Online Lecture Note

Introduction to Multiphysics CFD

Version 0.9

May 21, 2015

Satoru Yamamoto

Professor, Dr.Eng.

Laboratory of Mathematical Modeling and Computation
Dept. of Computer and Mathematical Sciences
Tohoku University
Sendai 980-8579, Japan

Email:yamamoto@caero.mech.tohoku.ac.jp

CONTENTS

Chapter A Fundamental Equations for Fluid Dynamics

1. Compressible Navier-Stokes Equations

Let me start from Compressible Navier-Stokes equations (CNS) using vector description as follows.

$$\rho_t + \nabla\cdot(\rho\boldsymbol{u}) = 0 \tag{1-1}$$

$$(\rho\boldsymbol{u})_t + \nabla\cdot\rho\boldsymbol{u}\boldsymbol{u} + \nabla p = \nabla\cdot\Pi \tag{1-2}$$

$$e_t + \nabla\cdot(e+p)\boldsymbol{u} = \nabla\cdot(\Pi\cdot\boldsymbol{u}) - \nabla\cdot\boldsymbol{q} \tag{1-3}$$

where ρ, $\boldsymbol{u}$, p, Π, e and $\boldsymbol{q}$ are density, velocity vector, pressure, viscous stress tensor, total internal energy per unit volume, and vector of heat flux. t is the time and the subscription t means the partial derivation with respect to time. First, second, and third equations are respectively mass conservation law, momentum conservation law, and energy conservation law.

These equations can be rewritten using tensor description:

$$\frac{\partial\rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \tag{1-4}$$

$$\frac{\partial}{\partial t}(\rho u_j) + \frac{\partial}{\partial x_i}(\rho u_i u_j + \delta_{ij} p) = \frac{\partial}{\partial x_i}(\tau_{ij}) \tag{1-5}$$

$$\frac{\partial e}{\partial t} + \frac{\partial}{\partial x_i}[(e+p)u_i] = \frac{\partial}{\partial x_i}\left(\tau_{ki}u_k + \kappa\frac{\partial T}{\partial x_i}\right) \tag{1-6}$$

where $(x_1, x_2, x_3) = (x, y, z)$ and $(u_1, u_2, u_3) = (u, v, w)$ for three dimensions in space. Originally for example, $\frac{\partial}{\partial x_i}(\rho u_i) = \sum_{i=1}^{3}\frac{\partial}{\partial x_i}(\rho u_i)$. T and κ are temperature and heat conductivity coefficient. τ_{ij} is viscous stress tensor and defined by

$$\tau_{ij} = \mu\left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right] \quad (i, j = 1,2,3) \tag{1-7}$$

where μ and δ_{ij} are molecular viscosity and Kronecker's delta. Second equation Eq. (1-5) is composed of three momentum equations along x, y, z directions if $j = 1,2,3$.

CNS is not a closed system itself because the pressure p as unknown variable is still unresolved. Assuming ideal gas, CNS can be closed by the equation of state:

$$p = \rho RT = (\gamma - 1)(e - \rho\boldsymbol{u}\boldsymbol{u}/2) = (\gamma - 1)(e - \rho u_i u_i/2) \tag{1-8}$$

where R and γ are specific gas constant and specific heat ratio ($\gamma = 1.4$).

CNS can be written using tensor description in vector form:

$$\frac{\partial Q}{\partial t} + \frac{\partial F_i}{\partial x_i} = \frac{\partial F_{vi}}{\partial x_i} \quad (i = 1,2,3) \tag{1-9}$$

$$Q = \begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ e \end{bmatrix}, \quad F_i = \begin{bmatrix} \rho u_i \\ \rho u_1 u_i + \delta_{1i} p \\ \rho u_2 u_i + \delta_{2i} p \\ \rho u_3 u_i + \delta_{3i} p \\ (e+p)u_i \end{bmatrix}, \quad F_{vi} = \begin{bmatrix} 0 \\ \tau_{1i} \\ \tau_{2i} \\ \tau_{3i} \\ \tau_{ki}u_k + \kappa\partial T/\partial x_i \end{bmatrix}$$

where Q, F_i and F_{vi} are vectors of unknown variables, convection and pressure terms (convection flux), and diffusion terms (diffusion flux). CNS in two dimensions may be easily derived from that of three dimensions as

$$Q=\begin{bmatrix}\rho\\ \rho u_1\\ \rho u_2\\ e\end{bmatrix},\qquad F_i=\begin{bmatrix}\rho u_i\\ \rho u_1u_i+\delta_{1i}p\\ \rho u_2u_i+\delta_{2i}p\\ (e+p)u_i\end{bmatrix},\qquad F_{vi}=\begin{bmatrix}0\\ \tau_{1i}\\ \tau_{2i}\\ \tau_{ki}u_k+\kappa\partial T/\partial x_i\end{bmatrix}$$

CNS may be originally defined in several books by the following description:

$$\frac{\partial Q}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}+\frac{\partial H}{\partial z}=\frac{\partial F_v}{\partial x}+\frac{\partial G_v}{\partial y}+\frac{\partial H_v}{\partial z} \tag{1-10}$$

$$Q=\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho w\\ e\end{bmatrix},\ F=\begin{bmatrix}\rho u\\ \rho uu+p\\ \rho vu\\ \rho wu\\ (e+p)u\end{bmatrix},\ G=\begin{bmatrix}\rho v\\ \rho uv\\ \rho vv+p\\ \rho wv\\ (e+p)v\end{bmatrix},\ H=\begin{bmatrix}\rho w\\ \rho uw\\ \rho vw\\ \rho ww+p\\ (e+p)w\end{bmatrix}$$

$$F_v=\begin{bmatrix}0\\ \tau_{xx}\\ \tau_{yx}\\ \tau_{zx}\\ \tau_{xx}u+\tau_{yx}v+\tau_{zx}w+\kappa\partial T/\partial x\end{bmatrix},\ G_v=\begin{bmatrix}0\\ \tau_{xy}\\ \tau_{yy}\\ \tau_{zy}\\ \tau_{xy}u+\tau_{yy}v+\tau_{zy}w+\kappa\partial T/\partial y\end{bmatrix},\ H_v=\begin{bmatrix}0\\ \tau_{xz}\\ \tau_{yz}\\ \tau_{zz}\\ \tau_{xz}u+\tau_{yz}v+\tau_{zz}w+\kappa\partial T/\partial z\end{bmatrix}$$

The viscous stresses are defined by

$$\begin{aligned}
\tau_{xx}&=\mu\left[\left(\frac{\partial u}{\partial x}+\frac{\partial u}{\partial x}\right)-\frac{2}{3}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right)\right]\\
\tau_{xy}&=\mu\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)=\tau_{yx}\\
\tau_{xz}&=\mu\left(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x}\right)=\tau_{zx}\\
\tau_{yy}&=\mu\left[\left(\frac{\partial v}{\partial y}+\frac{\partial v}{\partial y}\right)-\frac{2}{3}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right)\right]\\
\tau_{yz}&=\mu\left(\frac{\partial y}{\partial z}+\frac{\partial w}{\partial y}\right)=\tau_{zy}\\
\tau_{zz}&=\mu\left[\left(\frac{\partial w}{\partial z}+\frac{\partial w}{\partial z}\right)-\frac{2}{3}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right)\right]
\end{aligned} \tag{1-11}$$

2. Non-dimensionalization on CNS

Non-dimensionalization on CNS may be a crucial issue, because variables have different units and orders of magnitude. Especially it is quite crucial if we study multiphysics CFD(MCFD). MCFD solves flows with additional physics such as reaction, multiphase, the phase change, and external forces due to additional physics. Such external forces are modeled as a source term and added to CNS. Since generally the source terms have complicated units and the non-dimensionalization might be impossible. The following non-dimensionalization process may help the addition of source terms to CNS in which non-dimensionalization has been already conducted. Then we add source terms $s_j\left(j=1,\cdots,5\right)$ to CNS as

$$\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial x_i}\left(\rho u_i\right)=s_1 \tag{2-1}$$

$$\frac{\partial}{\partial t}\left(\rho u_j\right)+\frac{\partial}{\partial x_i}\left(\rho u_i u_j+\delta_{ij}p\right)=\frac{\partial}{\partial x_i}\left(\tau_{ij}\right)+s_{1+j} \tag{2-2}$$

$$\frac{\partial e}{\partial t}+\frac{\partial}{\partial x_i}\left[(e+p)u_i\right]=\frac{\partial}{\partial x_i}\left(\tau_{ik}u_k+\kappa\frac{\partial T}{\partial x_i}\right)+s_5 \tag{2-3}$$

First, all variables are non-dimensionalized as follows.

$$\begin{aligned}
&\bar{x}_j=\frac{x_j}{L},\ \bar{t}=\frac{t}{t_{ref}},\ \bar{\rho}=\frac{\rho}{\rho_\infty}\\
&\bar{u}_j=\frac{u_j}{V_\infty},\ \bar{e}=\frac{e}{\rho_\infty V_\infty^2},\ \bar{p}=\frac{p}{\rho_\infty V_\infty^2}\\
&\bar{T}=\frac{T}{T_\infty},\ \bar{\mu}=\frac{\mu}{\mu_\infty},\ \bar{\kappa}=\frac{\kappa}{\kappa_\infty}
\end{aligned} \tag{2-4}$$

The upper bar indicates the non-dimensionalized variable. L [m], ρ_∞ [kg/m^3] and V_∞ [m/s] are reference values of length, density and velocity. t_{ref} is a reference time and can be derived from other variables as $t_{ref}=L/V_\infty$. T_∞, μ_∞ and κ_∞ are reference values of temperature, molecular viscosity coefficient, and heat conductivity coefficient. These values are explained later.

Next Eqs. (2-1)-(2-3) are non-dimensionalized using the non-dimensionalized variables.

First, Eq. (2-1) as mass conservation law with a source term is non-dimensionalized as follows.

$$\begin{aligned}
&\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial x_i}\left(\rho u_i\right)=s_1\\
&\frac{\partial\left(\bar{\rho}\rho_\infty\right)}{\partial\left(\bar{t}t_{ref}\right)}+\frac{\partial}{\partial\left(\bar{x}_i L\right)}\left(\bar{\rho}\rho_\infty\bar{u}_i V_\infty\right)=s_1\\
&\frac{\rho_\infty}{t_{ref}}\frac{\partial\bar{\rho}}{\partial\bar{t}}+\frac{\rho_\infty V_\infty}{L}\frac{\partial}{\partial\bar{x}_i}\left(\bar{\rho}\bar{u}_i\right)=s_1\\
&\frac{\partial\bar{\rho}}{\partial\bar{t}}+\frac{\partial}{\partial\bar{x}_i}\left(\bar{\rho}\bar{u}_i\right)=\frac{L}{\rho_\infty V_\infty}s_1
\end{aligned} \tag{2-5}$$

The fourth equation has a final form. The form at left hand side (l.h.s.) is all the same with the original form except for the upper bar, while the source term s_1 at the right hand side (r.h.s.) was multiplied by $L/\rho_\infty V_\infty$. The value derived as $L/\rho_\infty V_\infty$ is quite important one. We have only to know this value if a dimensional source term s_1 is added to the mass conservation law even if the unit is unknown.

Eq. (2-2) as momentum equations with a source term are also non-dimensionalized as follows.

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\rho u_j\right)+\frac{\partial}{\partial x_i}\left(\rho u_i u_j+\delta_{ij}p\right)=\frac{\partial}{\partial x_i}\left(\tau_{ij}\right)+s_{1+j}\\
&\frac{\partial}{\partial\left(\bar{t}t_{ref}\right)}\left(\bar{\rho}\rho_\infty\bar{u}_j V_\infty\right)+\frac{\partial}{\partial\left(\bar{x}_i L\right)}\left(\bar{\rho}\rho_\infty\bar{u}_i V_\infty\bar{u}_j V_\infty+\delta_{ij}\bar{p}\rho_\infty V_\infty^2\right)=\frac{\partial}{\partial\left(\bar{x}_i L\right)}\left(\bar{\tau}_{ij}\frac{\mu_\infty V_\infty}{L}\right)+s_{1+j}\\
&\frac{\rho_\infty V_\infty}{t_{ref}}\frac{\partial}{\partial\bar{t}}\left(\bar{\rho}\bar{u}_j\right)+\frac{\rho_\infty V_\infty^2}{L}\frac{\partial}{\partial\bar{x}_i}\left(\bar{\rho}\bar{u}_i\bar{u}_j+\delta_{ij}\bar{p}\right)=\frac{\mu_\infty V_\infty}{L^2}\frac{\partial}{\partial\bar{x}_i}\left(\bar{\tau}_{ij}\right)+s_{1+j}\\
&\frac{\partial}{\partial\bar{t}}\left(\bar{\rho}\bar{u}_j\right)+\frac{\partial}{\partial\bar{x}_i}\left(\bar{\rho}\bar{u}_i\bar{u}_j+\delta_{ij}\bar{p}\right)=\frac{\mu_\infty}{\rho_\infty V_\infty L}\frac{\partial}{\partial\bar{x}_i}\left(\bar{\tau}_{ij}\right)+\frac{L}{\rho_\infty V_\infty^2}s_{1+j}
\end{aligned} \tag{2-6}$$

Since the Reynolds number is defined by $Re=\rho_\infty V_\infty L/\mu_\infty$, the coefficient of the viscous stress term is reduced as

$$\frac{\partial}{\partial\bar{t}}\left(\bar{\rho}\bar{u}_j\right)+\frac{\partial}{\partial\bar{x}_i}\left(\bar{\rho}\bar{u}_i\bar{u}_j+\delta_{ij}\bar{p}\right)=\frac{1}{Re}\frac{\partial}{\partial\bar{x}_i}\left(\bar{\tau}_{ij}\right)+\frac{L}{\rho_\infty V_\infty^2}s_{1+j} \tag{2-7}$$

The time derivative and the convection term are the same form with the original term except for the upper bar. $\bar{\tau}_{ij}$ is also derived as the same form:

$$\bar{\tau}_{ij} = \bar{\mu}\left[\left(\frac{\partial \bar{u}_i}{\partial \bar{x}_j} + \frac{\partial \bar{u}_j}{\partial \bar{x}_i}\right) - \frac{2}{3}\delta_{ij}\frac{\partial \bar{u}_k}{\partial \hat{x}_k}\right] \tag{2-8}$$

Non-dimensionalized process for Eq. (2-3) as energy conservation law with a source term is as follows.

$$\begin{aligned}
&\frac{\partial e}{\partial t} + \frac{\partial}{\partial x_i}\left[(e+p)u_i\right] = \frac{\partial}{\partial x_i}\left(\tau_{ik}u_k + \kappa\frac{\partial T}{\partial x_i}\right) + s_5 \\
&\frac{\partial\left(\bar{e}\rho_\infty V_\infty^2\right)}{\partial\left(\bar{t}t_{ref}\right)} + \frac{\partial}{\partial\left(\bar{x}_i L\right)}\left[\left(\bar{e}\rho_\infty V_\infty^2 + \bar{p}\rho_\infty V_\infty^2\right)\bar{u}_i V_\infty\right] = \frac{\partial}{\partial\left(\bar{x}_i L\right)}\left(\frac{\mu_\infty V_\infty^2}{L}\bar{\tau}_{ik}\bar{u}_k + \frac{\kappa_\infty T_\infty}{L}\bar{\kappa}\frac{\partial \bar{T}}{\partial \bar{x}_i}\right) + s_5 \\
&\frac{\rho_\infty V_\infty^3}{L}\frac{\partial \bar{e}}{\partial \bar{t}} + \frac{\rho_\infty V_\infty^3}{L}\frac{\partial}{\partial \bar{x}_i}\left[(\bar{e}+\bar{p})\bar{u}_i\right] = \frac{\mu_\infty V_\infty^2}{L^2}\frac{\partial}{\partial \bar{x}_i}\left(\bar{\tau}_{ik}\bar{u}_k + \frac{\kappa_\infty T_\infty}{\mu_\infty V_\infty^2}\bar{\kappa}\frac{\partial \bar{T}}{\partial \bar{x}_i}\right) + s_5 \\
&\frac{\partial \bar{e}}{\partial \bar{t}} + \frac{\partial}{\partial \bar{x}_i}\left[(\bar{e}+\bar{p})\bar{u}_i\right] = \frac{1}{Re}\frac{\partial}{\partial \bar{x}_i}\left(\bar{\tau}_{ik}\bar{u}_k + \frac{\kappa_\infty T_\infty}{\mu_\infty V_\infty^2}\bar{\kappa}\frac{\partial \bar{T}}{\partial \bar{x}_i}\right) + \frac{L}{\rho_\infty V_\infty^3}s_5
\end{aligned} \tag{2-9}$$

