

Analysis of Non-Equilibrium Thermo-Chemistry in Fire II Re-entry Flowfield

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Abstract

Rapid changes in a re-entry flowfield particularly at the bow shock wave, expansion corners, and neck regions can induce thermo-chemical non-equilibrium in the flowfield. Thermo-chemical non-equilibrium has significant effect on the aerothermodynamics of re-entry capsules. In the present paper, we investigate the non-equilibrium effects in Fire II re-entry flowfield. The re-entry flowfield is computed using five species (N_2 , O_2 , NO , N , O) and three dissociation and two exchange reactions. Two temperature model of Park is used to account for the vibrational non-equilibrium. Further we study the reactions that are effecting the gas composition in the flowfield. We find that thermo-chemical non-equilibrium brings changes in gas composition at the bow shock wave and first expansion corner. The gas chemistry in the separation bubble is frozen.

Keywords: Hypersonics, Re-entry capsules, Turbulent reacting flow, Thermo-chemical non-equilibrium

1 Introduction

Accurate prediction of aerodynamic heating experienced by re-entry capsule will eventually reduce the uncertainty levels associated with heating load on thermal protection system. However prediction of re-entry flows are complicated due to presence of high temperature effects. High temperature at the bow shock wave ahead of the capsule will induce thermal non-equilibrium among the translational, rotational and vibrational modes of the gas and finite rate chemical reactions. Hence appropriate non-equilibrium model should be used to model the high temperature effects. The thermo-chemical non-equilibrium model should consider the all relevant energy exchange mechanisms such as translation-dissociation, vibration-translation and vibration-dissociation in the flowfield. Thus non-equilibrium model has significant effect on computed flow structure, pressure and heat transfer [1].

The objective of the present paper is

to understand the non-equilibrium thermo-chemistry in different regions of a typical re-entry flow field and its effect on gas dynamic properties. The re-entry flowfield considered here is over Fire II re-entry configuration. The vehicle has a spherical forebody and conical afterbody with 66° included angle [2]. Present simulations are performed at 35 km altitude and corresponding freestream conditions are Mach number (M)=16, density (ρ)=0.0082 kg/m³, temperature (T)=237 K.

The paper is organized as follows. The details of the numerical method employed to compute the re-entry flowfield is given in simulation methodology. It is followed by results, in which description of the Fire II flowfield and non-equilibrium at the bow shock wave, expansion and separation bubble are given. Finally conclusion drawn from the current work are presented.

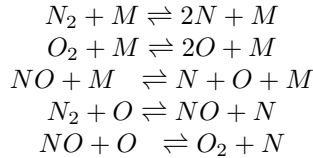
2 Simulation Methodology

The chemically reacting turbulent hypersonic flow around the Fire II re-entry configura-

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tion is simulated by solving the Reynolds-averaged Navier-Stokes equations along with the species conservation equations and the thermal non-equilibrium model. A five-species air chemistry model (N_2 , O_2 , NO , N and O) is used with three dissociation reactions and two exchange reactions [3]. Thermal non-equilibrium is modeled using a rotational-translational temperature and a single vibrational temperature. An additional equation is solved for the vibrational energy of the mixture with the Landau-Teller vibrational relaxation source terms given in Ref [4]. The Spalart-Allmaras model is used for turbulence closure. The governing equations are discretized using the finite volume approach. Inviscid fluxes are computed using a modified (low-dissipation) form of the Steger-Warming flux splitting approach [5], and the turbulence model equations are fully coupled to the mean flow equations [6]. The method is second order accurate both in stream-wise and wall normal directions. The viscous fluxes and turbulent source terms are evaluated using second order accurate central differencing and implicit Data Parallel Line Relaxation [3] is used to obtain steady-state solutions. No-slip, non-catalytic and isothermal wall boundary conditions are specified at the wall. Freestream conditions are specified at the outer boundary. Supersonic exit boundary conditions are specified at the exit section. Since vehicle had nearly zero angle of attack, axisymmetric simulations are performed. The five reactions considered in the present work are



The first three reactions represents dissociation of molecule nitrogen, oxygen and nitric oxide. In the dissociation reactions, M is collision partner, which provides the required energy, to break the chemical bond. The collision partner can be any of the five species, and it is unaltered in the reaction. The last two reactions are the Zeldovich exchange reactions. These Zeldovich reactions govern the concentration of NO in hypersonic flows.

