POLITECNICO DI TORINO
DOCTORAL PROGRAM IN ENERGETICS
Ph. D. THESIS PROPOSAL

Subject
BGK – type kinetic models and mesoscopic numerical schemes for multi – component gases undergoing chemical reactions and temperature gradients

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Description of the international background of the proposal

Chemically reactive gas mixtures play a relevant role in many meaningful physical applications, as for instance combustion, plasma physics and fuel cells, for which kinetic models of the extended Boltzmann equation can be used to improve the knowledge of the involved macroscopic phenomena, starting from a description of the system at the mesoscopic scale.

The influence of chemical reactions in rarefied flows has been analysed since the fifties by Prigogine and Xhrouet in the framework of the Boltzmann equation and more recently in the book by Bird at the level of direct simulation methods. On the other hand, after the paper by Prigogine, a wide literature on this topic has been produced, as documented in the book by Giovangigli, where the contribution to the generalization of the Boltzmann equation to reactive gas mixtures has been systematized. For a chemical mechanism with an arbitrary number of elementary reactions, the mathematical structure of chemistry source terms, conservation and equilibrium properties have been analyzed, where different chemical regimes have also been considered. In particular, the regimes corresponding to both slow and fast reactions, are challenging for many applications and they will be considered in the present proposal.

From the computational point of view, the lattice Boltzmann methods (LBMs) have been recently proposed in order to define mesoscopic simulation tools, which are affordable in terms of computational resources. LBMs are efficient numerical tools for investigating flow in highly complex geometries, such as porous media. Even though traditional Navier-Stokes solvers could be used to describe porous media flow, LBMs do not require pressure-velocity decoupling or the resolution of a large system of algebraic equations. They solve a simplified Boltzmann equation for an ensemble-averaged distribution of moving, interacting particles on a discrete lattice. The macroscopic quantities that describe the fluid flow can be calculated as moments of this distribution. Since the motion of particles is limited to fixed paths connecting lattice nodes, the resolution process needs only information about the nearest neighbour nodes. This feature, along with the explicit nature of the numerical scheme, makes LBMs very suitable for parallelization.

Lattice Boltzmann models seem to be very promising for the analysis of reactive mixtures in porous layers. For this reason, a lot of work has been performed in recent years in order to produce reliable lattice Boltzmann models for multi-component fluids and, in particular, for mixtures composed of reactive miscible species. The problems are (a) to find a proper way, within the framework of a simplified kinetic model, of describing the interactions among different

particles and (b) to do that by means of the minimum amount of microscopic velocities. Unfortunately, most existing lattice Boltzmann models for mixtures are based on heuristic assumptions or prescribe too many constraints for setting the microscopic parameters, the end result of which is an idealized (if correct) macroscopic description.

Research program objectives (intermediate and final) and expected results

The research program can be divided in two parts.

- The main objective of the first part consists in the derivation, in the framework of kinetic theory, of simple models which at the same time are capable to provide a good description of reactive gas flows in unbounded domains for two different chemical regimes, and are easy to handle numerical simulations. More in detail, for a reactive mixture, a BGK – type procedure is proposed in order to replace the complex form of the collision operators by a less detailed structure, based upon a simpler operator which retains the main properties of the true elastic and inelastic collision operator. Accordingly, two BGK-type terms are proposed for strong and kinetic chemical equilibrium regimes, following a unified procedure which is able to deal with strong temperature gradients. The basic idea is to develop a mesoscopic model which is able to consistently recover the macroscopic behaviour of the reactive mixture in the continuous limit (Maxwell – Stefan diffusion model, Law of the Mass Action, Quasi Steady State Approximation, …) and, at the same time, to take into account the rarefaction effects and the microscopic interactions among the mixture components.

- The second part aims to develop the numerical implementation of the previously defined model in a computational algorithm. In particular, this goal may be achieved by formulating first an LBM version of the previous theoretical model by considering only the minimum number of microscopic velocities. Essentially the key idea is to develop the optimal quadrature formula for the calculation the relevant statistical moments with the maximum accuracy up to a given order (fluidynamic regime and/or slightly rarefied regime). Then the developed truncated formula may be compared with the original formulation of the model, in order to evaluate the effects due to the poor discretization and eventually to partially suppress them.

