

## Sorption enhanced dimethyl ether synthesis: process analysis and reactor modelling

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### Highlights

- The direct DME synthesis from syngas obtained via biomass-gasification is investigated.
- Sorption enhancement allows to reach 90% DME yield removing water from the system.
- Main converter parameters have been tuned to optimize yield and control the hot-spot.

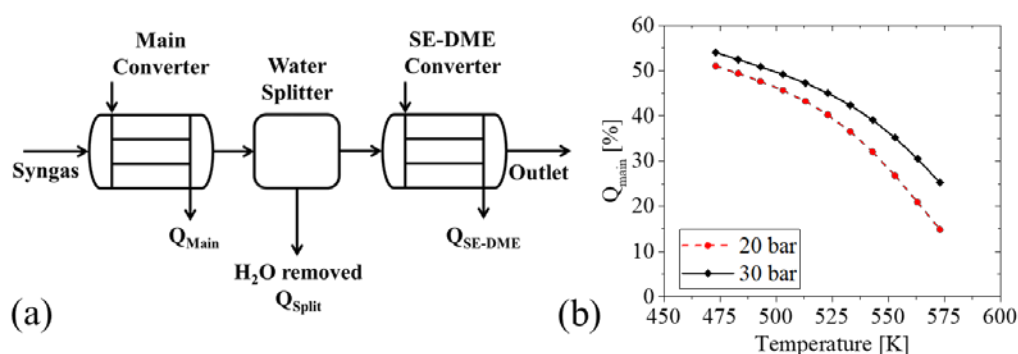
### 1. Introduction

The direct dimethyl ether (DME) synthesis from syngas is a process limited by thermodynamic equilibrium. Conversion limit can be overcome by removing produced water from the reacting system. In the sorption enhanced DME (SE-DME) process, in-situ water removal is achieved through a steam adsorbent added to the DME synthesis reactor. In this way, the single-pass DME yield is increased, also simplifying the downstream purification and eventually eliminating the recycle typically used in conventional processes. The DME synthesis is characterized by exothermic reactions: as consequence, heat management plays a key role in controlling the thermodynamics and the kinetics of the process. For this reason a proper reactor design is required in order to guarantee the desired selectivity and yield and to prevent catalyst deactivation.

### 2. Methods

A thermodynamic analysis of the process is performed by considering a DME synthesis train consisting of a conventional DME synthesis reactor (main converter, isothermal), a water splitter able to remove 90% of H<sub>2</sub>O produced and a SE-DME converter (isothermal) designed to achieve a target 90% DME yield (Figure 1a). Calculation are performed by adopting the SRK equation of state and data from [1,2].

A heterogeneous model of a single tube of a fixed bed multi tubular reactor for direct DME synthesis was developed. The model consists of *i*-species mass, energy and momentum balances written in 2D cylindrical coordinates, coupled with *i*-species mass and energy balances for the catalyst phase accounting for concentration gradients (1D) in an isothermal, isobaric pellet. A reaction scheme including CH<sub>3</sub>OH synthesis from CO<sub>2</sub>, Reverse Water Gas Shift and CH<sub>3</sub>OH dehydration is implemented with kinetics taken from the literature for a physical mixture of Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> CH<sub>3</sub>OH synthesis catalyst and  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> dehydration catalyst [3,4]. The model equations are implemented in gPROMS<sup>®</sup> for the numerical resolution of the boundary value problem. The model was validated by comparison with industrial CH<sub>3</sub>OH synthesis noted data.

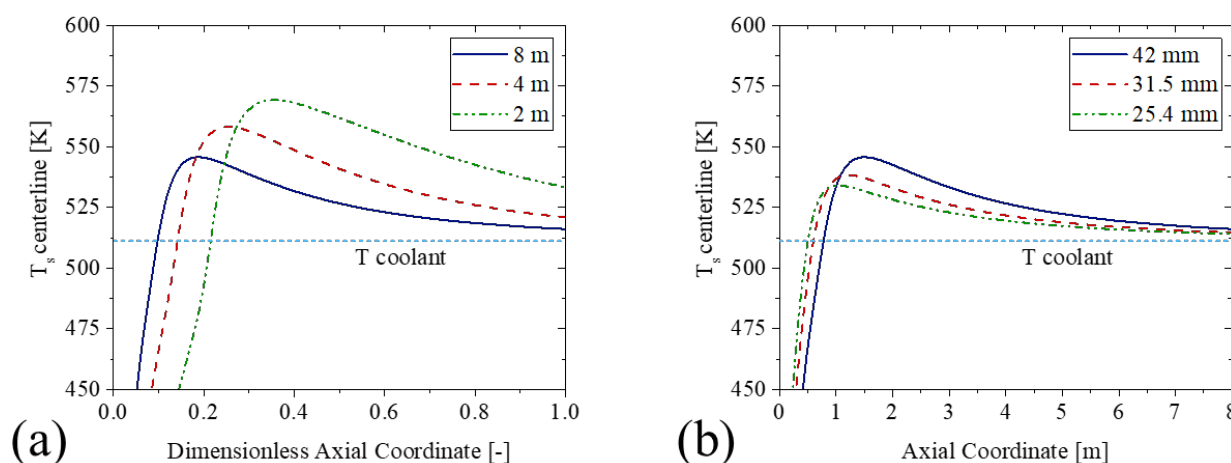


**Figure 1.** (a) Operating units layout of DME synthesis process; (b) percentage heat duty of the main converter as a function of temperature (473-573 K) at 20 and 30 bar pressure.

### 3. Results and discussion

Thermodynamic analysis shows that the single pass 90% DME target yield can be achieved when keeping H<sub>2</sub>O outlet molar fraction from the SE-DME converter at 10<sup>-4</sup>-10<sup>-3</sup> depending on temperature and pressure. Calculations also show (Figure 1b) that, for temperatures below 520 K and pressure over 20 bar, more than 40% of the overall heat duty is managed in the upstream converter, thus decreasing the thermal load of the SE-DME synthesis reactor.

Simulation results of the main converter confirm that temperature control is a critical issue, the combined exothermicity of CH<sub>3</sub>OH synthesis, WGS reaction and DME formation resulting in a marked hot-spot which may exceed safety temperature limit for product selectivity and catalyst stability. A sensitivity analysis on the operating conditions (pressure, temperature, composition, space velocity) and reactor geometry (tube diameter and length) has been performed in order to find the optimum parameter set which maximizes the DME yield and limits the hot-spot temperature (example in Figure 2).



**Figure 2.** Centerline temperature profile: (a) effect of reactor length; (b) effect of tube diameter.

The mathematical model of the SE-DME synthesis reactor is presently under development.

### 4. Conclusions

The thermodynamic analysis of the process has revealed that a main converter positioned upstream of the overall process is required to reduce the large heat duty to the SE-DME converter. The simulation of the main converter has shown indeed that heat management is a critical issue, and that the operating parameters have to be carefully selected in order to reduce the harshness of the hot-spot.

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### Keywords

DME synthesis; Sorption Enhancement; Catalytic multi tubular reactors; Reactor modelling.