



Framework for real-gas compressible reacting flows with tabulated thermochemistry



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ABSTRACT

Combustion in liquid rocket engines happens under severe thermodynamical conditions: pressure exceeds the critical pressure of injected propellants and temperature is cryogenic. Such a situation requires an important effort of modeling: real gas effects are incorporated through cubic equations of state along with pressure-correction terms, and transport properties follow specific rules. Modeling for turbulent combustion is also an issue and is presently considered with tabulated chemistry thus reducing the number of transported variables. In this study, a framework is provided to deal with real-gas compressible reacting flows with tabulated thermochemistry. As a consequence, a cubic equation of state for tabulated thermochemistry is derived with the adopted thermodynamic relations, and the temperature computation is adapted to incorporate real gas effects through the tabulated thermochemistry approach. Two-dimensional reactive and non-reactive theoretical test cases have been performed with success to demonstrate the capacity of the new method. Finally, the simulation of a three-dimensional non-reactive single injector derived from Mayer's experiment, that consists of a supercritical nitrogen jet injection into a warm nitrogen atmosphere, is also performed with success. The comparison between the tabulated approach and a fully coupled reference solution leads to similar results for the density values along the jet axis and for the spreading rate.

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1. Introduction

Many energetic systems operate at elevated pressures in order to improve the global system efficiency. For aero-engines, the pressure in the combustion chamber is between 20 and 30 bar, but it reaches 100 bar and above for rocket engines. In the last example, the pressure exceeds the thermodynamic critical pressure, p_c , of the injected propellants (typically H_2 and O_2 for the current Ariane 5 launcher) meaning that the fluid is in a supercritical state, *i.e.* there is no distinction between gas or liquid.

Pressure effects have a direct impact on the Reynolds number through the kinematic viscosity: the Reynolds number increases with pressure involving a decrease of the Kolmogorov scale with consequences on the mesh grid requirements [1]. In addition, for flows under these severe thermodynamical conditions, the flame becomes very thin. Ribert et al. [2] or Pons et al. [3] have shown that diffusion laminar flames are micrometric, meaning that direct numerical simulations (DNS) are definitively out of reach even for massively parallel computers. A way to reduce the numerical CPU

cost is to use tabulated chemistry [4–12]. With this technique, thermo-chemical quantities (Ψ_i) such as species mass fractions or reaction rates are tabulated as functions of a limited set of coordinates that describes physical phenomena like the chemical progress variable, mixture fraction, enthalpy, etc. Look-up tables are generated from canonical problems using complex chemical schemes solved under the low-Mach number assumption. Only few variables are then required to parametrize the whole chemical response compared to the detailed chemistry that needs a large number of species (N_s) and elementary chemical reactions. The set of coordinates, Ψ_i , is transported along with mass, momentum and energy equations. Introducing the tabulated chemistry into large eddy simulations (LES) has already been done with the ideal gas assumption [13–16] and the recent work of Vicquelin et al. [16] raises the issues and proposes solutions to address such coupling when using a full compressible code: temperature computation and boundary conditions treatment appear as crucial elements that must be carefully validated. The first attempt to consider real gas effects through this procedure has been recently performed by Lacaze and Oefelein [17]. Their ultimate goal is to develop a combustion model that reproduces the flame behavior in a rocket engine. Equations for mass, momentum, energy and mixture fraction are considered. A model is introduced into the energy equation

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to recover the correct temperature when using the classical cubic equation of state for real gases. The whole procedure is validated on two-dimensional laminar counterflow diffusion flames that mimic the work of Ribert et al. [2] performed with a one-dimensional low-Mach number code. However, several issues must still be addressed when a more realistic configuration that features real gas effects is simulated: as shown by Vicquelin et al. [16] the validation of the boundary conditions treatment is important for fully compressible codes. It becomes essential when real gas effects are considered because they may involve large density gradients that are challenging to capture [1,18]. Moreover the coupling between the equation of state (EoS) and the thermochemistry tabulated values must still be provided. Indeed, for ideal gases, the sole mean molecular weight of a mixture (W) is depending on the tabulated values (tab) of the species mass fractions Y_k^{tab} . It is then convenient to directly tabulate W^{tab} . The equation of state is then simply cast as $p = \rho RT/W^{tab}$ with ρ for density, T for temperature and p for pressure. \mathcal{R} is the ideal gas constant. Defining such new EoS for real gases based on a very small set of tabulated data has not been proposed yet and, as it will be shown in the next section, is more challenging.

In this study, a general framework is proposed to deal with the entire range of fluid thermodynamic states when a compressible code is coupled to a Ψ_l -dimensions look-up table for thermochemistry. In the next section, the formulation proposed by Vicquelin et al. is extended to a real gas formulation, and a new EoS is proposed to ensure the consistency between the stored information and the values of transported variables. Finally, in Section 3, reacting and non-reacting theoretical test cases are performed as well as the simulation of a non-reacting nitrogen injector under supercritical conditions to assess the whole methodology.

2. Framework for general fluid flows using a tabulated thermochemistry

As stated in Section 1, coupling a compressible solver with a tabulated thermochemistry that features real gas effects requires specific ingredients: a precise temperature computation, an equation of state that can manage together real gas features and data coming from the look-up table, and a robust treatment of boundary conditions. A complete derivation of the last point can be found in [19]: the mathematical development of needed matrixes follows the usual procedure [20], but the partial derivatives must be linked to the considered EoS as shown hereafter.

