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3D Modelling of Flow Dynamics in Packed Beds of Low Aspect Ratio

Faris Alzahrani [1] and Farid Aiouache [2]

1. PhD Candidate, Department of Engineering, University of Lancaster, (LA1 4YR), Lancaster, UK (email: m.aldehani@Lancaster.ac.uk).
2. Senior Lecturer, Department of Engineering, University of Lancaster, (LA1 4YR), Lancaster, UK (email: f.aiouache@Lancaster.ac.uk).

Aims

To investigate 3D fluid flow heterogeneity in packed beds of low aspect ratios and to compare the results with those from with 2D modelling

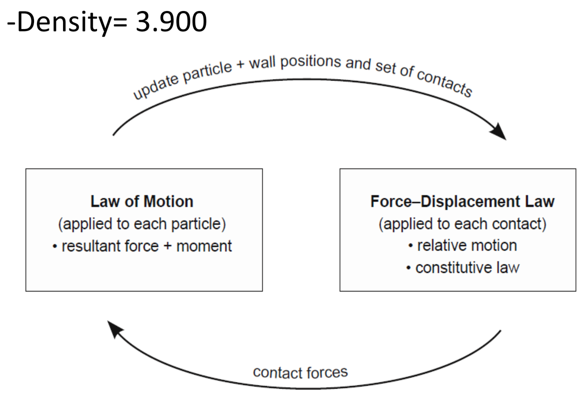
Abstract

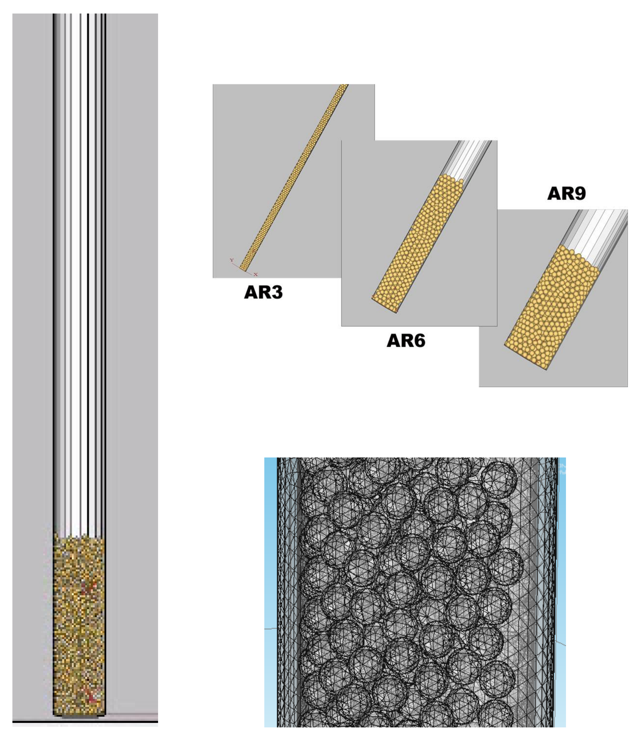
Computer fluid dynamics (CFD) was used to investigate non-uniform structure flow distributions in packed bed reactors of low aspect ratios. Detailed knowledge of flow dynamics in terms of local structure of the packed bed, pressure drops and interstitial flow distributions was examined. The discrete element method was used to generate various packing configurations. The porosity profiles from the CFD simulation results were in a good agreement with the semi-analytical models, especially, in the vicinity of the wall. Similar oscillation trends with damping profiles towards the centre of the packed beds were observed. The discrepancies in regions towards the centre would be caused by the loose structure of the generated packing. The simulation results were validated by pressure drop measurements. Both experimental and simulation results fitted well Reichelt and Zhavoronkov models at high Reynolds numbers and these results clearly demonstrated that the generated packing exhibited pressure drops which were close to relevant models at low aspect ratios allowing further investigations of mass transfer and chemical reactions. Flow heterogeneity was investigated by radial distribution of the velocity. At high aspect ratios of packed bed, the velocity profile had a thin peak near the wall and a dumped profile towards the centre.

