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# Computational Fluid Dynamics for Fixed Bed Reactor Design

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computational fluid dynamics, CFD, fixed bed, reactor modeling, particle-resolved, computer-generated packing, microkinetics

## Abstract

Flow, heat, and mass transfer in fixed beds of catalyst particles are complex phenomena and, when combined with catalytic reactions, are multiscale in both time and space; therefore, advanced computational techniques are being applied to fixed bed modeling to an ever-greater extent. The fast-growing literature on the use of computational fluid dynamics (CFD) in fixed bed design reflects the rapid development of this subfield of reactor modeling. We identify recent trends and research directions in which successful methodology has been established, for example, in computer generation of packings of complex particles, and where more work is needed, for example, in the meshing of nonsphere packings and the simulation of industrial-size packed tubes. Development of fixed bed reactor models, by either using CFD directly or obtaining insight, closures, and parameters for engineering models from simulations, will increase confidence in using these methods for design along with, or instead of, expensive pilot-scale experiments.

## 1. INTRODUCTION

A catalytic fixed bed reactor is a tube, usually cylindrical, filled with active elements such as particles, open foams, or structured inserts. The particles are often spheres, cylinders, or rings, but complex shapes, such as wagon wheels, multilobes, multichannel cylinders, and cylinders with external flutes or grooves, have been used for specific processes. If the reaction is accompanied by strong heat effects that require heat transfer through the tube, then the tube–to–particle diameter ratio ($N$) is quite low, typically 3–10, and wall effects play a major role in tube performance.

Models of fixed beds have been developed and used for many years. The conventional chemical reaction engineering model approach treats the catalyst bed as a homogeneous continuum with effective transport properties that reflect both the fluid and particulate phases. These models for many years assumed constant axial velocity, $v_z$, or plug flow. Recognizing the inadequacy of this assumption, researchers looked to include the radial variation of the axial velocity, $v_z(r)$, in 2D models. These types of treatment of the fixed bed velocity are not included in this review.

Computational fluid dynamics (CFD) for fixed beds has two main forms: the porous medium model (PMM) approach and the particle-resolved CFD (PRCFD) approach. Both are discussed in this article, with emphasis on the latter. There has been much interest in PRCFD (sometimes called detailed modeling, interstitial modeling, or pore-scale modeling) in recent years. In this approach, the fixed bed model includes individual particles, solving equations for the fluid flow around them coupled to pellet models for transport and reaction inside or on the surfaces of the pellets. This approach allows much more detailed study of fixed bed phenomena at different length and timescales than effective or continuous medium approaches, as **Figure 1** illustrates.

The interest in PRCFD is reflected in two review papers. Dixon et al. (1) covered work up to 2006, mainly studies of periodic bed segments and clusters of particles, and very low-$N$ tubes with few particles. The explosive growth of publications and methods since, up to 2017, has been comprehensively documented and interpreted by Jurtz et al. (2).

There has also been discussion on the role of PRCFD. Dixon & Nijemeisland (3) suggested that it could contribute to fixed bed design by improving the description of flow and by providing detailed information to develop improved reduced models for design and analysis. Wehinger & Kraume (4) asked if CFD was ready to be a design tool for low-$N$ tubular reactors. They concluded that despite heavy computational cost, PRCFD could replace classical approaches, advantages being that correlations for effective parameters would not be needed and that PRCFD allows algorithm-based design and optimization of new catalyst pellet shapes. Partopour & Dixon (5) suggested some areas of focus for future research, including the application of machine-learning methods to the large data sets produced by 3D PRCFD.

The present review attempts to identify recent trends over the past 10 years without giving a comprehensive literature survey, including as-yet-unresolved questions, disagreements, and needs for the future. To maintain focus, the scope of this article is limited. It does not present detailed model equations or discuss experimental techniques for validation of PRCFD or structured arrangements of particles. Only single-phase (usually gas) flow is covered; for CFD of multiphase flow, Wang et al.'s (6) review is recommended. For more detail on fixed bed CFD than is presented here, the reader is referred to References 1 and 2 and the specific references associated with each topic.

## 2. FIXED BED COMPUTATIONAL FLUID DYNAMICS: THE POROUS MEDIUM MODEL

We consider fixed bed CFD to consist of approaches that solve for the velocity field directly. In this section, we briefly discuss the PMM, which is the standard model available for porous flows in COMSOL®, ANSYS-Fluent/CFX, and STAR-CCM+.

