Computations of the Shock Waves at Hypersonic Velocities Taken into Account the Chemical Reactions that Appear in the Air at High Temperatures

Mihai Leonida NICULESCU*,[1], Marius Gabriel COJOCARU[1]
Mihai Victor PRICOP[1], Dumitru PEPELEA[1]

*Corresponding author
[1]INCAS − National Institute for Aerospace Research "Elie Carafoli",
Flow Physics Department, Numerical Simulation Unit,
B-dul Iuliu Maniu 220, Bucharest 061126, Romania
niculescu.mihai@incas.ro*, cojocaru.gabriel@incas.ro, pricop.victor@incas.ro
pepelea.dumitru@incas.ro

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Abstract: *The temperature in the nose region of a hypersonic vehicle can be extremely high, for example, reaching approximately 11 000 K at a Mach number of 36 (Apollo reentry). The bow shock wave is normal, or nearly normal, in the nose region of a blunt body, and the gas temperature behind this shock wave can be enormous at hypersonic speeds. In this case, the assumption of a calorically perfect nonreacting gas with the ratio of specific heats γ of 1.4 gives an unrealistically high value of temperature. Therefore, the proper inclusion of chemically reacting effects is vital to the calculation of an accurate normal shock wave temperature.*

Key Words*: Hypersonic flow, shock waves, chemical reactions, CFD, capsule reentry.*

1. INTRODUCTION

It is well known that at high temperatures, the air become to dissociate and ionize. For example, for air at one atmosphere, the molecular oxygen become to dissociate at about 2500 K and it is essentially totally dissociated at 4000 K.

At this temperature, molecular nitrogen begins and it is essentially totally dissociated at 9000 K. Above this temperature, ions are formed and the gas becomes a partially ionized plasma [1]. Unfortunately, the kinetics of these chemical reactions (cr) is quite, not very well understood and requires huge computational resources. For example, only the air dissociation requires at least 5 chemical reactions with third body efficiency and five species (O_2, O, N_2, N, NO) [2, 3].

For this reason, the present paper presents a simplified CFD method for computing the capsule reentry, which takes into account both the released or absorbed heat *Q* due to the chemical reactions and the modification of global gas constant *R*.

2. GOVERNING EQUATIONS FOR OBLIQUE SHOCK WAVES WITH CHEMICAL REACTIONS

The conservation laws of continuity, momentum and energy for oblique shock waves with chemical reactions could be written as follows [4]:

$$\rho_1 u_{1n} = \rho_2 u_{2n} \tag{1}$$

$$p_1 + \rho_1 u_{1n}^2 = p_2 + \rho_2 u_{2n}^2 \tag{2}$$

$$\rho_1 u_{1n} u_{1t} = \rho_2 u_{2n} u_{2t} \xrightarrow{(1)} u_{1t} = u_{2t} \tag{3}$$

$$\begin{aligned} &\frac{U_1^2}{2} + h_1 = \frac{U_1^2}{2} + c_p T_1 = \frac{U_1^2}{2} + \frac{\gamma R}{\gamma - 1} T_1 = \frac{U_2^2}{2} + h_2 - Q = \frac{U_2^2}{2} + c_{p2} T_2 - Q = \\ &\frac{U_2^2}{2} + h_{2\,cr} = \frac{U_2^2}{2} + c_{p2\,cr} T_2 = \frac{U_2^2}{2} + \frac{\gamma_{2\,cr} R_2}{\gamma_{2\,cr} - 1} T_2 = \frac{U_2^2}{2} + \frac{\gamma_{2\,cr}}{\gamma_{2\,cr} - 1} \frac{p_2}{\rho_2} \end{aligned} \tag{4}$$

Combining the above equations, one obtains the following link relation between the shock angle β and the flow deflection angle θ [1]

$$\tan\theta = 2\cot\beta \frac{M_1^2 \sin^2\beta - 1}{M_1^2(\gamma + \cos 2\beta) + 2} \tag{5}$$

for calorically perfect nonreacting air while for reacting air, the link relation is [1]

$$\tan(\beta - \theta) = \frac{u_{2n}}{u_{2t}} = \frac{u_{2n}}{u_{1n}} \frac{u_{1n}}{u_{2t}} = \frac{\rho_1}{\rho_2} \tan\beta \tag{6}$$

