

Analysis of differential diffusion phenomena in high enthalpy flows, with application to thermal protection material testing in ICP facilities

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This thesis presents the derivation of the theory leading to the determination of the governing equations of chemically reacting flows under local thermodynamic equilibrium, which rigorously takes into account effects of elemental (de)mixing [1, 2]. As a result, new transport coefficients appear in the equations allowing a quantitative predictions and helping to gain deeper insight into the physics of chemically reacting flows at and near local equilibrium. These transport coefficients have been computed for both air and carbon dioxide mixtures allowing the application of this theory to both Earth and Mars entry problems in the framework of a methodology for the determination of the catalytic activity of Thermal Protections Systems materials.

Firstly, we analyze the influence of elemental fraction variations on the computation of thermochemical equilibrium flows for both air and carbon dioxide mixtures [3]. To this end, the equilibrium computations are compared with several chemical regimes to better analyze the influence of chemistry on wall heat flux and to observe the elemental fractions behavior along a stagnation line. The results of several computations are presented to highlight the effects of elemental demixing on the stagnation point heat flux and chemical equilibrium composition for air and carbon dioxide mixtures. Moreover, in the chemical nonequilibrium computations, the characteristic time of chemistry is artificially decreased and in the limit the chemical equilibrium regime, with variable elemental fractions, is achieved. Then, we apply the closed form of the equations governing the behavior of local thermodynamic equilibrium flows, accounting for the variation in local elemental concentrations in a rigorous manner, to simulate heat and mass transfer in CO_2/N_2 mixtures. This allows for the analysis of the boundary layer near the stagnation point of a hypersonic vehicle entering the *true* Martian atmosphere. The results obtained using this formulation are compared with those obtained using a previous form of the equations where the diffusive fluxes of elements are computed as a linear combination of the species diffusive fluxes. This not only validates the new formulation but also highlights its advantages with respect to the previous one : by using and analyzing the full set of equilibrium transport coefficients we arrive at a deep understanding of the mass and heat transfer for a CO_2/N_2 mixture [4].

Secondly, we present and analyze detailed numerical simulations of high-pressure inductively coupled air plasma flows both in the torch [5] and in the test chamber using two different mathematical formulations: an extended chemical non-equilibrium formalism including finite rate chemistry and a form of the equations valid in the limit of local thermodynamic equilibrium and accounting for the demixing of chemical elements. Simulations at various operating pressures indicate that significant demixing of oxygen and nitrogen occurs, regardless of the degree of nonequilibrium in the plasma.

As the operating pressure is increased, chemistry becomes increasingly fast and the nonequilibrium results correctly approach the results obtained assuming local thermodynamic equilibrium, supporting the validity of the proposed local equilibrium formulation. A similar analysis is conducted for CO_2 plasma flows, showing the importance of elemental diffusion on the plasma behavior in the VKI plasmatron torch. As an example, in the following we present some results obtained for air plasmas. To assess the influence of finite rate chemistry on

