SCRIPTING AS AN APPROACH TO AUTOMATED CFD SIMULATION FOR PACKED BED CATALYTIC REACTOR MODELLING

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In CFD almost always multiple simulation runs are performed for a stated problem. This implies tedious and time-consuming case set-up typically with a lot of repetition work and little variation to the files. As an example from the field of chemical engineering, parameter studies on packed bed catalytic reactor models may include variations in reactor geometry or pellet design while the remaining case set-up remains unchanged. An efficient alternative to manual stepwise execution of the tasks involved can be the use of scripts to automatically conduct the simulation work flow covering pre-processing with geometry set-up, mesh generation and parameter variation as well as simulation and post-processing.

In this study an automation strategy covering an entire CFD simulation run is developed using `OpenFOAM` [1]. As suggested previously by Boccardo et al. [2] the packed bed is modelled with `Blender` [3] based on a rigid body simulation with the integrated Bullet physics library. Data analysis and visualisation are performed with `ParaView` [4].
Figure 1 gives an overview of the proposed automated simulation routine. It is composed of four main blocks, starting with the set-up of a case structure for the simulation files, followed by three blocks accounting for the actual simulation-run including mesh generation, flow simulation and reaction simulation. A bash script is utilised to execute these individual steps. In addition, python scripts are used where performance of file manipulations are required.
Since `OpenFOAM` cases have a distinctive directory and file structure a base case directory is set up in the beginning containing standard files in the appropriate directory structure. This includes information on case geometry, parameter values, initial conditions and boundary conditions as well as solver and discretisation settings. Furthermore, python scripts are included for the packed bed generation with `Blender` as well as for post-processing tasks involving `ParaView` functionality. Where applicable these base files have been parametrised to a high extend to allow for easy variation.
In the first step of the proposed simulation a python script is utilised to set-up the case structures by copying and modifying the base case directory according to user input.
Next, a loop over the cases is entered. Mesh generation is performed using the `OpenFOAM` tools `blockMesh` and `snappyHexMesh` as well as the software `Blender`. Using `Paraview's` python interface the mesh is evaluated in order to extract data for a radial porosity profile. The mesh generation step ends with the transfer of the final mesh of the reactors's flow domain to the corresponding case directories for flow and reaction simulation.
The next steps in the routine are the simulation of the flow field and the subsequent reaction simulation. These are treated separately, assuming that the reaction does not influence the flow field. `OpenFOAM's` CFD solver `simpleFOAM` is applied for the flow simulation. Once a satisfying solution for the flow field has been achieved, data for an axial pressure profile is extracted. To finish this block in the routine, the obtained steady-state flow field inside the packed bed is transferred to the corresponding case directory of the reaction simulation.
A modified version of the `OpenFOAM` solver `scalarTransportFOAM` is used for reaction simulation. When a steady-state solution has been reached, data for axial concentration profiles of the species involved in the reaction are extracted.

As an example the use of the presented simulation automation is demonstrated with a case study covering three catalytic fixed bed reactors with low to moderate aspect ratios of cylinder-to-pellet diameter. Diameter ratios of $N = 2 \,/\, 7.35 \,/\, 8.41$ are chosen, allowing the comparison of the obtained bed radial porosity profiles with an analytical solution by Govindarao et al. [5] for $N = 2$ and experimental results by Goodling et al. [6] for $N = 7.35 \,/\, 8.41$. To obtain the computational mesh for the flow domain a hexahedral background mesh with cylindrical geometry is used. The packed bed is based on spherical pellets with uniform size. The conditions are chosen such that a laminar flow is developed, setting a Hagen-Poiseuille profile as velocity inlet condition. An irreversible first order reaction is implemented as boundary condition on the catalytic pellet surface.
First results are shown for the radial porosity in Figure 2 and the magnitude of the fluid velocity in Figure 3 for a fixed bed with $N = 7.35$.

In this work the successful use of bash and python scripts to automatically conduct an entire CFD simulation run

was demonstrated, covering pre-processing with geometry set-up, mesh generation and parameter variation as well as simulation and post-processing. As a result the proposed automated simulation routine puts forward a time saving approach allowing for productivity gain in executing CFD simulations. In the next stage an optimisation step will be integrated as part of the automated routine. This would be a promising tool, paving the way for a number of possible research questions as for example the pellet geometry optimisation of packed beds.

