An unstructured shock-fitting solver for hypersonic plasma flows in chemical non-equilibrium

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ABSTRACT

A CFD solver, using Residual Distribution Schemes on unstructured grids, has been extended to deal with inviscid chemical non-equilibrium flows. The conservative equations have been coupled with a kinetic model for argon plasma which includes the argon metastable state as independent species, taking into account electron–atom and atom–atom processes. Results in the case of an hypersonic flow around an infinite cylinder, obtained by using both shock-capturing and shock-fitting approaches, show higher accuracy of the shock-fitting approach.

1. Introduction

CFD tools used in the aero-thermodynamic design and analysis of space vehicles entering planetary atmospheres rely upon the use of unstructured meshes: NASA's FUN3D [1,2] and DLR's TAU [3,4] codes are two such examples. Unstructured-grid codes offer greater flexibility than structured ones in tackling complex geometries allowing automatic adaption of the mesh to the local flow features. On the other hand, unstructured codes are less effective and accurate than structured ones especially when strong shocks occur in hypersonic regime due to the formation of stagnation point anomalies [5]. For this reason mesh-independent discretization schemes [6,7] and locally prismatic grids which mimic structured grids around the shocks [8] have been developed. In shock-capturing approach, the existence of an inner shock structure is a purely numerical artefact and the accuracy observed is reduced [9] within the entire shock-downstream region. In this paper a more radical approach based on the shock-fitting method within the unstructured-grid framework has been developed. Shock-fitting discretizations based on the so-called "boundary" variant have been in use until the mid 90s [10,11] to simulate supersonic and hypersonic flows: only the strong bow shock

was fitted and made to coincide with the upstream boundary of a structured mesh; all other shocks were captured. The "floating" variant of the shock-fitting technique, although more versatile since it enables embedded shock fitting, is algorithmically complex, so that only a few three-dimensional calculations have been reported in the literature [12]. Recent applications of the "boundary" shock-fitting technique in conjunction with high-order schemes on structured meshes have been reported in [13], where it is used to perform DNS of compressible turbulence in chemical and thermal non-equilibrium conditions. In recent years, some of the authors have developed an unstructured, shock-fitting algorithm that has been applied to the simulation of steady inviscid flows of a perfect gas in both two and three spatial dimensions [14–16]. This unstructured version of the shock-fitting technique combines features of both the "boundary" and "floating" variants proposed in the structured grid setting: it therefore enables fitting of both shock and embedded shocks. Moreover, the geometrical flexibility offered by the use of unstructured triangular and tetrahedral meshes allows to deal much more properly with interacting shock [17,18] than it was possible in the structured-grid context. The code has been extended to include a chemical non equilibrium description of an argon plasma, in which the continuity equation for the argon metastable state has been considered. Results show that the shock fitting technique can be adopted successfully also in these cases. In the following sections the descriptions of the model and of the numerical method have been reported together with results.

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2. Governing equations

Chemical non-equilibrium flows are governed by the multi-species Navier–Stokes equations, and neglecting viscous terms, by multi-species Euler equations. Given a control volume C, fixed in space and bounded by the control surface ∂C with inward[1] unit normal $\mathbf{n}$, the integral form of the governing conservation laws of mass, energy and linear momentum for an arbitrary mixture of thermally perfect gases in chemical non-equilibrium has the following form:

$$\frac{\partial}{\partial t}\int_C \rho_s dV - \oint_{\partial C} \rho_s \mathbf{u}\cdot\mathbf{n}\,dS = \int_C S_s dV, \tag{1a}$$

$$\frac{\partial}{\partial t}\int_C \rho E dV - \oint_{\partial C} \rho H \mathbf{u}\cdot\mathbf{n}\,dS = 0, \tag{1b}$$

$$\frac{\partial}{\partial t}\int_C \rho \mathbf{u} dV - \oint_{\partial C} \rho \mathbf{u}\mathbf{u}\cdot\mathbf{n}\,dS - \oint_{\partial C} p\mathbf{n}\,dS = \mathbf{0}. \tag{1c}$$

Introducing the vector of conservative variables $\mathbf{U} = (\rho_s, \rho E, \rho\mathbf{u})^t$ the Euler system (1) can be written in the following compact form:

$$\int_C \frac{\partial \mathbf{U}}{\partial t}\,dV = \oint_{\partial C} \mathbf{F}\cdot\mathbf{n}\,dS + \int_C \mathbf{S}\,dV \tag{2}$$

where $\mathbf{F}$ and $\mathbf{S}$ are respectively the inviscid flux and the chemical source terms defined as:

$$\mathbf{F} = \begin{pmatrix} \rho_s\mathbf{u} \\ \rho\mathbf{u}H \\ \rho\mathbf{u}\mathbf{u} + pI_{d\times d} \end{pmatrix}, \qquad \mathbf{S} = \begin{pmatrix} S_s \\ 0 \\ \mathbf{0} \end{pmatrix}. \tag{3}$$

