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DIFFUSION MODELS IMPLEMENTATION IN HYPERSONIC FLOW REGIMES

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ABSTRACT

This study highlights the diffusion phenomena in hypersonic flow regimes. It is an important event that has to be define in the flow field solutions. There are two famous diffusion model; Fick's Law of Diffusion and Stefan-Maxwell Diffusion Equation. Both are included in the calculations. The model differences are observed both physically and mathematically. Finally, their results are examined for each of the species.

INTRODUCTION

It is difficult to perform experiments in hypersonic wind tunnels, due to technical difficulties and cost related problems, and also expensive to do experiment during a real flight. Fortunately, advances in technology make computers more powerful. Nowadays, it is possible to simulate hypersonic flows in computers. Engineers use Computational Fluid Dynamics (CFD) to solve such flows.

One of the main purposes of hypersonic flow analysis is the safety of the space craft's crew. Due to high velocity and high temperature, extreme forces and heat act on the surface of the space craft. The gases which can be found in the atmosphere, tend to react with each other. These reactions can change the temperature and species distribution around the space craft. Therefore, the analysis without proper reaction models may yield inaccurate results. The properties of these gases can also change the aerodynamic characteristics of the space craft. Diffusion is one of the important phenomena that affects these changes.

Hypersonic flow usually occurs while a space craft passes through the atmosphere. It means that, the speed of flow is very high. Scalabrin specified that velocity of the flow can be between 7 and 12 km/s defined as hypersonic flow in his thesis [Scalabrin, 2009].

In hypersonic flows, shock is very strong so that, high temperature can be observed in upstream region and it cause intense heating environment [Mathews, 2015]. As an example, Stardust probe has reached 25,000 K in peak stagnation temperature, the photosphere of the Sun has temperature of 6000 K [Sekhar, 2012]. Also, there are some chemical reactions occur in the atmosphere due to temperature changing. Oxygen begins to dissociate if the temperature is between 2000 K to 4000 K [Anderson, 2010].

$$O_2 \longrightarrow 2O \qquad 2000 < T < 4000 \tag{1}$$

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If temperature is between 4000 K to 9000 K than Nitrogen starts to dissociate.

$$N_2 \longrightarrow 2N \qquad 2000 < T < 4000 \tag{2}$$

Finally, if temperature rises above 9000 K, both Oxygen and Nitrogen begins to ionize.

$$\begin{aligned} N \longrightarrow N^+ + e^- \qquad T > 9000 \\ O \longrightarrow O^+ + e^- \qquad T > 9000 \end{aligned} \tag{3}$$

It is stated in Gosse and Candler's paper that, diffusion models are needed [Gosse, 2005]. Yoon and Rasmussen defined that, multi-component mixtures can or cannot react with one another depending on the situation in most hypersonic flow regimes [Yoon, 1999], and this reactions play important role in space craft's safety. Desmeuzes, Duffa, Dubroca state that, diffusion modeling is needed in order to solve forces acting on the body precisely [Desmeuzes, 1997]. They defined that, diffusion is a physical process which, acting on the chemical species.

One of the simple diffusion model is Fick's Law of Diffusion and it can be used almost in every CFD code to model mass diffusion [Yoon, 1999]. Fick's Law is similar to theory of heat conduction by Fourier and it is old as Fourier's law [Patzek, 2006].

Fick's experiment is rather accurate [Patzek, 2006]. However, in his calculations, he took concentration differences as a driving force. Accordingly, there are no effect from other species and components [Bothe, 2009]. On the account of calculating physical forces more accurately, more complex and advanced diffusion models needed such as Stefan-Maxwell diffusion equation [Sutton, 1989]. In Stephan-Maxwell equation, the diffusion fluxes are calculated with respect to other diffusion fluxes. Solving the Stefan-Maxwell equations is gave an accurate and effective results in detailed equations [Sutton, 1989].