The coefficient of the heat flux is further transformed using some thermodynamic relations as

$$\begin{aligned}
\frac{\kappa_\infty T_\infty}{\mu_\infty V_\infty^2} &= \frac{c_{p\infty}T_\infty}{V_\infty^2 Pr} \\
&= \frac{\frac{\gamma}{\gamma-1}\frac{P_\infty}{\rho_\infty}}{V_\infty^2 Pr} \\
&= \frac{c_\infty^2}{(\gamma-1)V_\infty^2 Pr} \\
&= \frac{1}{(\gamma-1)M_\infty^2 Pr}
\end{aligned} \tag{2-10}$$

where $c_{p\infty}$ and Pr is a reference isobaric specific heat and the laminar Prandtl number. Reference values of speed of sound and the Mach number are $c_\infty^2 = \gamma P_\infty/\rho_\infty$, $M_\infty = V_\infty/c_\infty$. Finally non-dimensionalized form for energy conservation law with a source term is given by

$$\frac{\partial \bar{e}}{\partial \bar{t}} + \frac{\partial}{\partial \bar{x}_i}\left[(\bar{e}+\bar{p})\bar{u}_i\right] = \frac{1}{Re}\frac{\partial}{\partial \bar{x}_i}\left(\bar{\tau}_{ik}\bar{u}_k + \frac{\bar{\kappa}}{(\gamma-1)M_\infty^2 Pr}\frac{\partial \bar{T}}{\partial \bar{x}_i}\right) + \frac{L}{\rho_\infty V_\infty^3}s_5 \tag{2-11}$$

The non-dimensionalized CNS with source terms are summarized as follows (upper bar is removed).

$$\frac{\partial Q}{\partial t} + \frac{\partial F_i}{\partial x_i} = \frac{1}{Re}\frac{\partial F_{vi}}{\partial x_i} + S \quad (i = 1,2,3) \tag{2-12}$$

$$Q = \begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ e \end{bmatrix},\quad F_i = \begin{bmatrix} \rho u_i \\ \rho u_1 u_i + \delta_{1i}p \\ \rho u_2 u_i + \delta_{2i}p \\ \rho u_3 u_i + \delta_{3i}p \\ (e+p)u_i \end{bmatrix},\quad F_{vi} = \begin{bmatrix} 0 \\ \tau_{1i} \\ \tau_{2i} \\ \tau_{3i} \\ \tau_{ki}u_k + \frac{\kappa}{(\gamma-1)M_\infty^2 Pr}\frac{\partial T}{\partial x_i} \end{bmatrix},\quad S = \frac{L}{\rho_\infty V_\infty}\begin{bmatrix} s_1 \\ s_2/V_\infty \\ s_3/V_\infty \\ s_4/V_\infty \\ s_5/V_\infty^2 \end{bmatrix}$$

3. General Curvilinear Coordinates

We employ the general curvilinear coordinates (ξ,η,ζ) to solve CNS along a body fitted

coordinates.

(ξ,η,ζ) are the functions of (x,y,z) given by

$$\xi=\xi(x,y,z),\ \eta=\eta(x,y,z),\ \zeta=\zeta(x,y,z) \tag{3-1}$$

The total differentials of (ξ,η,ζ) and (x,y,z) are defined by

$$\begin{aligned} d\xi &= \xi_x dx+\xi_y dy+\xi_z dz \\ d\eta &= \eta_x dx+\eta_y dy+\eta_z dz \\ d\zeta &= \zeta_x dx+\zeta_y dy+\zeta_z dz \end{aligned} \tag{3-2}$$

$$\begin{aligned} dx &= x_\xi d\xi+x_\eta d\eta+x_\zeta d\zeta \\ dy &= y_\xi d\xi+y_\eta d\eta+y_\zeta d\zeta \\ dz &= z_\xi d\xi+z_\eta d\eta+z_\zeta d\zeta \end{aligned} \tag{3-3}$$

The metrics of (ξ,η,ζ) are derived from these relations as follows.

$$\begin{aligned} \begin{bmatrix} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{bmatrix} &= \begin{bmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{bmatrix}^{-1} \\ &= \frac{1}{J}\begin{bmatrix} y_\eta z_\zeta - y_\zeta z_\eta & -\left(x_\eta z_\zeta - x_\zeta z_\eta\right) & x_\eta y_\zeta - x_\zeta y_\eta \\ -\left(y_\xi z_\zeta - y_\zeta z_\xi\right) & x_\xi z_\zeta - x_\zeta z_\xi & -\left(x_\xi y_\zeta - x_\zeta y_\xi\right) \\ y_\xi z_\eta - y_\eta z_\xi & -\left(x_\xi z_\eta - x_\eta z_\xi\right) & x_\xi y_\eta - x_\eta y_\xi \end{bmatrix} \end{aligned} \tag{3-4}$$

where J is Jacobian for transformation and defined by

$$\begin{aligned} J &= \frac{\partial(x,y,z)}{\partial(\xi,\eta,\zeta)} = \begin{vmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{vmatrix} \\ &= x_\xi\left(y_\eta z_\zeta - y_\zeta z_\eta\right) - x_\eta\left(y_\xi z_\zeta - y_\zeta z_\xi\right) + x_\zeta\left(y_\xi z_\eta - y_\eta z_\xi\right) \end{aligned} \tag{3-5}$$

CNS are transformed to general curvilinear coordinates using the metrics and the Jacobian. The following original form of CNS is introduced again.

$$\frac{\partial Q}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}+\frac{\partial H}{\partial z}=\frac{\partial F_v}{\partial x}+\frac{\partial G_v}{\partial y}+\frac{\partial H_v}{\partial z} \tag{3-6}$$

The viscous terms are combined with the convection terms as follows.

$$\frac{\partial Q}{\partial t}+\frac{\partial(F-F_v)}{\partial x}+\frac{\partial(G-G_v)}{\partial y}+\frac{\partial(H-H_v)}{\partial z}=0 \tag{3-7}$$

Space derivative terms are redefined using F, G and H by

$$\frac{\partial Q}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}+\frac{\partial H}{\partial z}=Q_t+F_x+G_y+H_z=0 \tag{3-8}$$

The space derivatives of fluxes F, G and H are transformed to (ξ,η,ζ) coordinates as follows.

$$Q_t+\xi_x F_\xi+\eta_x F_\eta+\zeta_x F_\zeta+\xi_y G_\xi+\eta_y G_\eta+\zeta_y G+\xi_z H_\xi+\eta_z H_\eta+\zeta_z H=0 \tag{3-9}$$

$$\begin{aligned} &(JQ)_t+\left[J\left(\xi_x F+\xi_y G+\xi_z H\right)\right]_\xi - F\left[\left(J\xi_x\right)_\xi+\left(J\eta_x\right)_\eta+\left(J\zeta_x\right)_\zeta\right] \\ &+\left[J\left(\eta_x F+\eta_y G+\eta_z H\right)\right]_\eta - G\left[\left(J\xi_y\right)_\xi+\left(J\eta_y\right)_\eta+\left(J\zeta_y\right)_\zeta\right] \\ &+\left[J\left(\zeta_x F+\zeta_y G+\zeta_z H\right)\right]_\zeta - H\left[\left(J\xi_z\right)_\xi+\left(J\eta_z\right)_\eta+\left(J\zeta_z\right)_\zeta\right]=0 \end{aligned} \tag{3-10}$$

The metric terms in the bracket at the second term for each coordinate are disappeared, for example, as the following manner:

$$\begin{aligned}&\left(J\xi_x\right)_\xi+\left(J\eta_x\right)_\eta+\left(J\zeta_x\right)_\zeta\\&=\left(y_\eta z_\zeta-y_\zeta z_\eta\right)_\xi-\left(y_\xi z_\zeta-y_\zeta z_\xi\right)_\eta+\left(y_\xi z_\eta-y_\eta z_\xi\right)_\zeta=0\end{aligned}\tag{3-11}$$

Finally CNS in general curvilinear coordinates are obtained as

$$\hat{Q}_t+\hat{F}_\xi+\hat{G}_\eta+\hat{H}_\zeta=0\tag{3-12}$$

$$\hat{Q}=JQ$$

$$\hat{F}=J\left(\xi_x F+\xi_y G+\xi_z H\right)$$

$$\hat{G}=J\left(\eta_x F+\eta_y G+\eta_z H\right)$$

$$\hat{H}=J\left(\zeta_x F+\zeta_y G+\zeta_z H\right)$$

$$\hat{F}=J\begin{bmatrix}\rho U\\ \rho uU+\xi_x p-\left(\xi_x\tau_{xx}+\xi_y\tau_{yx}+\xi_z\tau_{zx}\right)\\ \rho vU+\xi_y p-\left(\xi_x\tau_{yx}+\xi_y\tau_{yy}+\xi_z\tau_{zy}\right)\\ \rho wU+\xi_z p-\left(\xi_z\tau_{yz}+\xi_y\tau_{yz}+\xi_z\tau_{zz}\right)\\ (e+p)U-\left(\xi_x\sigma_x+\xi_y\sigma_y+\xi_z\sigma_z\right)\end{bmatrix}$$

$$\hat{G}=J\begin{bmatrix}\rho V\\ \rho uV+\eta_x p-\left(\eta_x\tau_{xx}+\eta_y\tau_{yx}+\eta_z\tau_{zx}\right)\\ \rho vV+\eta_y p-\left(\eta_x\tau_{yx}+\eta_y\tau_{yy}+\eta_z\tau_{zy}\right)\\ \rho wV+\eta_z p-\left(\eta_z\tau_{yz}+\eta_y\tau_{yz}+\eta_z\tau_{zz}\right)\\ (e+p)V-\left(\eta_x\sigma_x+\eta_y\sigma_y+\eta_z\sigma_z\right)\end{bmatrix}$$

$$\hat{H}=J\begin{bmatrix}\rho W\\ \rho uW+\zeta_x p-\left(\zeta_x\tau_{xx}+\zeta_y\tau_{yx}+\zeta_z\tau_{zx}\right)\\ \rho vW+\zeta_y p-\left(\zeta_x\tau_{yx}+\zeta_y\tau_{yy}+\zeta_z\tau_{zy}\right)\\ \rho wW+\zeta_z p-\left(\zeta_z\tau_{yz}+\zeta_y\tau_{yz}+\zeta_z\tau_{zz}\right)\\ (e+p)W-\left(\zeta_x\sigma_x+\zeta_y\sigma_y+\zeta_z\sigma_z\right)\end{bmatrix}$$

where U, V and W are the contravariant velocities defined by

$$\begin{aligned}U&=\xi_x u+\xi_y v+\xi_z w\\V&=\eta_x u+\eta_y v+\eta_z w\\W&=\zeta_x u+\zeta_y v+\zeta_z w\end{aligned}\tag{3-13}$$

and σ_x, σ_y and σ_z are sets of diffusion terms:

$$\begin{aligned}\sigma_x&=\tau_{xx}u+\tau_{yx}v+\tau_{zx}w+\kappa\,\partial T/\partial x\\\sigma_y&=\tau_{xy}u+\tau_{yy}v+\tau_{zy}w+\kappa\,\partial T/\partial y\\\sigma_z&=\tau_{xz}u+\tau_{yz}v+\tau_{zz}w+\kappa\,\partial T/\partial z\end{aligned}\tag{3-14}$$

CNS in general curvilinear coordinates can be written using tensor description as follows.

$$\hat{Q}_t+\frac{\partial\hat{F}_i}{\partial\xi_i}=\frac{\partial\hat{F}_{vi}}{\partial\xi_i}\tag{3-15}$$

$$\hat{Q} = JQ = J\begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ e \end{bmatrix}, \qquad \hat{F}_i = J\frac{\partial \xi_i}{\partial x_j}F_j = J\begin{bmatrix} \rho U_i \\ \rho u_1 U_i + \dfrac{\partial \xi_i}{\partial x_1}p \\ \rho u_2 U_i + \dfrac{\partial \xi_i}{\partial x_2}p \\ \rho u_3 U_i + \dfrac{\partial \xi_i}{\partial x_3}p \\ (e+p)U_i \end{bmatrix},$$

$$\hat{F}_{vi} = J\frac{\partial \xi_i}{\partial x_j}F_{vj} = J\frac{\partial \xi_i}{\partial x_j}\begin{bmatrix} 0 \\ \tau_{j1} \\ \tau_{j2} \\ \tau_{j3} \\ \tau_{jk}u_k + \kappa\dfrac{\partial T}{\partial x_j} \end{bmatrix}$$

4. Conservation and non-conservation forms

CNS is basically defined by conservation laws for mass, momentum and energy. The conservation law means that fundamental equations satisfy also the conservation of mass. Mass conservation law proves the conservation of mass itself. Momentum and energy equations implicitly include the mass conservation law in them. Now conservation laws are divided to the conservation and the non-conservation parts. Conducting low-dimensionalization on Eq. (1-10) and releasing the viscous terms, the following equations are obtained as governing equations for one-dimensional inviscid flows called Euler equations:

$$Q_t + F_x = 0 \tag{4-1}$$

$$Q = \begin{bmatrix} \rho \\ \rho u \\ e \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (e+p)u \end{bmatrix}$$

The momentum equations are originally formed as the sum of the mass conservation law and a non-conservative momentum equation as

$$u\{\rho_t + (\rho u)_x\} + \rho\left\{u_t + uu_x + \frac{p_x}{\rho}\right\} = 0 \tag{4-2}$$

The energy equations implicitly include not only the mass conservation law but also the non-conservative momentum equations. This equation is originally formed as the sum among the mass conservation law, the non-conservative momentum equation and an equation for specific internal energy as

$$\frac{e}{\rho}\{\rho_t + (\rho u)_x\} + \rho u\left\{u_t + uu_x + \frac{p_x}{\rho}\right\} + \rho\left\{\varepsilon_t + u\varepsilon_x + \frac{p}{\rho}u_x\right\} = 0 \tag{4-2}$$

where ε is the specific internal energy per unit volume and $e = \rho\varepsilon + \rho u^2/2$.

The following is another description for conservative Euler equations:

$$\begin{bmatrix} 1 & 0 & 0 \\ u & \rho & 0 \\ e/\rho & \rho u & \rho \end{bmatrix}\begin{bmatrix} \rho_t + (\rho u)_x \\ u_t + uu_x + p_x/\rho \\ \varepsilon_t + u\varepsilon_x + pu_x/\rho \end{bmatrix} = 0 \tag{4-3}$$

Equations in the second matrix in Eq. (4-3) identify to non-conservative Euler equations.

Chapter B Fundamental of Computational Fluid Dynamics (CFD)

1. Euler Equations and the characteristic Speeds

Since compressible flows generate shock waves when the speed exceeds the speed of sound, accurately capturing shocks is crucial for the compressible flow simulation. The so-called shock capturing methods have been developed by a number of applied mathematicians and CFD research scientists for more than 60 years. Most of the methods were based on the theory of characteristics which is a theory for hyperbolic system. Exactly the theory can be applied to the system having an arbitrary number of independent variables, but actually the theory at most for two independent variables is standard for existing shock capturing methods. Such theory has been applied to multi-dimensional compressible flows which are governed by two- or three-dimensional Navier-Stokes equations. These equations have more than three independent variables such as (t, x, y, z). It suggests that the theory of characteristics for two independent variables is not exact for multi-dimensional Navier-Stokes equations. In addition, system of Navier-Stokes equations is not a hyperbolic one. We should keep in mind that most of current CFD methods for compressible flows employ shock capturing methods based on the theory for two independent variables.

