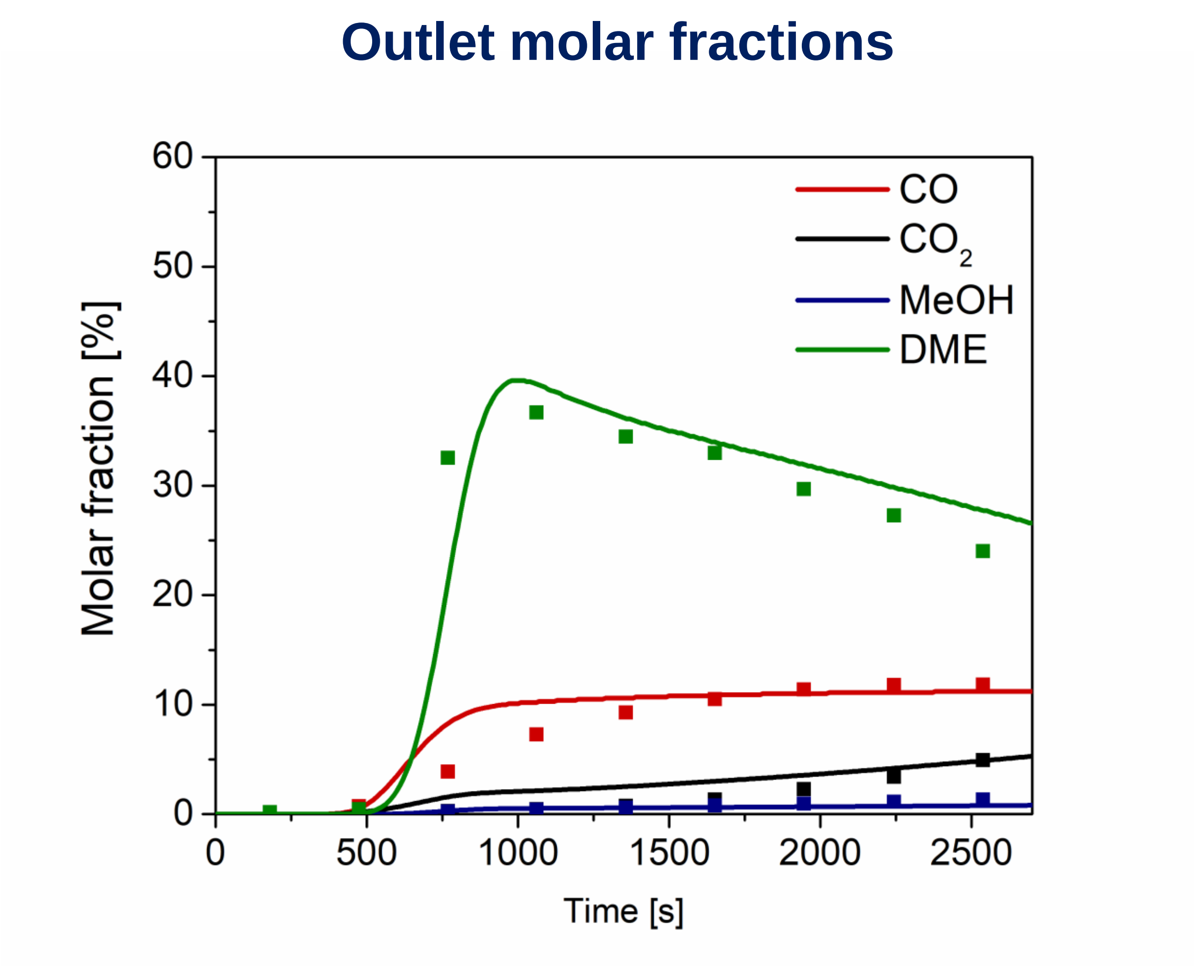
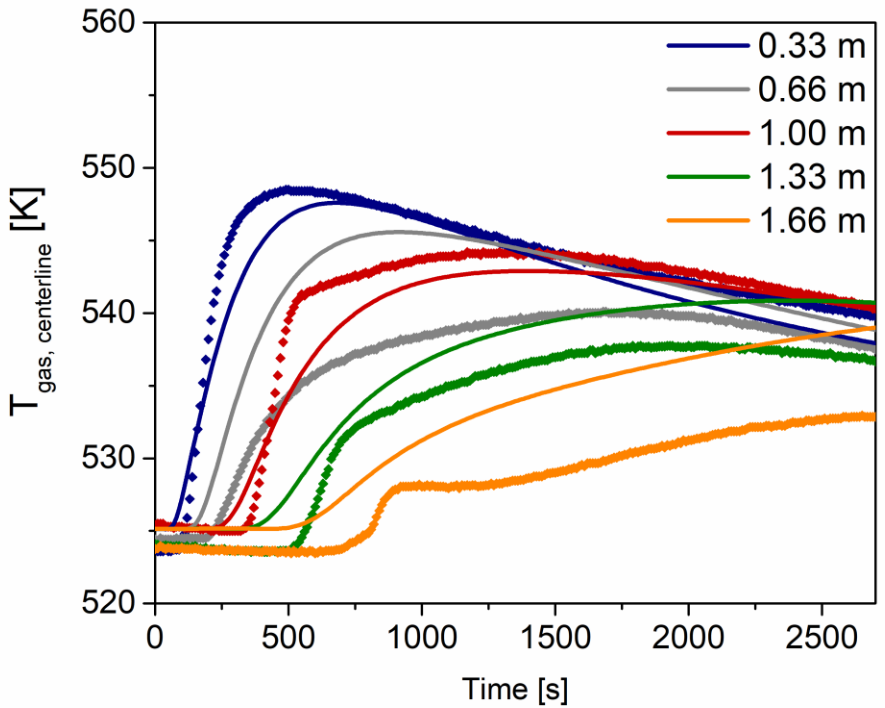
Model validation: outlet composition experimental vs. model

