DEM-CFD Modeling of a Packed Bed Reactor: Analysis of Local Transport & Deactivation Dynamics across Aspect Ratios

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ABSTRACT

Our thesis presents a three-dimensional computational investigation of coupled fluid flow (in an ANSYS 2-Way Fluent Coupling, student version), heat and mass transfer, and catalyst deactivation dynamics within a low aspect ratio packed bed reactor ($D/dp < 6$), where confining wall effects and packing heterogeneity govern local transport phenomena. The work bridges the gap between molecular-scale reaction kinetics and reactor-scale performance through an integrated Discrete Element Method–Computational Fluid Dynamics (CFD-DEM) modelling framework. The random packing of $M = 243$ spherical catalyst particles inside a cylindrical vessel (diameter $D = 0.15$ m, height $H = 1.2$ m) was generated using DEM with the Hertz-Mindlin contact model and Coulomb friction ($\mu s = 0.5$), replicating an industrial gravity-driven settling process.

The resulting geometry was transferred via Boolean subtraction to create the interstitial fluid domain, which was discretised using mixed tetrahedral-polyhedral elements (3,705 cells, minimum orthogonal quality 0.584). Particle-resolved Reynolds-Averaged Navier-Stokes (RANS) simulations were performed using the standard k–ε turbulence model under a pressure-based transient solver with the SIMPLE pressure-velocity coupling algorithm. Air at standard conditions ($\rho = 1.225$ kg/m³, $\mu = 1.7894 \times 10{-}5$ Pa·s, Pr = 0.71) served as the working fluid, with aluminium ($\rho = 2719$ kg/m³, $\lambda = 202.4$ W/(m·K)) representing the catalyst pellets. The principal findings of this investigation are as follows.

First, the radial porosity distribution exhibits the characteristic damped oscillatory behaviour, with porosity approaching unity at the confining wall and converging to $\varepsilon \approx 0.40$–0.42 in the bed interior, in agreement with established correlations by Mueller and de Klerk.

Second, near-wall velocity channelling is observed, with maximum interstitial velocities reaching approximately 3.27 m/s—confirming that the wall's influence permeates the entire bed cross-section at low aspect ratios.

Third, pressure-drop predictions agree with the Ergun, KTA, and Eisfeld-Schnitzlein correlations to within 25%, with the improved Reger formulation providing the closest match through its porosity-dependent form-loss correction.

Fourth, particle-to-fluid heat transfer analysis reveals Nusselt number variations between inner and outer bed regions, with Wakao's correlation demonstrating superior accuracy; at lower D/dp ratios, the inner and outer regions exhibit consistent heat transfer behaviour, whereas at higher ratios a significant reduction in outer-region Nusselt number is observed.

Fifth, the theoretical framework for Reynolds stress anisotropy characterisation—including Lumley triangle invariant maps and barycentric mapping—is

developed to quantify the departure from the isotropic Boussinesq assumption inherent in the k–ε model.

Sixth, catalyst deactivation patterns are shown to be markedly asymmetric along both axial and radial directions, with the dimensionless activation energy (γD) and Damköhler number (DaD) controlling the spatial heterogeneity and temporal evolution, respectively.

The "wrong-way" temperature behaviour and local thermal runaway conditions—phenomena entirely invisible to two-dimensional and pseudo-homogeneous formulations—are captured through the three-dimensional pore-level resolution. The comprehensive analysis demonstrates that particle-resolved CFD-DEM modelling is essential for capturing the local transport heterogeneities and deactivation dynamics that govern packed bed reactor performance, establishing a robust multi-scale framework for the design and safety assessment of industrial catalytic systems.