IN-SITU ADAPTIVE TABULATION FOR THE CFD SIMULATION OF HETEROGENEOUS FIXED BED REACTORS

Mauro Bracconi a, Alberto Cuoci b and Matteo Maestri a*

a Dipartimento di Energia, b Dipartimento di Chimica e Ingegneria Chimica
Politecnico di Milano
Milano, Italy

Abstract

The solution of chemical step in CFD simulations of heterogeneous reactive flows is the bottleneck of the entire simulation requiring up to 70-90 % of the total computational effort. In this contribution, we propose a numerical library, implementing the in-situ adaptive tabulation (ISAT) algorithm, to reduce the computational time spent in this step. The framework has been developed to efficiently evaluate computational expensive functions and has been specifically designed to deal with transient problems. The library can be easily interfaced to whatever CFD numerical reactive code adopting the operator splitting technique in order to solve the chemical sub-step. In particular, the capability of the library to solve the chemical sub-step, in the context of unsteady simulations of heterogeneous gas-solid catalytic systems, has been proved. The improvement of the performances obtained with our library assumes great relevance in the context of the advance design of catalytic converters, since broadens the field of application of CFD numerical codes by reducing the computation effort required.

Keywords

Operator-splitting, ISAT, Fixed bed reactor

Introduction

The detailed description and analysis of fixed bed reactor are relevant topics in chemical reaction engineering. An emerging and challenging methodology is based on the first principles multiscale approach which attempts to fully describe the system through the theoretical accessible phenomena, from the making and breaking of chemical bonds at level of the active sites to the rigorous description of the transport between the fluid and the surface. In this view, computational fluid dynamics (CFD) coupled with microkinetic descriptions of the surface reactivity is a crucial piece of information and have demonstrated an unprecedented potential in the fundamental understanding and analysis of the chemical transformation.

Recently, a numerical framework, implementing the operator splitting technique, has been proposed (Maestri and Cuoci, 2013) to efficiently solve the Navier-Stokes equations in general geometries with the accurate description of the surface reactivity by means of detailed microkinetic mechanism. The operator splitting approach accounts in separate fractional time step the transport phenomena and the chemistry. Nevertheless, a wide application of the envisioned approach is still hampered by the very high computational effort associated with the microkinetic model. In fact, most of the computational time is spent for the solution of the stiff ordinary differential equations (ODEs) system associated to the description of the chemical sub-step. An efficient treatment

* To whom all correspondence should be addressed
of this sub-step is expected to strongly improve the performances of the envisioned approach, closing the gap between such detailed multiscale simulations and real industrial work.

In this respect, we developed a numerical library implementing the in situ adaptive tabulation (ISAT) algorithm (Pope, 1997) and propose its application to the solution of the chemical sub-step in the context of transient simulation of heterogeneous catalytic processes based on microkinetic descriptions of the surface reactivity.

Results

ISAT is a storage and retrieval algorithm providing an efficient and accurate approximation to high-dimensional functions, which are computationally expensive to be directly evaluated.

We developed a numerical library, named ISATLib, which can be easily interfaced with any existing operator-splitting numerical tool. The library implements the main features of the ISAT algorithm and has been specifically conceived to efficiently deal with transient problems accounting dedicated solutions in table update procedures. In the present work, our library will be used to solve the chemical sub-step in the context of numerical simulation of heterogeneous devices by means of the operator-splitting approach.

The library has been successfully interfaced with the existent catalyticFOAM framework (Maestri and Cuoci, 2013) to efficiently solve the chemical sub-step. The accuracy of the ISATLib has been investigated by comparing the results of simulations carried out with ISAT treatment of the chemical sub-step and with direct integration (DI) of the ODE systems, adopting a large range of operative conditions. In Figure 1, the mean global error (Pope, 1997) is plotted against the tolerance value for both the adiabatic and isothermal simulations of methane partial oxidation carried out with a detailed microkinetic mechanism for the surface chemistry (Maestri et al., 2009). The library ensures a very good error control as the mean global error is generally below the respective tolerance value.

By comparing the ratio between the computational time required to solve a single chemical sub-step with and without ISAT, the capability of the library to reduce the chemical computational time up to 300 times, depending on the dimension and stiffness of the system, has been proved. Considering the ratio between the time spent to carry out the entire simulation with and without ISAT, a considerable decrease of the total computational time up to 15 times has been assessed, as depicted in the panel in Figure 1. Therefore, the simulation of large-scale industrial problems, such as fixed bed reactors, has been carried out with a reduced effort and in a feasible computational time.

Conclusions

In this work, we faced the problem of the reduction of the computational effort required in the solution of the chemical sub-step, in the context of heterogeneous reactive flow simulation. As a possible solution, we propose to exploit the features of the in-situ adaptive tabulation algorithm. In this view, a library implementing the methodology has been developed in order to be interfaced in whatever numerical tool requires the evaluation of multidimensional computational-demanding functions, as occurs in the resolution of the chemical sub-step in the context of the operator splitting technique.

The ISAT treatment of the chemical sub-step allows for a large computational gain in the solution of chemistry, resulting in an overall simulation speed-up at most of 15 times and ensuring accurate predictions for specie, temperature and site coverages.

On a more general basis, the development of ISATLib results in an innovative improvement to broaden the field of application of such solvers making them more attractive to the detailed analysis of large-scale problems.

References

