7
Conclusions and Suggestions

This chapter summarizes and highlights the main conclusions and contributions of this dissertation and suggest some paths for future works.

7.1
Contributions of this Dissertation

This dissertation presented and discussed some of the challenges that are encountered in the development of models for the numerical simulation of turbulent chemically reactive flows in industrial problems.

A literature review concerning the available techniques to reduce the size of a reaction mechanism and efficiently solve models for turbulent chemically reactive flows with detailed combustion thermochemistry is provided.

The chosen and implemented technique dubbed *in situ* adaptive tabulation (ISAT) is described in detail. Also, the ISAT technique was assessed for its accuracy, performance and memory usage in the numerical simulation of chemically reactive flows in homogeneous reactors using detailed thermochemistry mechanisms.

An *in house* modular code written in `ANSI C` and `Fortran 77` languages which implements the ISAT algorithm and the PMSR reactor model was developed in this work and has undergone series of verification tests. The results of the verification tests allowed to characterize the code in terms of computational performance and from the numerical analysis and computer programing point of view. The code is available under request on the email `americo.cunhajr@gmail.com`.

The ISAT technique shows good accuracy from a global point of view, with the absolute global error smaller than 1% for the reactor configurations studied. The analysis of ISAT accuracy also allows to identify the effect of the statistical seed on the control of the absolute global error, which decreases monotonically as ISAT error tolerance is reduced, when the simulations use the same statistical seed for ISAT and DI calculations. On the other hand, when different seeds are used, a limit value for ISAT error tolerance is observed.

Concerning the local error, ISAT technique achieves maximum error values of the instantaneous properties of the reactor of up to 20%, which could be unacceptable, depending on the application envisaged.

A strategy to avoid that the ellipsoid of accuracy degenerates as a single point is proposed. This modification in the half-lengths of ISAT ellipsoids constitutes a filter for chemical times scales. However, the performed tests shown that this modification does not offer any advantage in terms of ISAT technique accuracy.

In terms of performance, the ISAT technique allows to reduce the computational time of the simulations in all cases tested. For the test cases with the carbon monoxide/oxygen thermochemistry speed-up factors of 5.0 (case 1) and 1.0 (case 2) were achieved, whereas for case 3, which considers a system with a methane/air mixture, the algorithm allows to save 34% in terms of computational time. Moreover, the ISAT technique presented, in the cases studied the desired feature of speed-up factor increases with the complexity of the system analyzed.

Regarding the memory usage, ISAT technique is, as it could be expected, very demanding. In the simulation of the methane/air mixture using a binary search tree with 60,000 entries, the algorithm demanded 3.3 Gbytes of storage. This work confirms that memory expense is the major drawback of the ISAT technique.

Part of the results of this work were published in conference paper (Cunha and Figueira da Silva, 2010) [14], adjoined to this dissertation in appendix C.

The main results of this dissertation are being summarized in a paper, (Cunha and Figueira da Silva, in preparation), and will be submitted for publication in *Journal of Brazilian Society of Mechanical Sciences and Engineering*.

7.2 Suggestions for Further Works

A natural extension of this work is the characterization of the ISAT technique in the simulation of chemically reacting mixtures different from those used in this work. For example, it could be interesting to evaluate the ISAT behavior for a mixture of hydrogen with oxygen, which may be described by the reaction mechanism of Li et al. (2004) [48]; or a mixture of natural gas with air, which could be modeled by the mechanism of Le Cong & Dagaut (2008) [46].

Another natural extension of this work would be to incorporate the improvements of ISAT technique proposed by Lu & Pope (2009) [51] in the code developed. Also, performance gains would be possible if a parallelization strategy is implemented, such as those strategies proposed by Lu et al. (2009) [50].

A more sophisticated application would be the coupling of a detailed reaction mechanism, using the ISAT technique, with the hybrid LES/PDF model by Andrade (2009) [1] for description of turbulent combustion. This model currently uses a hybrid approach that combines large eddy simulation (LES), for description of fluid dynamics, and the transport of the PDF with a single step global kinetic for modeling the combustion. The incorporation of a detailed reaction mechanism would allow a better description of combustion, at the expense of a significant increase in computation time, which is not negligible in the case of a LES models. In this context, ISAT could be a viable option that may be able to decrease, to an acceptable level, the simulation time. It is also worth considering that LES calculations also spend a lot of memory, so that the coupling of LES with a detailed reaction mechanism with dozens of species, such as the GRI version 3.0 [89], is not yet feasible.

Finally, it is worth stressing that this study conducted verification tests of ISAT algorithm and PMSR reactor model only. No validation attempt was developed due to the difficulty of obtaining experimental data for such a homogeneous reactor configuration. This validation could be performed if carefully designed direct numerical simulations were available, or in more challenging flow problems, for instance.