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Comparison between detailed (CFD) and simplified models for the prediction of solid particle size distribution in fluidized bed reactors

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Introduction

The polyethylene polymerization process takes place in fluidized bed reactors containing a pressurized gas mixture, mainly ethylene, and growing polymer particles (Fig. 1 – l.h.s.). Such particles exhibit a multigrain structure, with catalyst fragments embedded in the polymer. Although many fluidization behaviors may occur depending on gas velocity and solid properties, fluidized bed reactors are built to work in the so-called "aggregative fluidization" regime (Fig. 1 – r.h.s, sketch (c)). The diameter of the final product is mainly determined by the residence time of the particles that is in turn given by the interplay between the reactor fluid-dynamics and the polymerization kinetics. Starting from the outcome of detailed CFD simulations, the aim of this work is the development of a simplified model suitable to effectively describe the fluidization behavior with minimal computational effort.

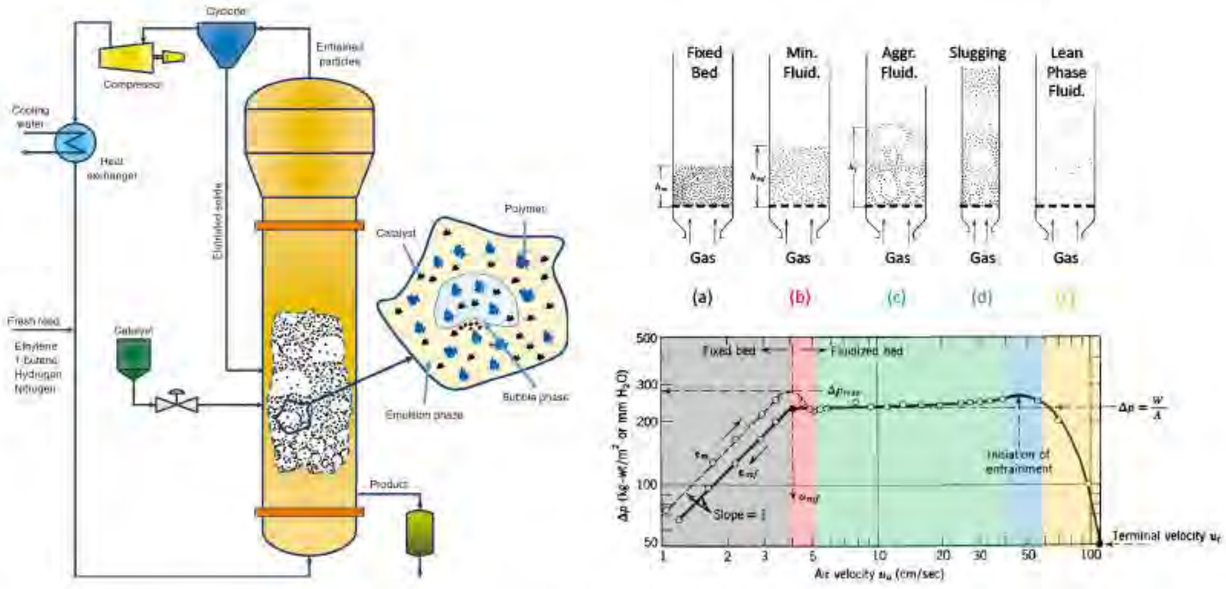

Fig. 1: Fluidized bed reactor (l.h.s. – Abbasi *et al.* [1]) and fluidization regimes (r.h.s. – adapted from Kunii & Levenspiel [2]).

CFD model

The fluidization behaviour and the solid phase distribution have been studied through monodisperse transient Euler-Euler CFD simulations using Fluent code from Ansys. The computational domain consists in a pilot-plant taken from literature [3] (Fig. 2 – l.h.s) represented as a 2D planar geometry with the dimensions depicted in Fig. 2 – r.h.s.. The reactor is initially filled with a given amount of particles packed at the bottom of the system. The motion of spherical polyethylene solid particles, with two different diameter values, has been analysed when expanded by a pressurized ethylene flow with three different velocities for 60 s of physical time, reaching a quasi steady-state behaviour. The solid phase volume fraction has been sampled over four heights from the reactor bottom (red lines of Fig. 2 – r.h.s.) to quantitatively determine the extent of fluidization and the resulting bed height.

