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Application of operator splitting and ISAT for the efficient coupling of an Eulerian-Lagrangian framework and microkinetic model for the simulation of fluidized beds

Riccardo Uglietti[1], Mauro Bracconi[1], Matteo Maestri[1]*

1 Laboratory of Catalysis and Catalytic Processes, Dipartimento di Energia, Politecnico di Milano, via La Masa 34, Milano, Italy

**Corresponding author: matteo.maestri@polimi.it*

Highlights

- Reactive Eulerian-Lagrange CFD framework for fluidized bed reactors
- Operator splitting approach enables efficient solution of particle dynamics
- In-situ adaptive tabulation boost the solution of the chemistry

1. Introduction

Fluidized bed reactors are characterized by strong interactions between the particles and the fluid flow resulting in a complex fluid dynamic characterized by several fluidization regimes depending on the inlet gas velocity, particles characteristics and reactor size. The fundamental understanding of such systems is still poor and mainly relies on phenomenological models based on empirical correlations. The adequacy and reliability of these models and parameters strongly depends on the local conditions. Moreover, their application might not be appropriate in some conditions experienced in industrial reactors. In this view, fundamental methodologies, such as CFD, can give a detailed insight in the system behavior by increasing the understanding in the complex phenomena involving gas and particles. The envisioned approach multiplies the opportunities of a deep understanding of these systems. However, several challenges have to be solved to directly employ this approach to the analysis of even lab scale reactors. In particular, the accurate description of the chemistry introduces a dramatic increase of the computational time. We propose the application of the operator splitting [1] and of the *In-Situ* Adaptive Tabulation (ISAT) algorithms [2] to a reactive CFD-DEM (Computational Fluid Dynamics - Discrete Element Method) framework aiming to an efficient management of the different phenomena involved and to a reduction of the computational cost. The proposed numerical tool combines the accurate description of complex fluid dynamic with the detailed modeling of the heterogeneous reactions at the catalytic particles.

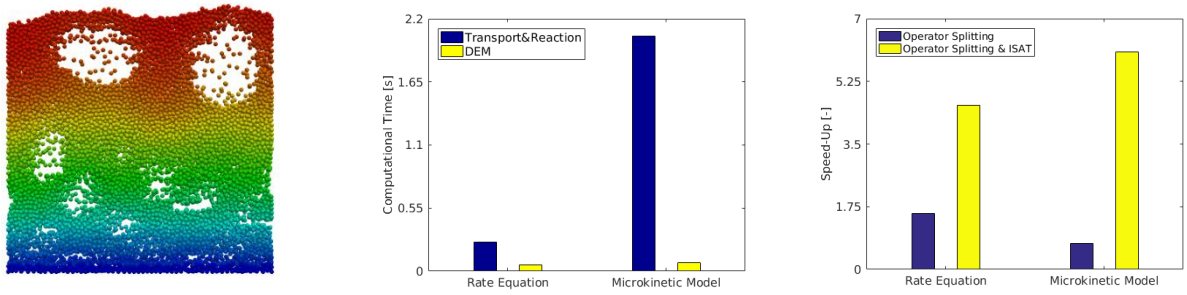
2. Methods

The framework uses a reactive CFD-DEM methodology to describe the fluidized bed, extending the non-reactive framework available in OpenFOAM. Solid and gas phases are solved sequentially according to the segregated approach. The solid phase is described by solving for each catalytic particle the energy and species balances along with site species conservation equations (i.e. transport/chemistry step), and the Newton's equations of motion (i.e. DEM step). At each time step, the gas-solid momentum, energy and mass transfer exchange rates are evaluated for each particle, accounting for the gas-particle interactions and collisional events. The gas phase is described by solving the Navier-Stokes equations together with the energy and species mass balances, where source terms are considered for the description of the gas-solid interactions. The operator splitting is applied to the transport/chemistry step. This algorithm accounts, in separate fractional time steps, for the gas-solid transport phenomena and for the chemical reactions [1]. In this perspective, the transport can be analytically solved, whereas the chemical sub-step requires the solution of a stiff Ordinary Differential Equations (ODE) system. Thus, ISAT algorithm [2] is applied to the reaction step allowing for a crucial reduction of the computational cost.

3. Results and discussion

The proposed framework is capable of describing the complex interaction between the particles and the fluid flow along with the description of the surface reactivity, as shown in Figure 1(a). Our analysis points out the

computational time spent in the solution of the particle dynamic depends on the contributions of the DEM and of the transport/reaction terms. The solution of latter requires most of the computational effort and becomes dominant when dealing with a microkinetic description of the chemistry, as shown in Figure 1(b). The extension of the operator splitting techniques, successfully proposed by our group for fixed bed reactor [1], enables to separately treat the contributions of the transport between the gas and the particle and of the chemical reaction occurring at the particle surface. The chemistry sub-step requires the solution of a stiff ODE system, whereas the transport sub-step is solved by means of an analytical expression. In this perspective, the operator splitting increases the performances of the system when the relative cost of transport and chemistry in the coupled approach is comparable. The analytical solution of the transport requires a negligible computational effort and strongly boosts the solution of reaction/chemistry step enabling an overall speed-up of the simulation around 1.5 and 4.6, with and without ISAT, respectively, for the case of lumped reaction rates [3], as shown in Figure 1(c). When a microkinetic model [4] is used, the cost of the solution of the chemistry is much larger than the one required for the solution of the transport. Thus, the beneficial effect of the analytical solution of the latter is hampered by the broad effort spent in the integration of the chemical sub-step. Thus, the operator splitting shows a negligible speed-up of the simulation where a microkinetic mechanism is considered. Nevertheless, the application of the splitting enables to exploit tabulation techniques which reduce the cost associated to the chemistry. In fact, ISAT is found to provide a speed-up of the solution of the chemistry sub-step of the order of 3-30 times, resulting in overall computational gain around 6 times, as shown in Figure 1(c).



(a) (b) (c)

Figure 1. Snapshot of the fluidized bed where the particles are colored as a function of the CO concentration (a); time spent in the solution of transport/reaction and DEM for rate equation chemistry and microkinetic model (b); simulation speed-up obtained by means of operator splitting and ISAT (c)

4. Conclusions

The operator splitting and ISAT algorithms have been applied to overcome the limitation imposed by the broad computational effort involved in the coupled solution of chemistry and transport in the particles. The speed-up has been quantified using both a reaction rate and a microkinetic model, obtaining an overall maximum speed-up of 4.6 and 6, respectively. This approach reduces the computational effort paving the way to the extension of such framework to industrially relevant reactors.

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Keywords
fluidized bed reactors; eulerian-lagrangian; CFD-DEM; microkinetic schemes; operator splitting; ISAT