Comparison of Particle-Resolved Direct Numerical Simulation and 1D modelling of catalytic reactions in cylindrical particle bed

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ABSTRACT

This work presents a comparative study of reactive flow in a realistically packed array of cylindrical particles on two widely different scales: particle-resolved direct numerical simulation (PR-DNS) and 1D modelling. PR-DNS directly simulates all transfer phenomena in and around the cylindrical particles, while 1D modelling utilizes closure models to predict system behaviour at a computational cost several orders of magnitude lower than PR-DNS.

PR-DNS is performed on a geometry of ~100 cylindrical particles generated using the discrete element method (Singhal et al. (2017)). Simulations are performed for a general catalytic reaction form (A(g) + B(s) → C(g) + B(s)) over a range of Thiele moduli, Prandtl numbers and reaction enthalpies. The geometry with particles of different aspect ratios (aspect ratio = 2, 4 and 6) are meshed with fine polyhedral elements both inside and outside the particles. Hence, we obtain accurate results for combined internal and external heat and mass transfer in the cylindrical particle array.

These results are compared with a 1D packed bed reactor model incorporating appropriate models for intra particle diffusion (verified for spherical particles) ([2],[3]) and for external heat transfer [1] (applicable to cylindrical particles). The differences and similarities between the two approaches are documented and recommendations are made to guide future 1D modelling works involving reactive flows in packed beds of cylindrical particles.

REFERENCES

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