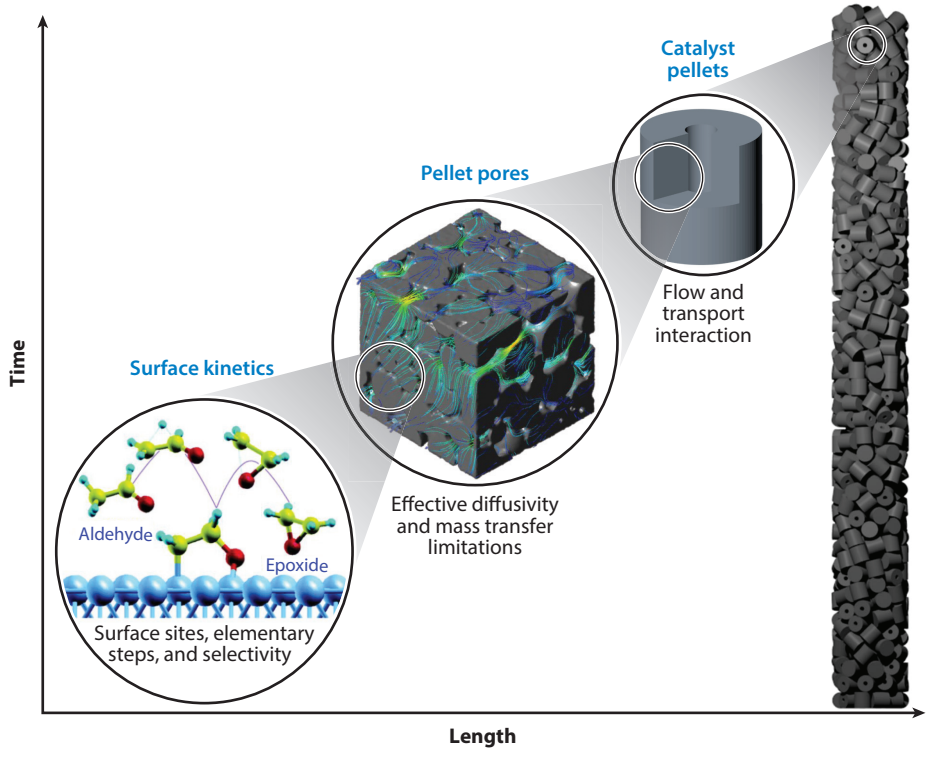


**Figure 1**

Multiscale nature of fixed bed transport and reaction processes, from molecular scale on catalyst surface to pore scale in catalyst pellets to bed scale in packed tubes of particles. Adapted in part with permission from Reference 145; copyright 2005 American Chemical Society.

The PMM treats the fixed bed as a continuum; the presence of the particles is included not explicitly but through source terms that account for momentum loss. The PMM adds the source terms into the incompressible Newtonian fluid Navier–Stokes equations. The source terms include viscous loss resistance and inertia loss resistance. Although source terms can account for the increase in resistance to flow owing to the particles, they cannot reproduce the radial variation in axial flow that is important in reactor modeling. To do this, a measure of bed structure must be used; the void fraction distribution $\varepsilon(r,z)$ is usually chosen. Often the axial variation is neglected, and a further simplification is to replace the oscillating voidage profile with an approximate exponential profile that captures only the increase in voidage near the tube wall.

Jakobsen et al. (7) provided an extended treatment of the PMM termed the 2D CFD model. They compared both 1D and 2D versions to classical 1D and 2D dispersion (effective parameter) models. The variations in velocity, pressure, and mixture density allowed in the 1D CFD model significantly affected chemical composition and conversion compared with dispersion models with fixed values for synthesis gas and methanol production processes. Including nonuniform $\varepsilon(r)$ in the 2D CFD model affected axial pressure drop and fluid velocity but had little influence on temperature and species mole fraction profiles.

Wu et al. (8) compared PRCFD (the realistic approach) to the porous medium approach. They noted that the PMM could not reproduce secondary flows and flow anisotropies, such as separation, oscillation, and vortex formation, but could capture average pressure drop and temperature

increase. The PRCFD approach was estimated at 3,000 times the computational cost of PMM. Gao et al. (9) and Zhuang et al. (10) used the two-temperature 2D PMM to simulate reactive processes in fixed beds with turbulent flow. They showed the two-temperature model gave better results compared with experiments than did a single-temperature model but did not present any results on the computed velocity field.

The 2D PMM solves for both velocity components $v_z$ and $v_r$, but because $v_r$ is driven by radial pressure gradients, which are zero across the entire bed diameter, $v_r$ is usually computed as negligible. This is a problem of scales; over a single particle, the radially displaced flow gives a significant $v_r$, but when averaged over the bed radius, the positive and negative variations cancel out. Recently, Hamzah et al. (11) used a form of the PMM to assist in the development of a new segmented continuum approach to radial heat and mass transfer.

The PMM is frequently used to include improved treatment of the velocity field compared with the simpler dispersion models, without incurring the high computational cost of full PRCFD models. There is a need to study whether the computed velocity field is realistic or, indeed, whether it needs to be for good reactor simulation.

## 3. COMPUTER GENERATION OF FIXED BEDS

Conducting accurate resolved particle CFD simulations of fixed beds without having proper packing geometry is impossible. Therefore, computer generation of fixed beds is essential for such studies and has been the subject of many investigations during the past three decades. Spherical particles are the simplest geometry. Soppe (12) showed that ballistic random deposition according to the rain model coupled with a Monte Carlo–based compression process can accurately reproduce the packing of spherical particles and evaluate its properties. Freund et al. (13, 14) used a similar algorithm to successfully generate and study fixed bed properties. Since then, there have been significant advances in the field. The discrete element method (DEM) is a powerful tool to generate packings of spherical and other particle shapes, such as cylinders. The method evaluates the trajectory and velocity of the particles in the system by calculating the forces on each particle owing to gravity and collision at each time step. Eppinger et al. (15) proposed an automated approach for numerical generation of packing spheres and cylinders based on the DEM algorithm. This approach was also capable of generating packings of rings, however, only by replacing the particles in the cylindrical packing. In conventional DEM methods, to have an accurate solution, specific contact detection and force models must be developed for different geometries. A workflow around this approach is to represent (estimate) complex particles with a glued spheres or clumped spheres model. In this approach, many spheres are glued together to represent cylinders, rings, and other shapes. Caulkin et al. (16) showed that this approach can significantly affect the accuracy of the models, especially owing to lack of true representation in the corners and edges. Therefore, in recent years, there have been numerous efforts to develop flexible DEM algorithms for arbitrary particle shapes.

Wachs and coworkers (17–19) conducted thorough investigations to develop generic DEM algorithms for complex particle shapes. Wachs et al. (17) introduced a new algorithm called Grains3D, which allowed simulation of flow dynamics of arbitrary particle shapes. The methodology is restricted to convex particle shapes and serial computing. However, it allows the user to have a combination of shapes and sizes in the simulation. Rakotonirina & Wachs (18) extended the algorithm to a parallel computing framework. Furthermore, Rakotonirina et al. (19) used glued convex particles to represent concave objects in Grains3D, which made the algorithm a very versatile methodology. Seelen et al. (20) also developed a unique methodology to simulate packings for different convex particle shapes. The algorithm advantage is its powerful method for identifying the contact points for the faces in contact.

Marigo & Stitt (21) conducted an extensive study on the accuracy and industrial applications of DEM methods. The authors emphasized calibration and validation as crucial tools for realistic DEM simulations. Furthermore, Yan et al. (22) studied the impact of DEM input parameters using a statistical approach. The authors showed that prior simulations carried out along with sensitivity analysis can help to identify important parameters that should be measured experimentally. Farsi et al. (23) studied the potential applications of the combined finite and discrete element methods (FEMDEM) in numerical packing generation. They suggested that FEMDEM can be used to study the effects of particle–particle interactions during the packing and the impact of the loading conditions on the final packing properties.