Now the forward and backward reaction rates for the above five reactions are given by

$$R_1 = \sum_m \left[k_{b1m} \frac{\rho_N}{M_N} \frac{\rho_N}{M_N} \frac{\rho_m}{M_m} - k_{f1m} \frac{\rho_{N_2}}{M_{N_2}} \frac{\rho_m}{M_m} \right]$$

$$R_2 = \sum_m \left[k_{b2m} \frac{\rho_O}{M_O} \frac{\rho_O}{M_O} \frac{\rho_m}{M_m} - k_{f2m} \frac{\rho_{O_2}}{M_{O_2}} \frac{\rho_m}{M_m} \right]$$

$$R_3 = \sum_m \left[k_{b3m} \frac{\rho_N}{M_N} \frac{\rho_O}{M_O} \frac{\rho_m}{M_m} - k_{f3m} \frac{\rho_{NO}}{M_{NO}} \frac{\rho_m}{M_m} \right]$$

$$R_4 = k_{b4} \frac{\rho_{NO}}{M_{NO}} \frac{\rho_N}{M_N} - k_{f4} \frac{\rho_{N_2}}{M_{N_2}} \frac{\rho_O}{M_O}$$

$$R_5 = k_{b5} \frac{\rho_{O_2}}{M_{O_2}} \frac{\rho_N}{M_N} - k_{f5} \frac{\rho_{NO}}{M_{NO}} \frac{\rho_O}{M_O}$$

In the above equation k_b and k_f are forward and backward reaction rate constants and these are functions of translational and vibrational temperature of mixture. The rate constants are evaluated using curve fits to experimental data by Park [7]. Suffix m indicates collision partner. ρ_i and M_i represents the i^{th} species density and molecular weight respectively. Translational and vibrational temperature are obtained by solving mixture total energy and vibrational energy equations. Species densities are obtained by solving species continuity equations. The species source term can be represented in terms of the reaction rates as shown below.

$$\begin{aligned}
w_{N_2} &= M_{N_2} (R_1 + R_4) \\
w_{O_2} &= M_{O_2} (R_2 - R_5) \\
w_{NO} &= M_{NO} (R_3 - R_4 + R_5) \\
w_N &= M_N (-2R_1 - R_3 - R_4 - R_5) \\
w_O &= M_O (-2R_2 - R_3 + R_4 + R_5)
\end{aligned}$$

3 Results

Main flow features in terms of the temperature contours are depicted in Fig 1. Detached bow shock ahead of the forebody decelerate the flow and causes sudden rise of temperature at the shock. High temperatures at the shock layer will excite the internal energy modes and chemical reactions in the shock, resulting in non-equilibrium flow downstream of the shock. The temperature in the stagnation region is about 5700 K and it varies less than 5% on the forebody. The flow on the entire forebody is subsonic with the Mach number approaching unity close to the first expansion corner. Flow will turn at the first corner due to expansion. This results in decrease of temperature to 4100 K . Flow