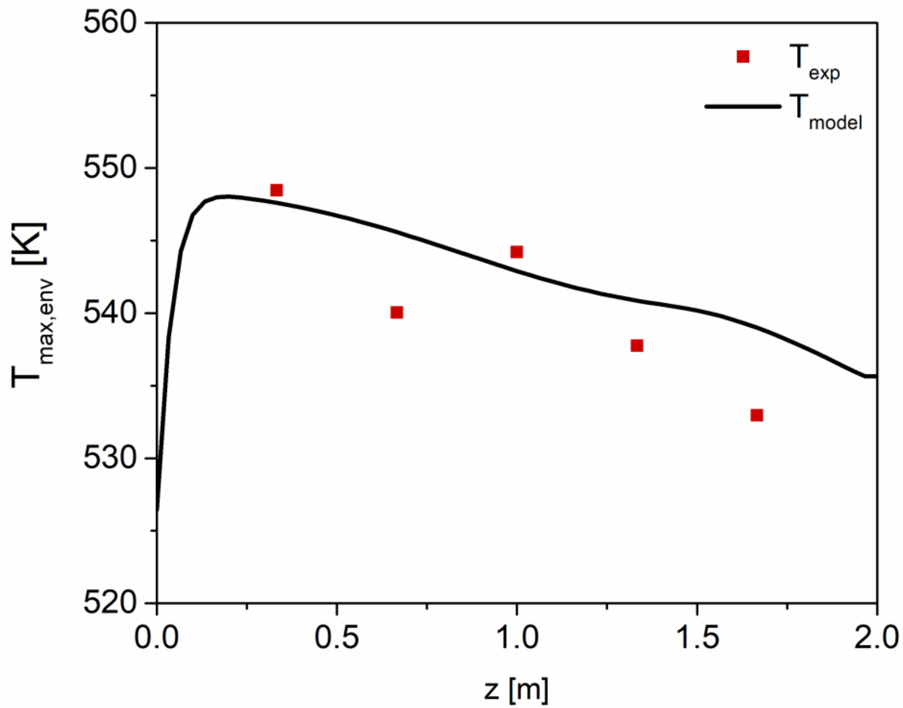


Model validation: temperature experimental vs. model

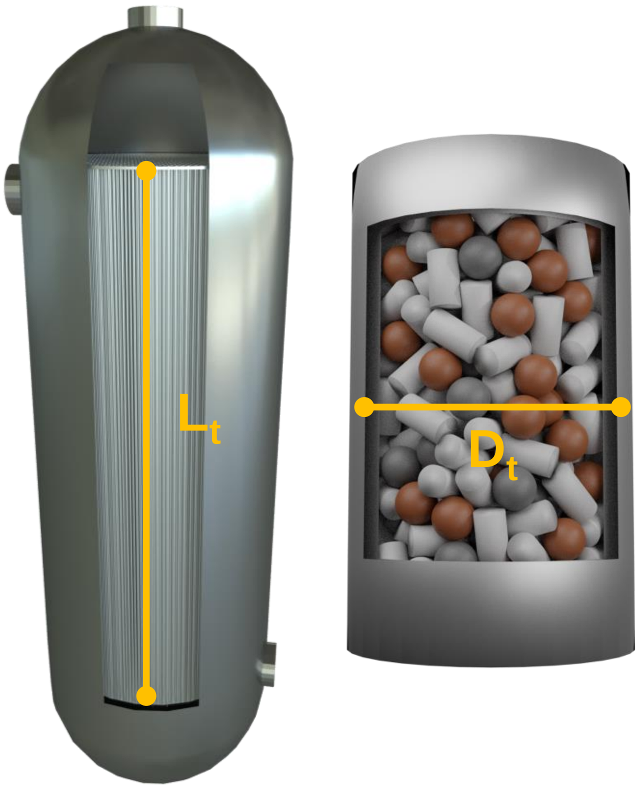
Temperature profiles



Envelope of maximum T

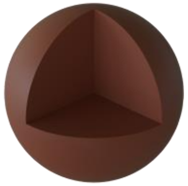


SEDMES reactor analysis and design

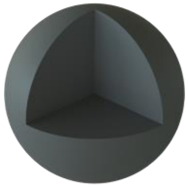