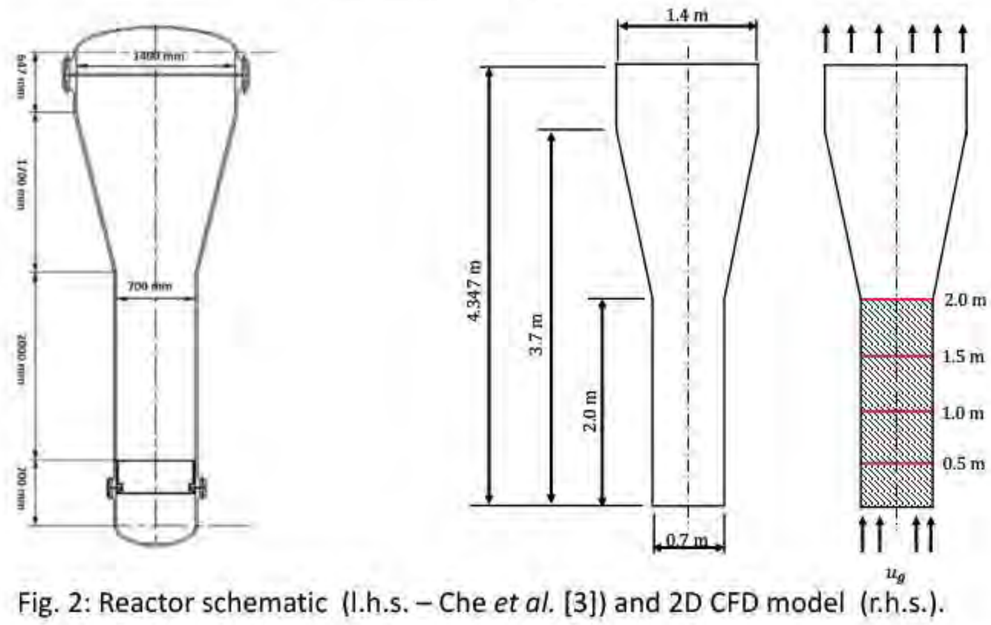

Fig. 2: Reactor schematic (l.h.s. – Che *et al.* [3]) and 2D CFD model (r.h.s.).

Simplified analytic model

The simplified model is based on population balance equations to evaluate the particle size distribution inside the bed. The bed is represented as N compartments in series, and each compartment contains three phases: emulsion, wake and bubble phase. Using the classical relationships by Kunii & Levenspiel [2], it is possible to evaluate the fluid-dynamics properties inside each compartment. This way, phase velocities, solid holdups and void fractions are estimated. Moreover, the distribution of the solid particles in each phase and compartment is evaluated using size dependant particle transfer constants as function of particle diameter and gas velocity. The resulting system of population balances and material balance equations is finally solved under steady-state conditions, thus obtaining the particle size distribution in each phase and position along the bed.

Results and conclusions

Solid phase distribution contours (Fig. 3) show that the fluidization behaviour is correctly described, especially in terms of interplay between particle size and gas velocity. Such results are also in agreement with experimental evidence. The solid level inside the bed decreases as the gas flow velocity is reduced while small particles (223 micron) undergo eultriation when fluidized at large velocity, *i.e.* 61 and 40 cm/s. The results of the two models (CFD and simplified) are in very good agreement for large particles at all velocity values (Fig. 4 – r.h.s.). On the other hand, the comparison is less satisfactory when considering smaller particle (Fig. 4 – l.h.s.), since the impact of the particle size is somehow underestimated by the simplified fluid-dynamics considered in the compartimentalized approach. Empirical refining of the literature equations is in progress, aimed at improving the prediction ability of the simplified model.