The expected results of the proposed project are the following.

- The main objective of the first part consists in the derivation, in the framework of kinetic theory, of **simple BGK – type kinetic models** which are consistent to the macroscopic behaviour of the reactive mixture in the continuous limit (Maxwell – Stefan diffusion model, Law of the Mass Action, Quasi Steady State Approximation,…)
- The objective of the second part is a **numerical code** based on some proper mesoscopic technique (for example LBM), implementing the previous theoretical model and which can eventually take advantage of parallel cluster computing, in order to fill the gap of the large computational demand required by practical applications in the energy engineering field (fuel cells, combustion, plasma physics,…).

List of publications of the proponents and/or specific references (with titles)

[1] Asinari P., von Spakovsky m. R., Cali' Quaglia M., Kasula B. V., Direct numerical calculation of the kinematic tortuosity of reactive mixture flow in the anode layer of solid oxide fuel cells by the Lattice Boltzmann Method, Journal Of Power Sources, ISSN: 0378-7753, (in press).

[2] Asinari P., Asymptotic analysis of multiple-relaxation-time lattice Boltzmann schemes for mixture modeling, Computers & Mathematics With Applications, ISSN: 0898-1221, (in press).

[3] Asinari P., Semi-implicit-linearized multiple-relaxation-time formulation of lattice Boltzmann schemes for mixture modeling, Physical Review E, Statistical, Nonlinear, And Soft Matter Physics, vol. 73, pp. 056705-1-056705-24, ISSN: 1539-3755, 2006.

[4] Asinari P., Viscous coupling based lattice Boltzmann model for binary mixtures, Physics of Fluids, vol. 17, pp. 067102-1-067102-22, ISSN: 1070-6631, 2005.

[5] Asinari P., Cali' Quaglia M., von Spakovsky M. R., Kasula B. V., Numerical simulations of reactive mixture flow in the anode layer of solid oxide fuel cells by the Lattice Boltzmann method, Proceedings of ESDA 8th Biennial ASME Conference on Engineering Systems Design and Analysis, vol. 1, pp. 1-15, ISBN/ISSN: 0-7918-3768-8, 2006.

[6] Asinari P., Coppo M., von Spakovsky M. R., Kasula B. V., Numerical simulations of gaseous mixture flow in porous electrodes for PEM fuel cells by the lattice Boltzmann method, Proceedings of III International Conference on Fuel Cell Science, Engineering and Technology, vol. 1, pp. 93-102, ISBN/ISSN: 0-7918-3757-2, 2005.

[7] L. Desvillettes, R. Monaco, F. Salvarani, A kinetic model for chemically reacting gases in Modeling and Numerics of Kinetic Dissipative Systems, Eds. L. Pareschi et al., Nova Science, New York, 119-132, 2006.

[8] R. Monaco, M. Pandolfi Bianchi, A.J. Soares, BGK-type models for slow and fast chemical reactions in Waves and Stability in Continuous Media, Eds. R. Monaco et al., World Scientific, Singapore, 378-389, 2006.

[9] R. Monaco, M. Pandolfi Bianchi, A.J. Soares, BGK-type models in strong reaction and kinetic chemical equilibrium regime J. Phys. A: Math. Gen., vol.38, 10413-10431, 2005.

[10] R. Monaco, M. Pandolfi Bianchi, A.J. Soares, A reactive BGK-type model: influence of elastic collisions and chemical interactions in Rarefied Gas dynamics, Ed. M. Capitelli, American Inst. of Phys., New York, 70-75, 2005.

[11] L. Desvillettes, R. Monaco, F. Salvarani, A kinetic model allowing to obtain the energy law of polytropic gases in the presence of chemical reactions, in Europ. J. Mech. B/Fluids, vol.24, 219-236, 2005.

[12] R. Monaco, M. Pandolfi Bianchi, S. Pieraccini, G. Puppo, Numerical simulations of a reacting gas mixture at the hydrodynamic scale, in Waves and Stability in Continuous Media, Eds. R. Monaco et al., World Scientific, Singapore, 334-340, 2004.