$$\alpha = \frac{CO}{CO + CO_2}$$

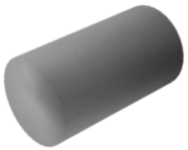
$$M = \frac{H_2 - CO_2}{CO + CO_2}$$



$Cu/ZnO/Al_2O_3$



γ-Al_2O_3



Zeolite 3A

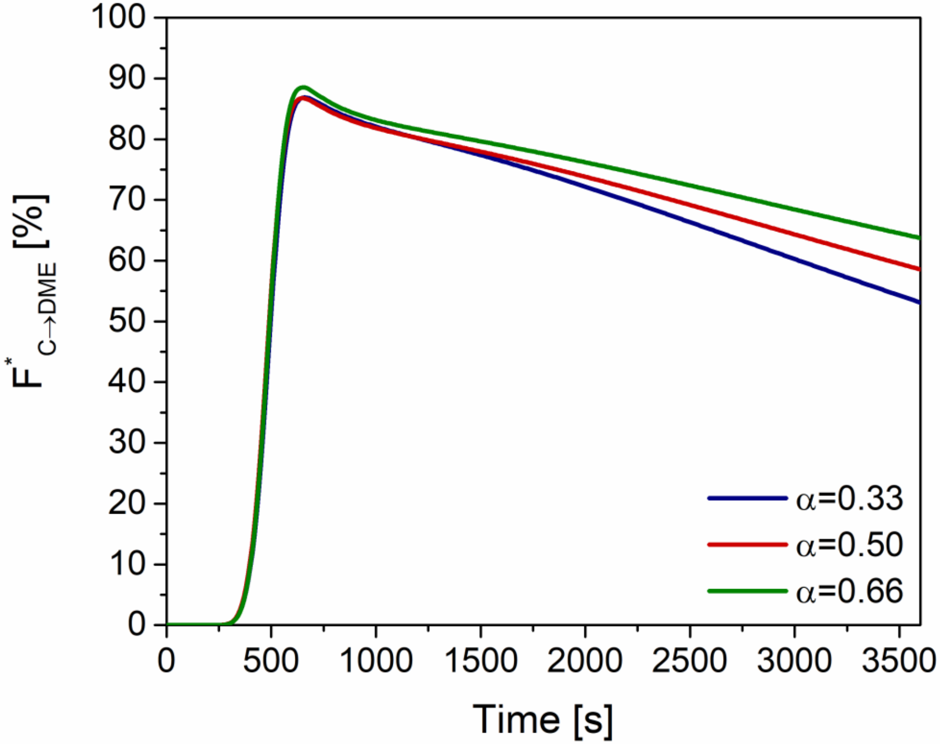
Input parameters

T_{inlet}	523 K
T_{cool}	523 K
P_{inlet}	25 bar
GHSV	140 h^{-1}
Ads:Cat.	4 : 1 w/w
CZA:γ-Al_2O_3	1 : 1 w/w
L_t	6 m
M	2