Marek (24) presented a numerical algorithm for filling a cylindrical column with equilateral cylinders based on simplified mechanics. The algorithm used sequential deposition and the frozen bed assumption—once a particle was at mechanical equilibrium, it could not be moved by later particles. Collision detection was performed by covering the particle surface with markers and checking their location. Good agreement with radial voidage profiles was obtained, and the orientation distributions were analyzed in a subsequent publication (25).

Boccardo et al. (26) and Partopour & Dixon (27) investigated a promising alternative to DEM for the numerical generation of packing of complex particle shapes. The methodology is based on rigid body dynamics (RBD) embedded in the Bullet Physics library and implemented in the open-source software Blender™. In the framework, particles are defined by surface meshes, and therefore, they can have any arbitrary shapes. The contact detection is carried out based on proximity queries for vertices in the objects. The computational space is usually divided into subspaces using octrees to speed up the calculation. Both studies (26, 27) showed that geometric properties of packings of complex particle shapes can be well reproduced using this methodology. Moghaddam et al. (28) have used very similar RBD methods and implemented an alternative method for transition between moving and resting particles. Fernengel at al. (29) have presented an automated workflow for random packing generation, mesh generation, flow simulation, and reaction simulation using bash and python scripts based on Blender™, OpenFOAM®, and ParaView®.

Fleischlen & Wehinger (30) conducted a comprehensive study to compare computer generation of fixed beds using RBD (in Blender™) and DEM (embedded in STAR-CCM+). They showed the two approaches are in very good agreement, although simulations carried out in Blender™ are less computationally expensive.

In most studies comparing experiments to computer-generated packings, the model generation is based on imaging of the bed. Baker et al. (31) have presented an interesting change to that process by creating the experimental bed using additive layer manufacturing or 3D printing from the computer-generated model. The authors suggest that this could be a new technique for studying flow in packed beds.

## 4. PARTICLE-RESOLVED COMPUTATIONAL FLUID DYNAMICS METHODOLOGY

The main methods for solving the PRCFD models are continuum Navier–Stokes approaches, such as finite volume (FV) and finite element (FE), and particle-based approaches, such as the lattice Boltzmann method (LBM). A third group is the network models based usually on a Delaunay tessellation of the bed structure (32), but this method is restricted to fluid flow at present.

The LBM method has the advantages that no partial differential equations need to be solved and it is computationally efficient and easy to parallelize. A related method, stochastic rotation dynamics, has recently been used (33) to determine the solvent hydrodynamics in a catalytic reactor.

The LBM is inherently transient in nature, and early versions could simulate only flow problems (with optional species) owing to the difficulty of including thermal relaxation times. Recent developments have led to the use of multiple–relaxation time collision operators to include thermal collisions (34). Unresolved problems are the inability of the LBM approach to include conjugate problems and high-*Re* turbulent flows owing to the wide variety of temporal and spatial scales needed. Li et al. (35) reported an application of LBM to a fixed bed, but the reaction was confined to the catalyst surface.

The continuum methods solve conservation equations of macroscopic quantities in the form of the Navier–Stokes equations defined on a region of space, which is discretized (along with time for unsteady problems) on a partition or mesh. This is the basis for most software packages; for example, FV is the most popular and is used in ANSYS-Fluent, ANSYS-CFX, Star-CCM+, and the open-source code OpenFOAM®. FE is preferred in the Multiphysics environment of COMSOL®. There have been very few uses of PRCFD in COMSOL®; for one example, see work by Touitou et al. (36). COMSOL® is a fine element–based solver that is more suited to PMM models, which generally have smaller meshes. Most published work uses ANSYS-Fluent or Star-CCM+. We focus mainly on continuum methods in this review, because at the moment they have the greatest potential for catalytic reactor simulations.

## 4.1. Meshing

The geometrical domain must be discretized or meshed into smaller regions for solution by one of the CFD algorithms. Many ways to do this have been developed, reflecting different balances between fidelity to the original geometry, ease of mesh generation, and accuracy/cost of the ensuing solution method. The two main classes of mesh are structured and unstructured. For a structured mesh, the distribution of nodes throughout the domain is known once the surface nodes are set, as the domain nodes are projected from the surfaces. For unstructured meshes, nodes are generated as a space-filling algorithm sweeps through the domain. A mixture of these, hybrid mesh, can be obtained by subdividing the domain.

For the LBM method, Cartesian structured meshes are used, and curved boundaries are accommodated using a cut-cell approach. This can lead to a staircase representation of a curved boundary, requiring refinement of the mesh. Structured meshes are easier to set up and require fewer cells.

For FV and FE solvers, many types of mesh are used. Most common in complex geometries is unstructured (usually tetrahedral) cells fitted as closely as possible to the original surfaces. Because there are usually strong boundary layer gradients and accurate fluxes are desired at interfaces, layers of thin hexahedral prism cells are frequently used in a body-fitted mesh. Recently, polyhedral cells have been used to reduce mesh size and increase computational stability.

One attempt to combine the advantages of both main mesh types is the so-called chimera grid (37), in which a hexahedral background mesh is overlaid by local body-fitted meshes. This requires increased computational overhead for the interpolations necessary to exchange information between meshes.

Several alternatives to the use of Cartesian grids for fixed beds have been suggested. Finn & Apte (38) compared body-conforming tetrahedral meshes to non-body-conforming fictitious domain approaches. Sulaiman et al. (39) coupled the sharp interface method to a fictitious domain two-phase flow solver to treat convective mass transfer around reactive particles. Das et al. (40) have used an immersed boundary method (IBM), originally applied to particulate flows, for simulations of foam and particle fixed beds. Most recently, Yuan et al. (41) put forward a method to combine immersed boundary and adaptive meshing methods.

The body-fitted grid combined with a FV approach is most common, as it can directly resolve the solid–fluid interface. Disadvantages are the resulting high cell count, more difficult mesh refinement for error estimation, and problems with particle–particle and particle–wall contact points, which can lead to highly skewed cells.