METHOD

It is not enough to use classical Navier-Stokes Equations in order to fully solve Hypersonic Flow Regimes. The Species Continuity Equations are essential beside Conservation of Mass, Momentum and Energy Equations. There are some assumptions that have to be clarified before defining any of the parameters. The flow domain must be satisfy the continuum approach in order to solve Navier-Stokes Equations. Therefore, the re-entry altitude is selected approximately 40 km, and Earth's atmosphere is selected as a outside domain. The equations are solved under the steady-state approach, so that the time has no effect on the flow parameters. Finally, heat fluxes are taken into account.

The mixture properties must be define before the diffusion law, due to atmosphere is consisted of mixtures (gases, ions, electrons, ie.).

$$\rho = \sum_{i=1}^{Ns} \rho_i \tag{4}$$

The species must be satisfied the Conservation of Mass Equation so that summation of all species' densities must be equal to mixture's density like in the Equation 4. In this formulation the maximum limit "Ns" is the number of species.

$$Y_i = \frac{\rho_i}{\rho} \tag{5}$$

The ratio of densities in the mixtures is called mass fraction and it can be seen in Equation 5. In addition to this, summation of the mass fraction must be equal to one.

$$x_i = \frac{M_i}{M} \tag{6}$$

The ratio of molar concentration is called mole fraction just like Equation 5, and it can be observed in Equation 6. Also, the summation of mole fraction must be equal to one.

Conservation Equations

There are four equations; namely, Conservation of Mass, Momentum, Energy and Mass of The Species Equations. In this study, 3-D Navier Stokes Equations are solved, so that there are 3 different Momentum Equations; x-Momentum, y-Momentum and z-Momentum Equations.

$$\frac{\partial Q}{\partial t}+\frac{\partial (F-F_v)}{\partial x}+\frac{\partial (G-G_v)}{\partial y}+\frac{\partial (H-H_v)}{\partial z}=S_{cv} \tag{7}$$

The equations can be written in the vector form as seen in Equation 7.

$$Q=\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho w\\ \rho E\\ \rho_1\\ \vdots\\ \rho_{N_s-1}\end{bmatrix}\quad S_{cv}=\begin{bmatrix}0\\0\\0\\0\\0\\ \omega_1\\ \vdots\\ \omega_{N_s-1}\end{bmatrix} \tag{8}$$

In Equation 8, Q is the variable vector, S_{cv} is the source vector.

$$F=\begin{bmatrix}\rho u\\ \rho u^2+P_x\\ \rho uv\\ \rho uw\\ (E+P)u\\ \rho_1 u\\ \vdots\\ \rho_{N_s-1}u\end{bmatrix}\quad G=\begin{bmatrix}\rho v\\ \rho uv\\ \rho v^2+P_y\\ \rho vw\\ (E+P)v\\ \rho_1 v\\ \vdots\\ \rho_{N_s-1}v\end{bmatrix}\quad H=\begin{bmatrix}\rho w\\ \rho uw\\ \rho vw\\ \rho w^2+P_z\\ (E+P)w\\ \rho_1 w\\ \vdots\\ \rho_{N_s-1}w\end{bmatrix} \tag{9}$$

The vectors which described in Equation 9 are inviscid flux vectors.

$$F_v=\begin{bmatrix}0\\ \tau_{xx}\\ \tau_{xy}\\ \tau_{xz}\\ \tau_{xx}u+\tau_{xy}v+\tau_{xz}w-q_x+\sum J_{x,s}h_s\\ -J_{x,1}\\ \vdots\\ -J_{x,N_s-1}\end{bmatrix},G_v=\begin{bmatrix}0\\ \tau_{yx}\\ \tau_{yy}\\ \tau_{yz}\\ \tau_{yx}u+\tau_{yy}v+\tau_{yz}w-q_y+\sum J_{y,s}h_s\\ -J_{y,1}\\ \vdots\\ -J_{y,N_s-1}\end{bmatrix}$$
$$H_v=\begin{bmatrix}0\\ \tau_{zx}\\ \tau_{zy}\\ \tau_{zz}\\ \tau_{zx}u+\tau_{zy}v+\tau_{zz}w-q_z+\sum J_{z,s}h_s\\ -J_{z,1}\\ \vdots\\ -J_{z,N_s-1}\end{bmatrix} \tag{10}$$

The vectors which described in Equation 10 are viscous flux vectors. In these vectors also, the term "J" is the diffusion flux term.

