A MULTI-SCALE APPROACH TO THE SIMULATION OF FLUIDIZED SYSTEMS: FROM PARTICLE TRACKING TO MICROKINETIC ANALYSIS

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Abstract

We present the application of a machine learning based multi-scale modeling approach to fluidized bed reactors. The solid phase is characterized by tracking each particle in the domain (DEM – Discrete Element Method), whereas the gas phase is solved by means of the Navier-Stokes, mass and energy balances. The gas-solid exchange terms are computed for each particle and exploited in the gas phase as source terms. The catalytic chemistry is solved by means of microkinetic models for each particle leading to a high computational cost. To reduce the computational load, machine learning methods, based on In Situ Adaptive Tabulation (ISAT) and Cell Agglomeration (CA) techniques, have been applied leading to a five-fold speed-up with a peak performance up to 25.

Keywords

MACHINE LEARNING, CFD-DEM, MICROKINETIC MODELS

Introduction

Fluidized systems are a key technology in the most challenging catalytic processes (e.g. anhydrides, FCC) and for the design of novel processes (e.g. OCM or the carbon nanotubes production). Nevertheless, the fundamental understanding of these units is hampered by the multi-scale nature of the involved phenomena (surface reactions, reactor scale transport phenomena, gas-solid interactions). In this context, the multi-scale modeling of catalytic systems has been acknowledged as a promising tool. In this work, we extend the methodology, successfully applied to fixed bed reactors (Maestri and Cuoci, 2013), to fluidized beds, by combining the microkinetic description of the heterogeneous chemistry with CFD-DEM (Uglietti et al., 2018). Despite its efficiency, the approach is limited by a high computational cost, which is linearly proportional to the number of particles. This practically limits the bed size to the order of 10^4 particles. In this contribution, we also apply machine learning techniques (ML) (Goldsmith et al., 2018) to reduce the computational cost of the chemistry. In particular, we implemented two machine learning methods based on In Situ Adaptive Tabulation (ISAT) and Cell Agglomeration (CA) algorithms. These methods, at each time step, are based on the selection of a small group of representative particles considering previous particles integrations (ISAT) or of particle similarities along the whole catalytic bed (CA). Kinetic evaluations are performed only on these selected particles, while the kinetic information on the rest of the particles derived from them, resulting in speed-up factors up to 25.

Methodology

According to CFD-DEM, the solid phase tracking, balances and collisional events are solved particle-wise. At each time step, the gas-solid exchange rates are evaluated for each particle. The gas phase is updated with

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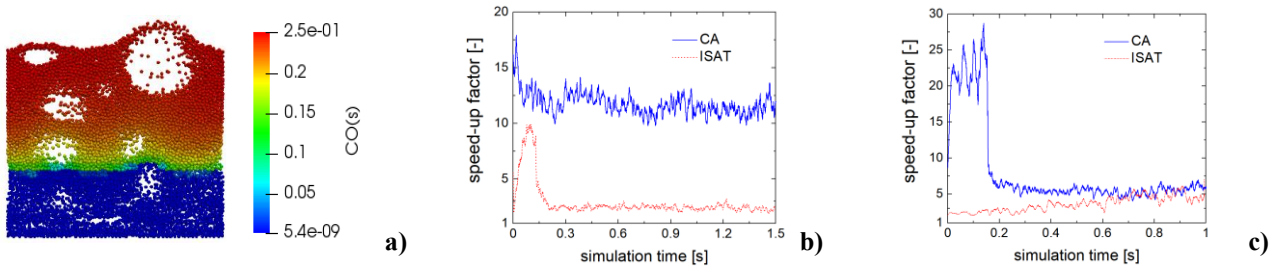

Figure 1 Machine learning speed-up in case of 10^4 pellets(a) for rate-equation model (b) and microkinetic model(c) of methane CPO

fundamental balances by means of the gas-solid transfer terms computed during DEM. The ISAT (Bracconi et al., 2017) and CA (Rebughini et al., 2016) algorithms have been applied to the mass and energy balances of the particles. ISAT has been implemented by means of the operator-splitting (OS), which accounts, in separate fractional time steps, for the gas-particle species and heat transport and the chemistry. Differently from fixed beds the transport can be analytically solved, whereas ISAT is applied to the more computationally-intensive chemical sub-step. ISAT is a storage and retrieval method which accurately approximates the reactivity of a catalytic particle based on previously stored information. At each time step, ISAT assesses if a pellet is similar to another one previously stored. If so, the results of the particle are approximated based on the stored one, otherwise the particle is solved and added to a table (built during the simulation). CA is an agglomeration algorithm which groups particles in a small number of bins. At each time step, each bin is solved considering the average properties and state variables of the underlying group, reducing the number of computationally-intensive calculations. CA has been applied for the first time without the operator-splitting algorithm, thus considering at the same time transport and reaction, differently from the current applications in fixed bed contexts.

Results and Discussion

We tested our method in an isothermal fluidized bed of 10^4 particles (Figure 1a). We tested both a rate-equation and a microkinetic model in case of the methane CPO as benchmark reaction. The results obtained by means of ISAT and CA have been compared with the one achieved without ML obtaining a maximum error of 3.7%. Figure 1b reports the speed-up obtained with ISAT and CA in case of rate-equation model. A relevant speed-up is obtained by means of both ISAT and CA. In particular, we found that the efficiency of the ISAT algorithm is limited by the efficiency of OS after the start of syngas production. In fact, OS alone is slower than the coupled transport and reaction whenever the smallest chemical characteristic time in the system is lower than the simulation time step (e.g. for the syngas combustion in methane CPO). In case of microkinetic model (Figure 1c), the OS is slower than the coupled approach during the whole simulation, due to the fast adsorption and desorption reactions (Uglietti et al, 2018), limiting the speed-up of ISAT. On the other hand, the CA is no more limited by OS, and we obtained a factor of 25 at the beginning of the simulation when the catalyst surface is almost completely covered by oxygen. On the other hand, when syngas production starts the surface composition becomes more complex, and the CA speed-up is lower (even if still higher than 5) due to the importance also of non-MARI low-content coverage species, when comparing the composition between two different particles. Additional tests will be performed by considering only the main non-adsorbed species and MARI when agglomerating particles to furtherly improve the computational gain provided by CA.

Conclusions

A multi-scale approach has been developed to integrate microkinetic modeling and fluidized reactive systems based on the detailed tracking of the particles of the bed. Two ML techniques, i.e. ISAT and CA, has been successfully applied, obtaining, respectively, an average speed-up of 2 and 12 in case of rate-equation, and of 4 and 5 with a peak of 25 for CA in case of detailed microkinetic model. As such, our framework enables the fundamental investigation of fluidized system, paving the way for bigger and more complex domains.

Acknowledgments

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