## 4.2. Contact Points

A meshing problem that is specific to PRCFD is that of contact points, either particle–particle or particle–wall. Packings of ideal spheres have point contacts, but packings of cylinders and other shapes can have point, line, and area contacts, which present many more difficulties. Mesh cells can be distorted or very small, which leads to large, expensive meshes.

Early approaches for spheres (3) shrank all particles by a fixed amount, e.g., 0.5–2% of diameter, the gap method. This is the easiest to implement and performs reasonably for flow simulations for 1% reduction or lower. Guardo et al. (42) suggested expanding the spheres, the overlap method. They reported no meshing problems, but this method does not eliminate a narrow fillet of fluid. The gap and overlap methods are termed global methods.

Local methods involve changing the geometry only in the vicinity of the contact points. The bridges method (43) replaces the fluid and a small portion of the particles with a small cylinder at the contact point. The caps method (44) introduced the idea of moving the surface nodes near a contact point to locally flatten the curved surface—equivalent to removing a spherical cap.

Several authors have compared these methods for spheres. Dixon et al. (45) found that global methods of gap and overlap at 1% changed the $\varepsilon$ and $\Delta P$ by too much. Local methods gave much smaller changes in $\varepsilon$ and $\Delta P$. For heat transfer, the caps method omits the finite area contact conduction, and so the bridges method was preferred. To obtain the correct heat flow, the correct bridge thermal conductivity must be used, and formulas were given for spheres. These conclusions were supported (46) in an investigation of flow and heat transfer; both studies recommended the bridge diameter should be smaller than 20% of the particle diameter. Rebughini et al. (47) extended the bridge method to cases of isothermal external surface reaction on the particles, at lower *Re*, and recommended bridge-to-particle ratios of 0.15 or higher to avoid skewness in the cells. They found conversion was unaffected for ratios up to 0.3.

For nonspherical particles, the problem is much more difficult. The main task is finding the contacts, which is easy for spheres. Contact algorithms have been developed for full cylinders (48), which Wehinger et al. (49) used to develop methods based on bridges and caps and to introduce a new united method.

For more complex particle shapes, it will be difficult to extend the bridges method, particularly the bridge thermal conductivity formulas. Methods based on local mesh rearrangement, such as Laplace smoothing, are easier to implement but may miss some heat-transfer pathways, especially at the tube wall where gradients are steep. There is considerable room for development of this topic.

## 4.3. Microkinetics for Particle-Resolved Computational Fluid Dynamics

There are two main methods to couple microkinetics models with PRCFD simulations. The traditional method is to add microkinetics as boundary conditions for the flow field on the fluid–solid interface. In this method, surface flux for each species is calculated using the detailed reaction mechanism presented by the microkinetics model based on the temperature and partial pressures of species at the solid–fluid interface. The method is reliable for very fast reactions where the rate is controlled by diffusion. In these systems, reaction mostly happens on the surface of catalyst

particles (e.g., methane partial oxidation on Rh). However, this framework could fail when reaction also happens inside the particles. Therefore, a second methodology (with different approaches) was introduced to include the reaction inside the solid catalyst particles. Maestri & Cuoci (50) introduced a transient multiregion operator splitting CFD approach to couple CFD with full microkinetics models, whereas Dixon et al. (51) presented a steady-state solid particle approach to couple microkinetics to transport and reaction inside the particle. Both methods are discussed in more detail in the following section. Matera et al. (52) developed a numerical framework to integrate first-principles kinetic Monte Carlo microkinetic models into stagnation flow and channel flow reactors, but this has not yet been applied to fixed beds. Partopour et al. (53, 54) suggested two different approaches based on full numerical solution of the microkinetics models learned by either multivariate splines or random forest trees. Votsmeier has also shown the computational savings gained by using multivariate splines to interpolate precomputed reaction rates (55). Rebughini et al. (56) proposed to use a cell agglomeration algorithm, whereas Blasi & Kee (57) used in situ adaptive tabulation for the task. All the approaches mentioned above successfully couple the reaction inside the catalyst particles with flow and transport. The second methodology (reaction inside the particles) is more reliable than traditional methods (reaction as flow boundary condition) when it comes to slow reactions. However, it is computationally more expensive than the traditional method.

It should be noted that when reaction is added via boundary conditions, usually, the mass and heat flux vectors only point outward into the fluid region. This is physically incorrect; in reality, the heat flux could be directed into the solid catalyst particles too.

## 4.4. Pellet Effective Medium Models

To model the reaction and diffusion inside the solid catalyst particles for PRCFD, effective medium models are necessary. The catalyst pores can range from nanometers to micrometers and are several orders of magnitude different in scale to the dimensions of the void space that determine transport and flow in the bed. Therefore, resolving pore geometry for fixed beds of several hundreds of particles is computationally extremely difficult if not impossible. Several studies have evaluated the accuracy of different effective medium models for species diffusion inside the particles. Dong et al. (58) showed that bimodal diffusion models with both macro and micro pore sizes could be used to study the overall performance of the fixed bed and tune important parameters such as selectivity and convergence. Wehinger et al. (59) compared three different approaches for incorporating transport into catalyst particles in fixed bed CFD: the instantaneous diffusion, effectiveness-factor, and 3D reaction–diffusion models. The authors suggested the instantaneous diffusion model results in significant error for reactor simulations. Furthermore, although the 3D reaction–diffusion model has superior accuracy, its computational time could be 200 times slower than the other approaches. The effectiveness-factor model, they believe, could perform reasonably well while keeping the computational cost manageable. They emphasize studying the catalyst structure (e.g., pore size distribution and bulk porosity) before choosing the right approach. Donaubauer & Hinrichsen (60) compared the three main effective multicomponent diffusion models: the dusty gas, binary friction, and mean transport pore models. Their results suggest that the discrepancy between these models is negligible. Furthermore, they identified porosity, tortuosity, and pore diameter as the most important parameters for effective diffusivity, respectively. Partopour et al. (61) studied the effects of flux dependency and anisotropic diffusion on the conventional Fickian simplification of the dusty gas model. The results showed that species flux changes inside the catalyst particles have considerable impact on the diffusion coefficient, whereas anisotropic effects owing to temperature and species gradient in 3D are negligible.