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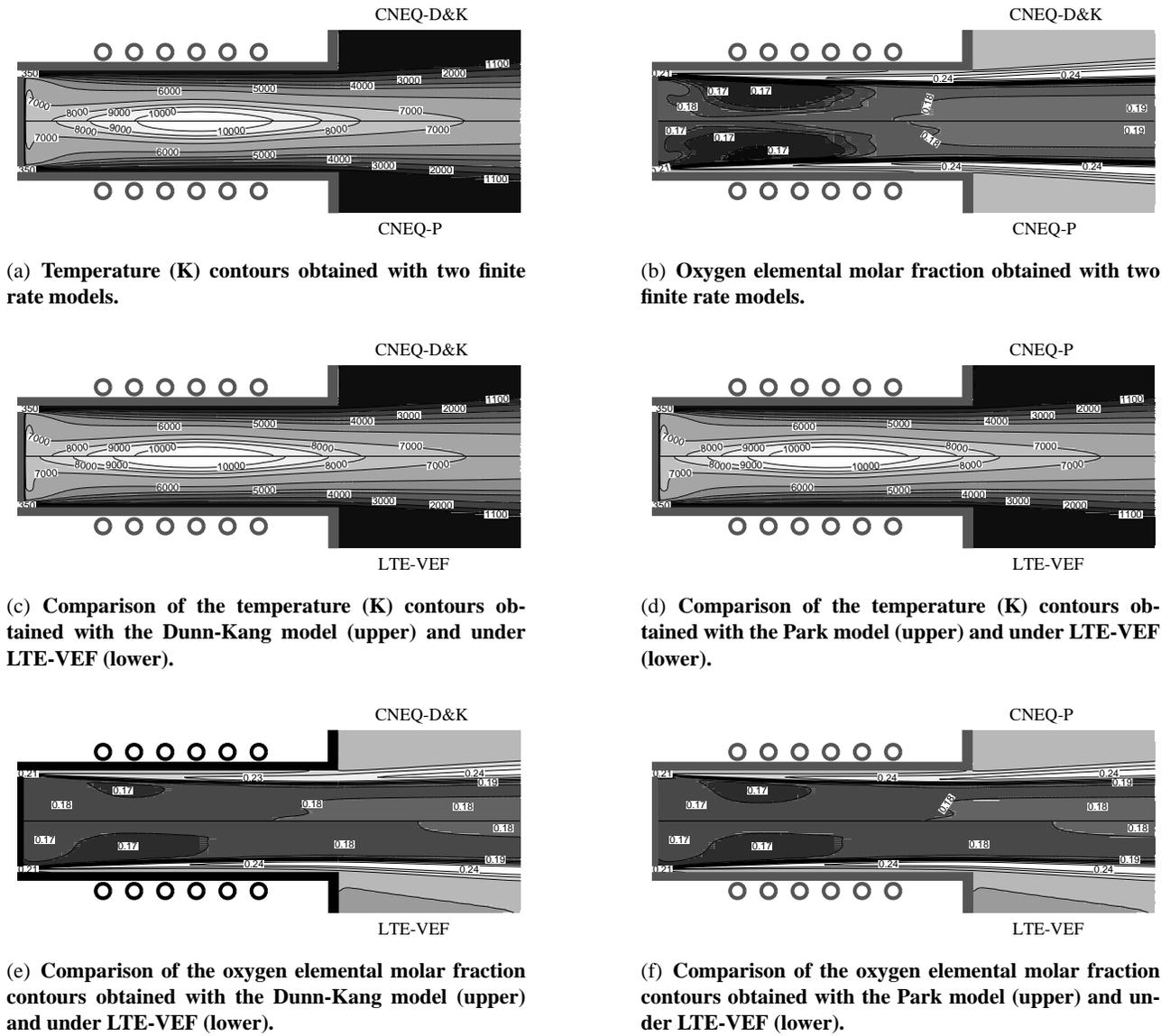


Figure 1: Air plasma flow within the VKI plasmatron facility under CNEQ and LTE-VEF conditions (30000 Pa).

the results of the simulation, two models have been selected as representative of Earth's atmosphere chemistry. Several numerical experiments have been conducted to assess how the operating pressure drives the flow behavior when one of the two models is used. As a result, we notice that the influence of the finite rate chemistry is only limited to low pressures (around 5000 Pa). Indeed, as the operating pressure is set to higher values, the results obtained under chemical non equilibrium (CNEQ) with both models are in very good agreement as shown in Fig. 1. The results presented in Fig. 1 have been obtained under local thermal equilibrium with variable elemental fraction (LTE-VEF) conditions and under CNEQ using two finite rate chemistry models: the

Park model, indicated as CNEQ-P, and the Dunn-Kang model named as CNEQ-D&K. Each non equilibrium result is compared with the respective one obtained with the other finite rate model but also with the result of the simulation carried out under thermochemical equilibrium with variable elemental fraction. This, at the same time, allows for the assessment of the influence of the finite rate chemistry model and to answer the question of whether or not equilibrium computations give the same results as non equilibrium simulations for high pressures in the chamber. A quick analysis of Fig. 1 shows the very good agreement between the temperature and elemental fraction profiles obtained using the chemical non equilibrium and local thermodynamics equilibrium formalisms. As a consequence, we can argue that for sufficiently high pressures the equilibrium formalism allows for the determination of results, both in the torch and in the chamber, characterized by an accuracy very close to the one we can achieve with non equilibrium simulations. This conclusion will allow researchers performing inductively coupled plasma flow simulations for the characterization of TPM, to obtain accurate results using an equilibrium formulation at a fraction of the cost required to simulate the same conditions under non equilibrium.

Thirdly, the extension of numerical tools developed at the von Karman Institute, required within the methodology for the determination of catalycity properties for thermal protection system materials, has been completed for CO₂ flows [6]. Non equilibrium stagnation line computations have been performed for several outer edge conditions in order to analyze the influence of the chemical models for bulk reactions. Moreover, wall surface reactions have been examined, and the importance of several recombination processes has been discussed. This analysis has revealed the limits of the model currently used, leading to the proposal of an alternative approach for the description of the flow-surface interaction. Finally the effects of outer edge elemental fractions on the heat flux map is analyzed, showing the need to add them to the list of parameters of the methodology currently used to determine catalycity properties of thermal protection materials.

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