ANALYSIS OF CHEMICALLY REACTING HYPERSONIC FLOW USING A MESHLESS METHOD

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Abstract

This study aims to develop a computational solver which is capable of calculating chemically reacting hypersonic flow based on meshless method. Governing equations for non-equilibrium flow which consists of 5 chemical species (N_2, O_2, NO, N, O) *are discretized using a meshless method based on Least squares method. AUSMPW+ scheme, which was developed to be used in a finite Volume Method for hypersonic flow analysis and adapted for the meshless method, is used for spatial discretization and LU-SGS scheme, which was also adapted for the meshless method, is used for time integration.*

1 Introduction

Heat is generated on the surface of the airplane due to aerodynamic heating in supersonic flight condition, and heat is transferred into the internal structure. When the temperature of the structure rises, structural failure can be occurred by aerodynamic heating. Therefore, accurate computational analysis on aerodynamic heating is essential in design process of thermal protection system. The purpose of this study is to develop a meshless method solver for hypersonic regime which includes non-equilibrium reactions of 5 species in high-temperature air.

2 Meshless Method

2.1 Least Squares Method

The Least Squares Method based on Taylor series expansion is used to calculate discretize the spatial derivative terms of Partial Differential Equations. The Taylor series is expanded up to the first orders term for discretization of the governing equations of hypersonic flow and is expanded up to the second order terms for discretization of the structural heat equation.

The Taylor series at a point with its point cloud is expanded as eq. (1)

$$\Delta\phi_{ij} = \Delta x_{ij}\frac{\partial\phi}{\partial x} + \Delta y_{ij}\frac{\partial\phi}{\partial y} + \Delta z_{ij}\frac{\partial\phi}{\partial z} + \frac{1}{2}\Delta x_{ij}^2\frac{\partial^2\phi}{\partial x^2} + \frac{1}{2}\Delta y_{ij}^2\frac{\partial^2\phi}{\partial y^2} + \frac{1}{2}\Delta z_{ij}^2\frac{\partial^2\phi}{\partial z^2} + \Delta x_{ij}\Delta y_{ij}\frac{\partial^2\phi}{\partial x\partial y} + \Delta y_{ij}\Delta z_{ij}\frac{\partial^2\phi}{\partial y\partial z} + \Delta z_{ij}\Delta x_{ij}\frac{\partial^2\phi}{\partial z\partial x} \quad (1)$$

The least squares method is expressed as eq. (2).

$$\min\sum_{j=1}^{n} w_{ij}\left[\Delta\phi_{ij} - \Delta x_{ij}\frac{\partial\phi}{\partial x} - \Delta y_{ij}\frac{\partial\phi}{\partial y} - \Delta z_{ij}\frac{\partial\phi}{\partial z} - \frac{1}{2}\Delta x_{ij}^2\frac{\partial^2\phi}{\partial x^2} - \frac{1}{2}\Delta y_{ij}^2\frac{\partial^2\phi}{\partial y^2} - \frac{1}{2}\Delta z_{ij}^2\frac{\partial^2\phi}{\partial z^2} - \Delta x_{ij}\Delta y_{ij}\frac{\partial^2\phi}{\partial x\partial y} - \Delta y_{ij}\Delta z_{ij}\frac{\partial^2\phi}{\partial y\partial z} - \Delta z_{ij}\Delta x_{ij}\frac{\partial^2\phi}{\partial z\partial x}\right] \quad (2)$$

$$\frac{\partial\varphi}{\partial x} \approx \sum_j a_{0j}(\varphi_j - \varphi_0) \quad (3)$$

$$\frac{\partial\varphi}{\partial y} \approx \sum_j b_{0j}(\varphi_j - \varphi_0) \quad (4)$$

$$\frac{\partial \varphi}{\partial z} \approx \sum_j c_{0j}(\varphi_j - \varphi_0) \qquad (5)$$

$$\frac{\partial^2 \varphi}{\partial x^2} \approx \sum_j d_{0j}(\varphi_j - \varphi_0) \qquad (6)$$

$$\frac{\partial^2 \varphi}{\partial y^2} \approx \sum_j e_{0j}(\varphi_j - \varphi_0) \qquad (7)$$

$$\frac{\partial^2 \varphi}{\partial z^2} \approx \sum_j f_{0j}(\varphi_j - \varphi_0) \qquad (8)$$

