SOME CHALLENGES AND METHODS FOR DIGITAL DEVELOPMENT OF NEW GENERATION FUELS

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New generation fuels, specifically those produced by renewable feedstocks and energy, are recognized as an unavoidable pillar to sustain the future economy, having important roles in long-term energy storage, clean energy production, heavy transport, energy-intensive industrial processes and even other applications. With the decline of fossil sources, traditional approaches for the study of the behaviour of new fuels are revealing inadequate for several reasons, among them the increased complexity of some new fuel molecules or because of the need to adopt new combustion regimes. Contemporary, both computational physics and mathematical methods, on one hand, and computational power and data management capabilities, are increasingly making it possible to develop new approaches for effective investigation of the properties of the new fuels and the design of the systems aiming at their adoption for energy conversion, both steps required for the development of digital twins of the new combustion systems. This presentation aims to give a brief overview of the challenges to face for an accurate representation of the new generation fuels and the correct reproduction by modelling their physical behaviour when employed in processes for energy conversion, together with an illustration of some new methodologies that are being developed at the CNR.

Keywords: *new generation fuels, detailed chemical mechanisms, bifurcation maps, community analysis, mechanisms reduction*

1. Introduction

The search for substitutes for fossil fuels is at the core of the energy transition dictated by the consequences of an increasing scarcity (for objective as well as political and economic factors) of these sources and the effect on the climate of their burning. Several programs are currently in development to find proper substitutes, and several options are on the table: use clean energy and abundant materials to produce small fuels molecules like hydrogen and ammonia, reprocess the sequestrated CO2 to produce fuels with medium size molecules like synthetic methane, or use/re-use renewable complex materials like bio-masses to produce complex fuel molecules, like drop-in substitutes of gasoline or jet fuels. In all these cases, technological challenges are open. For smaller molecules, new combustion processes must be envisaged for the clean combustion of the small molecules, whose characteristics are still far to be fully understood. In the case of complex molecules, the strict range of the properties required for the substitute fuels to be adopted in engines like jet turbofan is not easy to achieve and to stably maintain due to the continuous variation of the feedstock material. Not less important is the pursuit of a continuous improvement of the efficiency and emissions capabilities of the engines.

All these aspects claim for new and effective approaches to gain knowledge on the behaviour of the new combustion systems, and to design new combustors. With respect to the past, when refineries were optimized for the oil coming from a single well or a mix of well-established sources for decades, nowadays much more flexibility is required on both sources and engines that must accommodate varying properties of the final fuel product.

This challenge is further complicated by the need to adopt very detailed combustion mechanisms (up to thousands of species and tens of thousands of reactions) to catch the different behaviours of the new fuels and their mixing in the different operating conditions and mixture compositions. Figure 1 illustrates the evolution in the past years of the detailed chemical mechanisms developed for the description of combustion processes. Figure 1, left, indicates the number of species and reactions involved in the increasingly complex mechanisms, now easily

extending to close to 10,000 species and 30,000 reactions. Figure 1, right, estimate the computational effort in computing the number of exponential function evaluations to compute the contributions in the balance equations for a multicomponent mixture coming from the detailed mechanism in a single state. It clearly results that even with the most powerful high-performance computing facilities, the tout-court adoption of detailed chemical mechanisms is prohibitive.