Diffusion Models

There are three important non-dimensional numbers in order to calculate diffusion fluxes.

$$\begin{aligned} Sc &= \tfrac{\nu}{D} = \tfrac{\mu}{\rho D} \\ Le &= \tfrac{\alpha}{D} \\ Pe &= \tfrac{Lu}{D} = ReSc \end{aligned} \tag{11}$$

These numbers can be seen in Equation 11 and they are called Schmidt Number, Lewis Number and Peclet Number respectively. Two diffusion models are used in this study namely, Fick's Law of Diffusion and Stefan-Maxwell Diffusion Equation.

The Fick's Law of Diffusion calculates the diffusion fluxes in terms of concentration differences of the species.

$$J_i = -\rho \sum_{i=1}^{Ns} D_{ij} \bigtriangledown Y_i \tag{12}$$

The Fick's Law of Diffusion can be written in terms of mass fraction and the term D_{ij} in Equation 12 is called the Diffusion Constant or Diffusivity for short. In Fick's law this term is taken constant for all species.

Stefan-Maxwell Diffusion Equation is selected as a second diffusion model. In this equation, diffusion fluxes calculated not only for species concentration differences but also their effects with one and another.

$$J_i = -\rho D_{im} \bigtriangledown Y_i + \frac{Y_i}{(1-x_i)} D_{im} \sum_{j \neq i} (\rho \frac{M}{M_j} \bigtriangledown Y_j + \frac{M}{M_j} \frac{J_j}{Db_{ij}}) \tag{13}$$

The Stefan-Maxwell formulation can be observed in Equation 13. In this formulation the Diffusivity must be calculated for each species pair and the term Db_{ij} is called binary diffusion coefficient.

$$\rho Db_{ij} = 7.1613x10^{-25} \frac{M[T(\frac{1}{M_i} + \frac{1}{M_j})]^{1/2}}{\Omega_{ij}} \tag{14}$$

The Ω_{ij} is called collision cross section for mass diffusion in the calculation of Binary Diffusion Coefficient in Equation 14.

$$\Omega_{ij} = \pi (r_i + r_j)^2 \tag{15}$$

Diffusivity can be calculated easily if the Binary Diffusion Coefficient is known.

$$D_{ij} = Db_{ij}[1 + \frac{x_k(\frac{M_k}{M_j} Db_{ik} - Db_{ij})}{x_i Db_{jk} + x_j Db_{ik} + x_k Db_{ij}}] \tag{16}$$

Equation 16 can be modified to solve for 11 species system. Diffusivity can be written in terms of two different species. However, the combination of two in eleven species system is too much. Therefore, for each species, the effective diffusivity must be calculated.

$$D_{i,eff} = \sum_{j=1}^{n-1} D_{ij} \frac{\Delta x_j}{\Delta x_i} \tag{17}$$

RESULTS AND DISCUSSION

In this study, the Re-entry of Apollo AS-202 Command Module is studied since there are dozens of flight data can be found in the literature. The three dimensional representation can be observed in Figure 1. The half of the capsule is used in the solution due to the symmetric boundary condition. This helps the reduction of the computational time.