For a 3-D case, values of the meshless coefficients $a_{0j}, b_{0j}, c_{0j}, d_{0j}, e_{0j}, f_{0j}$ are calculated from eq. (9)-(11).

$$\mathbf{Ad} = \mathbf{b} \qquad (9)$$

$$(\mathbf{wA}^{\mathrm{T}})\mathbf{Ad} = (\mathbf{wA}^{\mathrm{T}})\mathbf{b} \qquad (10)$$

$$\mathbf{d} = \left(\mathbf{wA}^{\mathrm{T}}\mathbf{A}\right)^{-1}\mathbf{wA}^{\mathrm{T}}\mathbf{b} \qquad (11)$$

The matrices are defined as eq. (12)-(13).

$$\mathbf{A} = \begin{bmatrix} \Delta x_{i1} & \cdots & \Delta x_{in} \\ \Delta y_{i1} & \cdots & \Delta y_{in} \\ \Delta z_{i1} & \cdots & \Delta z_{i1} \\ \frac{1}{2}\Delta x_{i1}^2 & \cdots & \frac{1}{2}\Delta x_{in}^2 \\ \frac{1}{2}\Delta y_{i1}^2 & \cdots & \frac{1}{2}\Delta y_{in}^2 \\ \frac{1}{2}\Delta z_{i1}^2 & \cdots & \frac{1}{2}\Delta z_{in}^2 \\ \vdots & \vdots & \vdots \end{bmatrix}^{\mathrm{T}} \qquad (12)$$

$$\mathbf{w} = \begin{bmatrix} w_{i1} & \cdots & w_{in} \\ w_{i1} & \cdots & w_{in} \\ \vdots & \ddots & \vdots \\ w_{i1} & \cdots & w_{in} \end{bmatrix}^{\mathrm{T}} \qquad (13)$$

In eq. (13), inverse distance weighting function [1] is defined as eq. (14).

$$\omega_{ij} = \frac{1}{(\Delta x_{ij}^2 + \Delta y_{ij}^2 + \Delta z_{ij}^2)^{1/2}} \qquad (14)$$

2.2 Governing Equations for Chemically Reacting Hypersonic Flow

The 2-D Navier-Stokes equations with species equation in expressed in strong conservation law form.

$$\frac{\partial q}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = \frac{\partial f_v}{\partial x} + \frac{\partial g_v}{\partial y} + \mathrm{S} \qquad (15)$$

$$q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho_i \\ \vdots \end{bmatrix},\ f = \begin{bmatrix} \rho u \\ \rho u^2 + P \\ \rho uv \\ \rho uE \\ \rho_i u \\ \vdots \end{bmatrix},\ g = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + P \\ \rho vE \\ \rho_i v \\ \vdots \end{bmatrix}$$

$$f_v = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ -q_x + \phi_x \\ \rho D_i \frac{\partial \alpha_i}{\partial x} \\ \vdots \end{bmatrix},\ g_v = \begin{bmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ -q_y + \phi_y \\ \rho D_i \frac{\partial \alpha_i}{\partial y} \\ \vdots \end{bmatrix},\ S = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ W_i \\ \vdots \end{bmatrix} \qquad (16)$$

where $\phi_i = \tau_{ix}u + \tau_{iy}v$. The discretization of the equation is explained in next section. The spatial differential terms are can be discretized by meshless coefficients in eq. (6)-(8).