Packing generation by the Discrete Element Method

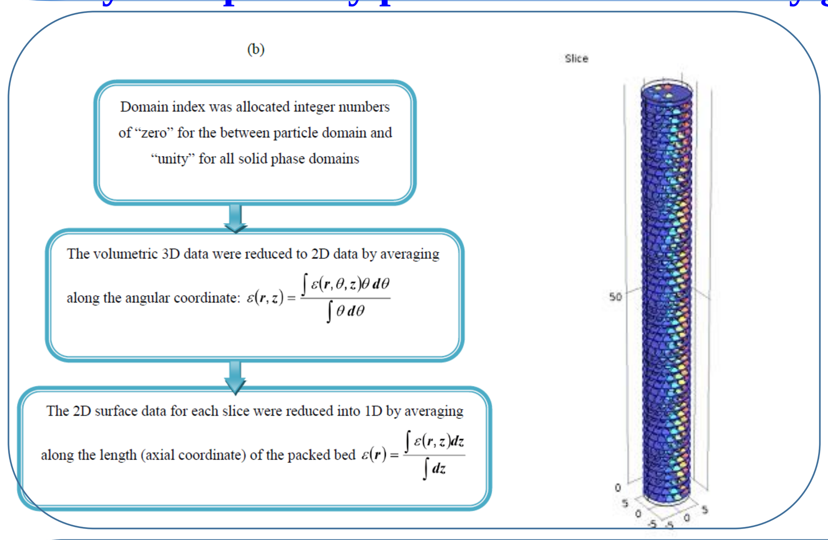
The overall setting parameters

- Wall parameters:
- Normal stiffness coefficient, kn =1*1013
- Tangential stiffness coefficient, ks=1*1013
- Friction coefficient, kfric=0.2;
- Particle parameters:
- Normal stiffness coefficient, kn =2.5*108
- Tangential stiffness coefficient, ks=2.5*108
- Friction coefficient, kfric=0.2
- Density= 3.900

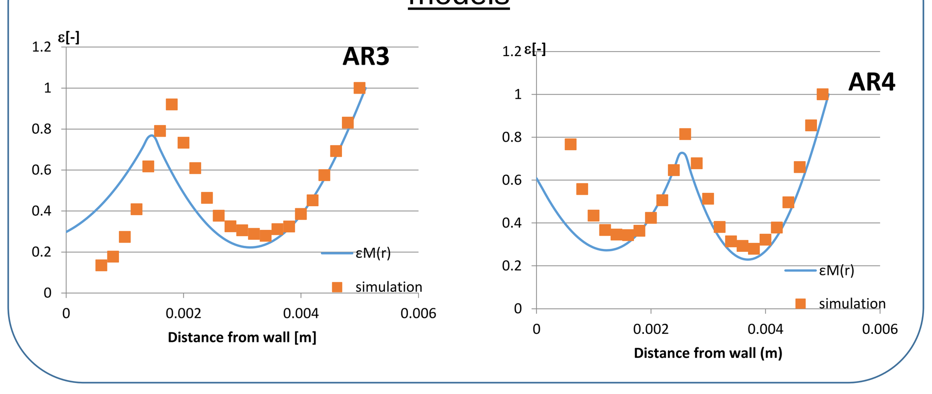




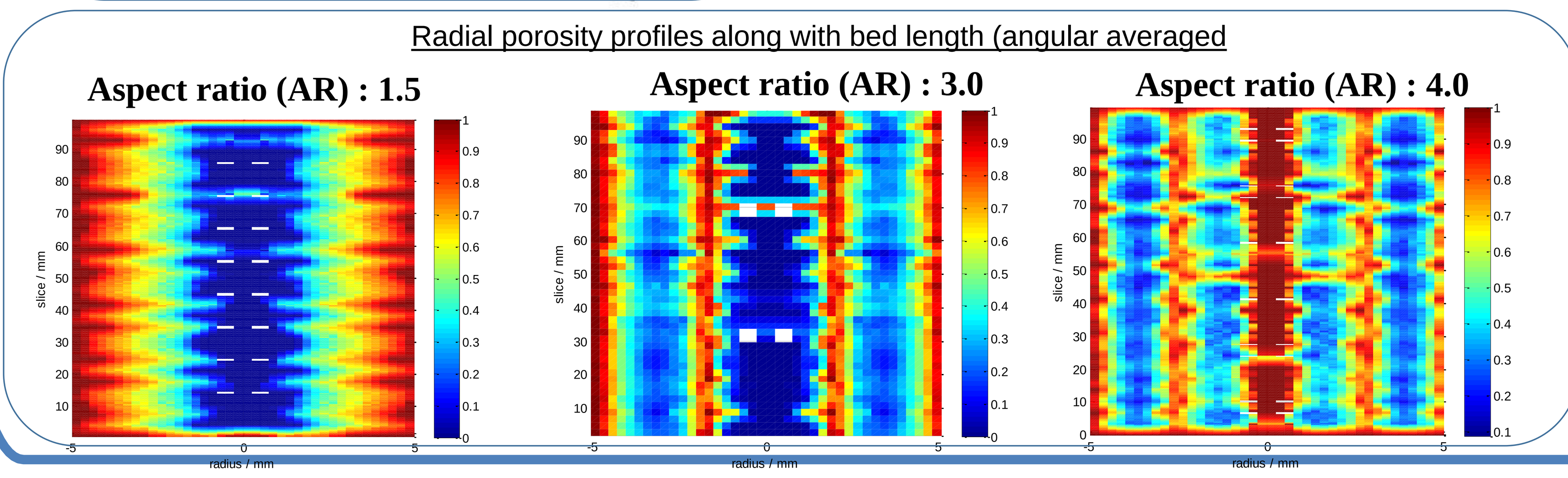
Analysis of porosity profiles of the randomly generated packings