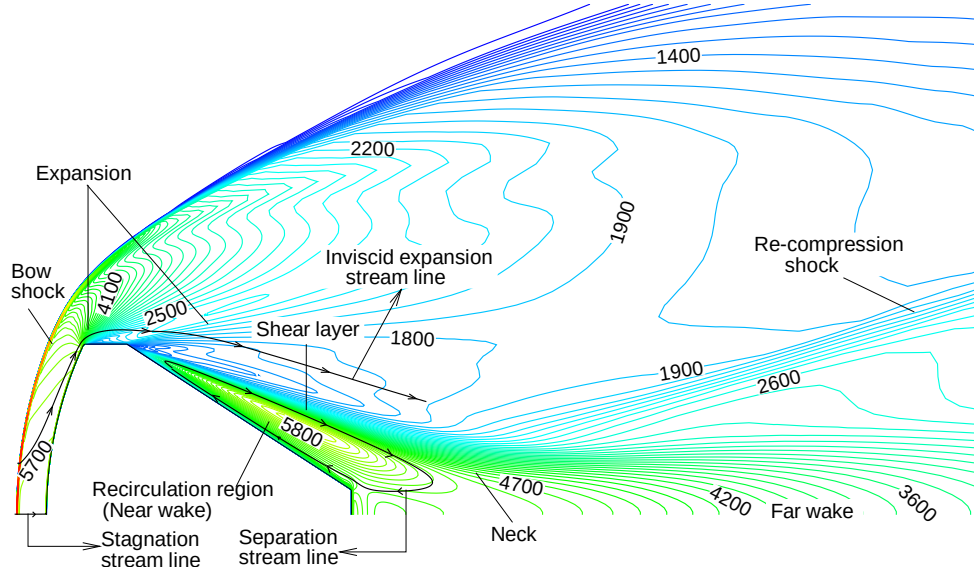


Figure 1: Temperature distribution in the flow around Fire II re-entry capsule at Mach 16 and altitude of 35 km

expansion around the second corner further decreases the temperature to about 2300 K.

Boundary layer separates immediately after the second corner and forms the recirculation region and is referred to the near wake region. The recirculation region consists of a single toroidal vortex and extends up to 0.4 times body diameter downstream of the base. The temperature at the vortex core is about 5800 K. The temperature in the outer inviscid region is about 2000 K and corresponding Mach number is ~ 3.5 . A free shear layer originates from the separation point and separates the inner recirculation region and outer inviscid expansion region. Flow in the separation bubble is subsonic. The outer inviscid flow is turned to freestream direction by a re-compression shock at the neck region. Re-compression shock increases the temperature of the gas to about 4900 K at the neck. Afterbody heat transfer rate predicted by SA turbulence model compared well with flight data and is presented in Ref [8]. Surface pressure predicted by SA model is higher than flight data.

Stagnation stream line

Fig 2(a) is magnified region at the bow shock wave which depicts the variation of the normalized (by freestream values) gas dynamic properties along the stagnation stream

line at the bow shock wave. As a result of strong bow shock wave Mach number suddenly decreases to 0.2 downstream of the shock, from a freestream value of 16. Pressure increases to 330 times freestream value at the shock wave. Density of the gas gradually increases to 12 times of freestream density. Fig 2(b) shows the translational and vibrational temperatures and species mass fractions on the stagnation streamline at the shock wave. Translational temperature peaks at about 8500 K immediately downstream of the shock, followed by a rapid decrease due to transfer of translational energy into the vibrational energy modes and chemical reactions. The vibrational temperature shows a gradual rise to about 6200 K. As the chemical reactions progress, there will be drain in vibrational and translational energy. This results in decrease of both temperatures to a equilibrium value of 5700 K downstream of the shock wave. Flow approaches thermal equilibrium for $s > 0.0075$.

The finite rate chemical reactions results in changes in the source terms which leads to changes in the mass fraction. Fig 2(c) and Fig 2(d) shows the source terms for five species and reaction rates for five reactions along the stagnation stream line at the shock wave. Negative (-ve) and positive (+ve) source terms represents destruc-