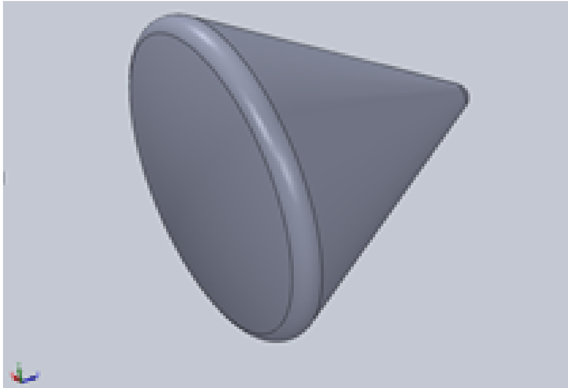

Figure 1: Three Dimensional Representation of Apollo AS-202 Command Module

The flow satisfied the continuum approach in this study as mentioned before. Therefore the free stream conditions selected in the altitude of 40 km which satisfies the continuum approach.

Table 1: Free Stream Conditions

Parameter	Value
Temperature(K)	220
Pressure (Pa)	664
Mach	10.18
Reynolds Number	$1.1x10^6$
Angle of Attack	0^o
Species	11 $(O_2, N_2, N, O, NO, O_2^+, N_2^+, N^+, O^+, NO^+, e^+)$

It is suitable to determine the grid size before starting any calculation. The solutions must be independent of the grid sizes, therefore, four different grids are selected and analyzed for grid independence study.

Table 2: Computational Time of Different Grid Sizes

Grid	i x j x k	Number of Cells	Computational Time (s)
Course	64 x 32 x 17	34816	238300
Medium	96 x 48 x 26	86112	736012
Fine	112 x 56 x 30	188160	1183129
Finer	128 x 64 x 34	278528	1896158

The grid sizes and the calculation time that the solution needs to convergence can be observed in Table 2. In addition to the table, the convergence characteristics of each grids can be seen in Figure 2

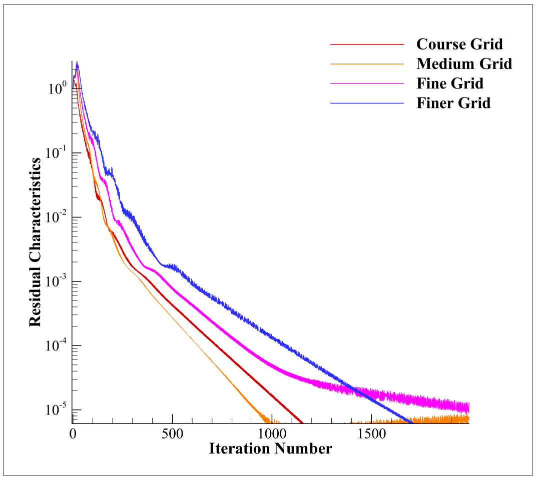

Figure 2: Convergence Characteristics

The grid can be selected with the data from Table 2 and Figure 2. The course grid is more advantageous then the rest in terms of computational time. However, residual characteristics show that it is not accurate as finer grid. The finer grid has higher accuracy as seen in Figure 2. Therefore, the finer grid is used for all calculations.

Firstly, the results for Fick's Law of diffusion are examined. It is important to validate the code with the experimental results. Therefore, for Fick's Law of diffusion is validated with the experiment of NASA.

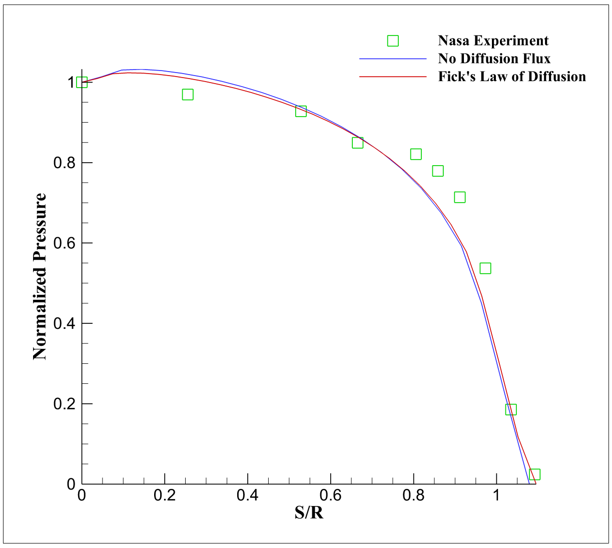

Figure 3: Validation of the Code with NASA's Experiment

The experiment and the code agrees with each other. Also, it can be seen in Figure 3 that addition of Diffusion fluxes are changing the pressure distribution around the stagnation point. The non-dimensional pressure around the stagnation point has a very smooth transition especially in the current study than the experiment. It can be said that since the experiment took place in almost five decades ago, the instruments were not accurate as todays. Therefore, there is a very big differences between experiment and analysis.