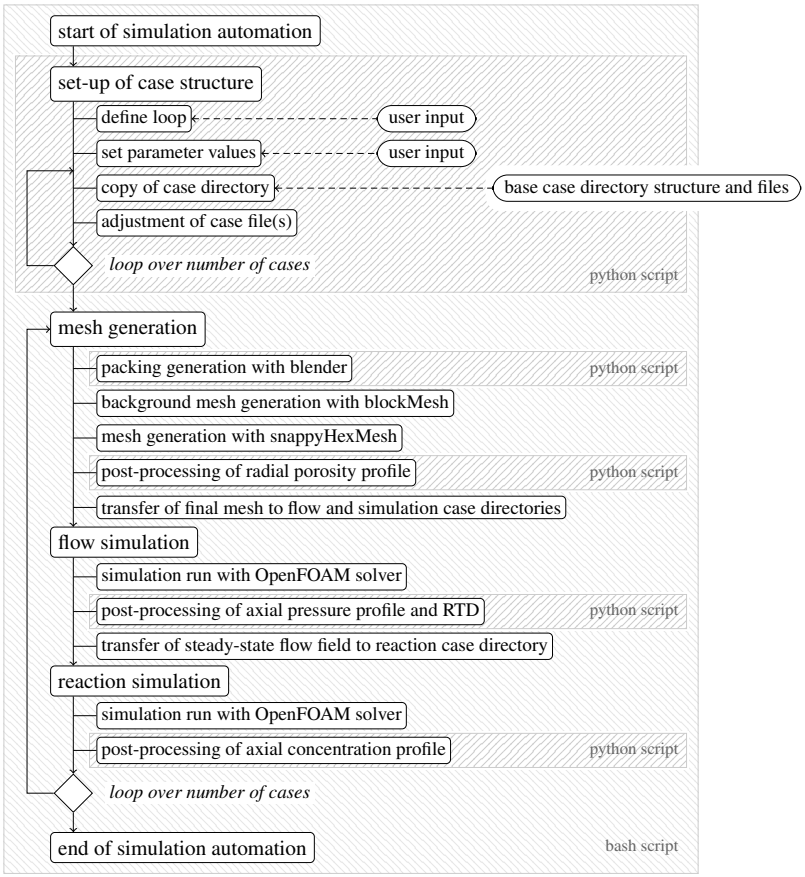

Figure 1: Flow chart of automated simulation routine.

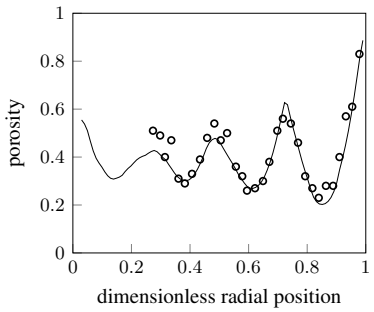

Figure 2: Radial porosity profile of packed bed with $N = 7.35$.
∘ data by Goodling et al. [6].

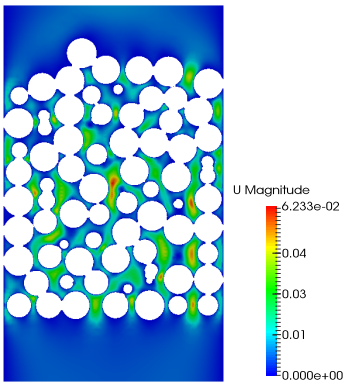

Figure 3: Contour plot of fluid velocity (in ms^{-1}) in planar cut through packed bed with $N = 7.35$. Inlet on top.

References

[1] OpenFOAM - The open source CFD toolbox. [Online]. Available: www.openfoam.com

[2] G. Boccardo, F. Augier, Y. Haroun, D. Ferré, and D. L. Marchisio, "Validation of a novel open-source work-flow for the simulation of packed-bed reactors," *Chemical Engineering Journal*, vol. 279, pp. 809–820, 2015.

[3] blender.org - Home of the Blender project. [Online]. Available: www.blender.org

[4] U. Ayachit, *The ParaView Guide: A Parallel Visualization Application*. Kitware, 2015.

[5] V. M. H. Govindarao, K. V. S. Ramrao, and A. V. S. Rao, "Structural characteristics of packed beds of low aspect ratio," *Chemical Engineering Science*, vol. 47, no. 8, pp. 2105–2109, 1992.

[6] J. S. Goodling, R. I. Vachon, W. S. Stelpflug, S. J. Ying, and M. S. Khader, "Radial porosity distribution in cylindrical beds packed with spheres," *Powder Technology*, vol. 35, pp. 23–29, 1983.