Numerical modeling of Partially Stirred Reactors (PASR) with arbitrarily complex kinetic mechanisms

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Highlights

- A stochastic model for describing a Partially Stirred Reactor (PaSR) was developed
- The model accounts for arbitrarily complex kinetic mechanisms
- The model was adopted for generation of look-up tables and for testing of skeletal mechanisms

1. Introduction

Combustion devices, such as internal combustion engines and gas turbines, can often significantly deviate from ideal mixing conditions. In particular, when the turbulent mixing rate is not fast compared to chemical kinetics, the performances ofa combustion device (or more in general of a reactor) can be strongly affected by the degree of mixing. The Perfectly Stirred Reactor (PSR) model, based on the hypothesis of fast mixing, cannot be adopted for describing such kind of situations. The assumption of fast mixing must be relaxed in order to have the so-called Partially Stirred Reactor (PaSR) model. In PaSR, the mean thermodynamic and chemical properties are assumed spatially homogeneous, but not perfectly mixed at the molecular level. The mixing process in PaSR is described through a mixing time (or equivalently, a mixing frequency), which is prescribed as an input parameter (usually equal to a turbulent time scale), because the fluid dynamics inside the system is not resolved.

In the present work, a stochastic model for numerically describing the PaSR was developed and implemented. The model was adopted for different purposes, from generation of look-up tables, testing of skeletal mechanisms and evaluation of turbulent combustion closure models.

2. Methods

Under the assumption that the mean thermo-chemical properties are spatially homogeneous, but imperfectly mixed at molecular level, it is possible to develop a balance equation describing the evolution of the joint-PDF (Probability Distribution Function) for a single reactive scalar [1]. Pope [2] generalized this approach to multiple reactive scalars, and the resulting equation describing the joint-PDF $\tilde{P}_{\bar{\phi}}(\bar{\psi},t)$ equation is:

$$\frac{\partial \tilde{P}_{\bar{\phi}}(\bar{\psi},t)}{\partial t} = -\sum_{\alpha=1}^{k}\frac{\partial}{\partial \psi_\alpha}\left\{S_\alpha(\bar{\psi})\tilde{P}_{\bar{\phi}}(\bar{\psi},t)\right\} + \frac{1}{\tau_{res}}\left\{\tilde{P}_{\bar{\phi},in}(\bar{\psi}) - \tilde{P}_{\bar{\phi}}(\bar{\psi},t)\right\} - \sum_{\substack{\alpha=1\\ \beta=1}}^{k}\frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta}\left\{<\varepsilon_{\alpha\beta}|\bar{\phi}=\bar{\psi}>\tilde{P}_{\bar{\phi}}(\bar{\psi},t)\right\}$$

The first two terms on the right hand side represent the effects of chemical reaction and the through-flow on the joint PDF, respectively. The last term represents the effect of micro-scale mixing on the PDF, which requires the use of a mixing model. The mixing model mimics the finite rate mixing of particles in the stochastic simulations. Two widely used mixing models are employed as options: the Coalescence-Dispersion (CD) [1] and the Modified Coalescence-Dispersion (MCD) [3] models.

In the present work, the equation above is solved according to the method developed by Pope [1], based on a Monte Carlo algorithm, and successively refined by Chen [4]. In particular, the dependent variable in the simulation is represented by an N-member ensemble (with N sufficiently large) and each of the members of the ensemble is referred to as a "particle". Although a unique number identifies each particle, no ordering is implied. All the operations for describing reactions, inlet/outlet and mixing are carried out either on all particles or particles selected at random. A time marching scheme with a prescribed time-step size is used and the Monte Carlo (stochastic) simulation is carried out by the following sequential steps with statistical particles: 1. convection, through which a proper number of fresh particles are fed to the system and the same number of particles, randomly selected, are forced to leave the system; 2. mixing, through which a proper number of particle pairs are randomly selected and mixed each other; 3. reaction, consisting in the numerical integration of species and energy equations for each individual particle, assumed as a batch reactor. The simplicity of using a Monte Carlo method and a scalar PDF allows performing simulations with detailed chemistry (hundreds of species and thousands of reactions) with reasonably small computational cost.

3. Results and discussion

The stochastic model here developed has been used for several purposes. One of the most relevant for CFD applications is the use of PaSR in the context of tabulated chemistry. Indeed, PaSR allows to explore a wide range of "feasible" conditions (in terms of temperature and composition), which allow to drastically reduce the computational cost behind the generation of look-up table to be used in complex CFD simulations (the alternative would be the discretization of N-space which is unfeasible, even for small values of N). The PaSR model has also been used for "a-priori" testing the ISAT (In Situ Adaptive Tabulation) technique [5], which is commonly used in CFD with detailed kinetics. Moreover, the PaSR is a valuable tool commonly used to evaluate reduced mechanisms in a realistic and demanding environment. Thus, the developed model was adopted also for "a-posteriori" testing of the quality of skeletal mechanisms, obtained from detailed mechanisms through conventional techniques, such as DRG, DRG-EP, etc. A final application, which is currently in progress, is the adoption of stochastic PaSR model for evaluation of turbulent combustion closure models.

4. Conclusions

A stochastic model for describing a Partially Stirred Reactor was developed and implemented. The model accounts for mixing and is computationally efficient for large coupled chemical reaction mechanisms involving many chemical species. The PaSR model represents an ideal test bed for evaluating mixing schemes for use in PDF method–based models. The model was adopted for several purposes, from generation of look-up tables, to testing of skeletal mechanisms in realistic conditions. Future applications will be focused on the adoption of the PaSR model to generate data for training neural networks to be used in CPU demanding CFD applications.

References

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Keywords
Detailed kinetics; turbulence-chemistry interactions; mixing; Monte Carlo.