Full packed bed radial porosity profiles along with literature models



Radial porosity profiles along with bed length (angular averaged)

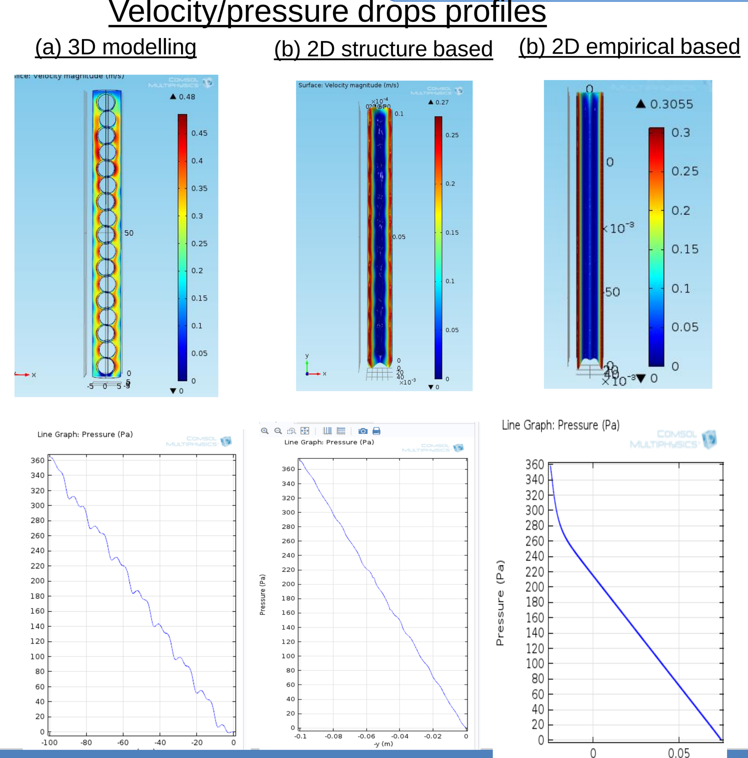


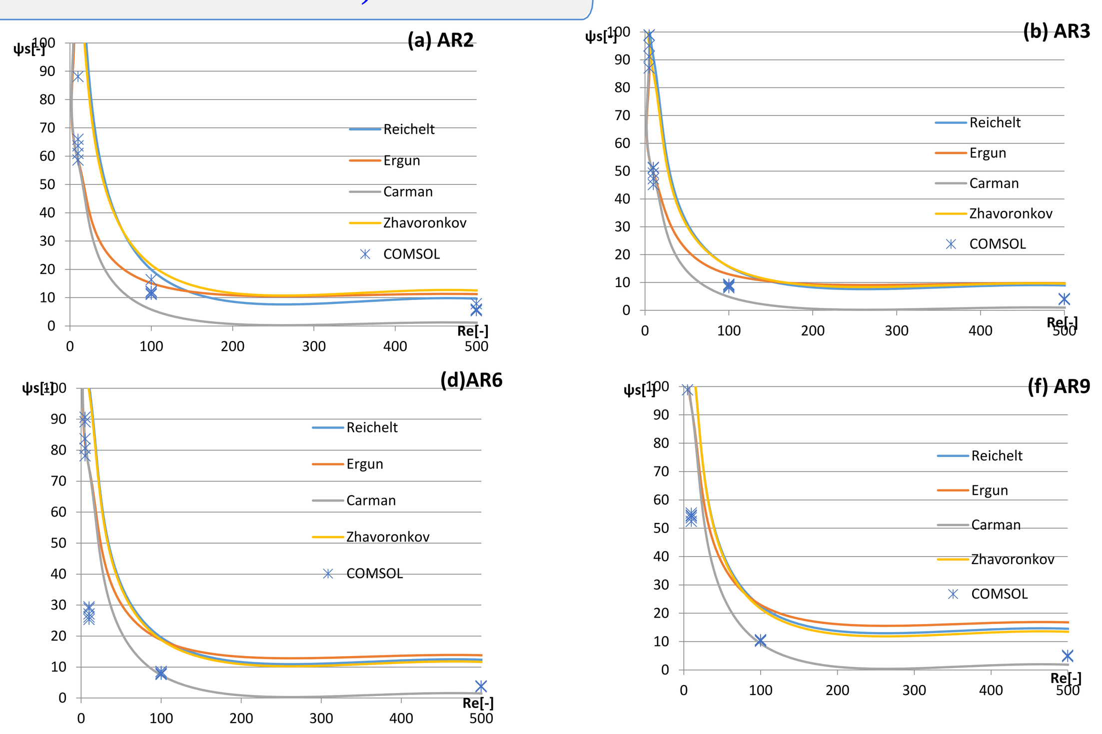
Results

Pressure drops by simulation and established models (Carman, Ergun, Zhavoronkov and Reichelt)

Velocity/pressure drops profiles

(a) 3D modelling (b) 2D structure based (b) 2D empirical based





Momentum balance

2D modeling (two missing data : porosity and/or porosity)

$$\varepsilon\rho_g u(\nabla u) = -\varepsilon\nabla P + \mu\nabla.\nabla u - \frac{2}{3}\varepsilon\mu\nabla.\nabla u + \varepsilon F$$

$$\nabla\cdot(\rho_g u) = 0$$

$$F = -\frac{\mu u}{K} - \beta\rho u^2$$

$$K = \frac{\varepsilon^3 dp^2}{A(1-\varepsilon)^2}, \quad \beta = \frac{B(1-\varepsilon)}{\varepsilon^3 dp}$$

$$where\ A = 150,\ B = 1.75$$

$$u\big|_{\tau=0} = u_0, \nabla u\big|_{\tau=1} = 0$$

$$\nabla u|_{r=0} = 0$$

1. Porosity by empirical models

$$\varepsilon_e(r') = 1 - \pi[R_{se}^2 - \alpha(r_e - r_{se})^2],$$

$$R_{se} = R_s^* - \frac{ar'^2}{r'^2+2},$$

$$with\ a = 0.045 - 0.55e^{-D/d_p}$$

$$r_e = \frac{(r_{se}+r)^2 - R_s^{*2}}{4r_{se}}, \quad r_{se} = [r_r + R_s^*],$$

