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Large Eddy Simulation of turbulent flow with multi-component of variable density

Takashi Maruyama [1], Takanori Uchida [2]

[1]*D.P.R.I. Kyoto University, Ujishi, Kyoto, Japan, tmaruyama540@gmail.com*
[2]*R.I.A.M. Kyushu University, Kasugashi, Fukuoka, Japan, takanori@riam.kyushu-u.ac.jp*

SUMMARY
Strong wind field causing disasters such as typhoon, tornado or volcanic eruption is a multi-component density flow including gases, liquid or solid particles such as raindrops or volcanic ash and so on. When multiple gases are mixed with dry air, density variations occur in both space and time even in an isothermal condition, and consequently, the flow field is affected by these variations. Furthermore, particles with significant differences in density are coexist in the atmosphere, they will move at a speed different from the atmosphere and entrain the surrounding flow. The calculation of flow near the ground is need the turbulent flow simulation. Therefore, we attempt to reproduce multi-component density turbulent flows using Large Eddy Simulation (LES) derived from space averaging operations that include solid and liquid particles. One-equation-type LES that use the sub-grid scale kinetic energy to predict the eddy viscosity is applied to account for the effect of turbulence explicitly. The filtered governing equations for the flow were derived by the filtering which can incorporate the effect of particle existence in the control volume. The examples of gas advection from the crater of Sakurajima are demonstrated.

Keywords: Large Eddy Simulation, multi-component density flow, turbulent flow

1. INTRODUCTIONS

Strong winds associated with typhoons, tornadoes and downbursts or volcanic ash fall associated with volcanic eruptions can sometimes trigger disasters. To simulate this kind of extreme atmospheric phenomena, we need the calculation method for the turbulent and density flow. Here the formulation of the governing equations to analyze the multi-component density flow including not only gas but also liquid or solid particles will be carried out. The equations were based on those for the low mac number density flow i.e. the flow speed is lower than that of sound (Rehm et al., 1978). The LES derived from the space averaging is commonly used to reproduce the turbulent flow. The filtering method (Hiraoka, 2014) to the control volume including different phases is adopted and the one-equation-type LES for the multi-component density flow will be derived.

2. FORMULATION

Temperature effect for density is not discussed here. Equations for the flow are based on the conservation of mass, momentum and kinetic energy. Filtered equations for the variable density flow including liquid or solid particles are obtained by the volume averaging. The one-equation-type LES is adopted.
Hiraoka (2014) proposed the volume averaging for the control volume including multi-phase components as follows. The space averaging of a function $f(\boldsymbol{x}, t)$ of position vector $\boldsymbol{x}(x_1,x_2,x_3)$ and

time t is defined as a convolution of f and a filter function ψ. The filter function is

$$\psi(\boldsymbol{x}) \to 0 \text{ when } \boldsymbol{x} \to \pm\infty, \tag{1}$$

and the control volume V_0 of the averaging is

$$V_0(\boldsymbol{x}) = \int_{-\infty}^{+\infty} \psi(\boldsymbol{x}) d\boldsymbol{x}. \tag{2}$$

The filter function is assumed to be constant in time and sufficiently smooth. The space averaged value $\overline{f}$ is defined as

$$\overline{f}(\boldsymbol{x}, t) = \frac{1}{V_F(x,t)} \int_{-\infty}^{+\infty} \{\psi(\boldsymbol{x} - \boldsymbol{y}) f(\boldsymbol{y}, t)\} d\boldsymbol{y}. \tag{3}$$

If the control volume includes liquid or solid particles, the integration is done in the volume of fluid. Therefore, the volume of the fluid V_F in the control volume is

$$V_F(\boldsymbol{x}, t) = \int_{-\infty}^{+\infty} \psi(\boldsymbol{x} - \boldsymbol{y}) d\boldsymbol{y}. \tag{4}$$

V_F is less than or equal to V_0 and varies in time and space. If the filter function is defined as a top hat function on V_0, V_F is equal to the fluid volume in V_0. The volume ratio of fluid is defined as

$$G_F(\boldsymbol{x}, t) = \frac{V_F}{V_0}, \qquad (0 \leq G_F \leq 1). \tag{5}$$