Two studies have examined resolved-pore simulations of thin catalyst layers: Bufe et al. (62) simulated diffusion and reaction in liquid-filled transport pores for Fischer–Tropsch synthesis to obtain optimal values of catalyst layer thickness and porosity, and Partopour & Dixon (63) simulated CO oxidation in a catalyst layer of $Rh/Al_2O_3$ where the macropore structure was explicitly modeled and the interaction between transport and reaction was shown. The coupling of resolved-pore modeling in catalyst pellets with resolved-particle modeling of the fixed bed is a level of simulation that is not yet achievable given present computational abilities.

## 4.5. Fluid-Particle Coupling

Early studies using PRCFD either ignored intraparticle transport or allowed only heat transfer inside the pellet. For heterogeneous catalytic reactor simulations, it is desirable to include chemical species inside the particle. A first approach to this treated the particles as porous regions (64, 65), with extra terms in the momentum balance to account for additional flow resistance. This method has been shown (51) to allow too much convective heat and mass transfer into the particles and cannot be used unless a prohibitively fine mesh is placed at the particle surfaces.

A new method was put forward that models the particles as solid regions (51) and that employs user-defined scalars to stand in for mass fractions of species inside the particles. Care must be taken to properly couple the mass fractions and the species fluxes across the particle–fluid interface. Several groups (66–70) have successfully used this method.

Maestri & Cuoci (50) put forward a different approach to the fluid–particle coupling problem. Their priority was solving large sets of species balances arising from detailed microkinetics models. They coupled microkinetics reactions with CFD simulations using an operator-splitting technique that separates the fluid transport and particle reaction timescales. The authors developed a new open source solver that works in the OpenFOAM® environment, called CatalyticFOAM. They applied it to a 3D model of a narrow bed of eight Raschig rings. In this initial work, only a surface layer of catalyst in contact with the flow was active. Maffei et al. (71) further developed the code to allow internal heat and mass transfer in the pellets. These were successfully tested on a packed bed of 50 spheres using a microkinetic model of $H_2$ combustion on Rh. Bracconi et al. (72) incorporated the in situ adaptive tabulation method into the operator-splitting algorithm to improve the handling of large sets of microkinetics equations and tested it on a packed bed of 25 spheres using methane steam reforming.

The operator-splitting method has been implemented in commercial software such as STAR-CCM+. Other approaches have been developed, such as the CAT-PP method for highly diluted heterogeneous catalytic systems (73) and DUO, which is an interface for OpenFOAM® and DETCHEM™ for elementary step kinetic modeling (74). DUO has been applied to coated honeycomb monoliths but not yet to fixed beds.

The operator-splitting method is inherently transient, although steady-state simulation is possible by pseudotime steps; the iterative structure makes it computationally expensive, and it is limited to surface kinetics, requiring a geometric correction factor for catalyst particles. The solid particle method can be slow to converge, owing to the longer timescale needed for intrapellet transport, and requires a nontrivial amount of user-defined coding. It can, however, represent reaction throughout the pellet. At present, both methods are in use.

## 4.6. Turbulence Models in PRCFD

Flow regimes in packed beds (75) range from viscous flow ($Re < 1$) to steady laminar inertial flow ($5 < Re < 60$), unsteady laminar inertial flow ($60 < Re < 120$), and turbulent flow

($Re > 120$). However, other studies (76) have suggested that turbulence does not appear until $Re > 900$, although the transition to turbulence can take place at different locations in the bed corresponding to different local flow rates.

Direct numerical simulation (DNS) in which all time- and length scales are resolved is not practical for anything more than small clusters of particles, as fine meshes and small time steps are needed. A compromise is large eddy simulation (LES), in which smaller length scales are modeled and only larger ones are resolved. The most common method is to use Reynolds-averaged Navier–Stokes (RANS) models in which all length scales are modeled, and which are based on the turbulent viscosity concept.

Lee et al. (77) found that LES was preferred in their study of pebble beds, along with the $k$-$\omega$ RANS model. Dixon et al. (78) compared turbulence models for drag and heat transfer on a single sphere and also found that LES and the shear stress transport (SST) $k$-$\omega$ model gave superior results. Shams et al. (79, 80) put forward their improved delayed detached eddy simulation method, which is a blend of LES and unsteady RANS. Note that LES and its derivatives are inherently unsteady methods, requiring time integration up to a statistically stable steady state, which can be computationally expensive.

Guardo et al. (81) compared the Spalart–Almaras, $k$-$\varepsilon$, $k$-$\varepsilon$ RNG, $k$-$\varepsilon$ Realizable, and $k$-$\omega$ RANS models and preferred the Spalart–Almaras model. Coussirat et al. (82) included Reynolds stress models and concluded they were no better. $k$-$\varepsilon$ models are the most common but are known to be poor for swirling and rotating flows and flows with strong separation, such as are found in PRCFD simulations, and do not perform as well as LES. More recently, Karthik et al. (69) confirmed these results for water flow in beds of spheres with different turbulence models compared with their experimental measurements. Jiang et al. (83) studied the local flow structure and turbulence quantities, such as the distribution of $k$ and $\varepsilon$ and the distribution of vortices with different intensities.

As important a decision as the choice of turbulence model is the choice of wall treatment, given the large amount of solid surface in fixed beds. The standard wall functions require $y^+ > 30$, but this is difficult to obtain in fixed beds, because flow over the particle surfaces varies strongly, and $y^+$ can range from one to several hundred over a single particle surface. A popular choice is some form of interpolation between using a resolved-layer approach for low $y^+$ and wall functions for larger $y^+$, embodied in enhanced wall treatments in most of the available commercial codes.

To date, there is no clear recommendation regarding choice of turbulence model. Good turbulence models (LES) are unsteady and expensive and are restricted to small beds of particles. More realistic beds can be simulated using RANS models, but all have shortcomings. More insight is needed as to what is gained in engineering predictions by using more refined turbulence models.