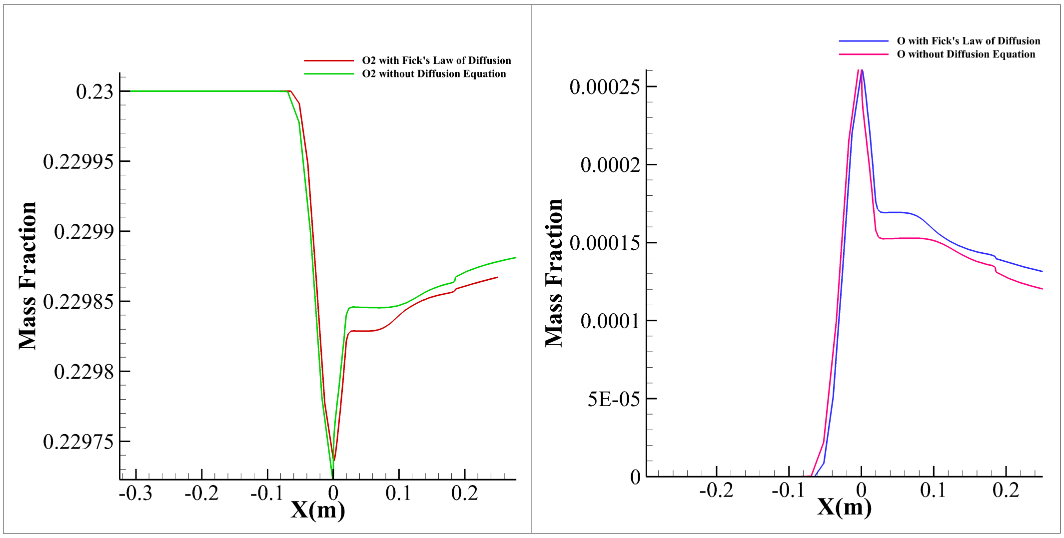

Figure 4: Mass Fraction of Species O and O_2 in the Stagnation Line

The mass fractions of species O_2 and O can be observed in Figure 4 respectively. The diffusion phenomena is effective near the stagnation point because the mass fraction of the species is constant before it.