2.3 AUSMPW+ scheme for Meshless Method

Left hand side of Eq. (15) can be discretized as eq. (17)

$$\frac{\partial q_i}{\partial t} + \sum_{j=1}^{n} a_{ij}\Delta f_{ij} + \sum_{j=1}^{n} b_{ij}\Delta g_{ij} = \frac{\partial q_i}{\partial t} + \sum_{j=1}^{n} \Delta F_{ij} \qquad (17)$$

where $F = af + bg$ is a directed flux along the metric weight vector (a, b). The midpoint flux at $\mathrm{j} + \frac{1}{2}$ instead of the flux at j is used for the convective term in the governing equations as eq. (18) [3].

$$\sum_{j=1}^{n} \Delta F_{ij} = 2\sum_{j=1}^{n} \Delta F_{ij+\frac{1}{2}} = 2\sum_{j=1}^{n}\left(F_{ij+\frac{1}{2}} - F_{ij}\right) \qquad (18)$$

$F_{ij+\frac{1}{2}}$ is calculated from AUSMPW+ scheme [2].

The numerical flux of AUSMPW+ is given by eq. (19)

$$F_{\frac{1}{2}} = \bar{M}^{+}{}_{L} c_{\frac{1}{2}} \Phi_L + \bar{M}^{-}{}_{R} c_{\frac{1}{2}} \Phi_R + (P_L^{+} P_L + P_R^{-} P_R) \qquad (19)$$

$\Phi = (\rho, \rho u, \rho H)^T$ and $\mathrm{P} = (0, p, 0)^T$. The subscripts 1/2 and (L,R) stand for quantities at a midpoint on the edge between point *i* and point *j*, and the left and right states across the edge, respectively. The Mach number at the midpoint is defined as eq. (20).

$$m_{\frac{1}{2}} = M_L^+ + M_R^- \quad (20)$$

If $m_{\frac{1}{2}} = M_L^+ + M_R^- \geq 0$, then

$$\overline{M_L^+} = M_L^+ + M_R^-[(1-w)(1+f_R) - f_L] \quad (21)$$

$$\overline{M_R^-} = M_R^- w(1+f_R) \quad (22)$$

If $m_{\frac{1}{2}} = M_L^+ + M_R^- < 0$, then

$$\overline{M_L^+} = M_L^+ + w(1+f_L) \quad (23)$$

$$\overline{M_R^-} = M_R^- + M_L^+[(1-w)(1+f_L) - f_R] \quad (24)$$

with

$$w(P_L, P_R) = 1 - min\left(\frac{P_L}{P_R}, \frac{P_R}{P_L}\right)^3 \quad (25)$$

The pressure-based weight function is

$$f_{L,R} = \left(\frac{P_{L,R}}{P_s} - 1\right), P_s \neq 0 \quad (26)$$

where

$$P_s = P_L^+ P_L + P_R^- P_R \quad (27)$$

The split Mach number is defined by

$$M^{\pm} = \begin{cases} \pm\frac{1}{4}(M \pm 1)^2, & |M| \leq 1 \\ \frac{1}{2}(M \pm |M|), & |M| > 1 \end{cases} \quad (28)$$

$$P^{\pm} = \begin{cases} \frac{1}{4}(M \pm 1)^2(2 \mp M), & |M| \leq 1 \\ \frac{1}{2}(1 \pm sign(M)), & |M| > 1 \end{cases} \quad (29)$$

The Mach number of each side is

$$M_{L,R} = \frac{U_{L,R}}{c_{1/2}} \quad (30)$$

and the speed of sound($c_{1/2}$) is

$$c_{1/2} = \begin{cases} min\left(\frac{c^{*2}}{max(|U_L|, c^*)}\right), \frac{1}{2}(U_L + U_R) > 0 \\ min\left(\frac{c^{*2}}{max(|U_R|, c^*)}\right), \frac{1}{2}(U_L + U_R) < 0 \end{cases} \quad (31)$$

where

$$c^* = \sqrt{2(\gamma - 1)/(\gamma + 1)H_{normal}} \quad (32)$$

$$H_{normal} = \frac{1}{2}(H_L - \frac{1}{2}V_L^2 + H_R - \frac{1}{2}V_R^2) \quad (33)$$

2.4 Chemical Reaction model and Transport Properties

Air with five species (N_2, O_2, NO, N, O) are considered and chemical reactions in eq. (34)-eq. (38), where M stands for collision partners, are considered.

