1D and 2D porous Media fixed bed reactor simulations with DUO

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Fixed (aka packed) bed reactors are the workhorse of the chemical process industry. As computational capabilities become less expensive, increasingly complex models are developed, like Particle Resolved CFD (PRCFD), to explore in detail the interaction between flow and chemistry. In some circumstances PRCFD may be the preferred analysis method, such as when ratio of the particle diameter to tube diameter, *N*, is small (e.g., when *N = Dp/Dt < ~5*). Unfortunately, PRCFD is computationally expensive, as discussed by [1], where DUO (DETCHEM [2] und OpenFOAM [3]) coupling was used to simulate Catalytic Partial Oxidation (CPOX) and Dry Reforming of Methane (DRM) in packed beds with 86 spherical catalyst particles. The typical calculation in [1] required ~8000-core hours without chemical acceleration (ISAT and/or cell agglomeration), and 200 to 800-core hours with chemical acceleration. For many practical engineering applications, even 200 core hours is too computationally intensive.

The DUO solver mentioned above extends OpenFOAM in several ways, including the implementation of surface reactions through the use of a shared library containing the DETCHEMTM surface reaction solver. In addition to chemical acceleration for surface reactions, prior work with DUO demonstrated mixture averaged and multicomponent diffusion along with a favorable comparison against ANSYS FLUENT [4], external coupling of 3D CFD to 2D and 1D DETCHEM solvers to accelerate the simulation of a monolith reactor with many individual flow channels [5], and integration with DAKOTA to optimize the placement and loading of catalyst to optimize hydrogen production in a surface coated reactor [6]. DUO is available for OpenFOAM v10 and OpenFOAM v2212, and all DUO calculations presented here were done with OpenFOAM v10. It is also noted that DETCHEM includes a 1D Packed Bed Reactor (DETCHEMPBR) tool that is extremely fast and also useful for comparisons against DUO.

With respect to the modeling fixed bed reactors, one way to reduce the computational intensity is to use a porous media model, which can reach a steady state solution in as little on the order of minutes to an hour on 2-4 cores. Although OpenFOAM presently has the capability to model heat transfer in porous media with separate fluid and solid energy balances via the *interRegionHeatTransfer* fvModel, heat transfer between the fluid and solid phases occurs via a fluid-solid heat transfer coefficient with a fixed value, and chemical reactions are evaluated at the fluid temperature. While this latter assumption may be appropriate for homogeneous reactions, for heterogeneous reactions, which occur at the fluid-solid interface, this assumption is often not appropriate. As such, the energy equation in DUO is extended so that the mixed phase (fluid + solid) energy equation is modelled with a single equation at steady state:

|  |  |
| --- | --- |
|  | (1) |

where is the sensible enthalpy, is the total sensible enthalpy ( = , is the enthalpy of formation (the term represents the heat of reaction), and is the sensible enthalpy of the specie. α*eff* is the effective thermal diffusivity, where , is the mass and porosity weighted heat capacity, and *keff* is obtained from literature correlations for packed bed heat transfer.

Meanwhile, the steady state species transport equation is:

|  |  |
| --- | --- |
|  | (2) |

where is density, *Yi* is mass fraction and is the source term for the specie, *u* is the superficial fluid velocity, is the mixture averaged diffusion coefficient for the ith species, and is the correction velocity, which ensures overall mass conservation according to Equation 3.

|  |  |
| --- | --- |
|  | (3) |

Here is the mass diffusion flux for the specie.

The results obtained using this porous media approach for modeling fixed bed reactors to can be very accurate as shown in Figure 1. In Figure 1 (left), DUO 3D PRCFD with 86 spherical particles (in a case setup similarly to the calculations described in [1], including the DRM microkinetic surface mechanism) is compared against a DUO 2D porous media model at the centerline in a 0.5 m length bed with *usuperficial* = 0.5 m/s. Here *N = 2* (i.e., a packed bed where the tube diameter is *2x* that of the particle diameter). As previously mentioned, low *N* values are challenging to model with 1D and porous media methods, but curves showing temperature, CO, H2 and CH4 mole fractions match closely between 2D and 3D PRCFD results. In another test (Figure 1, right), DETCHEMPBR and DUO 2D are compared against Steam Methane Reforming (SMR) experimental data presented in [7]. Here, the gas-phase pseudohomogeneous mechanism proposed by [7] is used to model SMR and Water Gas Shift reactions (WGS) reactions that occur in the 0.15 m length reactor. The parity plot (calculation CH4 conversion vs. experimental CH4 conversion) shows an excellent match against experimental data for both DETCHEMPBR and DUO 2D. The 2D cases in Figure 1 each required about 2 to 4-core hours.

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Figure 1: Comparisons of DUO 2D against 3D PRCFD for DRM (left) at N=2, and DUO 2D plus DETCHEMPBR (1D) versus experimental data from [7] for Steam Methane Reforming (right).

Even further acceleration can occur if DUO is configured to solve the porous media in one dimension. Presently, OpenFOAM is capable of solving 1D reactive flows if the boundary condition is adiabatic (i.e., *zeroGradient*) or isothermal. By further extending the energy equation to include an overall heat transfer coefficient (*U*), DUO can be used to model nonadiabatic nonisothermal fixed bed reactors. *U* is calculated according to [8]:

|  |  |
| --- | --- |
|  | (4) |

where *Rt* is the tube diameter, *hw* is the wall heat transfer coefficient, and *Bi* is the Biot number. Additional literature correlations are used to calculate *hw* and *Bi*.

As shown in Figure 2, for the DRM test case, the 1D DUO result (temperature as well as CO, CH4, and H2 mole fraction vs. axial distance) perfectly matches the 1D DETCHEMPBR result for a DRM case setup similarly to that shown in Figure 1 (left). However, the case shown in Figure 2 has a higher inlet and wall temperatures plus a lower solid particle thermal conductivity. The only discrepancy between DUO 1D and DETCHEMPBR is a slight increase in temperature near the front of the bed that is attributed to axial conduction, which is modelled in DUO but not in DETCHEMPBR. The DUO 1D case shown in Figure 2 took approximately 2 minutes to run on a single core (meanwhile DETCHEMPBR, which solves systems of ordinary differential equations, takes just a few seconds to run the case presented in Figure 2).

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Figure 2: DRM, mole fraction vs. axial distance, comparing DUO 1D and DETCHEMPBR (1D) simulations. The small difference in the temperature profile near the front of the bed is due to axial conduction, which is resolved in DUO 1D but not in DETCHEMPBR (N=2).

These porous media modeling developments greatly enhance OpenFOAM’s capabilities to evaluate the performance of fixed bed reactors, especially with respect to the reduction of calculation time relative to PRCFD (e.g., 100’s - 1000’s of core hours for 3D PRCFD, to ~2-4 core hours for 2D porous media, to core minutes for 1D porous media). For some applications, like optimization, where many cases need to be screened (preferably quickly), porous media modeling may be preferable over more advanced methods. Also, the developments presented here can be expanded upon to include fluid-solid heat transfer and mass transfer resistances, intra-particle diffusion resistances, and so on, in the future.

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