2.1. Mathematical formulation

The governing equations for reactive flows can be written as:

$$\frac{\partial U}{\partial t} + \frac{\partial F_c^j}{\partial x_j} + \frac{\partial F_d^j}{\partial x_j} = S, \quad (1)$$

where $U = [\rho, \rho u_i, \rho e_t, \rho \Psi_l]^T$ is the vector of conservative variables (unless stated otherwise, the tensor notation for repeated indices is adopted). u_i are the velocity components, ρe_t is the total energy decomposed as the sum of the internal ($\rho e = \rho h - p$) and kinetic ($\rho e_c = \rho u_i^2/2$) energies. h is the enthalpy of the N_s species mixture. Ψ_l is the l th coordinate used to describe the thermochemical database. F_c^j represents the conservative variables flux vectors and is given by: $F_c^j = [\rho u_j, \rho u_j u_i + \delta_{ij} p, \rho u_j e_t + u_j p, \rho u_j \Psi_l]^T$. F_d^j are the diffusive fluxes, $F_d^j = [0, -\tau_{ij}, -u_i \tau_{ij} + q_j, -\rho D(\partial \Psi_l / \partial x_j)]^T$. Assuming a unitary Lewis number, the diffusion coefficient, D , is defined based on the tabulated conductivity, λ^{tab} , and the heat capacity

at constant pressure, C_p^{tab} , as $D = \lambda^{tab}/(\rho C_p^{tab})$. The viscous stress tensor τ_{ij} is written:

$$\tau_{ij} = \mu^{tab} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu^{tab} \frac{\partial u_k}{\partial x_k} \delta_{ij}, \quad (2)$$

where μ^{tab} is the tabulated dynamic viscosity. The heat diffusion flux, q_i , is then expressed as $q_i = -\lambda^{tab}/C_p^{tab} (\partial h)/(\partial x_i)$. The source term vector $S = (0, 0, 0, 0, 0, \dot{\omega}_{\Psi_l})^T$ with $\dot{\omega}_{\Psi_l}$ the chemical rate of the variable Ψ_l .

For general fluid flows, cubic equations of state (EoS) [21] replace the classical ideal gas assumption. These EoS have three parameters (Eq. (3)) which quantify the attractive forces among particles ($a\alpha$), the co-volume of the particles (b), and the deviation from spherical symmetry in a molecule (namely the acentric factor (ω)).

$$p = \frac{\rho \mathcal{R} T}{W - \rho b} - \frac{\rho^2 a \alpha(\omega, T)}{W^2 + u b W \rho + w b^2 \rho^2}. \quad (3)$$

In Eq. (3), \mathcal{R} is the ideal gas constant and W , the molar mass of the mixture. (u, w) depend on the retained model for EoS: $(u, w) = (0, 0)$ for Van der Waals, $(u, w) = (1, 0)$ for Redlich–Kwong or Soave–Redlich–Kwong (SRK) and $(u, w) = (2, -1)$ for Peng–Robinson EoS, respectively [21]. The compressibility factor, Z , is written as $Z = p/(\rho \mathcal{R} T)$. Transport properties are replaced by accurate high-pressure relations such as the one proposed by Chung et al. [22] for viscosity, μ , and thermal conductivity, λ .

2.2. Temperature computation

Solving Eqs. (1)–(3) together requires to compute the temperature from the internal energy, e , and still be in agreement with the thermochemical database. However, the equations governing such database are usually isobaric and written under a low-Mach number assumption. They may not be exactly representative of compressible flows because acoustic waves locally generate energy fluctuations. As a consequence, the computed energy is then slightly different from the tabulated one, $e \neq e^{tab}$, and a special treatment must be done [15,16]. For conciseness, any variable \mathcal{Q}^{tab} will stand for $\mathcal{Q}(\Psi_l)$. For fluid flows featuring real-gas effects, the sensible energy depends on T , Y_k and p (or ρ). Assuming that the mixture composition is fixed and coming from the database ($Y_k = Y_k^{tab}$), i.e. the k transport equations are replaced by the transport of Ψ_l variables, the energy departure between transported and tabulated energies is given by $\Delta e = e(T, \rho) - e^{tab}(T^{tab}, \rho^{tab})$. The differential form of $e(T, \rho)$ is written

$$de = \left. \frac{\partial e}{\partial T} \right|_{\rho, Y_k} dT + \left. \frac{\partial e}{\partial \rho} \right|_{T, Y_k} d\rho \quad (4)$$

or

$$de = C_v dT + \kappa_T d\rho, \quad \text{with } C_v = \left. \frac{\partial e}{\partial T} \right|_{\rho, Y_k} \quad \text{and } \kappa_T = \left. \frac{\partial e}{\partial \rho} \right|_{T, Y_k}. \quad (5)$$

Using the integral form of Eq. (5), $\Delta e = e - e^{tab}$ becomes

$$\Delta e = e - e^{tab} = \int_{T_0}^T C_v(T', \rho) dT' + \int_{T_0}^T \kappa_T(T, \rho') d\rho' - \int_{T_0}^{T^{tab}} C_v(T', \rho^{tab}) dT' - \int_{T_0}^{T^{tab}} \kappa_T(T^{tab}, \rho') d\rho'. \quad (6)$$

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