3. NUMERICAL SIMULATIONS AND RESULTS

The main difficulty in the implementation of equations for shock waves with chemical reactions in an in-house code consists in obtainment of reliable data for the released or absorbed heat Q due to the chemical reactions. Usually, one gives the pseudo specific heat ratio $\gamma_{2\,cr}$ instead of released or absorbed heat Q because it is more convenient and efficient to implement it from the numerical point of view. Unfortunately, there are very few available works that give data for pseudo specific heat ratio $\gamma_{2\,cr}$, which is clearly a function of temperature and pressure. For example, the reference [1] recommends to use [5] to compute the specific heat ratio $\gamma_{2\,cr} = f(p_2,\rho_2)$ and temperature $T_2 = f(p_2,\rho_2) = p_2/\rho_2/R_2(p_2,\rho_2)$. These functions are quite complex because they have to take into account the chemical reactions (dissociation and ionization) that appear in the air at high temperatures. Unfortunately, our simulations have shown that the function $T_2 = f(p_2,\rho_2)$ given in [5] is not enough accurate and the function $\gamma_{2\,cr} = f(p_2,\rho_2)$ given in [5] is prone to spurious numerical oscillations that can induce the divergence of iterative numerical algorithm. For this reason, we prefer to use the formulas given in [6] that are more complex but they fix the above mentioned deficiencies.

In order to underline that the proper inclusion of chemically reacting effects is vital to the calculation of an accurate normal shock wave temperature, one presents the case of Apollo reentry, in Table 1.

Table 1 – Computation of normal shock wave for Apollo reentry

U_1= 10 972.8 m/s H = 51 816 m	for calorically perfect nonreacting air, γ = 1.4	for equilibrium chemically reacting air (CAL Report AG-1729-A-2 [7])	for equilibrium chemically reacting air (INCAS code)
p_2/p_1	1 233	1 387	1 463
ρ_2/ρ_1	5.972	15.19	15.40
h_2/h_1	206.35	212.8	223.0
T_2/T_1	**206.35**	**41.64**	**42.65**
R_2 [J/(kg.K)]	287	2.19 x 287	2.23 x 287
μ_2 (kg/kmol)	28.96	28.96/2.19	28.96/2.23

From Table 1, one clearly sees that the chemical reactions have the strongest effect on temperature. Moreover, the calorically perfect nonreacting model considerably overpredicts the temperature behind the normal shock wave T_2 by nearly 5 times, given a highly unrealistic value of 55 377 K. For this reason, it is impossible to use the calorically perfect nonreacting model even in the early stages of design because it is impossible to size the thermal shield of reentry vehicles. Instead, the pressure is governed mainly by the fluid mechanics of the flow, and not so much by the thermodynamics. Furthermore, there is a good agreement between the INCAS results and those published in [7].

Due to the dissociation of oxygen and nitrogen ($O_2 \rightarrow 2O$, $N_2 \rightarrow 2N$), the air weight μ decreases. When the dissociated air weight μ becomes 2 times smaller than that of the air at room temperature (28.96 kg/kmol), the air is practically totally dissociated. In the example presented in table 1, the value of temperature behind the normal shock wave T_2 is about 11300 K and air weight μ_2 is approximately 28.96/2.2 kg/kmol; therefore, the air is completely dissociated downstream to normal shock wave.

The bow shock wave is practically a normal one in the nose region of hypersonic reentry vehicles, after which it becomes an oblique shock wave. For this reason, it is very important and useful to study the oblique shock waves at hypersonic regime.

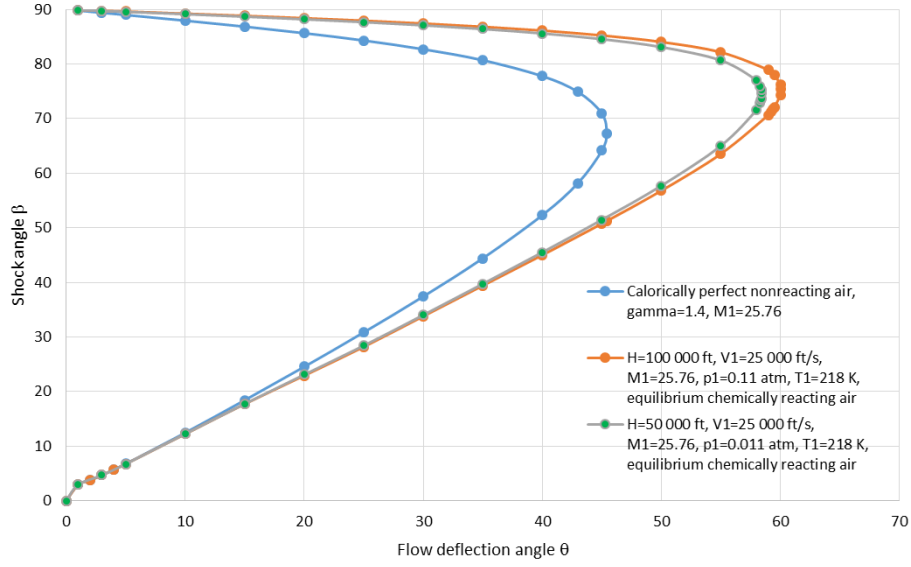

Fig. 1 – Influence of upstream pressure on oblique shock waves

In order to underline the importance of chemical reactions at hypersonic regime, even for oblique shock waves, Fig. 1 clearly shows the difference between the traditional calorically perfect nonreacting air model and equilibrium chemically reacting air model, especially for the maximum (detachment) flow deflection angle θ.