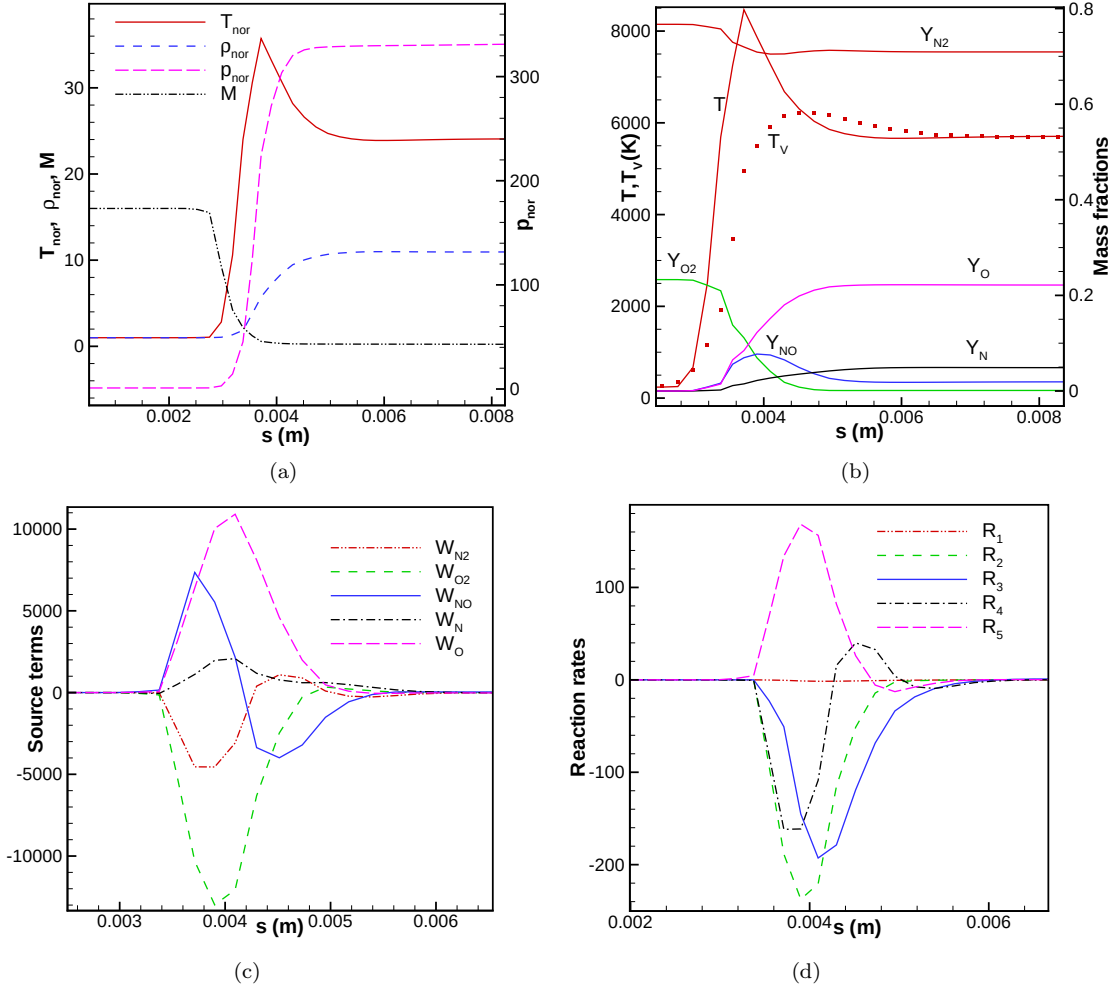


Figure 2: Gas dynamic and chemistry changes at the bow shock wave along the stagnation streamline: (a) Gas dynamic properties (b) Mass fractions (c) Source terms (d) Reaction rates, s represents running length along the stream line

tion and formation of the species respectively. -ve and +ve reaction rates represents dissociation and recombination reactions respectively. Due to finite source terms and reaction rates in the shock region ($s < 0.006$) species mass fractions changes. Hence gas is in chemical non-equilibrium state in this region. Species source terms and reaction rates asymptotically approaches zero for $s > 0.006$, resulting in a constant gas composition. Hence flow approaches chemical equilibrium state for $s > 0.006$. Oxygen is mostly dissociated in the non-equilibrium region which results in gradual increase of mass fraction of O to a maximum value of 0.22. In addition to dissociation of O_2 second Zel-

dovich reaction (R_5) also results in increase in magnitude of W_{O_2} . Hence dissociated oxygen molecules results in the formation of atomic oxygen as well as NO . We notice that the profiles of source terms of O_2 and O are symmetric, although their magnitudes are not equal.

