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# Numerical simulation of scale-up effects of methanol-to-olefins fluidized bed reactors

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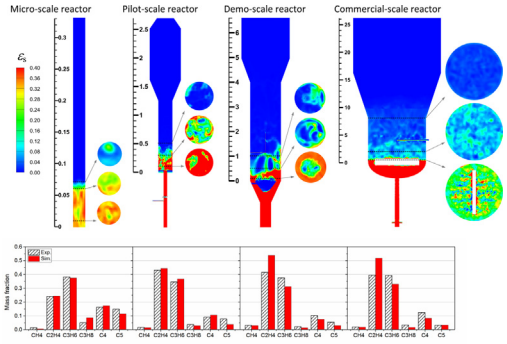
## HIGHLIGHTS

- The scale-up effects with varying reactor size are investigated with CFD simulations.
- Hydrodynamic behaviors in different MTO reactors are successfully predicted.
- Prediction of reaction behavior deviates from experiments gradually with reactor size.

## GRAPHICAL ABSTRACT

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## ABSTRACT

Scale-up of fluidized bed reactors has long been regarded as a big challenge in chemical reaction engineering. While traditional scaling theories are mostly based on hydrodynamics similarity, computational fluid dynamics (CFD) aided approach allows direct coupling between hydrodynamics and reaction factors and is expected to speed up the experiment-based scale-up process with lower cost. In this study, we aim to investigate the scale-up effects through simulations of a series of methanol-to-olefins (MTO) reactors of different sizes. The two-fluid model and energy-minimization multi-scale (EMMS)-based drag models are combined in simulations. The fluidization characteristics in terms of flow structures, velocity distribution, mass fractions of gaseous product and coke distribution are presented against available experimental data for different-sized reactors. It is found that typical hydrodynamic features can be reasonably predicted, while the prediction of reaction behavior shows growing discrepancy with increasing reactor size. Possible reasons are discussed in the last section along with future work presented for scale-up studies.



## 1. Introduction

Scale-up of fluidized bed reactors has long been regarded as a big challenge in chemical reaction engineering. Traditional approach focuses on searching scaling laws with various sets of dimensionless numbers (Rüdisüli et al., 2012; Glicksman, 1998),

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**Nomenclature**

| | |
|---|---|
| $a$ | inertial term, m/s$^2$ |
| $C$ | concentration, mol/L |
| $C_{D0}$ | standard drag coefficient for an individual particle |
| $d_b$ | bubble diameter, m |
| $d_p$ | particle diameter, m |
| $f$ | volume fraction of dense phase |
| $G_s$ | solid flux, kg/(m$^2$ s) |
| $H_D$ | heterogeneity index ($H_D = \beta/\beta_0$) |
| $I_s$ | solid inventory, g |
| $k_i$ | rate constant, L/($g_{cat}$ · s) |
| $M$ | molar weight, g/mol |
| $p$ | pressure, Pa |
| $R_i$ | reaction rate, g/($g_{cat}$ · s) |
| $Re$ | Reynolds number, $\rho_g \varepsilon_g \lvert \boldsymbol{u}_g - \boldsymbol{u}_s \rvert d_p/\mu_g$ |
| $\boldsymbol{u}$ | real velocity, m/s |
| $U_g$ | superficial velocity, m/s |
| $w_{coke}$ | coke content, % |
| $Y$ | mass fraction |

*Greek letters*

| | |
|---|---|
| $\beta$ | drag coefficient with structure in a control volume, kg/(m$^3$ s) |
| $\beta_0$ | drag coefficient without structure in a control volume, kg/(m$^3$ s) |
| $\varepsilon_g$ | voidage |
| $\varepsilon_s$ | solid volume fraction |
| $\eta$ | conversion ratio, % |
| $\mu$ | viscosity, Pa s |
| $\rho$ | density, kg/m$^3$ |

*Subscripts*

| | |
|---|---|
| c | dense phase |
| f | dilute phase |
| g | gas phase |
| s | solid phase |
| $i$ | lump in reaction kinetics model |

where the hydrodynamic similarity is mostly regarded. The coupling between reactions and hydrodynamics is however often neglected (Ye et al., 2015).