## 4.7. Newer Methodology in PRCFD

Despite many PRCFD simulations of flow and heat transfer in the literature, radiation has been included only recently. Behnam et al. (84) used the surface-to-surface (S2S) model in a validation study of a single-pellet-string reactor. Wehinger et al. (85) also used S2S radiation in a CFD model of dry reforming to compare with experiments. More extensive studies (86, 87) compared the S2S model, based on precomputing view factors, to solving the radiative transfer equation via the discrete ordinates method for a steam reforming gas mixture. The S2S model was recommended based on lower computational cost, with both models giving similar results. A strong argument was made that radiation should not be neglected in simulating this process, based on steam reforming simulations in a short 0.5-m length of packing representing the reformer tube inlet, at flow rates corresponding to $Re = 755$ and 7,554, with the tube wall temperature held constant

220 K above the inlet gas temperature. Results showed significant differences in temperature for the low reforming flow $Re = 755$ (up to 50 K), but less so for $Re = 7554$ (less than 20 K) and decreasing with tube length. This is to be expected for the higher $Re$, for which radial thermal dispersion will be larger and the relative contribution of radiation will be smaller. This is in accord with industrial experience on long reforming tubes at high flow rates (84).

Most PRCFD studies have been focused on steady-state operation. The dynamic behavior of the reactor is an important issue, as understanding the transient effects of process changes and disturbances is essential for safe and proper reactor operation. Simulations of an ethylene oxide reactor tube under unsteady conditions were run (88) using steady-state kinetics assuming rapid surface equilibration compared with transport processes, so a single timescale could be used. The mesh was made up of 24 M cells, and transients of wrong-way behavior, reactor shut-off, and reactor start-up were studied. These simulations were very demanding of computer time, taking approximately a week to simulate one second of real time. Routine use of dynamic PRCFD will need bigger, faster computers than were available in that study.

## 5. FIXED BED STRUCTURE AND HYDRODYNAMICS

To validate the computer generation of fixed beds, the radial void fraction profile caused by wall effects (89) is most frequently compared with experiments or standard correlations. This is usually done for spheres, as experimental data are scarce and correlations virtually nonexistent for nonspheres. Beyond voidage profiles, for cylinder-based shapes, the distribution of orientations (25–27, 90) of the particles with respect to the tube axis can be assessed.

As computer generation methods continue to improve, confidence in them increases, and we can consider using them for the development of new information. Correlations of $\varepsilon(r)$ for, e.g., cylinders, rings, and multihole particles could be developed for use in formulas for effective parameter models. New features of packed bed structure, such as coordination number, can be investigated as well.

The influence of filling methods is being studied (91) in producing loose or tight packings. Correlations of void fraction are needed for various packing states and different particle shapes. Agrawal et al. (92) have used computer generation of sphere packs to investigate whether packing defects observed at the top of the bed propagate through the bed, causing local flow variations. They suggested that measures of packing nonisotropy should be considered, in addition to measures of void fraction.

Virtually all PRCFD simulations of packed beds report the axial pressure drop and the radial profile of the axial velocity. These quantities are often compared with experiments for validation of CFD methodology, as well as being highly relevant for the development of dispersion-type reaction engineering models. Vollmari et al. (93) recently used PRCFD to assess pressure drop correlations for packings of complex shapes.

Unfortunately, quality data inside a packed bed are hard to obtain. Some recent examples are the magnetic resonance imaging studies of water flow of Robbins et al. (94) and Lovreglio et al. (95). Using near-infrared tomography, Alzahrani et al. (96) visualized gas flow in beds of spheres. Buwa and colleagues (69, 97) used particle image velocimetry, again for water as the working fluid with spheres. All of the above authors carried out PRCFD simulations in parallel with the experiments and obtained acceptable, if not perfect, agreement between them. There is a need for more velocity data for the gas phase and nonspheres.

Most PRCFD simulations of fluid flows have been for beds of spheres (83, 95, 98). Dorai et al. (99, 100) simulated flow through square ducts packed with spheres, cylinders, cubes, and tetrahedra to obtain probability distribution functions of velocity and to study the influence of microstructure

in the beds on pressure drop. Marek (101) simulated laminar flow in beds of Raschig rings by using the IBM, whereas in later work (102) gas flow maldistribution was investigated for similar beds of cylinders and rings. Pavlišič et al. (103) used PRCFD to develop pressure drop correlations for beds of cylinders, trilobes, and quadrilobes. Finally, Moghaddam et al. (104) have examined flow in beds of spheres and cylinders to contend that the usual azimuthal (angular) averaging for deriving velocity profiles from PRCFD fails to capture the effects of local flow features such as vortex regions.

## 6. FIXED BED HEAT, MASS, AND REACTION

Resolved particle CFD simulations are intended to study the interactions of transport phenomena (heat and mass transfer and flow field) with reaction kinetics. These phenomena impact each other simultaneously during the reactor operations. Often, chemical reactions are highly endothermic or exothermic. The heat generated or consumed affects the temperature of the flow field and particles, and most transport parameters are also temperature dependent. The temperature profile within the reactor is also highly affected by the flow patterns. Clearly an accurate model of fixed beds must consider all these variations and interactions. Therefore, many studies during the past years (for example, 105) have addressed these issues.

Yang et al. (106) studied the effects of the fixed bed geometrical properties (e.g., particle size and wall distance) on flow and temperature profile in packings of mono- and polydispersed spheres. The authors showed that for packing of uniform spheres with fixed heat flux at the wall, the velocity profile is higher and temperature is lower near the wall owing to high voidage. In packing of polydispersed particles, with smaller particles near the wall, the voidage near the wall was decreased, and therefore the temperature gradient owing to wall effects was improved. Although this method increased the radial heat transfer efficiency because of the smaller particles, pressure drop was increased. This study shows applications of resolved particle CFD simulations for optimal design. Zhang et al. (107) conducted a similar study for uniform randomly packed beds of cylindrical particles and showed similar flow and temperature gradients near the wall to the packing of spheres. The authors also proposed an improved 2D homogeneous model by incorporating the results of their 3D resolved particle model. Dong et al. (108) validated their resolved particle CFD simulations using novel profile reactor measurements. They studied the radial heat transfer for packings of spheres and rings. Although the simulations did not include the sampling capillary used in the experimental measurements, very good agreement between the simulations and the lab tests was found.