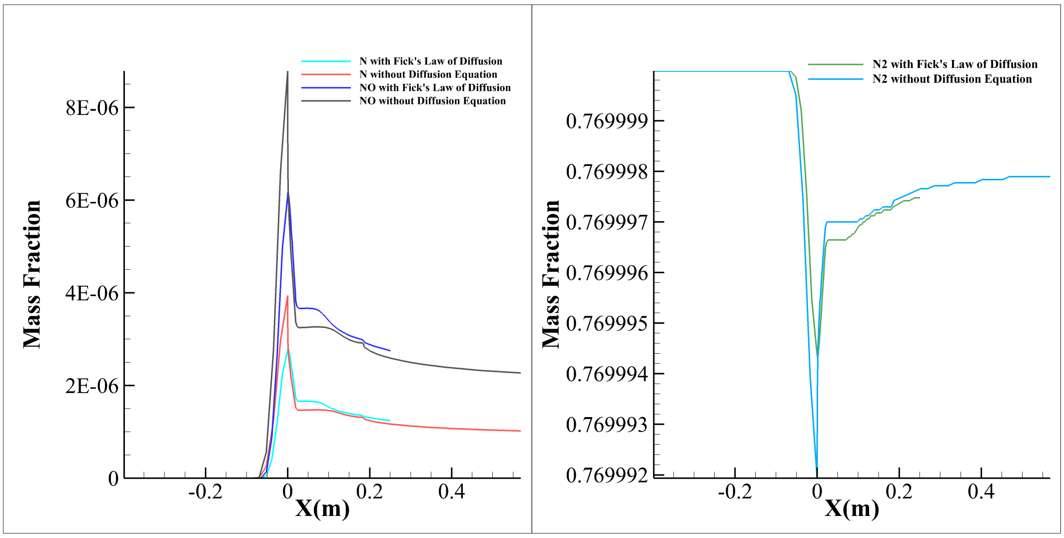

Figure 5: Mass Fraction of Other Species in the Stagnation Line

The mass fraction of the other species in the Stagnation Line can be seen in Figure 5. The Fick's Law of Diffusion helps the species spread even more in the leading edge of the space vehicle. The mass friction of each species is decreased when Fick's Law is applied. Therefore the chemical reactions between them are changed.

Secondly, the Stefan-Maxwell Equation is applied to the code. The same grid and same boundary conditions were used to see the differences between diffusion equations.

In the reentry, one of the important parameter is temperature. The temperature differences can bee seen in Figure 6 for Fick's Law and Stefan Maxwell Equation. The Fick's Law of Diffusion is the simplest diffusion method as mentioned before. It predicts the temperature distribution on the surface far greater than Stefan Maxwell Equation. It should be noted that temperature is one of the important parameter in chemical reactions.

The mass fraction distribution for O_2 and o can be observed for Stefan Maxwell, Fick's Law and

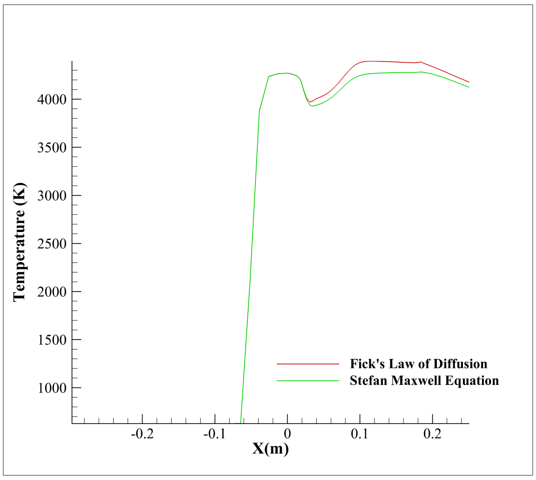

Figure 6: Temperature Distribution for two Diffusion Model in the Stagnation Line

