Automatic reduction and optimisation of chemistry for turbulent combustion modelling: Impact of the canonical problem

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ABSTRACT

In a preliminary part, reduced chemical schemes from the literature on methane/air turbulent combustion are tested in one-dimensional premixed flames at various equivalence ratios. As discussed by Peters (1985), for the very same number of chemical species transported with the flow, a scheme introducing essential intermediate species through analytical relations derived from quasi-steady state and equilibrium assumptions, provides much better predictions than the global schemes limited to the transported species. Along these lines, a fully automated reduction procedure is discussed. The calibration of reduced chemistry usually relies on canonical problems, also computed with reference detailed chemical schemes. To cover at once a given range of chemical compositions, equivalence ratios and temperatures, the chemical properties of stochastic particles, submitted to micro-mixing and chemical reactions, are combined with the computation of deterministic one-dimensional composition-space trajectories, issued from an arbitrary number of inlet conditions. Along these trajectories, well-established methods to reduce the numbers of species and reactions are applied, cast in a fully automated manner. The rates of the resulting reduced scheme are then optimised, following a genetic algorithm, to match the detailed chemistry response. The discussed strategy is applied to methane/vitiated-air combustion. The accuracy of the resulting reduced scheme is evaluated in the simulation of freely propagating one-dimensional premixed flames, at various equivalence ratios, and also in strained diffusion flames in a one-dimensional counterflowing jet configuration, up to the quenching point. The accurate reproduction of the flame speed response *versus* equivalence ratio requires adding premixed flames as target in the optimisation loop. Once the flame speed is captured, the quenching scalar dissipation rate of the diffusion flames is also well reproduced, as anticipated by Peters in a relation between the flame speed and the quenching scalar dissipation rate (Peters, 1991, 2000). Finally, the optimisation of the chemical rates is demonstrated under specific operating conditions, featuring four inlets with a large variety of flow compositions.

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1. Introduction

During the seventies, pioneer works paved the way for simulating numerically the physical properties of turbulent flames under the hypothesis of fast or very fast chemistry [4–14]. At that time, aside from a few attempts [15–18], the introduction of finite chemical rates into the modelling of turbulent flames was carefully avoided. Indeed, reduced and global chemical schemes were not that reliable and introducing the asymptotic limit of infinitely fast chemistry appeared as a safer choice, which allowed for understanding most of the basis of the interaction between flame and turbulence.

The gap between turbulent flame simulations and finite rate chemistry was, however, soon closed thanks to further works providing compact and predictive chemical models to progress in the simulation of turbulent flames [1,19], along with strategies to model the reaction zones in the case of unresolved fluctuations of species and temperature [20–23]. Peters contributed to this field in a major way. He discussed a rigorous strategy to derive reduced chemical schemes for hydrocarbon combustion [24], leading to a series of skeletal and reduced chemical kinetics based on a few steps. Peters introduced in his chemical kinetics the coupling between a reduced number of elementary steps and an analytical part, in which intermediate species are expressed from those transported with the flow via quasi-steady state and equilibrium hypotheses [25–28]. These skeletal, or reduced, kinetics were useful for conducting theoretical analysis of the inner structure of laminar flames and reaction zones [29,30] and the introduction of

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reduced kinetics became feasible for the numerical simulation of turbulent flames [23,31]. Then, up to very recently, further chemical schemes ready for turbulent flow simulations were derived by many groups, see for instance [32–35] and references therein.

Reduced chemical schemes have been met in a large variety of applications, as for instance in Large-Eddy Simulation (LES) of laboratory flames or complex systems (see [36–39] and references therein). They have also been used to fasten the building of chemical look-up tables, derived either from low-dimensional manifold projection [40] or from one- or multi-dimensional canonical combustion problems, such as laminar flamelets [41–46].

The complexity of the chemical schemes, which can be handled simultaneously with flow simulation, is continuously growing with the constant progress of computing tools. This complexity relates to the size of the schemes, in terms of number of species to be transported and reaction rates to be computed, and, to the stiffness of the differential system to be solved, both directly impacting on the numerical cost.

Because some species and reaction paths, which are physically involved in the flame, are missing after the reduction of the chemistry, the optimal values of the rate constants (pre-exponential factor, temperature exponent and activation energy) of the simplified scheme may not be exactly those of the fully detailed chemistry. Finding the best adjustment of the rate constants of a reduced kinetics is not an easy task. Part of the physics is missing in the reduced scheme and the values of the parameters of the rates must, at the same time, secure the expected evolution of given chemical species and compensate for the chemical paths which have been removed. To do so, many optimisation procedures have been proposed in the literature, to come up with the best set of constants, for given operating conditions [32,47–54].