$$O_2 + M \leftrightarrow O + O + M \quad (34)$$

$$N_2 + M \leftrightarrow N + N + M \quad (35)$$

$$NO + M \leftrightarrow N + O + M \quad (36)$$

$$N_2 + O \leftrightarrow NO + N \quad (37)$$

$$NO + O \leftrightarrow O_2 + N \quad (38)$$

The forward reaction rates are calculated by eq. (39) and the reaction rate coefficients by Park [4] are employed.

$$k_f(\bar{T}) = C_f \bar{T}^{\eta} \exp(-\theta_D/\bar{T}) \quad (39)$$

The backward reaction rates are calculated from the forward reaction rates and the equilibrium constants.

$$k_b(T) = k_f(T)/K_{eq}(T) \quad (40)$$

The molecular viscosity for each species is from Blottner's model [5], and the thermal conductivity is given by Eucken's model [6]. Wilke's mixture rule [7] is used to get the transport properties for air.

3 Shock stand-off distance problem

In order to verify the 5 species non-equilibrium flow solver, shock stand-off distance for a sphere in non-equilibrium hypersonic flow problem [14] is chosen as a test case.
Schemes and flow conditions are shown in table 1 and Table 2.

Table 1 Schemes

Computational method	Meshless
Spatial discretization	AUSMPW+
Limiter	Minmod
Time integration	LU-SGS

Table 2 Flow conditions

Sphere radius	mm	5
Pressure	mmhg	5
Velocity	m/s	4000
Mach		11.63
Mass fraction	N_2	0.767
	O_2	0.233

The results are compared with those of Furudate [8]. Translational and vibrational temperature along the stagnation streamline is plotted in figure 1. Calculated temperature plots in color is in a good agreement with Furadate's results in black. Figure 2 show the species mass fraction profiles along the stagnation streamline and they also matched well with the previous result.

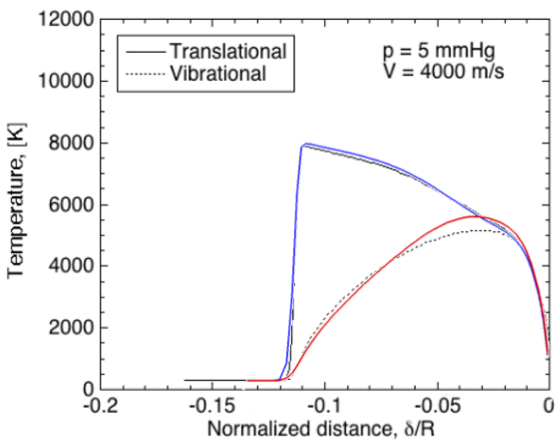

Figure 1 Temperature profile along the stagnation streamline

4 Conclusion

An aerothermal solver for calculation of hypersonic flow and structural thermal response is developed based on a meshless method. Non-equilibrium flow consists of 5 chemical species

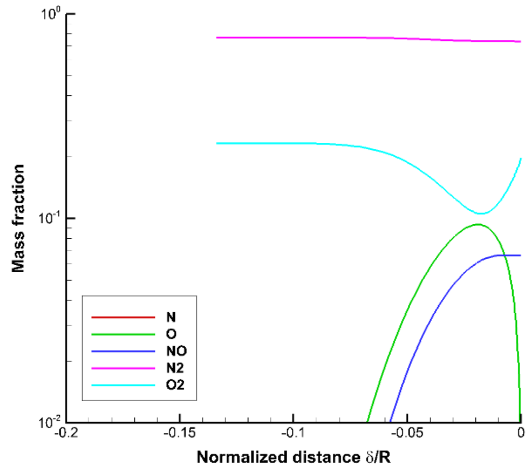

Figure 2 Species mass fraction profile along the stagnation streamline

(N_2, O_2, NO, N, O) is considered. Shock stand-off distance problem for a sphere in non-equilibrium hypersonic flow is chosen as a test case and the numerical results are similar to those from structured finite volume method.

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