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Numerical Investigation of High Enthalpy Flows

Francesco Bonelli^{a,*}, Michele Tuttafesta^b, Gianpiero Colonna^c, Luigi Cutrone^d,
Giuseppe Pascazio^a

^a*DMMM & CEMeC, Politecnico di Bari, via Re David 200, 70125, Bari, Italy*

^b*Liceo Scientifico Statale “L. da Vinci”, Via Cala dell’Arciprete 1 - 76011 Bisceglie (BT), Italy*

^c*CNR-IMIP, via Amendola 122/D - 70126 Bari (Italy)*

^d*Centro Italiano Ricerche Aerospaziali (CIRA), Capua, 81043, Italy*

Abstract

This work deals with fluid dynamic simulations of high enthalpy flows. Thermochemical non-equilibrium, typical of such flows, was modelled by using the well known multi-temperature model developed by Park. The non-equilibrium model was implemented in a 2D finite volume solver of the Euler equations and was assessed by comparing the results with available experimental measurements. Several test cases concerning 2D and axisymmetric expansion nozzles were performed by varying gas composition and stagnation temperature.

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1. Introduction

The analysis of high enthalpy flows is important for several engineering applications such as atmospheric entry problems, hypersonic transcontinental flights [1], combustion, flows through exhaust valves etc. Moreover, this subject is also relevant for fundamentals physics.

One of the main issue in modelling high enthalpy flows is that the relaxation time of internal states and chemical reactions can be comparable with the fluid dynamic characteristic time, making the flow a system in thermochemical non-equilibrium. One of the most popular approaches to thermochemical non-equilibrium is the multi-temperature model proposed by Park [2]. Such model assigns a single temperature to translational and rotational degrees of freedom (translational temperature), on the other hand, a different temperature (vibrational temperature) is assigned to vibrational levels which are supposed to follow a Boltzmann distribution and evolve according to a Landau-Teller

* Corresponding author. Tel.: +390805963221 ; fax: +390805963411.

E-mail address: bonellifra@alice.it

law. Moreover, reaction rate coefficients are supposed to follow the semiempirical Arrhenius law with a controlling temperature that is a weighted geometrical mean of translational and vibrational temperatures.

The aim of the present work is to assess the capability of the Park's model [2] and to investigate non-equilibrium effects in expansion nozzles. To this end, the Park's model for a neutral air mixture was integrated in a 2D finite volume solver of the Euler equations [3, 4]. Such model involves five neutral species, i.e., N_2 , O_2 , NO , N , O , which evolve following a kinetic mechanism of 17 reactions, and it considers three vibrational temperatures (one for each molecule).

The model was assessed by considering the experimental setup of Sharma and Ruffin [5], which deals with a high enthalpy nitrogen flow in a 2D nozzle. Moreover, a study of non-equilibrium effects by varying gas composition, stagnation temperature, and geometry configuration was also performed.

The work is organized as follow: in Section 2.1 the governing equations are presented. Then in Section 2.2 the Park's model implemented in this work is described. In Section 2.3 the numerical approach is summarized. The results are presented in Section 3. Finally, the conclusions are summarized.

2. Fluid dynamic model

2.1. Governing Equations

The flow field was simulated by solving the 2D Euler equations for a multicomponent mixture of reactive gases which in integral vector form read

$$\frac{\partial}{\partial t} \int_{V_0} \mathbf{U} dV + \oint_{S_0} \mathbf{F} \cdot \mathbf{n} dS = \int_{V_0} \mathbf{W} dV. \quad (1)$$

The vector of unknown conserved variables, the fluxes along x and y directions and the source term are defined as follows:

$$\mathbf{U} = [\rho_1, \dots, \rho_S, \rho u, \rho v, \rho e, \rho_1 \varepsilon_{vib,1}, \dots, \rho_M \varepsilon_{vib,M}]^T, \quad (2)$$

$$\mathbf{F} = (\mathbf{F}_x, \mathbf{F}_y), \quad (3)$$

$$\mathbf{F}_x = [\rho_1 u, \dots, \rho_S u, \rho u^2 + p, \rho uv, (\rho e + p)u, \rho_1 \varepsilon_{vib,1} u, \dots, \rho_M \varepsilon_{vib,M} u]^T, \quad (4)$$

$$\mathbf{F}_y = [\rho_1 v, \dots, \rho_S v, \rho uv, \rho v^2 + p, (\rho e + p)v, \rho_1 \varepsilon_{vib,1} v, \dots, \rho_M \varepsilon_{vib,M} v]^T, \quad (5)$$

$$\mathbf{W} = [\dot{\omega}_1, \dots, \dot{\omega}_S, 0, 0, 0, \dot{\omega}_{vib,1}, \dots, \dot{\omega}_{vib,M}]^T, \quad (6)$$

where ρ_s is the gas density of the species s , S is the total number of species, p is the gas pressure, u and v are the flow velocity component, respectively in the x and y directions, e is the specific total energy, $\varepsilon_{vib,m}$ is the specific vibrational energy of molecule m and M is the total number of molecules. The total density is given by $\rho = \sum_s \rho_s$. $\{\dot{\omega}_s\}$ are the chemical source terms, whereas $\{\dot{\omega}_{vib,m}\}$ are the vibrational energy source terms.

A relation between p and e is employed to close the system (1) [6]

$$p = (\bar{\gamma} - 1) \left[\rho e - \rho (\varepsilon_{vib} + \varepsilon_{chem}) - \rho \frac{u^2 + v^2}{2} \right], \quad (7)$$

where $\bar{\gamma}$ is the specific heats ratio of the gas mixture, ε_{vib} and ε_{chem} are the total contribution of vibrational and chemical energies given by

$$\varepsilon_{vib} = 1/\rho \sum_{s=1}^M \rho_m \varepsilon_{vib,m}, \quad (8)$$

$$\varepsilon_{chem} = 1/\rho \sum_{s=1}^S \rho_s h_s^f, \quad (9)$$

where h_s^f is the formation enthalpy per unit mass of species s . More details can be found in Refs. [4, 6].

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