$$r_r = br'^2 + r' + R_s^*, with\ b = 0.037 - 2.0e^{-D/d_p}$$

2. Porosity by angular (perimeter) averaging from 3D structures

3D modeling (no missing data but time computer power consuming)

$$\rho_g u\nabla u = -\nabla P + \mu\nabla.\nabla u - \frac{2}{3}\mu\nabla.\nabla u$$

$$\nabla\cdot(\rho_g u) = 0$$

$$\boldsymbol{u}\big|_{\tau=0} = \boldsymbol{u}_0, \boldsymbol{P}\big|_{\tau=1} = \boldsymbol{P}_0$$

Modelling of momentum, heat and mass balances in packed bed reactor (Pt/Alumina catalyst deactivation in CO oxidation)

Two-dimensional Modelling

Momentum balance in a homogenous porous medium

$$\varepsilon\rho_g u(\nabla u) = -\varepsilon\nabla P + \mu\nabla.\nabla u - \frac{2}{3}\varepsilon\mu\nabla.\nabla u + \varepsilon F$$

$$\nabla\cdot(\rho_g u) = 0$$

$$F = -\frac{\mu u}{K} - \beta\rho u^2$$

$$K = \frac{\varepsilon^3 dp^2}{A(1-\varepsilon)^2}, \quad \beta = \frac{B(1-\varepsilon)}{\varepsilon^3 dp}$$

$$where\ A = 150,\ B = 1.75$$

$$u\big|_{\tau=0} = u_0, \nabla u\big|_{\tau=1} = 0$$

$$\nabla u|_{r=0} = 0$$

Deactivation model

$$\frac{da}{dt} = A_D e^{\left(E_D/RT\right)} c_{CO}$$

Heat balance (both gas and solid phases)

$$(\varepsilon\rho_g Cp_g + (1-\varepsilon)\rho_s Cp_s)\frac{\partial T}{\partial t} +$$