Das and coworkers (40) followed a different approach for studying the flow and heat transfer in packing of spherical particles. The authors used fully resolved DNS with a sharp interface IBM. The advantage of the proposed coupling approach is the ability to avoid the meshing difficulties near the particle–particle and wall–particle contact areas. However, the mesh is not fully fitted to the particles; despite that, good agreement for heat transfer and pressure drop with existing correlations in the literature was found. Furthermore, the authors proposed new correlations for wall-to-bed heat transfer.

Several recent studies have also used fixed bed CFD simulations to investigate large-scale important industrial reactions, such as ethylene epoxidation, maleic anhydride production, and steam and dry reforming of methane. Karthik & Buwa (68) and Singhal et al. (109) studied fixed beds under methane steam reforming conditions using resolved particle simulations. The latter group studied spherical particles, whereas the former investigated several particle shapes, such as trilobe, hollow cylinder, and 7-hole. Both studies included only a limited number of particles and a short fixed bed length. Karthik & Buwa's (68) study results show that shaped particles, such as trilobe

and daisy, reduce the pressure drop and increase the dispersion in the methane steam reforming fixed bed, whereas particles with hollow sections improve the conversion owing to reduction in diffusion limitations. Singhal et al. (109) used the simulation to improve their 1D packed bed model and applied it to packed bed chemical looping reforming.

Partopour & Dixon (110) studied ethylene partial oxidation to ethylene oxide using resolved particle CFD. The study highlighted the failure of reduced microkinetics models under extreme temperature and species gradients that form in 3D CFD simulations of fixed bed reactors.

Both Partopour & Dixon (111) and Dong et al. (112) conducted studies of *n*-butane partial oxidation over iron molybdate catalyst. The former group focused on effects of temperature gradient on selectivity and surface oxygen profiles along a long bed of 800 spherical particles and showed that surface oxygen is highly correlated with temperature profile inside the fluid and solid particles and controls the reaction selectivity. The latter group studied the fixed bed behavior filled with Raschig rings and validated their study with profile reactor measurements. Furthermore, they developed an optimum wall temperature profile using their fixed bed CFD model and incorporated the temperature profile into their experimental setup whereby, as a result of the new temperature profile, selectivity was improved by 3% and the hot spot was removed from the bed.

Wehinger et al. (113, 114) studied dry reforming of methane using a similar methodology. In their first study, they showed the feasibility of coupling detailed surface kinetics with fixed bed CFD simulations, whereas in the second study they presented the effect of different particle shapes in the system. They showed that packing of the cylindrical particles resulted in superior yield and conversion compared with rings and spheres.

Behnam & Dixon (115) investigated local carbon formation in fixed beds under steam reforming conditions, which is one of the main industrial issues in fixed bed reactors. They showed the carbon formation is highly location dependent, where the maximum rate is on the outer surface of the particles and correlated with temperature profile in the particles. Alzahrani et al. (116) used a combination of PRCFD and near-infrared tomography to study the deactivation of CO in the preferential oxidation of CO and also found that deactivation was highest at the pellet surface.

## 7. PARTICLE-RESOLVED COMPUTATIONAL FLUID DYNAMICS AND CHEMICAL REACTION ENGINEERING MODELS

Given the high cost of PRCFD simulations, their routine use as design models may be some distance away, and their use for control or optimization is not likely to be feasible for a long time, if ever. A very significant role for these methods is therefore to provide baseline data to improve or develop parameters for use in simpler chemical reaction engineering models.

Particle-to-fluid heat and mass transfer coefficients are critical to models of catalytic reacting systems. Atmakidis & Kenig (117, 118) simulated dissolution of benzoic acid spheres in water and sublimation of naphthalene spheres in air. They showed that PRCFD gave good agreement with literature correlations. Bale et al. (119) used DNS simulations at $Re < 100$ to study the influence of the tube wall on the local mass transfer coefficient and found that it was higher for particles near the tube wall, owing to the higher velocity there. In a second study (120), they showed that $N$ affects the influence of exit and entrance regions on the mass transfer coefficient.

Kruggel-Emden and coworkers (121, 122) used LBM to study heat transfer; they used favorable comparisons of the heat transfer coefficient for benchmark simulations of single and small clusters of spheres to confirm their thermal lattice approach. A new correlation was derived for low $Re$ (20–100) and for random packings of spheres with high void fractions (0.6–1). Buist et al. (123) used IBM to obtain the heat transfer coefficient for some semistructured arrays of spheres to compare with their experimental studies. Sun et al. (124) also used a variation of IBM for spheres at

$Re < 100$ and $\varepsilon = 0.5$–$0.9$ to obtain a new correlation and develop a consistent two-fluid model. Singhal et al. (125, 126) used PRCFD to derive new heat transfer coefficient correlations for spheres and cylinders without wall effects at $\varepsilon \approx 0.4$ (spheres) and 0.5 (cylinders of aspect ratio 4), again at $Re < 100$. Based on the existing studies, there is a need for work at higher $Re$, for more complex particle shapes, and for a focus on dense packing typical of fixed beds.

The use of PRCFD for bed-scale longitudinal and transverse dispersion of mass in fixed beds has been less studied. This may be due to the need for longer beds of particles to obtain meaningful statistics of the dispersion processes. Jourak et al. (127) built a network model based on thousands of spherical particles. Their calculations simulated a breakthrough experiment for longitudinal dispersion and a coated wall dissolution experiment for transverse dispersion at low Peclet number values. Good agreement with experimental results reported in the literature was obtained.