Scale-up of the methanol-to-olefins (MTO) reactor that was developed by Dalian Institute of Chemical Physics (DICP) is a good example to understand such challenge (Tian et al., 2015). The MTO is a typical gas catalytic process, where both reactants and products are in gas phase, and the reactions take place over the surface of catalytic particles. The development of MTO process borrows ideas from the reaction-regeneration configuration of the modern fluid catalytic cracking (FCC) units. However, differences still exist between MTO and FCC processes, which constitute the challenge for scale-up (Lu et al., 2016; Ye et al., 2015). Firstly, different catalysts: SAPO-34 zeolite catalyst with small pores was used in DICP's MTO (or, DMTO) process, and it shows the highest selectivity to ethylene provided with certain coke deposition. In contrast, the FCC process employs the zeolite Y catalyst with larger pores which are not easily blocked by coke deposition. Secondly, different reactors: a densely fluidized bed reactor such as bubbling or turbulent fluidized bed with much longer residence time than that of the FCC riser reactor was preferred for DMTO. Thirdly, both the methanol-to-olefins reactions in reactor and coke burning in regenerator are exothermic, so there is no strict requirement for DMTO on heat-coupling between the reactor and regenerator as in FCC.

As shown in Fig. 1, before the commercialization, the scale-up of DMTO has experienced three-stage experiments on the micro-scale (or lab-scale), pilot-scale and demo-scale fluidized bed reactors, respectively. The micro-scale one was operated under the regime of bubbling fluidization in a batch manner without catalyst circulation. Its experimental results were used to evaluate catalyst performance, establish the network of reaction kinetics and help identify the optimal operation window for the design of pilot-scale fluidized bed reactor, such as the optimal gas-catalyst contact time. The operating regime of pilot-scale reactor is the same as the micro-scale one, reflecting their hydrodynamic similarity. In addition, a fluidized bed regenerator, which was connected with the reactor through a standpipe, was especially tested in the pilot-scale reactor to mimic the continual circulation of catalysts in industry. The fluidization performance and stripping attrition of catalyst were preliminarily investigated in this stage. In the demo-scale reactor, however, the operating velocity of gas was increased for high throughput. A different fluidization regime, i.e., turbulent fluidization, was hence adopted. Thus the catalyst circulation, stripping attrition and heat exchange and so on

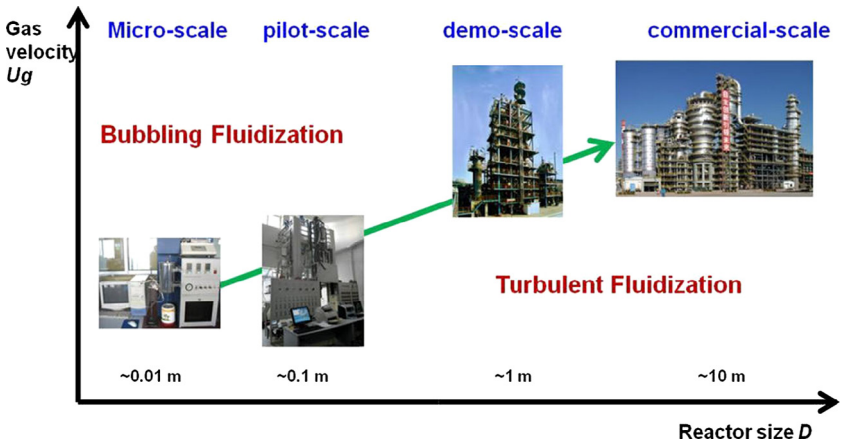


**Fig. 1.** Scale-up of DMTO (DICP's MTO) fluidized bed reactor (Tian et al., 2015).