The theory of characteristics for two independent variables is exact for one-dimensional Euler equations. Most of shock capturing methods are exact for the equations.

One-dimensional Euler equations are written in vector form:

$$Q_t + F_x = 0 \tag{1-1}$$

$$Q = \begin{bmatrix} \rho \\ \rho u \\ e \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (e+p)u \end{bmatrix} \tag{1-2}$$

Another vector form is also defined by

$$Q_t + AQ_x = 0 \tag{1-3}$$

where A is the Jacobian matrix defined by $A = \partial F / \partial Q$ and derived as the following matrix:

$$A = \begin{bmatrix} 0 & 1 & 0 \\ -(3-\gamma)u^2/2 & (3-\gamma)u & \gamma - 1 \\ (\gamma-1)u^3 - \gamma ue/\rho & \gamma e/\rho - 3(\gamma-1)u^2/2 & \gamma u \end{bmatrix} \tag{1-4}$$

Note that ρu should be defined as one unknown variable when the elements of A are derived.

Next relation is obtained when AQ is calculated.

$$F = AQ \tag{1-5}$$

Therefore, we can obtain the following relations called 'Euler's homogeneity relation' from Eqs. (1-1) and (1-3):

$$F_x = AQ_x = (AQ)_x \tag{1-6}$$

Eq. (1-6) indicates that A is independent to partial derivatives. This property is quite important for applying the theory of characteristics to Euler equations.

Now Eq. (1-3) is transformed from the conservation form to a non-conservation form as

$$\tilde{Q}_t + \tilde{A}\tilde{Q}_x = 0 \tag{1-7}$$

where $\tilde{Q}$ is the vector of unknown variables in non-conservation form (i.e., primitive variables) and $\tilde{A}$ is the Jabobian matrix in non-conservation form as follows.

$$\tilde{Q} = \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}, \quad \tilde{A} = \begin{bmatrix} u & \rho & 0 \\ 0 & u & 1/\rho \\ 0 & \rho c^2 & u \end{bmatrix} \tag{1-8}$$

where c is the speed of sound. Eq. (1-7) can be derived by the multiplication of a matrix $N = \partial\widetilde{Q}/\partial Q$ from the left on Eq. (1-3), where N is the matrix for transformation from conservation form to non-conservation form. Then $\widetilde{A}$ has a relation $\widetilde{A} = NAN^{-1}$ with A.

Now the eigenvalues of $\widetilde{A}$ are derived from the characteristic equation:

$$\left|\widetilde{A} - \lambda I\right| = 0 \tag{1-9}$$

where λ indicates the eigenvalue. We can obtain three different real eigenvalues: $\lambda_1 = u$, $\lambda_2 = u + c$ and $\lambda_3 = u - c$. Since the set of equations is hyperbolic when all eigenvalues of the characteristic equation are real, the set of one-dimensional Euler equations is proved as a hyperbolic system.

The eigenvalue is called 'characteristic speed' in CFD field. The matrix $\widetilde{A} - \lambda I$ has three row vectors or three column vectors, and the orthogonal vectors (i.e. eigenvectors) exist as

$$l^k\left(\widetilde{A} - \lambda_k I\right) = 0 \tag{1-10}$$

where $l^k\left(k = 1,2,3\right)$ are the left eigenvectors. From Eq. (1-10), we can define a matrix Λ for eigenvalues and a matrix $\widetilde{L}$ for left eigenvectors (note that different matrices can be also defined) :

$$\Lambda = \begin{bmatrix} u & & \\ & u+c & \\ & & u-c \end{bmatrix}, \quad \widetilde{L} = \begin{bmatrix} 1 & 0 & -1/c^2 \\ 0 & 1 & 1/\rho c \\ 0 & 1 & -1/\rho c \end{bmatrix} \tag{1-11}$$

Since $\widetilde{A} = \widetilde{L}^{-1}\Lambda\widetilde{L}$ and $\widetilde{A} = NAN^{-1}$, the following relation can be derived:

$$A = N^{-1}\widetilde{L}^{-1}\Lambda\widetilde{L}N \tag{1-12}$$

2. Flux Vector Splitting (FVS)

Eq. (1-1) is discretized by Finite Difference Method (FDM). First the convection flux vector F is discretized here as

$$Q_t = -\left(F_{j+1/2} - F_{j-1/2}\right)/\Delta x \tag{2-1}$$

where $F_{j\pm1/2}$ are the numerical flux vectors defined at the intermediate grid point $j+1/2$ between grid points j and $j+1$; that at $j+1/2$ between $j-1$ and j. Δx is the grid interval and a constant.

Steger and Warming [1] splits F to F^+ and F^- according to the signs of characteristic speed and redefined by

$$F = F^+ + F^- \tag{2-2}$$

where $F^\pm$ are obtained using Eq. (1-12) as

$$F^\pm = A^\pm Q = N^{-1}\widetilde{L}^{-1}\Lambda^\pm\widetilde{L}NQ \tag{2-3}$$

$\Lambda^\pm$ are the matrices composed of only positive and negative eigenvalues defined by

$$\Lambda^\pm = \begin{bmatrix} \lambda_1^\pm & 0 & 0 \\ 0 & \lambda_2^\pm & 0 \\ 0 & 0 & \lambda_3^\pm \end{bmatrix} \tag{2-4}$$

The eigenvalues are calculated from $\lambda_k^\pm = \left(\lambda_k \pm \left|\lambda_k\right|\right)/2 \ \left(k = 1,2,3\right)$.

The flux vectors $F^\pm$ are finally derived as the sum of three subvectors:

$$F^\pm = \frac{\gamma-1}{\gamma}\rho\begin{bmatrix} 1 \\ u \\ u^2/2 \end{bmatrix}\lambda_1^\pm + \frac{\rho}{2\gamma}\begin{bmatrix} 1 \\ u+c \\ h+cu \end{bmatrix}\lambda_2^\pm + \frac{\rho}{2\gamma}\begin{bmatrix} 1 \\ u-c \\ h-cu \end{bmatrix}\lambda_3^\pm \tag{2-5}$$

where total enthalpy $h = \left(e + p\right)/\rho$. The flux vectors $F_{j\pm1/2}$ are up-winded by the signs of characteristic speed in Eq. (2-5). For example, $F_{j+1/2}$ can be obtained at the first-order accuracy as the following

relation when all characteristic speeds are positive (i.e. supersonic flow)

$$F_{j+1/2} = F_j^+ = F_j \tag{2-6}$$

Note that the gradient of Eq. (2-5) is discontinuous at Mach number $M = -1, 0, 1$. Steger-Warming method cannot be used at subsonic region straightly. van Leer [2] proposed another flux vectors which are smoothly connected at the Mach numbers. But, another disadvantage for both Steger-Warming's method and van Leer's method as too dissipative in boundary layers was pointed out. Even though Steger-Warming's method has such restriction, this method is completely exact at supersonic region for one-dimensional Euler equations. It suggests that these FVS methods are not exact for multi-dimensional flows or viscous flows (i.e. Navier-Stokes equations).

3. Flux Difference Splitting (FDS)

Roe [3] proposed a FDS algorithm. FDS splits not flux vectors but the difference of flux vectors. The difference ΔF is defined by the sum of flux vectors $A^{\pm}\Delta Q$ as

$$\Delta F = A^+\Delta Q + A^-\Delta Q \tag{3-1}$$

where ΔQ is the difference of Q and $A^{\pm}$ are Jacobian matrices composed of elements obtained from only positive and negative eigenvalues.

Eq. (2-1) is rewritten using Eq. (3-1) as

$$Q_t = -\left\{\left(A^+\Delta Q\right)_{j-1/2} + \left(A^-\Delta Q\right)_{j+1/2}\right\}/\Delta x \tag{3-2}$$

where $\Delta Q_{j+1/2} = Q_{j+1} - Q_j$ and $A^{\pm}\Delta Q$ are obtained using Eq. (2-3) as

$$\begin{aligned} A^{\pm}\Delta Q &= L^{-1}\Lambda^{\pm}L\Delta Q \\ &= L^{-1}\Lambda^{\pm}\Delta \mathrm{W} \\ &= \sum_k \lambda_k^{\pm}\Delta w_k r^k \end{aligned} \tag{3-3}$$

$L = \tilde{L}N$ is the matrix composed of conservative left eigenvectors and $\Delta W = \left(\Delta w_1,\ \Delta w_2,\ \Delta w_3\right)$ are the vector of characteristic variables; $r^k\left(k = 1,2,3\right)$ is the conservative right eigenvectors. In Roe's method, $A^{\pm}_{j+1/2}$ are calculated only using Q_j and Q_{j+1}, and a special averaging called Roe's averaging is conducted to satisfy the conservation and the nonlinearity. Then the averaged values $\bar{\rho}$, $\bar{u}$, $\bar{h}$ and $\bar{c}^2$ are defined by

$$\begin{aligned} \bar{\rho} &= \sqrt{\rho_{j+1}\rho_j} \equiv R_{j+1/2}\rho_j \\ \bar{u} &= \frac{\left(u\sqrt{\rho}\right)_{j+1} + \left(u\sqrt{\rho}\right)_j}{\sqrt{\rho_{j+1}} + \sqrt{\rho_j}} = \frac{R_{j+1/2}u_{j+1} + u_j}{R_{j+1/2} + 1} \\ \bar{h} &= \frac{\left(h\sqrt{\rho}\right)_{j+1} + \left(h\sqrt{\rho}\right)_j}{\sqrt{\rho_{j+1}} + \sqrt{\rho_j}} = \frac{R_{j+1/2}h_{j+1} + h_j}{R_{j+1/2} + 1} \\ \bar{c}^2 &= (\gamma - 1)\left(\bar{h} - \bar{u}^2/2\right) \end{aligned} \tag{3-4}$$

Characteristic speeds and the right eigenvectors are calculated using Eq. (3-4) as

$$\begin{aligned} &\bar{\lambda}_1 = \bar{u},\quad \bar{\lambda}_2 = \bar{u} + \bar{c},\quad \bar{\lambda}_3 = \bar{u} - \bar{c} \\ &\bar{r}^1 = \begin{bmatrix} 1 \\ \bar{u} \\ \bar{u}^2/2 \end{bmatrix},\quad \bar{r}^2 = \frac{\bar{\rho}}{2\bar{c}}\begin{bmatrix} 1 \\ \bar{u} + \bar{c} \\ \bar{h} + \bar{c}\bar{u} \end{bmatrix},\quad \bar{r}^3 = -\frac{\bar{\rho}}{2\bar{c}}\begin{bmatrix} 1 \\ \bar{u} - \bar{c} \\ \bar{h} - \bar{c}\bar{u} \end{bmatrix} \end{aligned} \tag{3-5}$$

and characteristic values $\Delta w_k\left(k = 1,2,3\right)$ are defined by

$$\begin{aligned}\Delta w_1 &= \Delta\rho - \Delta p/\bar{c}^2 \\ \Delta w_2 &= \Delta u + \Delta p/\overline{\rho c}^2 \\ \Delta w_3 &= \Delta u - \Delta p/\overline{\rho c}^2\end{aligned} \tag{3-6}$$

where $\Delta(\cdot) = (\cdot)_{j+1} - (\cdot)_j$.

Roe's FDS approximates the flux vector using averaged variables as

$$Q_t = -\left\{\sum_k \left(\bar{\lambda}_k^+ \Delta w_k \bar{r}^k\right)_{j-1/2} + \sum_k \left(\bar{\lambda}_k^- \Delta w_k \bar{r}^k\right)_{j+1/2}\right\} \Big/ \Delta x \tag{3-7}$$

where $\bar{\lambda}_k^{\pm} = \left(\bar{\lambda}_k \pm \left|\bar{\lambda}_k\right|\right)/2$.

Roe's FDS guarantees the space accuracy even in boundary layers. However, this method may capture detached bow shocks inaccurately in supersonic flows. Liou [4] proposed Advection Upstream Splitting Method (AUSM) to improve the inaccuracy. But this method also has another trouble in the method.

Riemann Problem is known as a local one-dimensional shock tube problem. Roe' FDS belongs to the so-called approximate Riemann solver. A local cell is defined at the local region between the grid points $j-1/2$ and $j+1/2$. Riemann problem is solved at the interface between neighboring cells. This approach results in accurately capturing shocks. Primitive values obtained from the left side and the right side are defined as $\tilde{Q}_L$ and $\tilde{Q}_R$ at the interface $j+1/2$ of contacted two cells. Then the numerical flux of Roe's method can be redefined using $\tilde{Q}_L$ and $\tilde{Q}_R$ by

$$\begin{aligned}F_{j+1/2} &= \left\{F\left(\tilde{Q}_L\right) + F\left(\tilde{Q}_R\right)\right\}/2 + \left|A\left(\tilde{Q}_L,\ \tilde{Q}_R\right)\right|\left(\tilde{Q}_R - \tilde{Q}_L\right)/2 \\ &= \left\{F\left(\tilde{Q}_L\right) + F\left(\tilde{Q}_R\right)\right\}/2 + \sum_k \left|\bar{\lambda}_k\right| \Delta w_k \bar{r}^k /2\end{aligned} \tag{3-8}$$

Also this approach can be applied to FVS as

$$F_{j+1/2} = F^+\left(\tilde{Q}_L\right) + F^-\left(\tilde{Q}_R\right) \tag{3-9}$$

4. MUSCL Extrapolation

One of very popular methods obtaining the primitive variables $\tilde{Q}_L$ and $\tilde{Q}_R$ is Monotone Upstream-centered Schemes for Conservation Laws (MUSCL) [5]. These variables are calculated from the following interpolation:

$$\begin{aligned}\tilde{Q}_L &= \tilde{Q}_j + \frac{1-\alpha}{4}\Delta\tilde{Q}_{j-1/2} + \frac{1+\alpha}{4}\Delta\tilde{Q}_{j+1/2} \\ \tilde{Q}_R &= \tilde{Q}_{j+1} - \frac{1-\alpha}{4}\Delta\tilde{Q}_{j+3/2} - \frac{1+\alpha}{4}\Delta\tilde{Q}_{j+1/2}\end{aligned} \tag{4-1}$$

Eq. (4-1) results in second-order upwind and third-order biased upwind when $\alpha = -1$ and $\alpha = 1/3$. We proposed the fourth-order biased upwind version called Compact MUSCL [6] as follows.

$$\begin{aligned}\tilde{Q}_L &= \tilde{Q}_j + \frac{1}{6}\overline{\Delta}\tilde{Q}_{j-1/2} + \frac{1}{3}\overline{\Delta}\tilde{Q}_{j+1/2} \\ \tilde{Q}_R &= Q_{j+1} - \frac{1}{6}\overline{\Delta}\tilde{Q}_{j+3/2} - \frac{1}{3}\overline{\Delta}\tilde{Q}_{j+1/2} \\ \overline{\Delta}\tilde{Q}_{j+1/2} &= \Delta\tilde{Q}_{j+1/2} - \frac{1}{6}\Delta^3\tilde{Q}_{j+1/2} \\ \Delta\tilde{Q}_{j+1/2} &= \tilde{Q}_{j+1} - \tilde{Q}_j \\ \Delta^3\tilde{Q}_{j+1/2} &= \Delta\tilde{Q}_{j-1/2} - 2\Delta\tilde{Q}_{j+1/2} + \Delta\tilde{Q}_{j+3/2}\end{aligned} \tag{4-2}$$

5. TVD and Limiter Function

Not only accuracy but also robustness on Riemann solvers is crucial for capturing shocks. High-order finite differences may induce a numerical oscillation at the shock, while first-order upwind difference keeps the monotonicity even at the shock, resulting in no oscillation. von Neumann's stability analysis can find the stable condition for a linear scalar equation. TVD（Total Variation Diminishing）is a stability analysis for a nonlinear scalar equation and proposed by Harten [7]. Numerical schemes satisfying the TVD condition are called TVD scheme. In most of TVD schemes, a high-order accurate method is basically employed and the accuracy is reduced only at shocks to first order, because the first-order upwind difference unconditionally satisfies the TVD condition. Several limiter functions such as Minmod limiter [7], van Leer's limiter [8], Roe's Superbee limiter [9], and Chakravarthy-Osher's limiter [10] for switching the accuracy have been proposed.