At least two main types of reduced schemes may be found in the literature for simulating turbulent flames:

(i) Global schemes based on a few steps, which are anticipated in a more or less empirical manner and in which only major species are involved. The constants of these global chemical rates are adjusted to match experimental measurements or reference responses obtained with a detailed chemistry that was previously validated. Techniques have been discussed in the literature to adjust these constants, using well-established and automated optimisation tools [32,36,51].

(ii) Reduced schemes, also based on a few steps, but which have been obtained from a systematic downsizing of a detailed kinetics. Over the past decade, efficient methods have been discussed to perform this reduction procedure also in a fully automated manner. Indeed, numerical procedures have been set up to seek out, throughout the intricate chemical paths, the direct and indirect impact of species and elementary reactions on a given target set of chemical species, to be reproduced by the reduced scheme [35,55–59]. The intermediate species and elementary reactions with the least influence on the target species may then be removed. To this procedure, the formulation of quasi-steady state assumptions is usually added, to reduce even more the number of species, a step that may also be automated [32,60,61]. Part of the scheme is then said 'analytical', as introduced by Peters [1], because the subset of species in quasi-steady state will not be transported with the flow in the simulation. These species still enter the chemical rates, but they are obtained from the transported ones through algebraic relations derived from the steady state assumptions. Some of these relations may be non-linear in terms of species concentrations and a specific solution procedure is then required [62].

Whatever strategy is followed, a target model problem should be chosen to probe the chemical response along representative evolutions of chemistry from fresh to burnt gases. These chemical trajectories have been obtained in the literature *versus* time in homogeneous reactors, *versus* space in premixed and diffusion one-dimensional laminar flames, or again *versus* time and space in unsteady strained one-dimensional flames [63]. A severe limitation of these canonical problems lies in the number of boundary conditions restricted to two-inlets (fresh and burnt gases at a given equivalence ratio in 1D premixed flames; fuel-rich and fuel-lean in 1D non-premixed flames). The conditions locally feeding the reaction zones within a turbulent flame may actually be much more diverse, because of the local combustion regimes [64], or simply because real combustion systems sometimes operate simultaneously with three or four inlet conditions. A complementary approach is reported below, which features an unlimited number of potential inlets by construction, and which allows for covering at once a larger range of chemical compositions. The resulting reduced schemes are found to operate well for auto-ignition in the presence of micro-mixing, species profiles in premixed flames and strained diffusion flames, even though the diffusion flames were not part of the optimisation loop.

The evolution of the chemical composition of stochastic particles is considered. The particles are issued from inlets at various chemical compositions and the species concentrations of the particles vary according to a stochastic mixing closure and a chemical kinetics. Performing the scheme reduction and the optimisation on the numerous stochastic particles would be too costly. Also, to compact the information, still covering the given range of equivalence ratios and temperatures, the time evolving statistical properties of the stochastic particles enter a deterministic mixing closure, used to construct a set of one-dimensional composition space trajectories issued from each of the inlets. A fully automated reduction of the detailed chemical scheme is built along these chemical trajectories. The rates of the reduced scheme are then optimised with a genetic algorithm, coupled with the computation of the composition space trajectories.

The impact of the model problem is examined by further testing the reduced scheme obtained along the composition space trajectories, in the simulation of freely propagating one-dimensional and laminar premixed flames and strained diffusion flames in counterflowing jets. It is observed that a chemistry reduced under methane vitiated-air conditions with the stochastic approach, but without optimising the rates through the genetic algorithm (*i.e.* keeping for the retained reaction steps the constants of the detailed scheme), is sufficiently accurate to simulate species profiles in freely propagating premixed flames at various equivalence ratios, except for the richest conditions (*i.e.* $\phi > 1.3$). Major species in strained diffusion flamelets are also quite well captured. However, without applying the genetic algorithm to optimise the constants of the scheme, it lacks of generic character to fully reproduce the full set of composition space trajectories of the stochastic canonical problem and also the response of the maximum temperature *versus* strain rate in the counterflowing diffusion flamelet. Adding premixed flame profiles as target in the optimisation loop allows for better reproducing the flame speed and also the quenching point of the diffusion flamelet. Confirming the interest in selecting a series of model problems as generic as possible, along with the need for an optimisation procedure of the chemical rates of the reduced scheme, in order to handle flame propagation, diffusion flame-quenching, and situations more driven by auto-ignition and micro-mixing.

To introduce the context, results of existing global chemical schemes applied to one-dimensional premixed flames are first discussed in the next section, the results confirm Peters' vision on chemistry reduction based on an analytical part, to account for intermediate species. In the subsequent section, the focus is on the novel model problem for constructing reference chemical trajectories with a detailed chemical scheme. Then, a fully automated chemistry reduction/optimisation loop is reported, with a special emphasis on the practical implementation and calibration of a