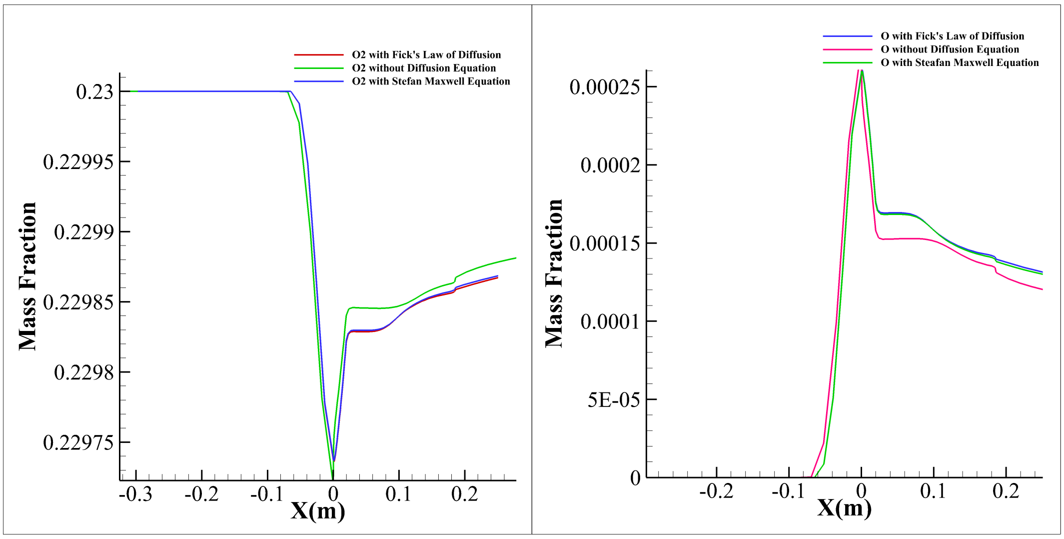

Figure 7: Mass Fraction of Species O and O_2 in the Stagnation Line

without Diffusion Equation respectively in Equation 7. Stefan Maxwell follows the trend for both of the results, but it is closer to Fick's Law of Diffusion.

The mass fraction distribution for other major species can be observed in Figure 8. First thing to notice is that for secondary species (N, O and NO) there is almost no differences. Since these species have less percentage in the flow field, the effect of diffusion is very small. However, in the primary species (N_2 and O_2) the differences can be observed. The Stefan Maxwell Equation gave very similar results to the Fick's Law. The important part is there are small differences between two diffusion models. Fick's Law is very basic model, therefore it is over predicted the mass fractions. On the other hand, Stefan Maxwell Equation is more complex and the results of it are not over predicted. In fact, they are in between Fick's results and no diffusion equation's one.

CONCLUSION

As a conclusion, diffusion models must be applied to the code, in order to get more physically realistic results. There are small differences between two current diffusion models. Fick's Law of Diffusion can be used to get a simple and fast results. On the other hand, Stefan Maxwell Equation gives more realistic results. In order to observe full differences use of the finest grid is required. Also, the experimental approach will improve the results and validation of the both cases.

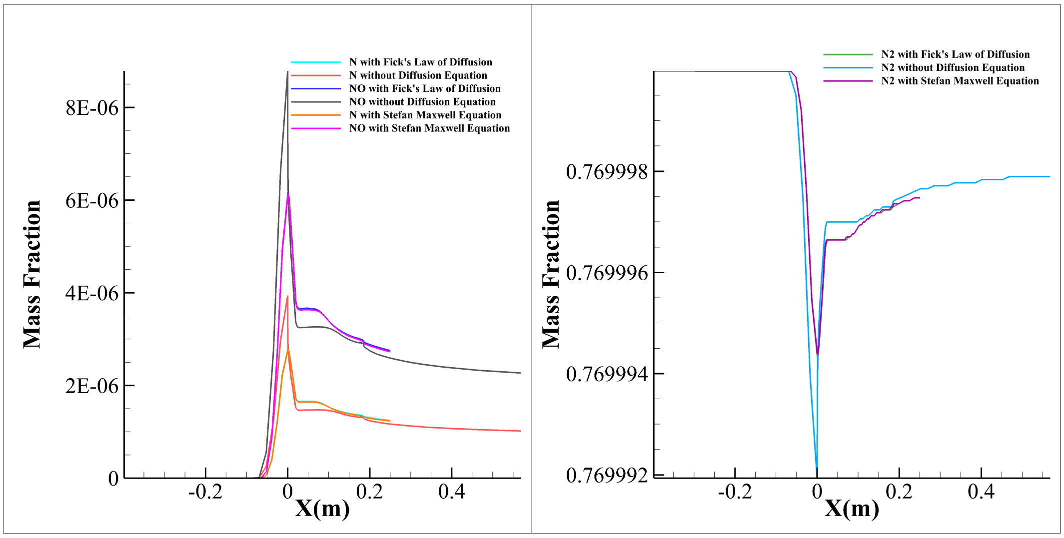

Figure 8: Mass Fraction of Other Species in the Stagnation Line

Finally, as a future work, more realistic diffusion models will be used and the Diffusivity in Fick's Law will be change with another diffusivity calculation. Therefore, it will not be constant in all species. Grid's size will be improved so that the effect will be observed more realistically. Also, the residual of the calculations will be improved.

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