Dixon & Medeiros (128) studied transverse dispersion with a focus on wall effects in narrow tubes of spheres. Simulations of dispersion from a coated wall were run for $87 < Re < 870$. The objective was to see what effective parameter models were needed to account for the experimentally observed decrease in transverse dispersion near the tube wall. A model with constant dispersion coefficient was inadequate to describe the radial concentration profile. Addition of a wall mass transfer coefficient improved agreement somewhat, but the best results were given by a three-parameter model of a radially varying dispersion coefficient. Extensions of these approaches to nonspherical particles and to longer tubes could yield interesting results.

Determination of reliable correlations for the effective radial thermal conductivity and the wall heat transfer coefficient in low-$N$ fixed beds has been a long-standing problem. The effective radial thermal conductivity is usually split into static and dynamic terms. Dixon et al. (129) used PRCFD in an annular bed of spheres with $N = 4$ to test literature correlations for the radial variation of stagnant thermal conductivity. Mathey (130) advocated the use of traditional models with CFD input. An upscaling approach was used in which dispersive kinetic energy was obtained from $k$-$\varepsilon$ CFD and used to model the thermal dispersion term. Channeling effects near the walls were also considered. The needed closures for the macroscopic equations were obtained from microscopic CFD of 3D periodic arrays of spheres and cylinders. Thiagalingam et al. (131) studied physical mechanisms contributing to wall heat transfer using 3D periodic packings of spheres and rings. They used CFD to get turbulent and dispersive mixing contributions to the overall heat transfer coefficient in a 1D model. In a subsequent contribution, Thiagalingam & Sagaut (132) used a similar strategy to derive a four-region formula for effective radial thermal conductivity, introducing the idea of a disrupted thermal boundary layer together with a channeling effect.

Dixon (133) used PRCFD simulation of steam methane reforming in a tube of $N = 5.96$ spheres to provide benchmark data to evaluate levels of model complexity, i.e., 1D and 2D effective medium models. The 1D model could not reproduce axial profiles without tuning the particle–fluid heat and mass transfer coefficients. The 2D model gave good agreement if local void fractions and axial velocity profiles were included.

PRCFD can also be crucial to the development of new model approaches to radial heat transfer. Behnam et al. (134) have suggested a 2D pseudocontinuum model in which the effective thermal dispersion contribution is replaced by direct inclusion of axial and radial velocity components obtained from PRCFD, along with radially varying stagnant thermal conductivity (129). A different new approach by Barreto and colleagues (135) develops a two-region, 2D model with a heat transfer coefficient between wall and core channels and includes a true wall-to-fluid heat transfer coefficient. They used PRCFD simulations on regular sphere arrays to evaluate these parameters for convection (136) and gave a new model for conduction under stagnant conditions (137). Similarly, Hamzah et al. (11) proposed porosity-dependent, segmented-continuum approaches, using PRCFD to obtain dispersion parameters.

## 8. NEW APPLICATIONS

Two relatively new types of packed beds in which PRCFD can play a role are micro packed bed reactors and packed foam reactors. Micro packed bed reactors are a configuration of small catalyst particles packed into the channels of metallic honeycomb matrices to enhance the heat transfer properties and increase the catalyst load per reactor volume of structured reactors. In packed foam reactors, either the empty pores of highly conductive metallic open-cell foams are filled with small catalytic particles or catalytic particles are made out of the foam. The presence of the particles increases radial and axial thermal dispersion to supplement the high thermal conductivity of the foam, as well as to increase the catalyst inventory in the reactor.

Maestri and coworkers (138, 139) have used PRCFD as the most detailed simulation and highest level in their proposed hierarchical approach to reaction model development. In the first study (138), detailed 3D simulations of a packed honeycomb channel provided suitable correlations for gas-to-particle mass and heat transfer in micro packed beds. Good agreement was obtained with a 1D heterogeneous effective parameter model showing the potential of hierarchical derivation of transport parameters using PRCFD. A follow-up study (139) treated the radial heat transfer properties, which are enhanced in a packed microchannel, and showed that a literature correlation for the overall heat transfer coefficient $U$ was applicable to a single packed channel of the honeycomb matrix. This was then used in a 2D model of the matrix to simulate the partial oxidation of *o*-xylene to phthalic anhydride, showing the use of the hierarchical approach when PRCFD would be too expensive.

Kolaczkowski et al. (140) suggested using catalyst pellets made out of actual foams as supports. Foam pellets have large open regions that allow reactants into the pellet, have lower pressure drop owing to higher void fraction, and increase heat transfer by both conduction and radiation. Das et al. (141) used the IBM to resolve flow around cubic porous particles, whereas flow through the particle was represented using closure terms. Wehinger et al. (142) took a similar approach to resolve fixed bed structure using FV CFD, whereas they used a PMM for flow and heat transfer in the foam cubes.

CFD has been used to resolve the structure of tubes containing open-cell foams; Dong et al. (143) provide an example with a comparison to spatial profiling data. Foams with particles filling the pores are a newer concept, and the available studies are experimental (144). This would appear to be an excellent opportunity to use PRCFD in combination with resolved-foam CFD to investigate the new configurations.

## 9. CONCLUDING REMARKS

The application of CFD to fixed bed modeling and design can be divided into two directions: PMM and PRCFD. The former is well accepted, although more extensive tests of its predictions would be useful. Most current research interest lies with PRCFD. Our review of the literature developments in the last 10 years or so reveals some areas in which satisfactory progress has been made and some in which more remains to be done.

One theme that emerges is the need for the field to move away from spheres to consider the complex particle shapes used in practice. This has been done in computer generation of packings, but problems remain in meshing and handling of contact points. Another area is the desire to include more realistic microkinetics reaction schemes; promising methods have been put forward, but often these lead to either restrictions in the reactor model or excessive computation time. Effective medium models must be used for the catalyst pellets; resolved-pore calculations are out of reach at present. Simulations of larger numbers of particles to approach industrial scales of tube

diameter and length, and improved turbulence approaches for high flow rates, also remain goals for the future.

Considerable activity and progress exist in using PRCFD to simulate reacting systems and to provide data and correlations for effective parameter models. These efforts will continue, with new applications such as foams and new methods such as radiation. It is not clear that PRCFD can replace effective parameter models for design in the near future, but it can contribute to new reactor development, new and better catalyst shapes, and improved understanding of fixed bed reactors.

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