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A general tool for LTE thermochemistry for adiabatic non-diffusive reactive fluid dynamics: Applications to 2D planar discontinuity flows in SPH

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ABSTRACT

Chemical reactions in fluid dynamics deeply modify physical flow conditions through the contribution of the energy from reactions, as well as through the variations of the mean molecular weight and of the ratio of specific heats. This occurs typically on time scales largely much smaller than the diffusive time scales of chemicals, especially for shock waves due to explosive events. In this work we show how it is possible to include a stand alone algorithm, dealing with both molecular and nuclear thermochemistry in a computational unreactive, non-diffusive, adiabatic flow dynamics in local thermal equilibrium (LTE) within an explicit scheme of integration, free of the adopted computational framework. To this purpose, we worked using the Free Lagrangian GASPHER framework, belonging to the smooth particle hydrodynamics methods (SPH). Assuming the same initial physical conditions, some comparisons are made among reactive to unreactive 2D planar discontinuity flows, assuming the same initial chemical compositions as simple as possible for a better understanding of the role not only of the thermochemical reaction energy, but also of the mean molecular weight and of the ratio of specific heats in fluid dynamics.

1. Introduction

Chemical reactions, essential in the transformation of matter, are fundamental in flow thermodynamics because of their contribution to the energy balance, as well as to the variation of the mean molecular weight and of the ratio of specific heats.

Reactive flows are a more and more challenging theme for the always wider fields of applications, because of their multidisciplinary content regarding real flows. Some textbooks have been written in the scientific literature [1–5] on the theoretical and experimental aspects, with a particular emphasis on atmospheric gases [6] and interstellar plasmas [7], as well as on a huge multitude of industrial and laboratory applications [8]. However, the description of how to implement a stand alone molecular and nuclear chemistry tool, in a fluid dynamics numerical code is an enterprise that has not yet been accomplished.

Therefore, the main aim of this paper is to give a detailed description of the stand alone algorithm we wrote, relative to a gas phase molecular and nuclear thermochemistry in those numerical codes in which a Predictor-Evaluator-Corrector (PEC), or a Predictor-Evaluator-Corrector-Evaluator (PECE), numerical integration technique are used. In particular, this effort is here made in the Smoothed Particle Hydrodynamics (SPH) framework [9], and particularly in its GASPHER version [10].

In this paper, the system of equations for reactive flows, as well as its numerical conversion in the SPH Lagrangian framework, refer to a non-diffusive, adiabatic LTE fluid dynamics. The algorithm we discuss could also be implemented in a wider scenario because those stand alone code sections, dealing with the thermochemistry, strictly concern the reactive fluid dynamics, simply adding the time derivatives of reactive contributions to the density and to the energy time derivatives in the equations of unreactive fluid dynamics. This means that both unreactive fluid dynamics spatial derivatives and time integration algorithms stay unchanged.

Non-diffusive LTE adiabatic reactive flows are meaningful in reactive fluid dynamics in which diffusive time scales are normally much longer than reaction and dynamic time scales. Any chemical quenching of reactions, due to any flow cooling (either radiative or because of the adiabatic expansion), and the successive diffusive transport of reaction products deal with other themes of fluid dynamics, not considered here.

To this purpose, in Section 2 of this paper we recall the system of equations to be solved. Although the new stand alone thermochemistry does not concern a specific scheme of description of fluid dynamics, in the same section we describe how a PEC-PECE

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GASPHER technique works. In Section 3 we use the rate of the local reactive mass density for gases both for molecular and for nuclear reactive flows. In the same section we also show how the specific energy rate, produced by reactive thermothermochemistry processes, is calculated. In Section 4, we discuss the essential algorithm steps on thermochemistry, also showing some flow charts explaining how it is merged within the structure of an unreactive PEC or PECE integration scheme of flow dynamics. In Section 5 we show results relative to 2D planar discontinuity flow structures and to their dynamic evolutions, considering either a molecular or a nuclear thermochemistry. A comparison of each reactive discontinuity flow profile is made with that relative to the simpler unreactive modelling, adopting the same initial conditions, limiting our results to a small number of reactions and of chemicals. In so doing it is better possible to understand the role of physical parameters within the assumed state equation (EoS). After indicating some caution required in dealing with reactive flows, conclusions are reported in Section 6, also considering the existence of other numerical reactive fluid dynamics codes, working with plasma nuclear thermochemistry flows.

2. Adiabatic non-viscous reactive flows in LTE: how a stand alone algorithm is set in the GASPHER approach

2.1. The equations of adiabatic non-viscous reactive flows in LTE

In the physically adiabatic, non-diffusive and non-viscous flows, the hyperbolic Euler system of equations in the Lagrangian scheme in LTE for reactive flows:

$$\frac{d\rho}{dt} + \rho\nabla\cdot\mathbf{v} = \sum_{k=1,r=1}^{K,R} \left.\frac{d\rho_k}{dt}\right|_r \quad \text{continuity equation} \tag{1}$$

$$\frac{d\mathbf{v}}{dt} = -\frac{\nabla p}{\rho} + \mathbf{f} \quad \text{momentum equation} \tag{2}$$

$$\frac{d}{dt}\left(\epsilon + \frac{1}{2}v^2\right) = -\frac{1}{\rho}\nabla\cdot(p\mathbf{v}) + \mathbf{f}\cdot\mathbf{v} + \sum_{k=1,r=1}^{K,R} \left.\frac{d\epsilon_k}{dt}\right|_r \quad \text{energy equation} \tag{3}$$