Compact MUSCL employs two-step minmod limiters:

$$
\begin{aligned}
&\widetilde{Q}_L = \widetilde{Q}_j + \frac{1}{6}\overline{\Delta}\widetilde{Q}_j^L + \frac{1}{3}\overline{\Delta}\widetilde{Q}_j^R \\
&\widetilde{Q}_R = Q_{j+I} - \frac{1}{6}\overline{\Delta}\widetilde{Q}_{j+1}^L - \frac{1}{3}\overline{\Delta}\widetilde{Q}_{j+1}^R \\
&\overline{\Delta}\widetilde{Q}_j^L = \mathrm{minmod}\left(\overline{\Delta}\widetilde{Q}_{j-1/2}, b_1\overline{\Delta}\widetilde{Q}_{j+1/2}\right) \\
&\overline{\Delta}\widetilde{Q}_j^R = \mathrm{minmod}\left(\overline{\Delta}\widetilde{Q}_{j+1/2}, b_1\overline{\Delta}\widetilde{Q}_{j-1/2}\right) \\
&\overline{\Delta}\widetilde{Q}_{j+1/2} = \Delta\widetilde{Q}_{j+1/2} - \frac{1}{6}\Delta^3\widetilde{Q}_{j+1/2} \\
&\Delta\widetilde{Q}_{j+1/2} = \widetilde{Q}_{j+1} - \widetilde{Q}_j \\
&\Delta^3\widetilde{Q}_{j+1/2} = \Delta\widetilde{Q}_L - 2\Delta\widetilde{Q}_M + \Delta\widetilde{Q}_R \\
&\Delta\widetilde{Q}_L = \mathrm{minmod}\left(\Delta\widetilde{Q}_{j-1/2}, b_2\Delta\widetilde{Q}_{j+1/2}, b_2\Delta\widetilde{Q}_{j+3/2}\right) \\
&\Delta\widetilde{Q}_M = \mathrm{minmod}\left(\Delta\widetilde{Q}_{j+1/2}, b_2\Delta\widetilde{Q}_{j+3/2}, b_2\Delta\widetilde{Q}_{j-1/2}\right) \\
&\Delta\widetilde{Q}_R = \mathrm{minmod}\left(\Delta\widetilde{Q}_{j+3/2}, b_2\Delta\widetilde{Q}_{j-1/2}, b_2\Delta\widetilde{Q}_{j+1/2}\right)
\end{aligned}
\tag{5-1}
$$

where $1 < b_1 \le 4, \quad b_2 \cong 2$ and the minmod function is defined by

$$
\mathrm{minmod}(a_1, \cdots, a_n) = \mathrm{sign}(a_1)\max\left\{0, \min\left(|a_1|, \mathrm{sign}(a_1)\cdot a_2, \cdots, \mathrm{sign}(a_1)\cdot a_n\right)\right\} \tag{5-2}
$$

6. Time integration

Eq. (2-1) can be solved by the so-called time-marching method. The simplest method is called Euler Forward Method defined by

$$
\frac{Q^{n+1} - Q^n}{\Delta t} = -\frac{F_{j+1/2}^n - F_{j-1/2}^n}{\Delta x} \tag{6-1}
$$

where n and Δt are the time step and the time interval. Q^{n+1} is the updated vector of unknown variables and is obtained from all known values at n time step by the time integration in first-order accuracy as

$$
Q^{n+1} = Q^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^n - F_{j-1/2}^n\right) \tag{6-2}
$$

The time-marching method in which Q^{n+1} is obtained from only known values at n time step is called explicit method. The time interval Δt is limited by CFL (Courant-Friedrichs-Lewy) number defined by $c\Delta t/\Delta x$, where c is a convection speed. This number should be $\mathrm{CFL} \le 1$ for explicit methods to keep the linear stability, otherwise no stable solutions are obtained. To remove the limitation, implicit methods have been proposed. Since Q^{n+1} is integrated using the values at the same $n+1$ time step for the implicit

methods, basically the inversion of a matrix should be solved.

Approximate Factorization (AF) method [11] is one of typical implicit methods which has been well used until around 1990.

Two-dimensional Euler equations are given by

$$Q_t + \partial F_i / \partial x_i = Q_t + A_i \, \partial Q_i / \partial x_i = 0 \ \ (i = 1,2) \tag{6-3}$$

Appling the AF method to Eq. (6-3), the following equation is derived:

$$\left(I + \theta \Delta t \partial A_1 / \partial x_1\right)\left(I + \theta \Delta t \partial A_2 / \partial x_2\right)\Delta Q^n = -\Delta t \, \partial F_i^n / \partial x_i \equiv RHS \tag{6-4}$$

where $\theta = 1$ for fully implicit method and $\theta = 1/2$ for Crank-Nicholson method. Twice inversions of a block diagonal matrix should be solved for the time integration in Eq. (6-4). This equation can be further rewritten using Eq. (2-3) as follows [12].

$$\left\{I + \theta \Delta t\left(\Lambda_1^+ \nabla_1 + \Lambda_1^- \Delta_1\right)\right\}\widetilde{L}_1 \widetilde{L}_2^{-1}\left\{I + \theta \Delta t\left(\Lambda_2^+ \nabla_2 + \Lambda_2^- \Delta_2\right)\right\}\widetilde{L}_2 N \Delta Q^n = \widetilde{L}_1 N \, RHS \tag{6-5}$$

where ∇_i and Δ_i are forward and backward difference operators. Since two inversions of a scalar diagonal matrix are only solved in Eq. (6-5), the computational cost can be significantly reduced from that for Eq. (6-4).

We proposed a maximum second-order accurate AF method [13] based on Crank-Nicholson method and Newton iteration given by

$$\left\{I + \theta \Delta t\left(\Lambda_1^+ \nabla_1 + \Lambda_1^- \Delta_1\right)\right\}^m \left(\widetilde{L}_1 \widetilde{L}_2^{-1}\right)^m \left\{I + \theta \Delta t\left(\Lambda_2^+ \nabla_2 + \Lambda_2^- \Delta_2\right)\right\}^m \left(\widetilde{L}_2 N\right)^m \Delta Q^m = \left(\widetilde{L}_1 N\right)^{\mathrm{m}} \, RHS^m \tag{6-6}$$

where

$$\begin{aligned} \Delta Q^m &= Q^{m+1} - Q^m \\ RHS^m &= -\left(Q^m - Q^n\right) - \Delta t\left(\partial F_i^m / \partial x_i + \partial F_i^n / \partial x_i\right)/2 \end{aligned} \tag{6-7}$$

m is the Newton iteration. $Q^m = Q^n$ if $m = 0$ and $Q^m \to Q^{n+1}$ $\left(\Delta Q^m \to 0\right)$ if $m \to \infty$. Then a solution with maximum second-order in time can be obtained.

Another implicit method which is also well-known and now employed by our group is LU-SGS (Lower-upper Symmetric Gauss-Seidel) method [14]. This method is defined by the following two-step process:

$$\begin{aligned} D\Delta Q^* &= RHS - \theta \Delta t\left\{\left(A_1^+\right)_{i-1,j} + \left(A_2^+\right)_{i,j-1}\right\}\Delta Q^* \\ \Delta Q^n &= \Delta Q^* - D^{-1}\theta \Delta t\left\{\left(A_1^-\right)_{i+1,j} + \left(A_2^-\right)_{i,j+1}\right\}\Delta Q^n \end{aligned} \tag{6-8}$$

where $\left(A_k^{\pm}\right)_{i,j}$ $(k = 1,2)$ are the Jacobian matrices split by the sign of characteristic speed in x_k direction at the grid point (i, j). These matrices are approximately defined by

$$\left(A_k^{\pm}\right)_{i,j} = \left\{\left(A_k\right)_{i,j} \pm \left(r_k\right)_{i,j} I\right\}/2 \tag{6-9}$$

$\left(r_k\right)_{i,j}$ is the spectral radius of $\left(A_k\right)_{i,j}$ obtained from

$$\left(r_k\right)_{i,j} = \alpha \max\left[\left(\lambda_k\right)_{i,j}\right] \tag{6-10}$$

$\alpha \geq 1$ and $\left(\lambda_k\right)_{i,j}$ are the characteristic speeds of $\left(A_k\right)_{i,j}$.

The operator D is defined as the following algebraic equation:

$$D = I\theta \Delta t \sum_k \left(r_k\right)_{i,j} \tag{6-11}$$

No matrix inversions should be solved for LU-SGS even though it is an implicit method. A forward and a backward sweeps for solving Eq. (6-8) on the so-called hyper plane which is a skew line (plane) across grid points are only requested. Conclusively LU-SGS method may accept a large CFL number far beyond one.

We also apply Crank-Nicholson method and Newton iteration to Eq. (6-8). The maximum second-order accurate LU-SGS method [15] is given by

$$\begin{aligned} D^m \Delta Q^* &= RHS^m - \theta \Delta t\left\{\left(A_1^+\right)_{i-1,j}^m + \left(A_2^+\right)_{i,j-1}^m\right\}\Delta Q^{*m} \\ \Delta Q^m &= \Delta Q^{*m} - \left(D^{-1}\right)^m \theta \Delta t\left\{\left(A_1^-\right)_{i+1,j}^m + \left(A_2^-\right)_{i,j+1}^m\right\}\Delta Q^m \end{aligned} \tag{6-12}$$

References

1. Steger, J.L. and Warming, R.F., Flux Vector Splitting of the Inviscid Gas-dynamic Equation with Applications to Finite Difference Methods, *J. Comp. Phys.*, Vol.40, (1981), pp.263-293.
2. van Leer, B., Flux Vector Splitting for the Euler Equations, Proc. 8th Int. Conf. on Numerical Methods. in Fluid Dynamics, *Lecture Notes in Phys.*, Vol.170, (1982), pp.507-512, Springer-Verlag.
3. Roe, P. L., Approximate Riemann Solver, Parameter Vectors and Difference Schemes, *J. Comp. Phys.*, Vol.43, (1981), pp.357-372.
4. Liou, M.-S. and Steffen, C.J., A New Flux Splitting Scheme, *J. Comp. Phys.*, Vol.107, (1993), pp.23-39.
5. van Leer, B., Towards the Ultimate Conservative Difference Scheme. V. A Second-order Sequel to Godunov's Method, *J. Comp. Phys.*, Vol.32, (1979), pp.101-138.
6. Yamamoto, S. and Daiguji, H., Higher-order-accurate Upwind Schemes for Solving the Compressible Euler and Navier-Stokes Equations, *Computers and Fluids*, Vol.22, (1993), pp.259-270.
7. Harten, A., High Resolution Schemes for Hyperbolic Conservation Laws, *J. Comp. Phys.*, Vol.49, (1983), pp.357-393.
8. van Leer, B., Towards the Ultimate Conservative Difference Scheme II. Monotonicity and Conservation Combined in a Second Order Scheme, *J. Comp. Phys.*, Vo.14, (1974), pp.361-370.
9. Roe, P.L., Some Contributions to the Modelling of Discontinuous Flows, *Proc. 1983 AMS-SIAM Summer Seminar on Large Scale Computing in Fluid Mechanics*, *Lecture Notes in Applied Mathematics*, Vol.22, (1983), pp.163-193.
10. Chakravarthy, S.R. and Osher, S., High Resolution Applications of the Osher Upwind Scheme for the Euler Equations, AIAA Paper 83-1943, (1983).
11. Beam, R.M. and Warming, R.F., An Implicit Factored Scheme for the Compressible Navier-Stokes Equations, *AIAA J.*, Vol.16, (1978), pp.393-402.
12. Pulliam, T.H. and Chaussee, D.S., A Diagonal Form of an Implicit Approximate Factorization Algorithm, *J. Comp. Phys.*, Vol.39, (1981), pp.347-363.
13. Yamamoto, S. and Daiguji, H., Numerical Simulation of Unsteady Turbulent Flow through Transonic and Supersonic Cascades, *Lecture Notes in Phys.*, Vol.371, (1990), pp.485-486, Springer-Verlag.
14. Yoon, S. and Jameson, A., Lower-upper Symmetric-Gauss-Seidel Method for the Euler and Navier-Stokes Equations, *AIAA J.*, Vol.26, (1988), pp.1025-1026.
15. Yamamoto, S. and Kano, S., An Efficient CFD Approach for Simulating Unsteady Hypersonic Shock-shock Interference Flows, *Computers and Fluids*, Vol.27, (1998), pp.571-580.

Chapter C Modeling for Condensation

1. General Dynamic Equation (GDE) [1]

GDE which governs nucleation and growth of small particle; the coagulation due to Brownian motion is defined by

$$\frac{Df}{Dt} = I\delta\left(v - v^*\right) + f_{coag} \tag{1-1}$$

where f is a distribution function with respect to time t, space x_j and volume v for a small sphere particle with radius r, i.e. $f = f\left(v, x_j, t\right)$. L.h.s. of Eq. (1-1) is expanded to the following equation:

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \frac{\partial}{\partial v}\left(\frac{\partial v}{\partial t} f\right) + \frac{\partial}{\partial x_j}\left(u_j f\right) \tag{1-2}$$

u_j is particle velocities. The first term at r.h.s. in Eq. (1-1) is a function composed of nucleation rate I, Dirac's delta function, volume v and a particle volume v^* with the critical radius r^*. The second term f_{coag} is for coagulation due to Brownian motion.

2. Method of Moments (MoM) [2]

MoM has been widely used for solving GDE. MoM first multiplies $v^\ell\ (\ell = 1,2,3,\cdots)$ to Eq. (1-1) as

$$\frac{\partial}{\partial t}\left(\int_0^\infty v^\ell f dv\right) + \int_0^\infty v^\ell \frac{\partial}{\partial v}\left(\frac{\partial v}{\partial t} f\right) dv + \frac{\partial}{\partial x_j}\left(u_j \int_0^\infty v^\ell f dv\right) = I\int_0^\infty v^\ell \delta\left(v - v^*\right) dv + \int_0^\infty v^\ell f_{coag} dv \tag{2-1}$$

The first term at r.h.s. results in $I\int_0^\infty v^\ell \delta\left(v - v^*\right) dv = I v^{*\ell}$.

Defining $n_\ell = \int_0^\infty v^\ell f dv$, Eq. (2-1) can be transformed to the following equation:

$$\frac{\partial n_\ell}{\partial t} + \frac{\partial}{\partial x_j}\left(n_\ell u_j\right) = I v^{*\ell} + \ell\int_0^\infty v^{\ell-1} \frac{\partial v}{\partial t} f dv + \int_0^\infty v^\ell f_{coag} dv \tag{2-2}$$

n_ℓ is called ℓ th moment. The second term at r.h.s. in Eq. (2-2) is derived from the second term at l.h.s. in Eq. (2-1). Hill [3] introduced an averaged particle radius into GDE. Here we introduce an averaged particle volume $\overline{v}$. Then $\partial v/\partial t = \partial \overline{v}/\partial t$. This relation simplifies the second term at r.h.s. in Eq. (2-2) to

$$\int_0^\infty v^{\ell-1} \frac{\partial v}{\partial t} f dv = \frac{\partial \overline{v}}{\partial t}\int_0^\infty v^{\ell-1} f dv = \frac{\partial \overline{v}}{\partial t} n_{\ell-1} \tag{2-3}$$

Finally Eq. (2-2) is redefined by

$$\frac{\partial n_\ell}{\partial t} + \frac{\partial}{\partial x_j}\left(n_\ell u_j\right) = I v^{*\ell} + \ell \frac{\partial \overline{v}}{\partial t} n_{\ell-1} + S_\ell \tag{2-4}$$

For example, Eq. (2-4) includes the following equations for 0th, 1st and 2nd moments:

$$\frac{\partial n_0}{\partial t} + \frac{\partial}{\partial x_j}\left(n_0 u_j\right) = I + S_0 \tag{2-5}$$

$$\frac{\partial n_1}{\partial t} + \frac{\partial}{\partial x_j}\left(n_1 u_j\right) = I v^* + \frac{\partial \overline{v}}{\partial t} n_0 + S_1 \tag{2-6}$$

$$\frac{\partial n_2}{\partial t} + \frac{\partial}{\partial x_j}\left(n_2 u_j\right) = I v^{*2} + 2\frac{\partial \overline{v}}{\partial t} n_1 + S_2 \tag{2-7}$$

where $S_\ell = \int_0^\infty v^\ell f_{coag} dv$ (S_ℓ is derived later). These moments have units: n_0 [1/m^3], n_1 [m^3/m^3] and n_2 [m^3].