Mass fraction of NO gradually increases to 0.08 at $s \sim 0.004$ and then decreases to a equilibrium value of 0.05. Initially both exchange reactions proceed in a direction such that, they result in the formation of NO . This results in increase of Y_{NO} and W_{NO} up to $s \sim 0.004$. For $s > 0.004$ dissociation of NO occurs and it dominates other two exchange reactions, resulting in -ve source

term for W_{NO} . This results in decrease of mass fraction of NO to 0.05 in the equilibrium region. The change in the sign of source term for NO in the non-equilibrium zone is a combined effect of two exchange reactions (R_4 , R_5) and dissociation of NO (R_3). In addition to the formation of NO , exchange reactions results in the formation of O , N and consumption of N_2 , O_2 . Due to this mass fraction of N_2 decreases to a minimum value of 0.7 at $s \sim 0.004$ and increases to 0.71 in the equilibrium region. Mass fraction of N gradually attains equilibrium value of 0.05. Dissociation of N_2 is negligible compared to other reactions. Hence R_3 , R_4 , R_5 are the reactions that effects the concentration and source terms of N_2 and N .

Inviscid expansion region

Fig 3(a) shows the variation of normalized gas dynamic properties along a stream line that passes through the bow shock wave and expansion region at the shoulder. Variation of the properties at the shock wave are similar to that occurred at the shock region of the stagnation stream line. As the gas turns around the first expansion corner, flow undergoes rapid expansion resulting in a decrease in pressure, temperature and density. Due to expansion, Mach number increases from 0.4 to 3. Flow experiences mild adverse pressure gradient on the shoulder ($s \sim 0.368$) due to which slight increase in pressure, temperature and density can be observed. Further expansion of the flow at the second corner ($0.4 < s < 0.5$) results further decrease of pressure, density and temperature. Mach number increases from 2.8 to 3.7 due to expansion around the second corner. However the changes in all gas dynamic properties around the second expansion corner are less compared to first expansion corner.

Fig 3(b) depicts the variation of the translational and vibrational temperatures and species mass fractions along the expansion stream line. Vibrational temperature differs from the translational temperature at the shock region as well as for $s > 0.25$. The energy exchange mechanism at the shock region is similar to that explained on the stagnation streamline. Downstream of the shock both temperatures equilibrate with each other resulting in thermal equilibrium flow up to

$s \sim 0.209$. Due to expansion of the flow, both temperatures continue to decrease. However T decreases at much faster rate than T_v resulting in thermal non-equilibrium state for $0.209 < s < 0.311$. For $s > 0.311$ the T_v remains constant about 4820 K where as T decreases to about 1650 K. T_v is not sensitive to the expansion at the second corner. Low density in this region ceases the vibrational-translational energy transfer and results in the thermally frozen flow.

Similar behavior can be observed in mass fractions also. Downstream of the shock chemical equilibrium exist up to $s < 0.22$ and chemical non-equilibrium exist for $0.22 < s < 0.27$ where mass fraction of species changes. For $s > 0.27$ mass fractions of species remains constant resulting in the frozen flow. In the non-equilibrium zone Y_{N_2} increases from 0.72 to 0.75 with a corresponding decrease in Y_N (0.04 to 0.01). The predominant reaction for this change in composition is R_4 which results in the formation of the N_2 while consuming N and NO . Recombination reaction of NO (R_3) occurs to a smaller extent than R_4 . This results in -ve source term for NO . Hence Y_{NO} also decreases. Recombination of O_2 also occurs. However R_5 consumes the newly formed oxygen molecules resulting in formation of NO and O . Hence Y_{O_2} is unaffected and Y_O increases. The gas composition is not sensitive to the local changes occurring in the gas dynamic properties at the second expansion corner. Low density in the expanded region ceases chemical reactions resulting in the frozen flow.

