Kinetic models and hydrodynamic limits for reacting mixtures of polyatomic gases

M. Bisi[1], R. Monaco[2], A.J. Soares[3]

[1]Università di Parma, Italy

[2]Politecnico di Torino, Italy

[3]Universidade do Minho, Portugal

Gases involved in real world applications, for instance in simple dissociation and recombination problems or in the evolution of dust in the atmosphere, are usually composed of polyatomic particles. In the paper [1], a possible generalization to polyatomic gases of the classical Boltzmann model has been proposed. Non-translational degrees of freedom of polyatomic molecules are modelled allowing the distribution function to depend even on a continuous internal energy variable. Proper options for the internal energy measure allow to reproduce the well known energy laws for polytropic or non polytropic gases. However, Boltzmann collision operators turn out to be quite awkward to deal with, especially in reactive frames. For this reason, we are proposing a consistent BGK relaxation approximation, able to retain most properties of the original Boltzmann equations (correct conservation laws, collision equilibria, H-theorem). We follow the lines of papers [2, 3], where the BGK equation for each gas shows a unique collision operator of relaxation type (towards a suitable Maxwellian attractor), which takes into account all collisional (mechanical and reactive) effects on the gas itself. Auxiliary parameters appearing in the attractor are made explicit in terms of actual macroscopic fields of the gas mixture by imposing that the BGK model preserves the correct collision invariants. In collision dominated regimes, by applying a Chapman-Enskog asymptotic procedure to our BGK model it is possible to analytically derive consistent hydrodynamic equations for the main macroscopic fields. We focus our attention on balance equations for species number densities, which are not preserved by chemical reactions (only suitable combinations of them are collision invariants). At the Euler level, the main analytical steps leading to the computation of the pertinent collision contributions are presented, while at the Navier-Stokes accuracy even constitutive equations for diffusion velocities and number density corrections are required.

[l] Desvillettes, Monaco, Salvarani, Europ. J. Mech. B **24**, 219 (2005).

[2] Andries, Aoki, Perthame, J. Stat. Phys. **106**, 993 (2002).

[3] Bisi, Càceres, Comm. Math. Sci. **14**, 297 (2016).