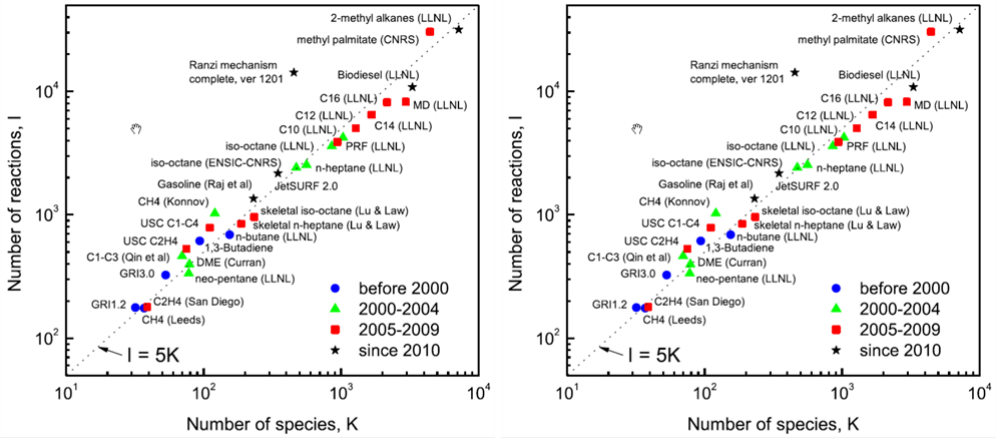

Figure 1: On the left, number of species and reactions of the detailed combustion reaction mechanisms. On the right, the corresponding computational complexity measured in terms of the computation of exponential functions for a single state determination. Source: ref. [1].

2. New directions of development

Several approaches are being developed to deal with these challenges. Most of them are devoted to reducing the computational effort by both reducing the dimension of the problem [2] or by making more efficient the computational efficiency [3]. Here the focus will be given to some original contributions developed at CNR-STEMS in cooperation with other scientific partners.

At the base for a correct reproduction of the physical phenomena by a virtual representation is a correct knowledge of its behaviour at least in the conditions aimed to be reproduced. In the case of combustion processes, the strong non-linearity of the chemical and physical interactions makes risky the attempt to derive unknown conditions as interpolation of known ones. This is essentially the procedure adopted even with the most advanced machine learning methods, also when based on experimental observations. This kind of procedure can be safely adopted only if prior knowledge of the regions in the parameters space where the system behaves sufficiently smooth has been gained, thus limiting the application of the virtual representation to the safe regions [4].

To gain this kind of knowledge, the bifurcation analysis offers the theoretical bases and the computational tools to systematically investigate the regions of the parameter spaces where “catastrophic” changes in the system behaviour occur, thus indicating the regions where “digital twins” can safely operate. In the case of systems represented by detailed chemical mechanisms, the use of tools like parametric continuation is not straightforward and is computationally extremely demanding. Special procedures have been developed to make affordable this type of analysis even for the most complex chemical mechanisms [5]. Even if they have been adopted up to now only for simple archetypal reactors, like the perfectly stirred reactor, thanks to the parallelism existent between this type of reactor and the computational cell of a finite volume CFD representation of a complex reactor, important information can be gained. In terms of knowledge gain, recognizing among such a large number of species and reactions, those mainly contributing to the observed behaviour of the system, is also important. Being manual inspection prohibitive, automatic methods must be envisaged. This aspect is being pursued by developing algorithms based on the representation of the detailed chemical mechanism as a bipartite network and thus employing concepts and methods of networks analysis, like community partitions and coarse-grained states. This approach

appears, in conjunction with the bifurcation analysis, very promising to recognize how the evolution of a chemical mechanism changes while varying the actual conditions, allowing the identification of the regions where potentially very reduced mechanisms can be developed and safely applied to make affordable the computation of a digital twin [6].

The knowledge of the most critical regions in the parameter spaces also allows the development of robust and accurate reduced chemical mechanisms. This objective has been pursued by developing a systematic procedure for the reduction of detailed chemical mechanisms based on the weighting of the contribution of the species and reactions with respect to thermodynamic functions [7]. Specifically, the adoption of the entropy production rate as the weighting function has already permitted the development of efficient skeletal mechanisms for synthetic aviation fuels. The computational efficiency of this approach has been adopted also for developing the on-the-fly reduction of detailed mechanisms in CFD codes [8]. More recently, for the development of ultra-reduced mechanisms, named virtual chemistry [9], the possibility of reproducing with just a very few reactions the complex behaviour observed close to the ignition and extinction points of a reactive mixture, identified with the methods of bifurcation analysis, is being investigated.

3. Conclusions

Some of the challenges to face in some aspects of the development of Digital Twins for the design and control of energy systems involving combustion processes have been outlined. The presentation will deepen the here shortly illustrated arguments, furnishing practical examples of application of the proposed methods.

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