The averaging of partial derivative in time is defined as

$$\overline{\frac{\partial f}{\partial t}} = \frac{1}{V_F} \frac{\partial}{\partial t}\left(V_F \overline{f}\right) - \frac{1}{V_F} [\![f^s v_k^s n_k]\!], \tag{6}$$

where $[\![f^s v_k^s n_k]\!]$ is the inter-phase transfer term caused by the motion and deformation of particles defined as

$$[\![f^s v_k^s n_k]\!] = \int_S \psi(\boldsymbol{x} - \boldsymbol{y}) f(\boldsymbol{y}, t) v_k(\boldsymbol{y}, t) n_k(\boldsymbol{y}, t) dS(\boldsymbol{y}), \tag{7}$$

where v_k is the x_k-directional velocity component of the boundary between fluid and the particle and n_k is the normal vector component directing from fluid to particle on the boundary. The averaging of partial derivative in space is defined as

$$\overline{\frac{\partial f}{\partial x_j}} = \frac{1}{V_F} \frac{\partial}{\partial x_j}\left(V_F \overline{f}\right) + \frac{1}{V_F} [\![f^s n_j]\!], \tag{8}$$

where $[\![f^s n_j]\!]$ is the inter-phase transfer term caused by the in/out-flow across the boundary between the particle and the fluid defined as

$$[\![f^s n_j]\!] = \int_S \{\psi(\boldsymbol{x}-\boldsymbol{y}) f(\boldsymbol{y},t) n_j(\boldsymbol{y},t)\} dS(\boldsymbol{y}). \tag{9}$$

We get the filtered equations for the variable density follow. The governing equations of mass (density $\overline{\rho}, \overline{\rho}_n$), momentum $\overline{U}_i$ and sub-grid scale kinetic energy $\overline{E}_S$ are described as follows:

Mass (density),
$$\frac{\partial}{\partial t}\left(G_F\overline{\rho}_n\right) + \frac{1}{V_0}\frac{\partial}{\partial x_j}\left(V_0 G_F \overline{U}_j\right) = -G_F\frac{\partial \overline{Q}_{\rho n j}}{\partial x_j} + G_F\overline{S}_{\rho n} + \frac{1}{V_0}\left([\![\rho_n^S v_k n_k]\!] - [\![(\rho_n u_j)^s n_j]\!] - [\![Q_{\rho n j}^S n_j]\!]\right), (\overline{\rho}_n, n\text{th-component}) \tag{10}$$

$$\frac{\partial}{\partial t}\left(G_F\overline{\rho}\right) + \frac{1}{V_0}\frac{\partial}{\partial x_j}\left(V_0 G_F \overline{U}_j\right) = \frac{1}{V_0}\sum\nolimits_n\left([\![\rho_n^S v_k n_k]\!] - [\![(\rho_n u_j)^s n_j]\!]\right). (\overline{\rho}, \text{all component}) \tag{11}$$

Momentum,
$$\frac{\partial}{\partial t}\left(G_F\overline{U}_i\right) + \frac{1}{V_0}\frac{\partial}{\partial x_j}\left(V_0 G_F \overline{U}_i\tilde{u}_j\right) = -G_F\frac{\partial}{\partial x_i}\overline{P} + G_F\frac{\partial}{\partial x_j}\left(\overline{F_{ij}} - \overline{T_{ij}}\right) + G_F\overline{B}_i + \frac{1}{V_0}\left([\![(\rho u_i)^s v_k n_k]\!] - [\![(\rho u_i u_j)^s n_j]\!] - [\![P^s n_i]\!] + [\![F_{ij}^S n_j]\!]\right). \tag{12}$$