Moreover, there is a quite good agreement between our results obtained with in-house INCAS codes and those published in [8].

Furthermore, one sees that the upstream pressure has a small influence on chemical reactions because the results for upstream pressure of 0.11atm and 0.011atm are almost identical.

This observation is very important because it suggests that it is possible to assume that the pseudo specific pressure heat $c_{p\ cr}$ is function of temperature only in certain pressure ranges.

Unfortunately, there are very few available works that give data for pseudo specific pressure heat $c_{p\ cr}$. Moreover, our simulations have shown that the relations for $c_{p\ cr}$ =f(T) given in [9] are not enough accurate because the numbers that appear in these relations have too few digits.

Even the preliminary simulations of Earth reentry vehicles require a lot of computational work [10]. For this reason, it is useful to have a fast CFD method but it has to be enough accurate.

The real gas model requires more computational effort than the ideal gas model but it is more accurate.

For this reason, we proposed a method based on ideal gas model that takes into account the chemical reactions through introduction of pseudo specific pressure heat $c_{p\ cr}$ =f(T) given in [9] or in another work, instead of classical specific pressure heat c_p and through the modification of classical air constant R_{air} = 287 J/kg/K:

- Compute the normal/oblique shock wave with chemical reactions using equations (1-6)
- use as global air constant R the average mean of R_2 and classical air constant R_{air} = 287J/kg/K, see Table 1
- use pseudo specific pressure heat $c_{p\ cr}$ =f(T) given in [9] or in another work, instead of classical specific pressure heat c_p

Some results using this methodology are given in Figs. 2 and 3.

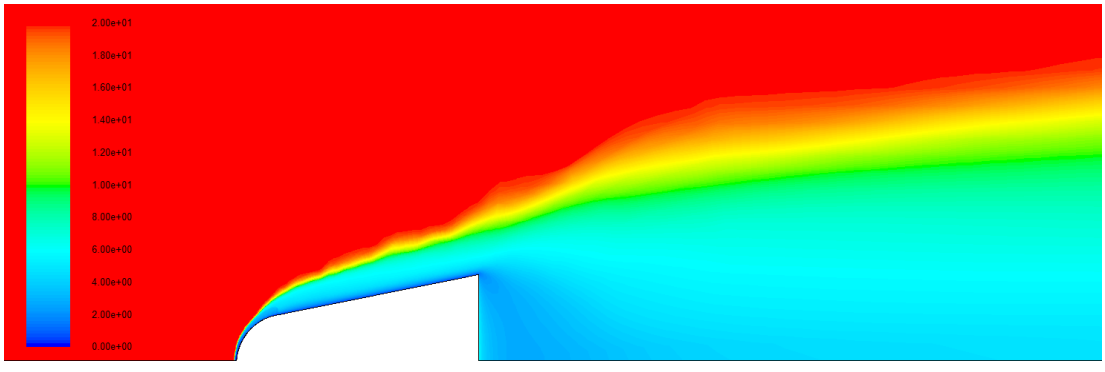

Fig. 2 – Mach number distribution for a reentry capsule, M_∞ = 20, p_∞ = 0.8627 Pa, $c_{p\ cr}$ are taken from [9] using ANSYS Fluent 15 [11] and AUSM scheme

Fig. 3 – Pressure distribution for a reentry capsule, $M_\infty = 20$, $p_\infty = 0.8627$ Pa, $c_{p\,cr}$ are taken from [9] using ANSYS Fluent 15 [11] and AUSM scheme

4. CONCLUSIONS

The present paper presents a CFD methodology that has been successfully implemented in Ansys Fluent to compute the hypersonic vehicles reentry. The chemically reactions that appear in the air at high temperatures are taken into account only through the introduction of pseudo specific pressure heat $c_{p\,cr}(T)$ and the globally changing of air constant R, see Table 1. Further work is necessary to be done in order to diminish the spurious numerical oscillations that appear, see Figs 2 and 3. Moreover, the authors of this paper has succeeded in developing 2 in-house codes written in Fortran that compute normal and oblique shock waves at hypersonic regime taking into account the chemical reactions that appear in the air at high temperatures. Furthermore, there is a good concordance between the results obtained with in-house codes and those published in [7, 8], see Table 1.

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