Separation bubble

Fig 4(a) shows the variation of gas dynamic properties along a stream line in the separation bubble. Pressure, density and translational temperatures increases from $s = 0$ to $s \sim 0.5$ and then decreases. $s \sim 0.5$ corresponds to the point where velocity direction changes (hereafter referred to as point B). Entire flow on this stream line is subsonic with maximum M of 0.9 at $s \sim 0.15$ and minimum M of 0.08 near point B. Mach number profile attains local peaks at $s \sim 0.15$ and $s \sim 0.879$ compared to single peak in other gas dynamic properties at $s \sim 0.5$. Compared to the temperature variation, pressure and density changes are steeper towards

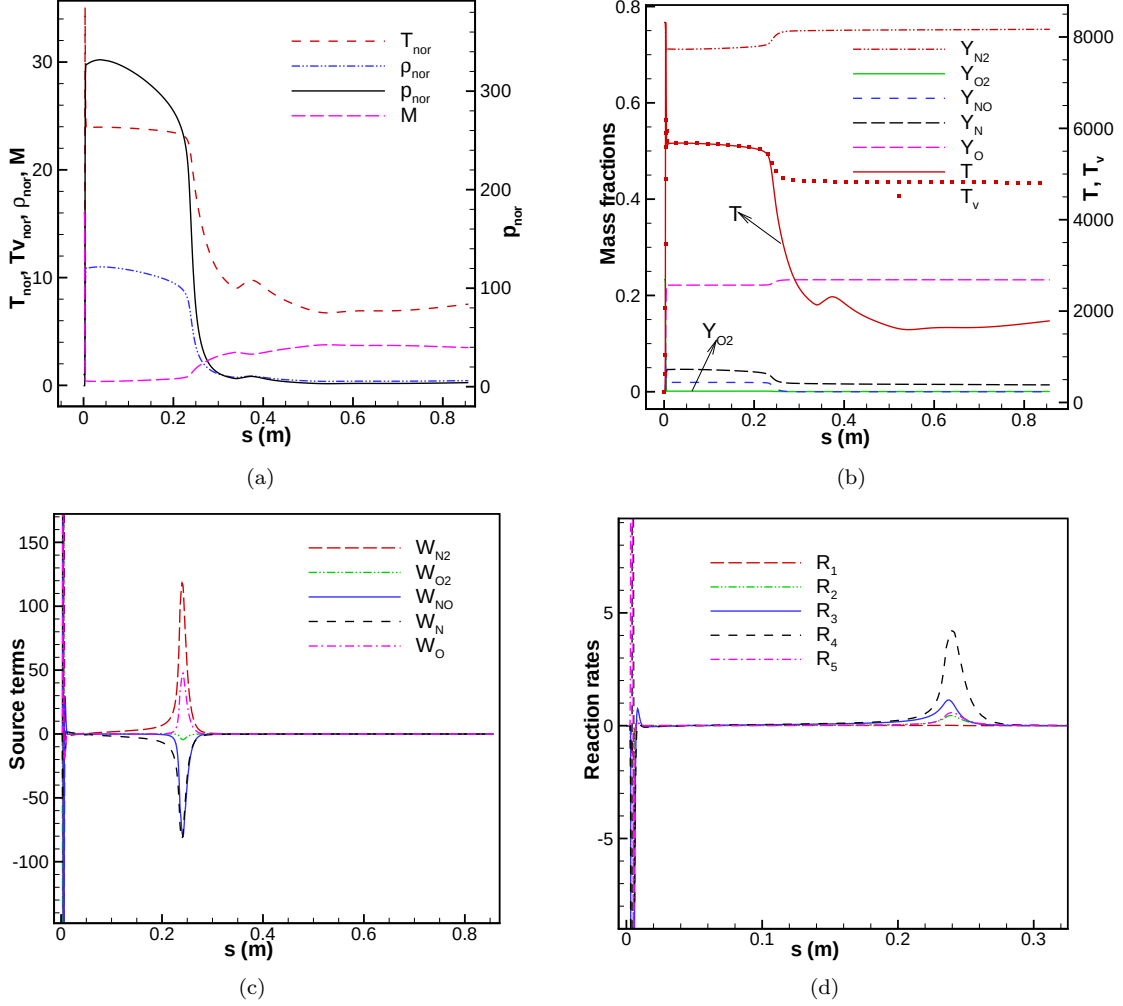


Figure 3: Gas dynamic and chemistry changes along the expansion streamline: (a) Gas dynamic properties (b) Mass fractions (c) Source terms (d) Reaction rates