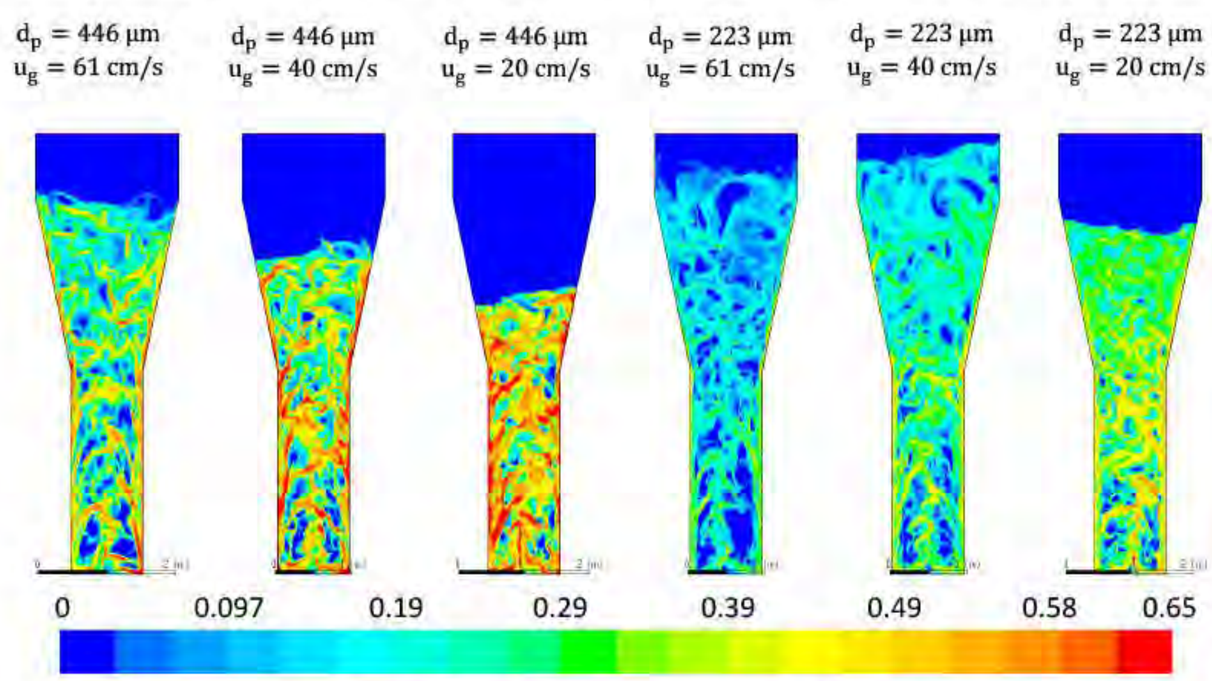

Fig. 3: CFD solid phase distribution contours at 60 s of physical time.

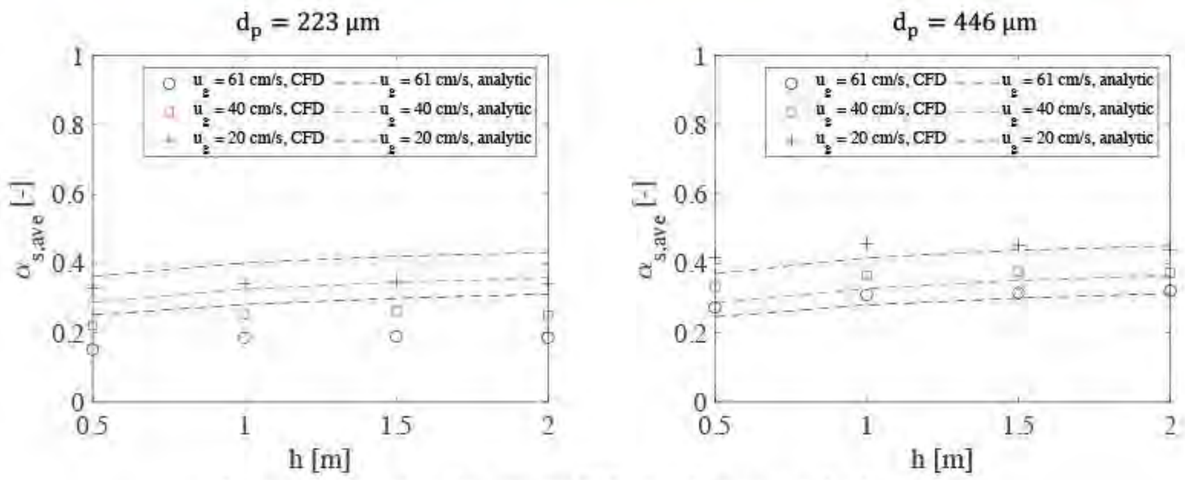

Fig. 4: Comparison between CFD simulation results (markers) and analytic model (dashed lines) for $d_p = 223$ µm and $d_p = 446$ µm.

Acknowledgments

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References

[1] M.R. Abbasi, A. Shamiri, M.A. Hussain, 2019. A review on modeling and control of olefin polymerization in fluidized-bed reactors. Reviews in Chemical Engineering, 35(3), 311-333.

[2] D. Kunii, O. Levenspiel, 1991. Fluidization Engineering, second ed. Boston, MA: Butterworth-Heinemann.

[3] Y. Che, Z. Thian, Z. Liu, Y. Gao, E. Zou, S. Wang, P. Liu, 2015. CFD prediction of Scale-up Effect on the Hydrodynamics Behaviors of a Pilot-Plant Fluidized Bed Reactor And Preliminary Exploration of Its Application For Non-Pelletizing Polyethylene Process. Powder Technology, 278, 94-110.

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