In (3) $I_{d\times d}$ is the identity matrix of order d, where d is the geometrical dimension of the problem, i.e. $d = 2$ for two-dimensional (2D) flows and $d = 3$ for three-dimensional (3D) flows. Eq. (2), can be rewritten in a differential form as follows:

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla\cdot\mathbf{F} = \mathbf{S} \tag{4}$$

whereas the corresponding quasi-linear form reads:

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}\cdot\nabla\mathbf{U} = \mathbf{S} \tag{5}$$

where the Jacobian matrix of the inviscid fluxes is defined as $\mathbf{A} = \partial\mathbf{F}/\partial\mathbf{U}$.

The expressions of the fluxes $\mathbf{F} = \mathbf{F}_i\mathbf{e}_i$ and of the corresponding Jacobian matrices $\mathbf{A} = \mathbf{A}_i\mathbf{e}_i$ are reported in Appendix A, see Eqs. (A.1) and (A.2).

At high temperature, the effects of intermolecular force on particles motion can be neglected, so that it is possible to consider a mixture of thermally perfect gases [19], and the equation of state is given by Dalton's law:

$$p = \sum_{s=1}^{N_s} \rho_s R_s T = \rho R T. \tag{6}$$

The total internal energy per unit mass $E = e + \frac{\mathbf{u}\cdot\mathbf{u}}{2}$ is the sum of the kinetic energy and the mixture internal energy:

$$e = \sum_{s=1}^{N_s} \alpha_s e_s(T). \tag{7}$$

For high temperature flows it is not possible to neglect the electronic, vibrational and rotational energy excitation, which implies that it is not any longer possible to assume that the gas is calorically perfect. The internal energy is given by the sum of a translational contribution e_s^t, a contribution due to the excitation of the internal energy modes e_s^i and the formation enthalpy h_s^f [20–23]:

$$e_s = e_s^t + e_s^i + h_s^f. \tag{8}$$

The translational energy is assumed to be completely excited, it reads:

$$e_s^t(T) = \frac{3}{2}R_s T, \tag{9}$$

while the internal energy can be sub-divided (as a first approximation [22]) into three contributions: rotational (r), electronic (e) and vibrational (v):

$$e_s^i = e_s^r + e_s^e + e_s^v. \tag{10}$$

Concerning the atomic species, the internal energy is only due to the electronic energy while electrons do not have an internal structure. We obtain the following expressions for the internal energy per unit mass:

$$e_s = \frac{3}{2}R_s T + e_s^e + h_s^f \tag{11}$$

being zero the formation energy of electrons. In a state-to-state model, each excited internal state is convected as a single chemical species, which implies that there is no internal contribution to the energy of each individual chemical species [24,25]. For the kth excited level of the sth chemical species, the internal energy is given only by the sum of the roto-translational and formation energies:

$$e_s^i = \frac{3}{2}R_s T + h_{s,k}^f. \tag{12}$$

The internal energy of a given species is given by the sum of the level energy weighted by the internal distribution.

Chemical source terms S_s in Eq. (1) are given by the well known mass action law [20]:

$$S_s = M_s \sum_{r=1}^{N_r} (v_{sr}'' - v_{sr}')\dot{\xi}_r \tag{13}$$

where the velocity for the rth chemical reaction is:

$$\dot{\xi}_r = k_{fr}\prod_{i=1}^{N_s}\left(\frac{\rho_i}{M_i}\right)^{v_{ir}'} - k_{br}\prod_{i=1}^{N_s}\left(\frac{\rho_i}{M_i}\right)^{v_{ir}''}. \tag{14}$$

The reaction rates k_{fr} and k_{br} in Eq. (14) depend upon the selected collisional model [22].

2.1. Kinetic model for an ionized argon mixture

In this work a quasi-neutral argon plasma has been considered in which heavy species and electrons are in thermal equilibrium ($Te = T$). A non-equilibrium plasma would require a detailed collisional–radiative model, considering all possible transitions involving the atomic electronic excited levels [26] and electron energy distribution function (EEDF) may follow a non-Maxwellian distribution [27–29]. This approach could be the subject of future investigations. In this work we considered a reduced number of electronic excited levels, taking into account only three chemical species: the neutral atoms Ar, the positive ions Ar$^+$ and the electrons e^-. Following [30], we consider a two-levels system for the neutral atom, with the ground state Ar^0 and the $4s$ metastable state Ar* and only the ground state for the positive ion Ar$^+$. The

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[1] The use of inward normals is a convention in use since the early developments of this class of schemes.