Sub-grid scale kinetic energy,
$$\frac{\partial}{\partial t}\left(G_F\overline{E}_S\right) + \frac{1}{V_0}\frac{\partial}{\partial x_j}\left(V_0 G_F \overline{E}_S\tilde{u}_j\right) = G_F\frac{\partial}{\partial x_j}\left\{\left(\overline{v}_F + \frac{\overline{v}_{SF}}{\sigma_S}\right)\frac{\partial \overline{E}_S}{\partial x_j}\right\} - G_F\left(\overline{\varepsilon}_S + \overline{T_{ij}}\widetilde{d_{ij}}\right). \tag{13}$$

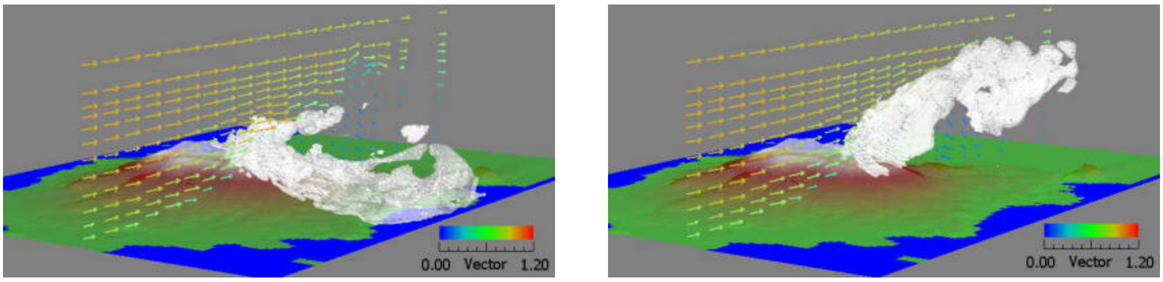
where the nomenclature is as follows: The density $\overline{\rho} = \sum_n \overline{\rho}_n$, $\overline{\rho}_n$(nth-component), the momentum of x_i direction $\overline{U}_i = \overline{\rho}\tilde{u}_i$, the Favre averaging (denoted by superscript tilde) of velocity u_i is $\tilde{u}_i = \frac{\overline{\rho u_i}}{\overline{\rho}}$, the mass flux and the source of nth-component of density as $\overline{Q}_{\rho n j}$ and $\overline{S}_{\rho n}$, the pressure $\overline{P}$, the body force $\overline{B}_i$, the sub-grid scale kinetic energy $\overline{E}_S = \overline{\rho}\tilde{e}_S = \overline{\rho}\left(\frac{1}{2}\widetilde{u_i' u_i'}\right)$ using the fluctuation velocity $u_i' = \tilde{u}_i - u_i$. The newly emerging terms are modeled with the coefficient of diffusion $\overline{\kappa}_{\rho n}$, the kinematic viscosity of nth-component of fluid $\overline{v}_{Fn}$, the eddy kinematic viscosity $\overline{v}_{SF}$, the turbulent Schmidt number σ_S , Coriolis parameter f_{Ci}, the coefficient of friction c_{fm} and the wind pressure c_{dm} and the area a_{pm} and velocity $\boldsymbol{v}_{pm}$of mth-particle as follows: the mass flux $\overline{Q}_{\rho n j} = -\overline{\kappa}_{\rho n}\overline{\rho}\frac{\partial}{\partial x_j}\left(\frac{\overline{\rho}_n}{\overline{\rho}}\right)$, the momentum flux $\overline{F_{ij}} = \overline{v}_F\left\{\left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\frac{\partial \overline{U}_k}{\partial x_k}\right\}$, $\overline{T_{ij}} = -\left\{\overline{v}_{SF}\left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_i}\right) - \frac{2}{3}\overline{E}_S\right\}$, the body force $\overline{B}_i = \overline{\rho}(\delta_{i3}g + f_{Ci})$, the kinematic viscosity $\overline{v}_F = \frac{\sum_n \overline{v}_{Fn}\overline{\rho}_n}{\overline{\rho}}$, the drag $[\![P^s n_i]\!] = -\sum_m\left[a_{pm}c_{dm}\frac{1}{2}\overline{\rho}\left(v_{pmi} - \tilde{u}_i\right)\left|\boldsymbol{v}_{pm} - \tilde{\boldsymbol{u}}\right|\right]$, $[\![F_{ij}^S n_j]\!] = \sum_m\left[a_{pm}c_{fm}\overline{\rho}\left(v_{pmi} - \tilde{u}_i\right)\right]$, the velocity difference $\left|\boldsymbol{v}_{pm} - \tilde{\boldsymbol{u}}\right| = \left|(v_{pm1} - \tilde{u}_1)^2 + (v_{pm2} - \tilde{u}_2)^2 + (v_{pm3} - \tilde{u}_3)^2\right|^{1/2}$. The turbulence effect terms were modeled (Okamoto et al., 1999) with the model coefficients c_v, c_ε and c_K as follows: the eddy kinematic viscosity $\overline{v}_{SF} \cong c_v\Delta_v\sqrt{\tilde{e}_S}$, the energy dissipation rate $\overline{\varepsilon}_S = \frac{c_\varepsilon}{\Delta_L}\overline{E}_S\sqrt{\tilde{e}_S} + 2\overline{v}_F\frac{\partial\sqrt{\overline{E}_S}}{\partial x_j}\frac{\partial\sqrt{\overline{E}_S}}{\partial x_j}$, $\Delta_v = \frac{\Delta_L\tilde{e}_S}{\tilde{e}_S + c_K{\Delta_L}^2{\widetilde{d_{ij}}}^2}$, $\Delta_L = V_F^{1/3}$ and $\widetilde{d_{ij}} = \frac{1}{2}\left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_i}\right)$. The pressure can be decomposed into the mean environmental component $\overline{P}_0$, the static equilibrium component $\delta_{i3}\overline{\rho}_0 g$ and the residual P' with the mean environmental density $\overline{\rho}_0$ and the gravitational acceleration g as