point B. We can note that density of the gas is much lower than freestream density (with peak density of 0.0024 kg/m^3 at point B). Fig 4(b) illustrates the variation of species mass fraction and translational and vibrational temperature. All along the streamline, vibrational temperature differs from translational temperature resulting in the thermal non-equilibrium state. Translational temperature attains a peak of 5100 K at $s \sim 0.5$. Vibrational temperature attains a peak of 4800 K at $s \sim 0.70$. T is greater than T_v up to $s \sim 0.63$ and in the remaining part of the separation bubble T_v is greater than T .

Y_{NO} gradually increases from 0 at the beginning of the stream line to 0.05 at point B, and then decreases rapidly. O_2 follows simi-

lar behavior of NO , but attains a peak 0.03 much ahead to the point B. Slight changes in the mass fraction of other species can be observed towards point B. The source terms and reaction rates are much smaller in the separation bubble. Although slight change in gas composition can be observed in the separation bubble, the density of the gas is much lower than the expansion region. Hence the change in the gas composition in the separation bubble can be due to molecular and turbulent diffusion effects.

Conclusions

In the present paper we study the thermochemical non-equilibrium at the bow shock

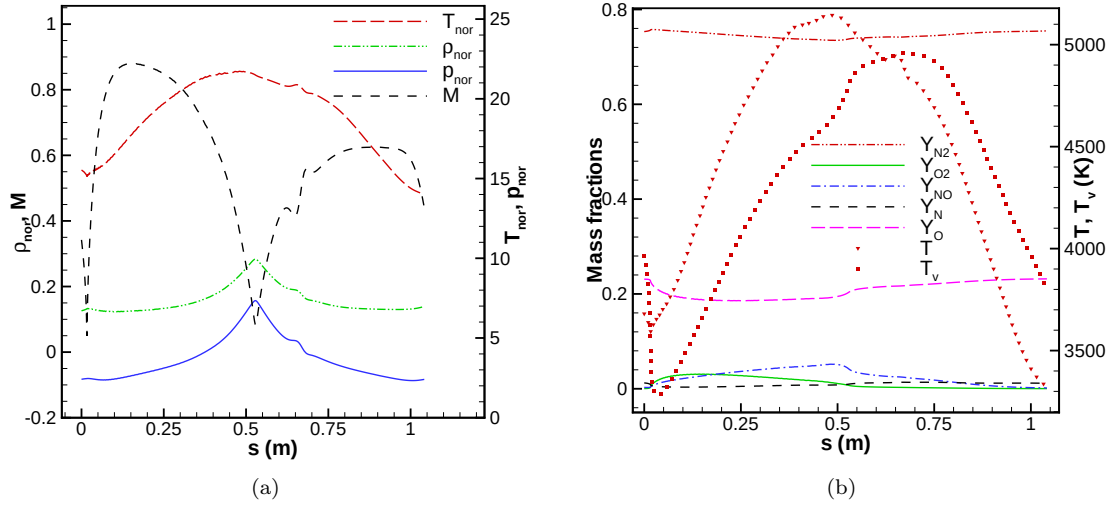


Figure 4: Flow variation along a stream line in the separation bubble: (a) Gas dynamic properties (b) Mass fractions

wave, inviscid expansion region and separation bubble in Fire II re-entry flowfield. High temperature at the shock initiates the non-equilibrium phenomena among the translational and vibrational modes and chemical reactions resulting in decrease of temperature and increase of density. Rapid expansion around shoulder also induces non-equilibrium in the flowfield. However as the flow expands density decreases and as a result, the chemical reactions and vibration-translation energy transfer cease to result in a frozen flow. The gas composition and vibrational temperature remains constant subsequently. Along the expansion stream line flow experiences equilibrium, non-equilibrium and frozen states as it turns around the expansion corners. Contrary to the bow shock wave and inviscid expansion regions, the chemistry is frozen in the separation bubble. However slight changes in composition can be observed in the separation bubble. This can be due to molecular and turbulent diffusion effects.

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