Let me further transform Eqs. (2-5)-(2-7) to another description. n_0 is number density of particle per unit volume. Here n_0 is replaced by ρn, where n is the number density of particle per unit mass [1/kg] and ρ is total density of fluid [kg/m^3]. Then Eq. (2-5) is rewritten as

$$\frac{\partial \rho n}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho n u_j\right)=I+S_0 \tag{2-8}$$

Density of particles is defined by $\rho\beta$, where β is the mass fraction of particle. Also density of a particle ρ_p [kg/m^3] multiplied by $\bar{v}$ [m^3] and the number density ρn [1/m^3] identifies to the mass of particles per unit volume. Then we obtain the following relation:

$$\rho\beta=\rho_p\bar{v}\rho n \tag{2-9}$$

Assuming the averaged volume of particles, $n_1=\int_0^\infty \bar{v} f dv=\bar{v}n_0=\bar{v}\rho n$. Then Eq. (2-8) is further transformed to the equation for density of particles as

$$\frac{\partial \rho\beta}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho\beta u_j\right)=\rho_p\left(Iv^*+\frac{\partial \bar{v}}{\partial t}\rho n+S_1\right) \tag{2-10}$$

$\bar{v}=4\pi\bar{r}^3/3$ in which $\bar{r}$ is the averaged radius of a particle, and the time derivative is $\partial\bar{v}/\partial t=4\pi\bar{r}^2\,\partial\bar{r}/\partial t$, giving another form of Eq. (2-10) as

$$\frac{\partial \rho\beta}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho\beta u_j\right)=\rho_p\left(\frac{4}{3}\pi r^{*3}I+4\pi\bar{r}^2\frac{\partial \bar{r}}{\partial t}\rho n+S_1\right) \tag{2-11}$$

Locally assuming averaged volume of particles identifies to the assumption of monodisperse system. We've employed the same equation with Eq. (2-11) for moist-air and wet-steam flow simulations [4]. Then, local averaged radius of particles is obtained from $\rho\beta=4\rho_p\pi\bar{r}^3\rho n/3$ as the following equation:

$$\bar{r}=\left(\frac{3\beta}{4\pi\rho_p n}\right)^{1/3} \tag{2-12}$$

On the other hand, system locally including particles with a different radius is called polydisperse system.

3. Nucleation Model

We know primary two types for nucleation of particles. One is homogeneous nucleation where condensation suddenly starts without nucleus. Another is heterogeneous nucleation starting from already existing nucleus. Former nucleation induces a strong nonequilibrium condensation due to a high saturation (supercooled) condition; the condensation is called nonequilibrium condensation. For example, wet-steam flows in steam turbines are governed by such nonequilibrium condensation, while aerosol in atmosphere is formed by condensation based on the heterogeneous nucleation in which a small particulate in atmosphere may be the nucleus.

Here we introduce the nucleation rate I governing homogeneous nucleation based on the classical nucleation theory [5].

First, a well-known model of nucleation rate [6] which we usually employ is defined by

$$I=\alpha_c\left(\frac{2\sigma}{\pi m^3}\right)^{1/2}\frac{\rho_v{}^2}{\rho_p}\exp\left(-\frac{4\pi r^{*2}\sigma}{3k_BT}\right) \tag{3-1}$$

where α_c, m, σ, ρ_v, ρ_p, k_B and T are respectively condensation coefficient, mass of a molecular composing particles, surface tension of a particle, density of vapor, density of a particle and Boltzmann constant and temperature of a particle. r^* is critical radius of a particle.

Nucleation rates for not only that of wet steam but also that of aerosol, metal nanoscale particle, and polymer nanoscale particle have already been modeled.

Let me explain the process of the derivation. First, the primary underlying thermodynamics is governed by Gibbs's free energy (GFE) based on the first and second laws of thermodynamics defined by

$$G=U+pV-Ts \tag{3-2}$$

where U, p, V, T and s are internal energy, pressure, volume, temperature and entropy in a closed system.

Differential of Eq. (3-2) are given by

$$dG = dU + pdV + Vdp - Tds - sdT \tag{3-3}$$

Also differential of internal energy U is defined by

$$dU = Tds - pdV \tag{3-4}$$

and Eq. (3-4) is substituted into Eq. (3-3). Then the following relation is obtained:

$$dG = Vdp - sdT \tag{3-5}$$

GFE identifies to the required energy for phase change from uniform vapor condition to nucleus of a particle like an energy wall which must be climbed over. The difference of GFE can be defined using those under vapor and nucleus conditions by

$$\begin{aligned}\Delta G = G_{particle} - G_{vapor} &= \left(n_{total} - n_{liquid}\right)g_{vm} + n_{liquid}g_{lm} + 4\pi r_p^2\sigma - n_{total}g_{vm} \\ &= n_{liquid}\left(g_{lm} - g_{vm}\right) + 4\pi r_p^2\sigma\end{aligned} \tag{3-6}$$

where g_{lm} and g_{vm} are GFE for one molecule in liquid and vapor states. n_{total} and n_{liquid} are the number of total molecules which phase can be changed and the number which phase was changed to liquid. $4\pi r_p^2\sigma$ identifies to GFE originating from the surface tension σ for a particle with radius r_p. dg_{lm} and dg_{vm} are obtained from Eq. (3-5) assuming an equal temperature field as

$$dg_p = v_{lm}dp, \quad dg_v = v_{vm}dp \tag{3-7}$$

where v_{lm} and v_{vm} are the volumes for one liquid molecule and one vapor molecule. Eq. (3-7) can be approximated assuming $v_{vm} >> v_{lm}$ as

$$d\left(g_{lm} - g_{vm}\right) = \left(v_{lm} - v_{vm}\right)dp \cong -v_{vm}dp \tag{3-8}$$

Vapor is assumed as ideal gas; substituting the equation of state $pv_{vm} = k_BT$ into Eq. (3-8), then

$$d\left(g_{lm} - g_{vm}\right) = -k_BT\frac{dp}{p} \tag{3-9}$$

Integrating Eq. (3-9) from a vapor pressure p_s to a particle pressure p_p for the particle with radius r_p derives the following equation:

$$g_{lm} - g_{vm} = -k_BT\int_{p_s}^{p_p}\frac{dp}{p} = -k_BT\ln\frac{p_p}{p_s} \tag{3-10}$$

Eq. (3-6) can be redefined using Eq. (3-10) by

$$\Delta G = -n_{liquid}k_BT\ln\frac{p_p}{P_s} + 4\pi r_p^2\sigma \tag{3-11}$$

$S = p_p/p_s$ as saturation ratio and $v_{lm}n_{liquid} = 4\pi r_p^3/3$ rewrite Eq. (3-11) as

$$\Delta G = -\frac{4}{3}\pi r_p^3\frac{k_BT}{v_{lm}}\ln S + 4\pi r_p^2\sigma \tag{3-12}$$

Eq. (3-12) is always positive when $S < 1$, while the first term at r.h.s. is negative when $S > 1$.

Partially differencing Eq. (3-12) with respect to r_p can find the maximum value of GFE as

$$\frac{\partial\Delta G}{\partial r_p} = -4\pi r_p^{*2}\frac{k_BT}{v_{lm}}\ln S + 8\pi r_p^*\sigma = 0 \tag{3-13}$$

where r_p^* is the radius of particle at the maximum GFE obtained by

$$r_p^* = \frac{2\sigma v_{lm}}{k_BT\ln S} \tag{3-14}$$

r_p^* identifies to the critical radius of liquid particle. Then GFE has a maximum value ΔG^* and the phase changing is under a metastable condition. GFE decreases soon when r_p is larger or smaller than r_p^*.

GFE is also smaller when S is larger because of smaller r_p^*.

Pressure of liquid particle can be derived from Eq. (3-14) as

$$p_p = p_s \exp\left(\frac{2\sigma v_{lm}}{k_B T r_p}\right) \tag{3-15}$$

This equation is well known as Kelvin's equation for obtaining the pressure of liquid particle p_p from the saturation pressure at liquid surface p_s. p_p increases while increasing r_p and reaches p_s.

ΔG^* is finally obtained as the following equation:

$$\Delta G^* = \frac{4}{3}\pi r_p^{*2}\sigma \tag{3-16}$$

We know some processes introducing nucleation rate I based on mechanical and statistical approaches. Those processes are generally too complicated to understand. Passing such process, let me start the following definition proposed by Volmer [7] assuming that the rate of nucleation due to homogeneous nucleation has a Boltzmann distribution:

$$I = C \exp\left(-\frac{\Delta G}{k_B T}\right) \tag{3-17}$$

On the other hand, I is proportional to the product of the number of molecules n_{eq} in particles which can be in equilibrium state at the critical radius r_p^* and the collision frequency C^* for vapor molecules colliding to liquid molecules given by

$$I = C^* n_{eq} \tag{3-18}$$

where

$$n_{eq} = n_{total} \exp\left(-\frac{\Delta G^*}{k_B T}\right) \tag{3-19}$$

n_{total} is the total number of vapor molecules which can be changed to liquid molecules. C^* is defined according to kinetic theory of molecule by

$$C^* = \alpha_c u_m \pi r_p^{*2} n_{total} = \alpha_c \sqrt{\frac{8k_B T}{\pi m}} \pi r_p^{*2} n_{total} \tag{3-20}$$

where u_m is mean averaged molecular speed and m is mass of a molecule. Using Eqs. (3-18)-(3.20), the following nucleation rate is derived:

$$I = \alpha_c \sqrt{\frac{8k_B T}{\pi m}} \pi r_p^{*2} n_{total}^2 \exp\left(-\frac{\Delta G^*}{k_B T}\right) \tag{3-21}$$

Helfgen [8] modified Eq. (3-21) to

$$I = z\alpha_c \sqrt{\frac{8k_B T}{\pi m}} \pi r_p^{*2} n_{total}^2 \exp\left(-\frac{\Delta G^*}{k_B T}\right) \tag{3-22}$$

where z is Zeldvich nonequilibrium factor. Hill [3] and Kotake [9] defined the similar equation:

$$I = z\alpha_c \frac{p_v}{\sqrt{2\pi m k_B T}} 4\pi r_p^{*2} \frac{p_v}{k_B T} \exp\left(-\frac{\Delta G^*}{k_B T}\right) \tag{3-23}$$

Since vapor pressure $p_v = n_{total} k_B T$, Eq.(3-23) can be rewritten as the same equation to Eq. (3-22). The detail derivation of z is explained in Refs. [5][10]. z is a correction coefficient to take the second-order term of ΔG^* into account given by

$$z = \frac{v_{lm}}{2\pi r_p^{*2}} \sqrt{\frac{\sigma}{k_B T}} \tag{3-24}$$

Substituting Eq. (3-24) to Eq. (3-23), then

$$I = 2\alpha_c \frac{p_v}{\sqrt{2\pi m k_B T}} \sqrt{\frac{\sigma (v_{lm})^2}{k_B T}} n_{total} \exp\left(-\frac{\Delta G^*}{k_B T} \right) \tag{3-25}$$

Eq. (3-25) identifies to the equation proposed by Debenedetti [11].
Also substituting Eq. (3-24) to Eq. (3-22),

$$I = \alpha_c \sqrt{\frac{2\sigma}{\pi m}} v_{lm} n_{total}^2 \exp\left(-\frac{\Delta G^*}{k_B T} \right) \tag{3-26}$$

Since $v_{lm} = m/\rho_p$, $n_{total} = \rho_v / m$, Eq. (3-27) can be rewritten as

$$I = \alpha_c \sqrt{\frac{2\sigma}{\pi m^3}} \frac{\rho_v^2}{\rho_p} \exp\left(-\frac{\Delta G^*}{k_B T} \right) \tag{3-27}$$

Eq. (3-27) identifies to the equation employed by Young [6] and Schnerr [12].

After all, we get a conclusion that nucleation rates defined for wet-steam flows, aerosol particles, metal nanoscale particles and polymer particles are basically the same model.

It should be noted here that all the existing models for nucleation rate assume ideal gas, i.e. $pv_v = k_B T$. Debenedetti [11], Kwauk [13], Helfgen [8] and Türk [14] studied Rapid Expansion of Supercritical Solutions (RESS) based on the nucleation rate model for polymer nanoscale particles. RESS is a process for producing small polymer particles. Supercritical carbon dioxide (SCO_2) is employed as a solvent. SCO_2 with a solute material streaming in a capillary nozzle is expanded in an expansion chamber, resulting in the loss of solvent power and hence precipitation of the solute. Debenedetti [11] found that non ideality of SCO_2 increases the free energy barrier against nucleation of solute material, and the increase may reduce the number density of particles; the classical nucleation theory originally derived assuming an ideal gas is not accurate for SCO_2. It suggests that EOS for ideal gas applied to nucleation rate should be replaced by a general EOS which is accurate even for SCO_2.

For example, we know a EOS for SCO_2 proposed in IUPAC [15] defined by

$$p_{real} = \rho_v RT \left[1 + \omega \sum_{i=0}^{9} \sum_{j=0}^{J_i} b_{ij} (\tau - 1)^j (\omega - 1)^i \right] \tag{3-28}$$

where parameters in Eq. (3-28) were also defined in IUPAC.

Now the difference between EOS for ideal gas and that by Eq. (3-28) is defined by ϕ, then $p_{real} = \rho_v RT\phi = n_{total} k_B T\phi$ or $p_{real} v_{lm} = k_B T\phi$. Eq. (3-14) may be redefined by

$$r_p^* = \frac{2\sigma v_{lm}}{k_B T \phi_s \ln S} \tag{3-29}$$

where $S = p_{real,p} / p_{real,s} = p_p \phi_p / p_s \phi_s$.

4. Condensation Model

Here the growth rate $d\bar{v}/dt$ for condensation of particles is modeled. Averaged number of incoming and outgoing molecules on a liquid particle with an averaged radius $\bar{r}$ per unit time is defined by

$$\alpha_c \sqrt{\frac{8k_B T}{\pi m}} \pi \bar{r}^2 n = \alpha_c 4\pi \bar{r}^2 \frac{p}{\sqrt{2\pi m k_B T}} \tag{4-1}$$

Assuming that liquid particles grow (evaporate) due to the collision (separation) of vapor molecules and the radius of liquid particles are sufficient smaller than mean-free path of molecules, then condensation follows Hertz-Knudsen's law. The growth rate $d\bar{v}/dt$ is derived using $\bar{v} = v_{lm} n$ as

$$\frac{d\bar{v}}{dt} = v_{lm} \frac{dn}{dt} = \alpha_c v_{lm} 4\pi \bar{r}^2 \left(\frac{p_v}{\sqrt{2\pi m k_B T}} - \frac{p_s}{\sqrt{2\pi m k_B T_p}} \right) \tag{4-2}$$

where T_p is particle temperature. Assuming $T = T_p$,

$$\frac{d\bar{v}}{dt} = \alpha_c v_{lm} 4\pi \bar{r}^2 \frac{p_s}{\sqrt{2\pi m k_B T}} (S-1) \tag{4-3}$$

Since $4\pi\bar{r}^2 = (36\pi)^{\frac{1}{3}} \bar{v}^{2/3}$ from $\bar{v} = 4\pi\bar{r}^3/3$ and $p_s = n_{total} k_B T$, Eq. (4-3) can be written as

$$\frac{d\bar{v}}{dt} = \alpha_c v_{lm} (36\pi)^{1/3} \bar{v}^{2/3} n_{total} \sqrt{\frac{k_B T}{2\pi m}} (S-1) \tag{4-4}$$

Eq. (4-4) identifies to the equation proposed by Pratsinis [2].