$$\varepsilon\rho_g Cp_g u\cdot\nabla T = \nabla\cdot(k\nabla T) + Q$$

$$k\nabla T|_{r=R} = 0$$

$$Q = \Delta H_R R$$

$$\nabla T|_{r=0} = 0$$

Mass balance (both gas and solid phases)

$$\frac{\partial\varepsilon C_i}{\partial t} + \nabla\cdot(-D_i\nabla C_i) + \varepsilon u\cdot\nabla C_i = R_i$$

$$\nabla c|_{r=0} = 0$$

$$R_i = aAe^{\left(E/RT\right)} c_{CO}$$

Three-dimensional Modelling

1. **Momentum balance**

$$\rho_g u\nabla u = -\nabla P + \mu\nabla.\nabla u - \frac{2}{3}\mu\nabla.\nabla u$$

$$\nabla\cdot(\rho_g u) = 0$$

$$\boldsymbol{u}\big|_{\tau=0} = \boldsymbol{u}_0, \boldsymbol{P}\big|_{\tau=1} = \boldsymbol{P}_0$$

2. **Mass balance**

2.1. **in the gaseous phase**

$$\frac{\partial c_i}{\partial t} + \nabla.(-D_i\nabla c_i) + u\nabla c_i = 0$$

2.2. **in the catalytic phase**

$$\frac{\partial c_i}{\partial t} + \nabla.(-D_{ie}\nabla c_i) = R_i$$

$$D_{ie} = \frac{\varepsilon_c D_i}{\tau_c}a \qquad R_i = aAe^{\left(E/RT\right)} c_{CO}$$

3. **Heat balance in the gas phase**

3.1.Heat balance in the gas phase

$$\rho_g Cp_g\frac{\partial T}{\partial t} + \rho_g Cp_g u\nabla T = \nabla(k\nabla T)$$

3.2. in the catalytic phase

$$\rho_g Cp_s\frac{\partial T}{\partial t} = \nabla(k_s\nabla T) + Q$$

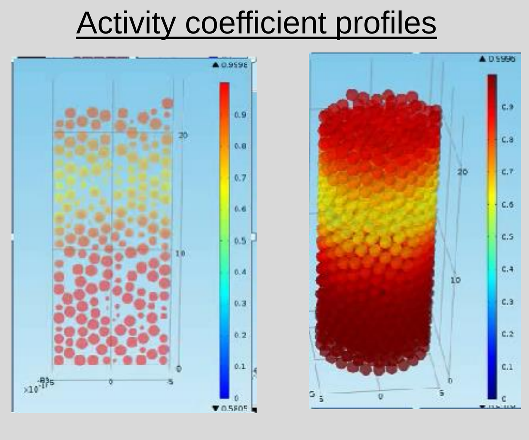
$$Q = R\Delta H_R$$

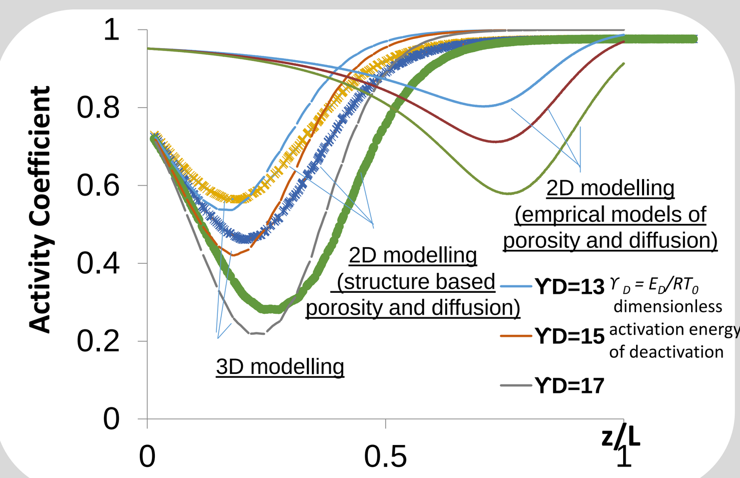
4. Deactivation rate

$$\frac{da}{dt} = A_D e^{\left(E_D/RT\right)} c_{CO}$$

Local deactivation results

Activity coefficient profiles





Conclusions

- This work used the 3D CFD modelling to investigate non uniform (local) deactivation in packed bed reactors of low AR under dynamic operations.
- The modelling was justified by pressure drops tests and *in situ* sampling by moving capillary and mass spectrometry
- Good agreements in terms of pressure drops and porosity profiles with established models
- 2D modelling based on averaged distribution structures of 3D modelling is promising approach to substitute large computation consuming 3D mdoelling.

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Acknowledgement

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