Analyzed parameters

α	0.33-0.66
D_t	25.6-46.6 mm

SEDMES reactor: effect of α=CO/CO_x on DME yield



$$F^*_{C\rightarrow DME} = \frac{2F_{DME_{out}}}{F_{CO_{in}} + F_{CO_{2_{in}}}}$$

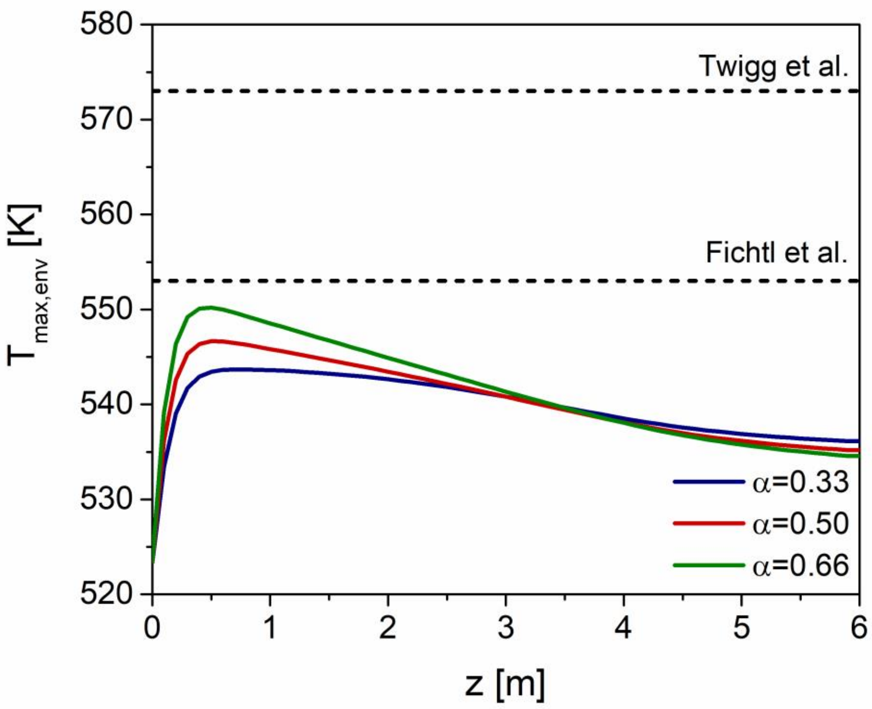
DME yield

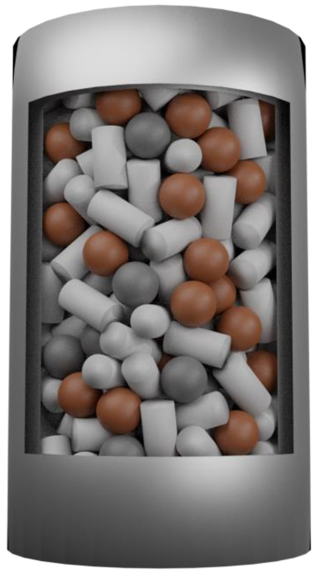
$$Y_{DME} = \frac{2\left(\int_0^{t_{end}} F_{DME_{out}} dt + \int_0^{V_t} C_{gas,DME}(t_{end}) dV_t\right)}{\int_0^{t_{end}}\left(F_{CO_{in}} + F_{CO_{2_{in}}}\right) dt}$$

