A method for the direct numerical simulation of hypersonic boundary-layer instability with finite-rate chemistry

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ABSTRACT

A new numerical method is presented here that allows to consider chemically reacting gases during the direct numerical simulation of a hypersonic fluid flow. The method comprises the direct coupling of a solver for the fluid mechanical model and a library providing the physio-chemical model. The numerical method for the fluid mechanical model integrates the compressible Navier–Stokes equations using an explicit time advancement scheme and high-order finite differences. This Navier–Stokes code can be applied to the investigation of laminar-turbulent transition and boundary-layer instability. The numerical method for the physio-chemical model provides thermodynamic and transport properties for different gases as well as chemical production rates, while here we exclusively consider a five species air mixture. The new method is verified for a number of test cases at Mach 10, including the one-dimensional high-temperature flow downstream of a normal shock, a hypersonic chemical reacting boundary layer in local thermodynamic equilibrium and a hypersonic reacting boundary layer with finite-rate chemistry. We are able to confirm that the diffusion flux plays an important role for a high-temperature boundary layer in local thermodynamic equilibrium. Moreover, we demonstrate that the flow for a case previously considered as a benchmark for the investigation of non-equilibrium chemistry can be regarded as frozen. Finally, the new method is applied to investigate the effect of finite-rate chemistry on boundary layer instability by considering the downstream evolution of a small-amplitude wave and comparing results with those obtained for a frozen gas as well as a gas in local thermodynamic equilibrium.

1. Introduction

The accurate prediction of the location of laminar-turbulent transition in the boundary layer is a critical step in the design of hypersonic flight vehicles. In comparison to laminar flows, turbulent flows induce much higher thermal load on the surface of vehicles moving through a planetary atmosphere at high speed [1].

1.1. Boundary-layer dynamics

Depending on the type of vehicle and its mission, the gas surrounding the vehicle may heat up significantly. For slender bodies at hypersonic speeds, the temperature at the boundary-layer edge may be comparable to the temperature of the

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environment through which the vehicle moves, owing to the small deflection angle of the leading edge shock produced by the vehicle. The temperature inside the boundary layer may be very high owing to a conversion of kinetic energy into thermal energy. For blunt re-entry vehicles a strong increase in temperature is expected in the shock layer as a result of the severe bow shock in front of the vehicle. Hence, it is the edge temperature that may be highest in this case; for an example see Fig. 4 in [2]. Here, we consider only the former case, i.e. low temperature at the boundary-layer edge.

Laminar-turbulent transition for flows of a high-temperature gas has been considered experimentally [3,4] and using linear theories for parallel [5–9] and non-parallel flow [10]. The theoretical calculations must be preceded by a numerical simulation in order to obtain a steady-state boundary-layer flow, which is then used as a base flow in the theoretical approach. A number of low-order numerical methods exist for this purpose (see for instance [11,12]).

1.2. Chemically reacting gases at high temperature

High-temperature gas effects may influence boundary-layer dynamics. For instance, chemical reactions in a gas mixture may affect the thermodynamic and transport properties of the fluid, the flow, and hence the process of laminar-turbulent transition [13]. If the reaction rates are much smaller compared to the convective mass transport rate, the fluid is frozen. If the reaction rates are much larger compared to the convective mass transport rate, the fluid is in chemical equilibrium. The regime of finite-rate chemistry, or non-equilibrium chemistry, lies in between these two limiting states.

A gas of a single species is called a calorically perfect gas if its internal energy is proportional to the temperature and hence its specific heat is constant. For a thermally perfect gas of a molecular species, however, the internal energy is a non-linear function of a single temperature due to the excitation of vibrational and electronic modes of the molecules. Below we will only consider gases in thermal equilibrium, for which thermal-relaxation characteristic time scales are very small.

In most practical applications, the fluid is a mixture of gases, for example air composed of atomic and diatomic species. At low temperature, vibrational and electronic modes are not excited and the gas mixture behaves as a calorically perfect gas. As temperature increases, these modes get excited and the specific heat becomes a function of temperature. If the temperature remains below a certain threshold, chemical reaction rates are low and the composition of the gas mixture does not change: the gas mixture is frozen. Eventually for even higher temperature chemical reactions may cause the molecules to dissociate and hence change the composition of the mixture. The surface can also influence the gas composition due to catalycity effects. The details of these effects are neglected here, i.e. we consider only non-catalytic surfaces. Finally, a gas in thermal non-equilibrium is described by multiple temperatures.

The dissociating gas is in local thermodynamic equilibrium only if the characteristic time based on the flow velocity is large compared to all chemical-reaction and thermal-relaxation characteristic time scales. In equilibrium, the gas composition depends on only two thermodynamic quantities, such as the temperature and the pressure, provided that the elemental composition is constant. The composition of a gas in chemical non-equilibrium is governed by transport equations for the chemical species densities, and this complicates the numerical treatment significantly. Our objective here is to develop and verify a numerical method applicable for the chemical non-equilibrium regime.

1.3. Numerical methods

Numerical methods for finite-rate chemistry have been reported for time-dependent flows involving combustion. While the expression 'finite-rate chemistry' is commonly used as a synonym for 'non-equilibrium chemistry' or 'real gas effects' in the literature on hypersonic flow, the combustion community uses the expressions 'detailed chemistry' or 'complete chemical scheme' instead. An overview of methods used for combustion is given in [14]. A number of second-order methods are described in the literature [15–17], but only few methods with higher order are reported [18]. All the cited methods for combustion have in common that they rely on a low Mach number formulation. They are therefore not applicable to the hypersonic flow regime.

Several numerical simulations of hypersonic boundary layer instability and laminar-turbulent transition have been performed for calorically perfect gases. On the other hand, only a few numerical methods for non-equilibrium chemistry have been reported in which an unsteady solution to the compressible Navier–Stokes equations at hypersonic speeds has been sought [19,20]. The complexity associated with the combination of unsteady boundary-layer instability waves that cause transition [21], high Mach numbers, and high temperatures makes such time-dependent simulations challenging.

Numerical methods based on a high-order discretization are particularly well suited for simulations of unsteady phenomena occurring during laminar-turbulent transition. These methods require low dispersion and dissipation in order to preserve the character of the underlying flow. Examples for these high-order numerical methods that are capable of handling the high-temperature regime including finite-rate chemistry can be found only in the recent literature, such as [22–24].

As stated above, the state of boundary layer is strongly influenced by the freestream conditions arising from vehicle geometry and its mission. The boundary layer could be in local thermodynamic equilibrium, chemical non-equilibrium and thermal equilibrium, or even in full thermo-chemical non-equilibrium including gas–surface interaction. For this reason, studies for all these conditions are justified at present. The condition of local thermodynamic equilibrium has previously been considered by Marxen et al. [25]. In order to study the chemical non-equilibrium regime for complex, transitional test cases, a simulation method capable of handling this regime must be developed and verified.