Also $d\bar{v}/dt = 4\pi\bar{r}^2 \, d\bar{r}/dt$ changes Eq. (4-4) to the following equation:

$$\frac{d\bar{r}}{dt} = \alpha_c v_{lm} \left(\frac{p_v}{\sqrt{2\pi m k_B T}} - \frac{p_s}{\sqrt{2\pi m k_B T_p}} \right) \tag{4-5}$$

Using $k_B = mR$, Eq. (5-5) can be rewritten as

$$\frac{d\bar{r}}{dt} = \alpha_c \frac{v_{lm}}{m} \left(\frac{p_v}{\sqrt{2\pi R T}} - \frac{p_s}{\sqrt{2\pi R T_p}} \right) = \frac{\alpha_c}{\rho_p} \left(\frac{p_v}{\sqrt{2\pi R T}} - \frac{p_s}{\sqrt{2\pi R T_p}} \right) \tag{4-6}$$

Eq. (4-6) identifies to the equation employed by Young [5]. Eqs. (4-4), (4-5) and (4-6) are conclusively the same equation. Note that these models can only be used to condensation under Hertz-Knudsen's law. Condensation in wet-steam flows may not follow Hertz-Knudsen's law. We know Gyarmathy's model [16] and Kantrowitz's modification [17] for such dense condensation. The detail for nucleation and condensation are explained in some books and reviews [18]-[20].

References

1. Seinfeld, J.H., Atmospheric Chemistry and Physics of Air Pollution, (1986), Wiley.
2. Pratsinis, S.E., Simultaneous Nucleation, Condensation, and Coagulation in Aerosol Reactors, *J. Colloid and Interface Science*, Vol.124. No.2 (1988), pp.416-427.
3. Hill, P. G., Condensation of Water Vapour during Supersonic Expansion in Nozzles, *J. Fluid Mech*., Vol.25, No.3 (1966), pp.593-620.
4. Ishizaka, K., Ikohagi, T. and Daiguji, H., A High-Resolution Numerical Method for Transonic Non-Equilibrium Condensation Flow through a Steam Turbine Cascade, *Proc. of the 6th ISCFD*, Vol.1, (1995), pp. 479-484.
5. Frenkel, J., Kinetic Theory of Liquids, (1955), Dover.
6. Young, J.B., The Spontaneous Condensation of Steam in Supersonic Nozzle, *PhysicoChemical Hydrodynamics*, Vol. 3, No.1(1982), pp.57-82.
7. Volmer, M., Kinetik der Phasenbuildung, (1939), Steinkopff.
8. Helfgen, B., Türk, M. and Schaber, K., Hydrodynamic and Aerosol Modeling of the Rapid Expansion of Supercritical Solution (RESS-Process), *J. Supercritical Fluids*, Vol.26, (2003), pp.225-242.
9. Kotake, S. and Glass, I.I., Flow with Nucleation and Condensation, *Progress of Aerospace Sciences*, Vol.19 (1981), pp.129-196.
10. Bakhtar, F., Young, J.B., White, A.J., and Simpson, D.A., Classical Nucleation Theory and its Application to Condensing Steam Flow Calculations, *Proc. IMechE*, Vol.219 , Part C (2005), pp.1315-1333.
11. Debenedetti, P.G., Homogeneous Nucleation in Supercritical Fluids, *AIChE Journal*, Vol.36, No.9 (1990), pp.1289-1298.
12. Schnerr, G. H. and Dohrmann, U., Transonic Flow around Airfoils with Relaxation and Energy Supply by Homogeneous Condensation, *AIAA Journal*, Vol.28, No.7 (1990), pp.1187-1193.
13. Kwauk, X. and Debenedetti, P.G., *J. Aerosol Science*, Vol.24, No.4(1993), pp.445-469.
14. Türk, M, Influence of Thermodynamic Behaviour and Solute Properties on Homogeneous Nucleation in Supercritical Solutions, *J. Supercritical Fluids*, Vol.18, (2000), pp.169-184.

15. Angus, S. et al., International Thermodynamic Table of the Fluid State-3 Carbon Dioxide, IUPAC, Vol.3, (1976).
16. Gyarmathy, G., Bases for a Theory for Steam Turbine, *Bulletin*, *Institute for Thermal Turbomachines*, *Federal Technical University*, *Zurich, Switzerland*, Vol.6, (1964).
17. Kantrowitz, A., Nucleation in Very Rapid Vapour Expansions, *J. Chem. Phys.*, Vol.19 , (1951), pp.1097-1100.
18. Wegener, P.P., Nonequilibrium Flows I, Gasdynamics, ed. by P.P.Wegener, (1969), pp.162-243, Marcel Dekker Publishers.
19. Wegener, P.P. and Mack, L.M., Condensation in Supersonic and Hypersonic Wind Tunnels, Advances in Applied Mechanics, eds. by H.L.Dryden and T.von Karman, (1969), pp.307-447, Academic Press.
20. Abraham, F.F., Homogeneous Nucleation Theory, (1974), Academic Press.

Chapter D Modeling for Condensate Flows

1. Equations for moist-air flows

Actual atmosphere includes a finite amount of water vapor. It plays an important role in weather conditions and in the earth's various environments. Water vapor occasionally condenses over aircrafts which is cruising in a high humid condition. Condensation of water vapor results in a change of pressure distributions on the wing surface and it may reduce the lift/drag ratio.

A typical onset of condensation over a wing in atmospheric wind tunnel conditions is started by a rapid flow expansion in supersonic region. Then, both the local pressure of water vapor p_v and the local saturation pressure of water vapor p_s decrease. Since p_s soon reaches a lower value than p_v according to the decrease of local temperature, the supersaturation ratio S (the relative humidity Φ is $\Phi = S$ x 100), defined by the ratio of p_v and p_s, increases. The ratio S may soon go beyond the saturation ratio S =1 through the inlet of the wind tunnel, and it reaches S »1 rapidly over the wing without condensation. A huge amount of nuclei is produced from pure water vapor at such a sufficiently high-supersaturated condition.

On the other hand, the phase change in atmospheric flight conditions may be generally dominated by a heterogeneous nucleation of water vapor, because small particulates, such as soot or aerosols may behave as a nucleus of condensation.

Two-dimensional transonic flows of moist air over an airfoil in atmospheric wind tunnel conditions have been experimentally and numerically studied by Schnerr and Dohrmann [1][2]. The experimental Schlieren photographs present a condensation shock associated with the heat release of water ahead of an intrinsic shock wave. Our group has studied numerical simulation of three-dimensional transonic viscous flows over ONERA M6 wing assuming atmospheric wind tunnel conditions [3] and those flows over a delta wing assuming atmospheric flight condition [4]. Comparison between atmospheric wind tunnel and flight conditions were also discussed in our previous paper [5].

We developed the fundamental equations for simulating three-dimensional compressible viscous flows of moist-air in general curvilinear coordinates. Flows are supposed to be a homogeneous fluid without any slip between air and water droplets assuming that condensed water droplets are smaller than 1μm and the mass fraction β is less than 10%.

These equations are written with SST turbulence model [6] as follows.

$$Q_t + \frac{\partial F_i}{\partial \xi_i} = \frac{\partial F_{vi}}{\partial \xi_i} + S \tag{1-1}$$

$$Q = J\begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ e \\ \rho_v \\ \rho\beta \\ \rho n \\ \rho k \\ \rho\omega \end{bmatrix},\ F_i = J\begin{bmatrix} \rho U_i \\ \rho u_1 U_i + \partial\xi_i/\partial x_1 p \\ \rho u_2 U_i + \partial\xi_i/\partial x_2 p \\ \rho u_3 U_i + \partial\xi_i/\partial x_3 p \\ (e+p)U_i \\ \rho_v U_i \\ \rho\beta U_i \\ \rho n U_i \\ \rho k U_i \\ \rho\omega U_i \end{bmatrix},\ F_{vi} = J\frac{\partial\xi_i}{\partial x_j}\begin{bmatrix} 0 \\ \tau_{1j} \\ \tau_{2j} \\ \tau_{3j} \\ \tau_{kj}u_k + \kappa\partial T/\partial x_j \\ 0 \\ 0 \\ 0 \\ \sigma_{kj} \\ \sigma_{\omega j} \end{bmatrix},\quad S = J\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -\Gamma_c \\ \Gamma_c \\ I \\ S_k \\ S_\omega \end{bmatrix}$$

where ρ, ρ_v, β and n are total density of moist-air, density of water vapor and mass fraction of condensed water droplets and number density of water droplets per unit mass. k and ω are the turbulent kinetic energy and the dissipation rate. Γ_c and I in source term S are mass generation rate due to condensation which was basically the same with that at Chapter C, Eq. (2-11) and the homogeneous nucleation rate [7] [Chap. C, Eq. (3-2)]. σ_{kj} and $\sigma_{\omega j}$ are the diffusion terms for SST

model, and S_k and S_ω are the source term.

our group derived the following approximate equation of state for moist air considering the release of latent heat.

$$p = \rho R_m T(1-\beta) = \frac{(1-\beta)R_m}{C_{pm} - (1-\beta)R_m}\left[e - \rho \boldsymbol{uu}/2 - \rho h_{0m}\right] \tag{1-2}$$

where h_{0m}, R_m and C_{pm} are heat of formation, specific heat ratio and isobaric specific heat for moist air. These values are obtained from linear combination between those of gas and liquid.

2. Numerical method

FDS derived as Eq. (3-8) in Chapter B is basically employed for discretizing Eq. (1-1) with Compact MUSCL [Chap. B, Eq.(5-1)] for convection term and the second-order central difference is applied to viscous term.

The numerical flux $(F_i)_{\ell+1/2}$ for F_i defined at the interface between the control volume ℓ and $\ell+1$ in each coordinate $i\,(i=1,2,3)$ can be written by FVS form as

$$(F_i)_{\ell+1/2} = (F_i^+)_{\ell+1/2} + (F_i^-)_{\ell+1/2} = (A_i^+)_{\ell+1/2} Q^L_{\ell+1/2} + (A_i^-)_{\ell+1/2} Q^R_{\ell+1/2} \tag{2-1}$$

where Q^L and Q^R are the primitive vectors extrapolated by the Compact MUSCL from left and right directions. FVS form for $(A_i^\pm)_{\ell+1/2} Q^M_{\ell+1/2}$ is given in general curvilinear coordinates by

$$(A_i^\pm)_{\ell+1/2} Q^M = (L_i^{-1}\Lambda_i^\pm L_i)_{\ell+1/2} Q^M = \lambda_{i1}^\pm Q^M + \frac{\lambda_{ia}^\pm}{c\sqrt{g_{ii}}} Q_{ia} + \frac{\lambda_{ib}^\pm}{c^2} Q_{ib} \tag{2-2}$$

g_{ii} are the metrics ($=\nabla\xi_i \cdot \nabla\xi_i$). Upper subscript M is replaced by L and R. L_i and Λ_i are the matrices composed of eigenvectors and characteristic speeds (eigenvalues). $\lambda_{ia}^\pm$ and $\lambda_{ib}^\pm$ are defined by

$$\begin{aligned} \lambda_{ia}^\pm &= \left(\lambda_{i4}^\pm - \lambda_{i5}^\pm\right)/2 \\ \lambda_{ib}^\pm &= \left(\lambda_{i4}^\pm + \lambda_{i5}^\pm\right)/2 - \lambda_{i1}^\pm \end{aligned} \tag{2-3}$$

where $\lambda_{ij}^\pm\ (j=1,4,5)$ are calculated from

$$\lambda_{ij}^\pm = \left(\lambda_{ij} \pm |\lambda_{ij}|\right)/2 \tag{2-4}$$

$\lambda_{ij}\ (j=1,4,5)$ are the characteristic speeds defined by

$$\begin{aligned} \lambda_{i1} &= U_i \\ \lambda_{i4} &= U_i + c\sqrt{g_{ii}} \\ \lambda_{i5} &= U_i - c\sqrt{g_{ii}} \end{aligned} \tag{2-5}$$

c is the speed of sound. Q_{ia} and Q_{ib} are the subvectors given by

$$\begin{aligned} Q_{ia} &= \bar{p} Q_{ic} + \Delta\bar{m}_i Q_d \\ Q_{ib} &= \left(\Delta\bar{m}_i c^2 / g_{ii}\right) Q_{ic} + \bar{p} Q_d \\ \bar{p} &= Q_e \cdot Q^M \\ \Delta\bar{m}_i &= Q_{im} \cdot Q^M \end{aligned} \tag{2-6}$$

where the subvectors Q_{ic}, Q_p, Q_{im} and Q_d are derived as

$$\begin{aligned} Q_{ic} &= \left[0 \quad \partial\xi_i/\partial x_1 \quad \partial\xi_i/\partial x_2 \quad \partial\xi_i/\partial x_3 \quad U_i \quad 0 \quad 0 \quad 0 \quad 0 \quad 0\right]^T \\ Q_e &= \left[\phi^2 \quad -\tilde{\gamma}u_1 \quad -\tilde{\gamma}u_2 \quad -\tilde{\gamma}u_3 \quad -\tilde{\gamma} \quad 0 \quad 0 \quad 0 \quad 0 \quad 0\right]^T \\ Q_{im} &= \left[-U_i \quad \partial\xi_i/\partial x_1 \quad \partial\xi_i/\partial x_2 \quad \partial\xi_i/\partial x_3 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0\right]^T \\ Q_d &= \left[1 \quad u_1 \quad u_2 \quad u_3 \quad (e+p)/\rho \quad \rho_v/\rho \quad \beta \quad n \quad k \quad \omega\right]^T \end{aligned} \tag{2-7}$$

$\tilde{\gamma} = \gamma - 1$ and $\phi^2 = \tilde{\gamma} u_j u_j / 2 - h_{0m}$.

Eq. (2-1) can be alternatively written by FDS form as

$$(F_i)_{\ell+1/2} = \frac{1}{2}\left[F_i\left(Q^L_{\ell+1/2}\right) + F_i\left(Q^R_{\ell+1/2}\right) - \left|(A_i)_{\ell+1/2}\right|\left(Q^R_{\ell+1/2} - Q^L_{\ell+1/2}\right)\right] \tag{2-8}$$

$\left|(A_i)_{\ell+1/2}\right|Q^M_{\ell+1/2} (i = 1,2,3; M = L, R)$ is calculated from the following subvectors:

$$\left|(A_i^{\pm})_{\ell+1/2}\right|Q^M = \left|\bar{\lambda}_{i1}\right|Q^M + \frac{\left|\bar{\lambda}_{ia}\right|}{\bar{c}\sqrt{g_{ii}}}Q_{ia} + \frac{\left|\bar{\lambda}_{ib}\right|}{\bar{c}^2}Q_{ib} \tag{2-9}$$

where

$$\begin{aligned} \left|\bar{\lambda}_{ia}\right| &= \left(\left|\bar{\lambda}_{i4}\right| - \left|\bar{\lambda}_{i5}\right|\right)/2 \\ \left|\bar{\lambda}_{ib}\right| &= \left(\left|\bar{\lambda}_{i4}\right| + \left|\bar{\lambda}_{i5}\right|\right)/2 - \left|\bar{\lambda}_{i1}\right| \end{aligned} \tag{2-10}$$

and

$$\begin{aligned} \bar{Q}_{ia} &= \bar{p}\bar{Q}_{ic} + \Delta\bar{m}_i\bar{Q}_d \\ \bar{Q}_{ib} &= \left(\Delta\bar{m}_i\bar{c}^2/g_{ii}\right)\bar{Q}_{ic} + \bar{p}\bar{Q}_d \\ \bar{p} &= \bar{Q}_e \cdot \bar{Q}^M \\ \Delta\bar{m}_i &= \bar{Q}_{im} \cdot \bar{Q}^M \end{aligned} \tag{2-11}$$

Variables with upper bar are obtained by Roe's averaging.