$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \quad \text{kinematic equation} \tag{4}$$

must be solved, together with the state equation (EoS) of the fluid

$$p = f(\gamma, \rho, \epsilon, \mathbf{r}, \mathbf{v}) \quad \text{state equation.} \tag{5}$$

$k = 1, \ldots, K$ is an index relative to the specific chemical component among the totality of K chemicals, and $r = 1, \ldots, R$ is an index relative to the rth chemical reaction. d/dt stands for the Lagrangian derivative, ρ is the total gas mass density, ϵ is the thermal energy per unit mass, p is the gas pressure, here generally expressed as a function $f(\ldots)$ of local properties, $\mathbf{v}$ and $\mathbf{r}$ are the vectors velocity and position, $\mathbf{f}$ is the external force field per unit mass. The adiabatic index $\gamma = c_p c_V^{-1}$ is the ratio of specific heats.

$$\sum_{k=1,r=1}^{K,R} \left.\frac{d\rho_k}{dt}\right|_r = 0 \tag{6}$$

for a molecular chemistry, while

$$\sum_{k=1,r=1}^{K,R} \left.\frac{d\rho_k}{dt}\right|_r \neq 0 \tag{7}$$

for a nuclear chemistry.

For nuclear reactions, the mass to the binding energy conversion (and vice versa) should also be taken into account.

In LTE conditions, a molecular chemistry contributes only with the algebraic summation term to the right side of Eq. (3), while the continuity equation could also be involved for a nuclear chemistry. For each chemical component k, the specific continuity equation is:

$$\frac{d\rho_k}{dt} + \rho_k\nabla\cdot\mathbf{v} = \sum_{r=1}^{R} \left.\frac{d\rho_k}{dt}\right|_r, \tag{8}$$

being $d\rho_k/dt|_r$ the explicit algebraic contribution due to the rth reaction to the kth chemical component. Moreover, $\sum_{k=1}^{K}\rho_k = \rho$. In so doing, the summation over k of Eq. (8) gives exactly Eq. (1). If ε_k is the energy contribution per unit mass corresponding to the kth chemical component (e.g. its formation enthalpy $\Delta H^0_{f,k}$ or its rest-mass-energy q_k), for the rth reaction

$$\left.\frac{d\epsilon_k}{dt}\right|_r = -\frac{\varepsilon_k}{\rho}\left.\frac{d\rho_k}{dt}\right|_r. \tag{9}$$

Notice that ϵ_k and ε_k are not conceptually equal with each other, the first being a computed energy per unit mass, while the second being an assigned energy per unit mass for the same kth chemical component.

It is important to note that the temporal variations due only to the reaction rates can indifferently be either Lagrangian derivatives d/dt or Eulerian derivatives $\partial/\partial t$, being any chemistry strictly local. Henceforth, we will indistinctly adopt the $\dot{A}$ formalism to identify the reaction rate of the chemical species A, instead of $\partial A/\partial t$ or dA/dt. This implies that any stand alone numerical algorithm to calculate the flow chemical composition could be directly implemented in any numerical scheme. In that regard, we adopt a finite volume Lagrangian scheme of moving smooth domains, based on the well-known SPH framework [9], formulated on the basis of the mathematical error function as a profile of the spatial distribution of the smooth physical properties [10].

2.2. The GASPHER interpolation-integration Kernel in the SPH framework

The SPH method is a nonlinear Free Lagrangian scheme [11] depicting the fluid into interacting and interpolating domains called "particles" [12,13], moving according to pressure and body forces. The method makes use of a Kernel W useful to smoothing interpolate a physical quantity $Q(\mathbf{r})$ related to a gas particle at position $\mathbf{r}$ according to:

$$\bar{Q}(\mathbf{r}) = \int_D Q(\mathbf{r}')W(\mathbf{r}, \mathbf{r}', h)d\mathbf{r}'. \tag{10}$$

$W(\mathbf{r}, \mathbf{r}', h)$, the interpolation-integration Kernel, is a continuous function – or even two or more connecting continuously differentiable functions at their connecting point – defined within a spatial window, whose spatial resolution length limit for $h \to 0$ is the Dirac delta distribution function. All physical quantities are described as extensive properties, smoothly distributed in space, and computed by interpolation at $\mathbf{r}$. Therefore, in the SPH formalism:

$$\bar{Q}(\mathbf{r}_i) = \bar{Q}_i = \sum_{j=1}^{N} \frac{Q_j}{n_j} W(\mathbf{r}_i, \mathbf{r}_j, h) = \sum_{j=1}^{N} \frac{Q_j}{n_j} W_{ij} \tag{11}$$

at the position $\mathbf{r}_i$ of the ith particle. The sum is extended to all neighbour particles included within the domain D, $n_j = \rho_j m_j^{-1}$ is the number density relative to the jth particle. $W(\mathbf{r}_i, \mathbf{r}_j, h)$ is the adopted interpolation-integration Kernel, whose value is determined by the relative distance between particles i and j. $\int W(\mathbf{r}_i, \mathbf{r}_j, h)d^3\mathbf{r}' = 1$, that is: $\sum_j W(\mathbf{r}_i, \mathbf{r}_j, h)n_j^{-1} = 1$.