	α=0.33	*α=0.50*	*α=0.66*
SEDMES	64.9%	67.6%	70.7%
Equilbrium	27.5%	35.4%	43.9%

J. van Kampen et al., J. CO_2 Util. 37 (2020) 295–308.

SEDMES reactor: effect of $\alpha=CO/CO_x$ on thermal stresses





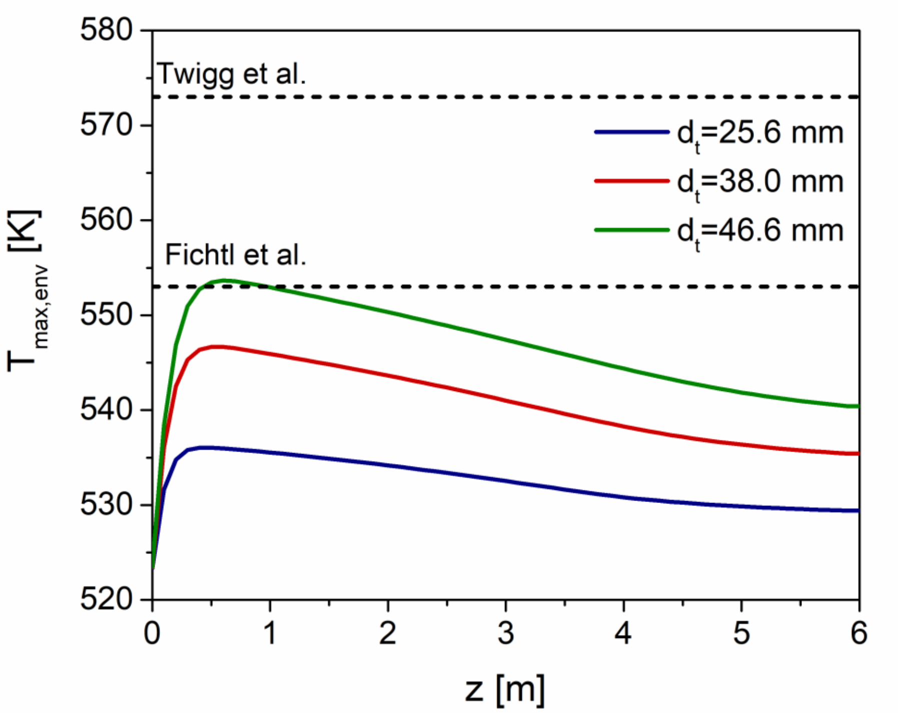
Ads./Cat. = 4/1 w/w

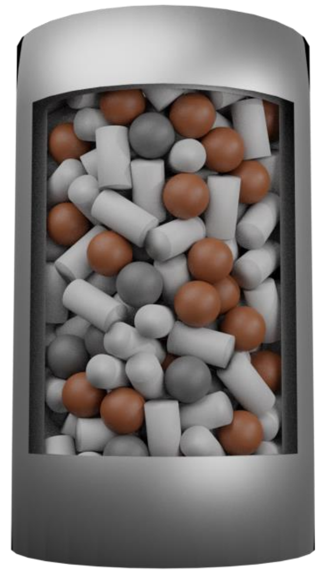
M. V. Twigg et al., Appl. Catal. A Gen. 212 (2001) 161–174.
M.B. Fichtl et al, Appl. Catal. A Gen. 502 (2015) 262–270.

$$2\,CO + 4\,H_2 \leftrightarrow CH_3OCH_3 + H_2O \downarrow_{ads} \qquad \Delta H_r^0 = -250.0\ \mathrm{kJ/mol}_{DME}$$

$$2\,CO_2 + 6\,H_2 \leftrightarrow CH_3OCH_3 + 3\,H_2O \downarrow_{ads} \qquad \Delta H_r^0 = -259.7\ \mathrm{kJ/mol}_{DME}$$

SEDMES reactor: effect of the tube diameter on thermal stresses





Ads./Cat. = 4/1 w/w

S. Guffanti et al., NGCS12, (2019), San Antonio (Texas – USA). → **25.6 mm**

$$2\ CO + 4\ H_2 \leftrightarrow CH_3OCH_3 + H_2O \downarrow_{ads} \qquad \Delta H_r^0 = -250.0\ \mathrm{kJ/mol}_{DME}$$

$$2\ CO_2 + 6\ H_2 \leftrightarrow CH_3OCH_3 + 3\ H_2O \downarrow_{ads} \qquad \Delta H_r^0 = -259.7\ \mathrm{kJ/mol}_{DME}$$

Conclusions

- A SEDMES 2D reactor model validated against bench scale experimental data has been developed.

- Model results confirm that with SEDMES, high DME yields, are obtained independently of syngas CO/CO_x ratio, which is particularly advantageous at high CO_2 content.

- The thermal dilution of catalyst in adsorbent material (1/4 w/w) allows to operate with larger tube diameters with respect to the conventional synthesis.

Thank you for your attention!

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