LU-SGS method [Chap.B, Eq. (6-8)] is employed for time integration. The following two-step processes are executed:

$$\begin{aligned} D\Delta Q^* &= RHS + \Delta t G^+\left(\Delta Q^*\right) \\ \Delta Q &= \Delta Q^* - D^{-1}\Delta t G^-\left(\Delta Q\right) \end{aligned} \tag{2-12}$$

where

$$\begin{aligned} G^+\left(\Delta Q^*\right) &= \left(A_1^+\Delta Q^*\right)_{i-1,j,k} + \left(A_2^+\Delta Q^*\right)_{i,j-1,k} + \left(A_3^+\Delta Q^*\right)_{i,j,k-1} \\ G^-\left(\Delta Q\right) &= \left(A_1^-\Delta Q\right)_{i+1,j,k} + \left(A_2^-\Delta Q\right)_{i,j+1,k} + \left(A_3^-\Delta Q\right)_{i,j,k+1} \end{aligned}$$

$A_\ell^{\pm}\,\Delta Q(\ell = 1,2,3)$ may be calculated from Eq. (2-2) by replacing Q^M to ΔQ.

3. Equations for wet-steam flows in turbomachinery

Condensation observed in steam turbines is of quite important in engineering. The phase change may be governed by homogeneous nucleation and the nonequilibrium process of condensation. The latent heat of water is released to surrounding non-condensed vapor, increasing temperature and pressure. It is known that condensed water droplets affects the performance of the steam turbine. The blade of the steam turbine is occasionally damaged by the erosion due to the interaction with the condensed water droplets. However, the accurate mechanism of the erosion is still unknown.

Transonic wet-steam flows in a steam turbine cascade channel have been studied by Bakhtar and Mohammadi Tochai [8], Moheban and Young [9], and Young [10]. Young [10] calculated two-dimensional wet-steam turbine cascade flows by solving Euler equations with a Lagrangian method for integrating the growth equation of a water droplet through each streamline.

Flows are supposed to be a homogeneous fluid without any slip between water vapor and water droplets assuming that condensed water droplets are smaller than 1μm and the mass fraction β is less than 10%. In addition, centrifugal and Coriolis forces are added for three-dimensional flows through turbine rotor blade rows. $\boldsymbol{u} = \boldsymbol{w} + \boldsymbol{\Omega} \times \boldsymbol{r}$ is a relation between flow velocities in rotors (relative velocities) $\boldsymbol{w} = (w_1\ w_2\ w_3)$ and those in stators (absolute velocities) $\boldsymbol{u} = (u_1\ u_2\ u_3)$, where $\boldsymbol{\Omega}$ and $\boldsymbol{r}$ are the vectors of rotational angular velocity and the radius. Eq. (1-1) is transformed to the equations for relative velocity field as

$$Q_t + \frac{\partial F_i}{\partial \xi_i} = \frac{\partial F_{vi}}{\partial \xi_i} + S \tag{3-1}$$

$$Q = J\begin{bmatrix} \rho \\ \rho w_1 \\ \rho w_2 \\ \rho w_3 \\ e \\ \rho\beta \\ \rho n \\ \rho k \\ \rho\omega \end{bmatrix},\ F_i = J\begin{bmatrix} \rho W_i \\ \rho w_1 W_i + \partial\xi_i/\partial x_1 p \\ \rho w_2 W_i + \partial\xi_i/\partial x_2 p \\ \rho w_3 W_i + \partial\xi_i/\partial x_3 p \\ (e+p)W_i \\ \rho\beta W_i \\ \rho n W_i \\ \rho k W_i \\ \rho\omega W \end{bmatrix},\ F_{vi} = J\frac{\partial\xi_i}{\partial x_j}\begin{bmatrix} 0 \\ \tau_{1j} \\ \tau_{2j} \\ \tau_{3j} \\ \tau_{kj}w_k + \kappa\partial T/\partial x_j \\ 0 \\ 0 \\ \sigma_{kj} \\ \sigma_{\omega j} \end{bmatrix},\quad S = J\begin{bmatrix} 0 \\ 0 \\ \rho\left(\Omega^2 x_2 + 2\Omega w_3\right) \\ \rho\left(\Omega^2 x_3 - 2\Omega w_2\right) \\ 0 \\ \Gamma_c \\ I \\ S_k \\ S_\omega \end{bmatrix}$$

where ρ is total density of wet-steam (note that the equation for ρ_v in Eq. (1-1) is removed). W_i is the vectors of contravariant relative velocities. Source terms of momentum equations in ξ_2 and ξ_3 directions corresponds to centrifugal and Coriolis forces. Eq. (1-2) as EOS is transformed to that for relative velocities as

$$p = \rho R_m T(1-\beta) = \frac{(1-\beta)R_m}{C_{pm} - (1-\beta)R_m}\left[e - \rho\left(\boldsymbol{w}^2 - r^2\Omega v_u\right)/2 - \rho h_{0m}\right] \tag{3-2}$$

v_u is tangential velocity of rotation.

Numerical methods are basically the same with those for moist-air flows. But, $\lambda_{ij}\ (j = 1,4,5)$ are the characteristic speeds defined using relative contravariant velocities by

$$\begin{aligned} \lambda_{i1} &= W_i \\ \lambda_{i4} &= W_i + c\sqrt{g_{ii}} \\ \lambda_{i5} &= W_i - c\sqrt{g_{ii}} \end{aligned} \tag{3-3}$$

and velocities in subvectors Q_{ic}, Q_p, Q_{im} and Q_d are also replaced by relative velocities as

$$\begin{aligned} Q_{ic} &= \left[0 \quad \partial\xi_i/\partial x_1 \quad \partial\xi_i/\partial x_2 \quad \partial\xi_i/\partial x_3 \quad W_i \quad 0 \quad 0 \quad 0 \quad 0 \quad 0\right]^T \\ Q_e &= \left[\phi^2 \quad -\tilde{\gamma}w_1 \quad -\tilde{\gamma}w_2 \quad -\tilde{\gamma}w_3 \quad -\tilde{\gamma} \quad 0 \quad 0 \quad 0 \quad 0 \quad 0\right]^T \\ Q_{im} &= \left[-W_i \quad \partial\xi_i/\partial x_1 \quad \partial\xi_i/\partial x_2 \quad \partial\xi_i/\partial x_3 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0\right]^T \\ Q_d &= \left[1 \quad w_1 \quad w_2 \quad w_3 \quad (e+p)/\rho \quad \rho_v/\rho \quad \beta \quad n \quad k \quad \omega\right]^{\mathrm{T}} \end{aligned} \tag{3-4}$$

where $\phi^2 = \tilde{\gamma}w_j w_j/2 - h_{0m}$.

Currently our group is developing an in-house code called 'Numerical Turbine' which can simulate not only wet-steam flows but also moist-air flows considering nonequilibrium condensation through multi-stage stator-rotor blade rows in turbomachinery. Recent progresses have been reported at ASME Turbo Expo [11]-[15].

References

1. Schnerr, G. H. and Dohrmann, U., Transonic Flow around Airfoils with Relaxation and Energy Supply by Homogeneous Condensation, *AIAA Journal*, Vol.28, No.7 (1990), pp.1187-1193.
2. Schnerr, G. H. and Dohrmann, U., Drag and Lift in Nonadiabatic Transonic Flow, *AIAA J.*, Vol.32, (1994), pp.101-107.
3. Yamamoto, S., Hagari, H. and Murayama, M., Numerical Simulation of Condensation around the 3-D Wing, *Trans. the Japan Society of Aeronautical and Space Science*, Vol.42, No.138 (2000),

pp.182-189.
4. Yamamoto, S., Onset of Condensation in Vortical Flow over Sharp-edged Delta Wing, *AIAA Journal*, Vol.41, No.9 (2003), pp.1832-1835.
5. Yamamoto, S., Computation of Practical Flow Problems with Release of Latent Heat, *Energy*, Vol.30, (2005), pp.197-208.
6. Menter, F.R., Two-equation Eddy-viscosity Turbulence Models for Engineering Applications, *AIAA J.*, Vol.32, No.8(1994), pp.1598-1605.
7. Frenkel, J., Kinetic Theory of Liquids, (1955), Dover.
8. Bakhtar, F. and Mohammadi Tochai, M.T., An Investigation of Two-Dimensional Flows of Nucleating and Wet Steam by the Time-Marching Method, *Int. J. Heat Fluid Flow*, Vol.2, No.1(1980), pp.5-18.
9. Moheban, M. and Young, J.B., A Study of Thermal Nonequilibrium Effect in Low-Pressure Wet-Steam Turbine Using a Blade-to-Blade Time-Marching Technique, Int. J. Heat and Fluid Flow, Vol.6, (1985), pp.269-278.
10. Young, J. B., Two-Dimensional, Nonequilibrium, Wet-Steam Calculations for Nozzles and Turbine Cascades, *Trans. ASME, J. Turbomachinery*, Vol.114, (1992), pp.569-579.
11. Yamamoto, S., Sasao, Y., Kato, H., Satsuki, H., Ooyama, H. and Ishizaka, K., Numerical and Experimental Investigation of Unsteady 3-D Wet-steam Flows through Two-stage Stator-rotor Cascade Channels, *Proc. ASME Turbo Expo 2010*, GT2010-22796, (2010).
12. Miyake, S., Sasao, Y., Yamamoto, S., Tabata, S., Miyawaki, T. and Ooyama, H., Simulation of Unsteady 3-D Wet-steam Flows through Three-stage Stator-rotor Blade Rows with Equilibrium and Nonequilibrium Condensations, *Proc. ASME Turbo Expo 2012*, GT2012-68828, (2012).
13. Miyake, S., Yamamoto, S., Sasao, Y., Momma, K., Miyawaki, T. and Ooyama, H., Unsteady Flow Effect on Nonequilibrium Condensation in 3-D Low Pressure Steam Turbine Stages, *Proc. ASME Turbo Expo 2013*, GT2013-94832, (2013).
14. Miyake, S., Koda, I., Yamamoto, S., Sasao, Y., Momma, K., Miyawaki, T. and Ooyama, H., Unsteady Flow Effect on Nonequilibrium Condensation in 3-D Low Pressure Steam Turbine Stages, *Proc. ASME Turbo Expo 2014*, GT2014-25491, (2014).
15. Miyake, S., Miyazazwa, H., Yamamoto, S., Sasao, Y., Momma, K., Ooyama, H. and Miyawaki, T., Unsteady 3-D Wet-steam Flows through Low Pressure Turbine Final Three Stages considering Blade Number, *Proc. ASME Turbo Expo 2015*, GT2015-42366, (2015).

Chapter E Preconditioning Method

1. Preconditioned equations

Ordinary compressible flow solvers cannot be applied to the calculation for very slow flows such as natural convection. One of the reasons is the so-called stiff problem that occurs when flows at a very low Mach number are calculated by compressible flow solvers. The relatively high speed of sound compared with physical velocities in these flows restricts the Courant-Friedrich-Lewy (CFL) number. Then, we need a huge number of time-marching iterations to get a solution Turkel [1], Choi and Merkle [2], and Weiss and Smith [3] have developed a preconditioning method that is a numerical approach to overcome the stiff problem. A numerical speed of sound has been derived and applied to the pseudo-compressibility method. Fundamental equations are smoothly switched to different equations according to the value of the numerical speed of sound. The equations are completely the same with the CNS when the value is set to the physical speed of sound, while the incompressible Navier-Stokes equations with the pseudo-compressibility term and the temperature equation are formed by setting the value to that in a same order of local physical velocity. We have employed the same approach for simulating natural convective flows.

CNS modified by the preconditioning method are written in general curvilinear coordinates as

$$\Gamma\frac{\partial\hat{Q}}{\partial t}+\frac{\partial F_i}{\partial\xi_i}=\frac{\partial F_{vi}}{\partial\xi_i} \tag{1-1}$$

where Γ is the preconditioning matrix. The elements in Γ are fundamentally the same as those of the formulation by Weiss and Smith [3], represented by

$$\Gamma=\begin{bmatrix}\theta & 0 & 0 & 0 & \rho_T\\ \theta u_1 & \rho & 0 & 0 & \rho_T u_1\\ \theta u_2 & 0 & \rho & 0 & \rho_T u_2\\ \theta u_3 & 0 & 0 & \rho & \rho_T u_3\\ \theta h-1 & \rho u_1 & \rho u_2 & \rho u_3 & \rho_T h+\rho C_p\end{bmatrix} \tag{1-2}$$

where θ is the preconditioning parameter defined by

$$\theta=1/U_r^2-\rho_T/\rho C_p \tag{1-3}$$

$h=(e+p)/\rho$ and $\rho_T=\partial\rho/\partial T$. $\rho_T=-\rho/T$ if ideal gas is taken into account. U_r is a switching parameter. If U_r equals the physical speed of sound, θ is to be zero and the equations are reduced to CNS. $\hat{Q}$ is the vector of unknown primitive variables defined by $\hat{Q}=[p\ \ u_1\ \ u_2\ \ u_3\ \ T]^T$.

2. Preconditioned flux-vector splitting form [4]

The numerical flux $(F_i)_{\ell+1/2}$ for F_i in Eq. (1-1) defined at the interface between the control volume ℓ and $\ell+1$ in each coordinate $i(i=1,2,3)$ can be written by FVS form as

$$(F_i)_{\ell+1/2}=\left(F_i^+\right)_{\ell+1/2}+\left(F_i^-\right)_{\ell+1/2}=\left(\hat{A}_i^+\right)_{\ell+1/2}\hat{Q}^L_{\ell+1/2}+\left(\hat{A}_i^-\right)_{\ell+1/2}\hat{Q}^R_{\ell+1/2} \tag{2-1}$$

$\hat{A}_i^{\mp}$ are preconditioned Jacobian matrices composed of only positive or negative characteristic speeds. $\hat{Q}^L$ and $\hat{Q}^R$ are unknown vectors extrapolated by Compact MUSCL from left and right directions. The preconditioned FVS (PFVS) form [4] for $\left(\hat{A}_i^{\mp}\right)_{\ell+1/2}\hat{Q}^M_{\ell+1/2}$ is derived as

$$\left(\hat{A}_i^{\mp}\right)_{\ell+1/2}\hat{Q}^M=\left(\Gamma L_i^{-1}\Lambda_i L_i\right)_{\ell+1/2}\hat{Q}^M=\hat{\lambda}_{i1}^{\mp}\Gamma\hat{Q}^M+\frac{\hat{\lambda}_{ia}^{\mp}}{\hat{c}_i\sqrt{g_{ii}}}\hat{Q}_{ia}+\frac{\hat{\lambda}_{ib}^{\mp}}{\hat{c}_i^2}\hat{Q}_{ib} \tag{2-2}$$

L_i and Λ_i are the matrices composed of preconditioned eigenvectors and preconditioned characteristic speeds (eigenvalues). $\hat{\lambda}_{ia}^{\mp}$ and $\hat{\lambda}_{ib}^{\mp}$ are defined by

$$\hat{\lambda}_{ia}^{\mp} = \left(\hat{\lambda}_{i4}^{\mp} - \hat{\lambda}_{i5}^{\mp}\right)/2$$
$$\hat{\lambda}_{ib}^{\mp} = \left(\ell_i^- \hat{\lambda}_{i4}^{\mp} - \ell_i^+ \hat{\lambda}_{i5}^{\mp}\right)/\left(\ell_i^- - \ell_i^+\right) - \hat{\lambda}_{i1}^{\mp} \tag{2-3}$$

where $\hat{\lambda}_{ij}^{\mp}\ (j=1,4,5)$ and $\ell_i^{\mp}$ are calculated by

$$\hat{\lambda}_{ij}^{\mp} = \left(\hat{\lambda}_{ij} \pm \left|\hat{\lambda}_{ij}\right|\right)/2 \tag{2-4}$$

$$\ell_i^{\mp} = \rho U_r^2 \Big/ \left(U_i(1-\alpha)/2 \mp \hat{c}_i\sqrt{g_{ii}}\right) \tag{2-5}$$