$$\frac{\partial}{\partial x_i}\overline{P} = \frac{\partial}{\partial x_i}\left(\overline{P}_0 + P'\right) + \delta_{i3}\overline{\rho}_0 g \tag{14}$$

If the particle is enough small to control volume, has no deformation and no in/out-flow across the boundary between the particle and the fluid, the inter-phase transfer terms $\llbracket \rho_n^s v_k n_k \rrbracket$, $\left\llbracket (\rho_n u_j)^s n_j \right\rrbracket$, $\llbracket (\rho u_i)^s v_k n_k \rrbracket$ and $\left\llbracket (\rho u_i u_j)^s n_j \right\rrbracket$ are assumed to be zero, and $\overline{P}_0$ and $\overline{\rho}_0$ are assumed to be constant in the atmosphere near the ground.

3. CALCULATION

The calculations of density flow around Sakurajima volcano were carried out. To examine the effect of the density of contained gas, the flow is assumed to be isothermal and eliminate the influence of temperature. The program which was developed for the analysis of density flow over complex terrain (Uchida et al., 2020) was modified and used for the numerical calculation. A turbulent boundary layer was developed numerically over a rough surface and used the turbulent flow in the boundary was used for the inlet boundary condition. The no-slip condition was used for the ground boundary and the free outlet boundary for the rest boundaries. Flows with heavier gas than dry air and with lighter gas were numerically calculated as shown in Figure 1. The heavier gas flows down the mountainside, on the other hand the lighter gas does not.



a. With heavier gas **b.** With lighter gas

Figure 1. Numerical simulation of air flows around Sakurajima with gas erupting from the crater. Arrows are velocity vectors ($\widetilde{\boldsymbol{u}}/|\widetilde{\boldsymbol{u}}_0|$), white surfaces are iso-surfaces of density (a: $\overline{\rho}_{gas}$=1.002$\overline{\rho}_0$, b: $\overline{\rho}_{gas}$=0.998$\overline{\rho}_0$)

4. CONCLUSIONS

The filtered governing equations of one-equation-type Large Eddy Simulation were derived. The filtering functioned to the control volume including different phases, i.e. gases and particles, was adopted to the multi-component density flow. Examples of gas eruption from the crater of Sakurajima is demonstrated. The difference of the flow with density of gas were reproduced.

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