$\hat{\lambda}_{ij}\ (j=1,4,5)$ are preconditioned characteristic speeds defined by

$$\hat{\lambda}_{i1} = U_i$$
$$\hat{\lambda}_{i4} = (1+\alpha)U_i/2 + \hat{c}_i\sqrt{g_{ii}} \tag{2-6}$$
$$\lambda_{i5} = (1+\alpha)U_i/2 - \hat{c}_i\sqrt{g_{ii}}$$

$\hat{c}_i$ is the numerical speed of sound. It is derived as

$$\hat{c}_i = \sqrt{U_i^2(1-\alpha)^2/g_{ii} + 4U_r^2}\,/2 \tag{2-7}$$

and $\alpha = U_r^2\left(\rho_p + \rho_T/\rho C_p\right)$, where $\rho_p = \partial\rho/\partial p$. $\rho_p = 1/(RT)$ if ideal gas is assumed. If U_r equals the physical speed of sound, α is reduced to unit. Then, characteristic speeds and the physical speed of sound for compressible flows are recovered. $\hat{Q}_{ia}$ and $\hat{Q}_{ib}$ are subvectors derived as

$$\hat{Q}_{ia} = \hat{q}_1^M Q_{ic} + \rho\hat{U}_i Q_d$$
$$\hat{Q}_{ib} = \left(\rho\hat{U}_i\hat{c}_i^2/g_{ii}\right)Q_{ic} + \left(\hat{q}_1^M\hat{c}_i^2/U_r^2\right)Q_d \tag{2-8}$$

$\hat{q}_j^M$ and $\hat{U}_i$ $[=(\partial\xi_i/\partial x_j)\hat{q}_{j+1}^M\ (j=1,2,3)]$ are the j-th element of $\hat{Q}$ and the contravariant velocities extrapolated by Compact MUSCL. Q_{ic} and Q_d are subvectors given by

$$\hat{Q}_{ic} = \left[0 \quad \partial\xi_1/\partial x_1 \quad \partial\xi_1/\partial x_2 \quad \partial\xi_1/\partial x_3 \quad U_i\right]^T \tag{2-13}$$

$$\hat{Q}_d = \left[1 \quad u_1 \quad u_2 \quad u_3 \quad (e+p)/\rho\right]^T \tag{2-14}$$

3. Preconditioned FDS form [4]

FDS method based on Roe's approximate Riemann solver [Chap. B, Eq. (3-8)] is employed for discretizing convection terms. The numerical flux Eq. (2-1) is rewritten as

$$(F_i)_{\ell+1/2} = \frac{1}{2}\left[F_i\left(\hat{Q}_{\ell+1/2}^L\right) + F_i\left(\hat{Q}_{\ell+1/2}^R\right) - \left|\left(\hat{A}_i\right)_{\ell+1/2}\right|\left(\hat{Q}_{\ell+1/2}^R - \hat{Q}_{\ell+1/2}^L\right)\right] \tag{3-1}$$

The FDS term $\left|\left(\hat{A}_i\right)_{\ell+1/2}\right|\hat{Q}^M$ is derived using PFVS form Eq. (2-2) as

$$\left|\left(\hat{A}_i\right)_{\ell+1/2}\right|\hat{Q}^M = \left|\hat{\lambda}_{i1}\right|\Gamma\hat{Q}^M + \frac{\left|\hat{\lambda}_{ia}\right|}{\hat{c}_i\sqrt{g_{ii}}}\hat{Q}_{ia} + \frac{\left|\hat{\lambda}_{ib}\right|}{\hat{c}_i^2}\hat{Q}_{ib} \tag{3-2}$$

All the components in Eq. (3-2) are the same with those for FVS form.

4. Preconditioned LU-SGS method [4]

LU-SGS method [Chap. B, Eq. (6-8)] can be modified to the following preconditioned form:

$$\Gamma D\Delta\hat{Q}^* = RHS + \Delta t G^+\left(\Delta\hat{Q}^*\right)$$
$$\Delta\hat{Q} = \Delta\hat{Q}^* - \Gamma^{-1}D^{-1}\Delta t G^-\left(\Delta\hat{Q}\right) \tag{4-1}$$

where G^+ and G^- are functions composed of time derivatives of numerical flux at neighboring grid points defined by

$$
\begin{aligned}
G^{+}\left(\Delta\hat{Q}^{*}\right) &= \left(\hat{A}_1^{+}\Delta\hat{Q}^{*}\right)_{i\text{-}1,j,k} + \left(\hat{A}_2^{+}\Delta\hat{Q}^{*}\right)_{i,j-1,k} + \left(\hat{A}_3^{+}\Delta\hat{Q}^{*}\right)_{i,j,k-1} \\
G^{-}\left(\Delta\hat{Q}\right) &= \left(\hat{A}_1^{-}\Delta\hat{Q}\right)_{i+1,j,k} + \left(\hat{A}_2^{-}\Delta\hat{Q}\right)_{i,j+1,k} + \left(\hat{A}_3^{-}\Delta\hat{Q}\right)_{i,j,k+1}
\end{aligned}
\tag{4-2}
$$

$\hat{A}_i^{\mp}\Delta\hat{Q}\ (i=1,2,3)$ may be calculated from Eq. (2-2) in which $\hat{Q}^{M}$ is replaced by $\Delta\hat{Q}$.

As applications of preconditioning method, we simulated natural convection and that coupled with heat conduction in solid [5], those with condensation [4], and very slow flows of moist-air in a cooled pipe [6].

References

1. Turkel, E., Preconditioned Methods for Solving the Incompressible and Low Speed Compressible Equations, *J.Comp.Phys.* Vol.72, (1987), pp.277-298.
2. Choi, Y.H., and Merkle, C.L., The Application of Preconditioning in Viscous Flows, *J. Comp. Phys*. Vo.105, (1993), pp.207-223.
3. Weiss, J.M. and Smith, W.A., Preconditioning Applied to Variable and Constant Density Flows, *AIAA Journal*, Vol.33, (1995), pp.2050-2057.
4. Yamamoto, S., Preconditioning Method for Condensate Fluid and Solid Coupling Problems in General Curvilinear Coordinates, *J. Comp. Phys.*, Vol.207, (2005), pp.240-260.
5. Yamamoto, S., Niiyama, D., and Shin, B.R., A Numerical Method for Natural Convection and Heat Conduction around And in A Horizontal Circular Pipe, *Int. J. Heat and Mass Transfer*, Vol.47, (2004), pp.5781-5792.
6. Sakakura, K. and Yamamoto, S., Numerical and Experimental Predictions of Heterogeneous Condensate Flow of Moist air in Cooled Pipe, *Int. J. Heat and Fluid Flows*, Vol.27, (2006), pp.220-228.

Chapter F Modeling for Thermophysical Flow

1. Modification of preconditioned equations

CNS equations with a source term modified by the preconditioning method are written in general curvilinear coordinates as

$$\Gamma\frac{\partial\hat{Q}}{\partial t}+\frac{\partial F_i}{\partial\xi_i}=\frac{\partial F_{vi}}{\partial\xi_i}+S \tag{1-1}$$

where all the terms in Eq. (1-1) except for source term S is the same with those of Eq. (1-1) in Chapter E. Source term includes some additional physics, for example gravitational force toward $x_2(=y)$ is taken into account as $S=J[0\quad 0\quad(\rho_s-\rho)g\quad 0\quad(\rho_s-\rho)u_2 g]^T$, where ρ_s and g are referenced density and gravitational acceleration.

To consider accurate thermophysical properties such for supercritical fluids, not only the variation of properties with respect to temperature but also that with respect to pressure should be taken carefully into consideration. The preconditioning matrix Γ is slightly modified [1] to

$$\Gamma=\begin{bmatrix}\theta & 0 & 0 & 0 & \rho_T\\ \theta u_1 & \rho & 0 & 0 & \rho_T u_1\\ \theta u_2 & 0 & \rho & 0 & \rho_T u_2\\ \theta u_3 & 0 & 0 & \rho & \rho_T u_3\\ \theta h-(1-\rho h_p) & \rho u_1 & \rho u_2 & \rho u_3 & \rho_T h+\rho h_T\end{bmatrix} \tag{1-2}$$

where $h=(e+p)/\rho$. The preconditioning parameter θ is also redefined by

$$\theta=\frac{1}{U_r^2}-\frac{\rho_T(1-\rho h_p)}{\rho h_T} \tag{1-3}$$

$\rho_T=\partial\rho/\partial T$, $h_T=\partial h/\partial T$ and $h_p=\partial h/\partial p$.

2. Thermophysical models

Substances have their own thermophysical properties. The values are changed according to the values of temperature and pressure. The phase is occasionally changed among gas, liquid, and solid. In addition, substances become supercritical fluids if the temperature and pressure are beyond the critical points. Especially, supercritical fluids have anomalous properties near the critical point: maximum peak of isobaric specific heat and that of reaction rate; rapid change of solubility, zero surface tension, and so on. These anomalous properties are utilized for the decomposition of waste, the fabrication of nanoscale particles, heat exchangers, and so on, by chemical, material and mechanical engineers. Eckert et al. [2] reviewed the research works of supercritical fluids in the *Nature*.

Ordinary CFD solvers employing the equation of state (EOS) for ideal gas cannot predict actual thermophysical values in flows of arbitrary substance. Fortunately, primary thermophysical properties such as density, viscosity and thermal conductivity have been mathematically modelled by chemical engineers for most of substances. For examples, we know several EOSs based on cubic-type and virial-type models. Cubic-type EOS is formed by a cubic equation based on the van der Waals EOS. The form is not so complicated as compared with that of virial-type EOS. We simulated thermal convection of supercritical carbon dioxide [3] using our preconditioning method coupled with Peng-Robinson EOS (P-R EOS) [4] which is a modified EOS from the van der Waals EOS. The obtained results suggest that the solution is essentially different from ordinary solutions obtained by assuming an ideal gas. P-R EOS could be applied to the carbon dioxide reasonably. However, P-R EOS could not predict water accurately. It suggests that cubic-type EOS cannot be used as a general-purpose EOS for arbitrary substance.

Virial-type EOS is formed by a polynomial equation. Even though the computational cost is relatively higher than that of cubic-type EOS, the accuracy is sufficiently preserved even if the temperature and pressure are changed between two phases. For example, a virial-type EOS for carbon dioxide was standardized in IUPAC [5] defined as a polynomial equation by

$$p = \rho RT\left[1 + \omega\sum_{i=0}^{9}\sum_{j=0}^{J_i} a_{ij}(\tau-1)^j(\omega-1)^i\right] \tag{2-1}$$

where $\omega = \rho/\rho^*$, $\tau = T^*/T$ and actually $\rho^* = 468\,[\mathrm{kg/m^3}]$ and $T^* = 304.21\,[\mathrm{K}]$ for carbon dioxide. Parameters a_{ij} and J_i are referred from IUPAC [5]. Using Eq. (2-1), isobaric and isometric specific heats are obtained from the following equations:

$$C_v = \int_0^\rho \frac{T}{\rho^2}\left(\frac{\partial^2 p}{\partial T^2}\right)_\rho d\rho + C_v^{ideal} \tag{2-2}$$

$$C_p = C_v + \frac{T}{\rho^2}\frac{(\partial p/\partial T)_\rho^2}{(\partial p/\partial\rho)_T} \tag{2-3}$$

where C_v^{ideal} is the isometric specific heat for ideal gas.

EOS for water was also defined in IAPWS IF97 [6]. Density is obtained by the virial-type EOS as a function of temperature and pressure. Not only specific heats but also the related partial derivatives can be derived from the EOS.

As other properties, molecular viscosity μ and thermal conductivity κ were further modeled using a polynomial equation as

$$\ln\frac{\mu}{\mu_x} = \sum_{i=1}^{4}\sum_{j=0}^{1} b_{ij}\tau^j\omega^i \tag{2-4}$$

$$\ln\frac{\kappa}{\kappa_x} = \sum_{i=1}^{5}\sum_{j=0}^{2} d_{ij}\tau^j\omega^i \tag{2-5}$$

where $\mu_x = \sum_{i=1}^{3} c_i\tau^{i-3/2}$ and $\kappa_x = \sum_{i=1}^{3} e_i\tau^{i-3/2}$. The coefficients b_{ij}, c_{ij}, d_{ij} and e_{ij} were defined in IUPAC.

We know some databases for thermophysical properties such as that developed by NIST. Currently we use the thermophysical database PROPATH [7] developed by Kyushu University: a database of thermophysical properties for 48 substances. Most of the mathematical models for EOS, molecular viscosity, thermal conductivity, isobaric and isometric specific heats and so on, are programmed as a polynomial equation which has been standardized by an authorized conference or society. Since the anomalous property is quite deeply related to the flow feature near the critical point, the accurate evaluation is absolutely necessary for simulating supercritical-fluid flows. Our preconditioning method was fully coupled with PROPATH. Thermophysical properties are programmed as functions for each substance in PROPATH. The set of the functions are contained in a same file as the library file for each substance. The names of the functions are all the same in the different libraries even if the substance is different. This feature enables us to change the substance quite easily. Only if the library file is replaced to the other, we can simulate thermophysical flows of different substance, such as carbon dioxide, water, nitrogen, hydrogen, methane, and so on.

Currently we are developing another in-house code called 'Supercritical-fluids Simulator (SFS)' which is based on such preconditioning method and PROPATH for simulating not only very slow flows but also high-speed flows beyond supersonic of gas, liquid, and supercritical fluid considering the phase change. As one of the final destinations of SFS, we simulated Rapid Expansion of Supercritical Solution (RESS) [8] process using SFS [9][10]. We seamlessly simulated supercritical CO_2 (SCO_2) entering the nozzle, SCO_2 crossing the critical pressure in the nozzle, supersonic CO_2 gas expanding into the expansion chamber, shocks and CO_2 condensation in the chamber, nucleation, condensation, and coagulation of polymer particles. Finally all physics expected in RESS could be totally simulated [10].

1. Yamamoto, S., Furusawa, T. and Matsuzawa, R., Numerical Simulation of Supercritical Carbon Dioxide Flows across Critical Point, *Int. J. Heat and Mass Transfer*, Vol.54, No.4(2011), pp.774-782.
2. Eckert, C.A., Knutson, P.G. and Debenedetti, P.G., Supercritical Fluids as Solvents for Chemical and Material Processing, *Nature*, Vol.383, No.26 (1996), pp.313-318.
3. Yamamoto, S., Toratani, M. and Sasao, Y., Preconditioning Method Applied to Near-Critical Carbon-Dioxide

Flows in Micro-Channel, *JSME Int. J., Series B*, Vol.48, (2005), pp.532-539.
4. Peng, D.-Y. and Robinson, D.B., A New Two-Constant Equation of State, *Ind. Eng. Chem. Fundam.,* Vol.15, (1976), pp.59-64.
5. Angus, S., et al., International Thermodynamic Table of the Fluid State-3 Carbon Dioxide, IUPAC, Vol.3 (1976).
6. 1999 Steam Table, JSME, (1999).
7. A PROGRAM PACKAGE FOR THERMO-PHYSICAL PROPERTIES OF FLUIDS, Vol.12.1, PROPATH group.
8. Matson, W., Fulton, J.L., Petersen, R.C. and Smith, R.D., Rapid Expansion of Supercritical Fluid Solutions: Solute Formation of Powders, Thin Films, and Fibers, *Ind. Eng. Chem. Res.*, Vol. 26, (1987) , pp.2298-2306.
9. Yamamoto, S., Matsuzawa, R. and Furusawa, T., Simulation of Thermophysical Flow in Axisymmetric Nozzle with Expansion Chamber, AIChE Journal, Vol.57, No.10(2011), pp.2629-2635.
10. Yamamoto, S. and Furusawa, T., Thermophysical Flow Simulations of Rapid Expansion of Supercritical Solutions (RESS), *Journal of Supercritical Fluids*, Vol.97, (2015), pp.192-201.
(Featured online on 'Advances in Engineering': https://advanceseng.com/general-engineering/, April.28, 2015)