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DEVELOPMENT OF NUMERICAL ANALYSIS METHOD BASED ON STAGGERED GRID FOR ARBITRARY 3-DIMENSIONAL MESH SHAPE FOR TWO-PHASE THREE-FIELD MODEL

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ABSTRACT

Numerical analysis method for an unstructured staggered grid system for 3-field two-phase flow model was developed. Because of the complex definition of staggered volume and corresponding variables, commercial computational fluid dynamics codes usually adopt a collocated grid system for the analysis of complicated domain. In the conventional staggered grid system the staggered cell takes the halves of the neighboring two scalar cells. However, this study takes the whole of the two neighboring cells for the definition of the staggered cell. Finite volume method over this staggered grid system was implemented with some creative vector algebra and calculus. Time advancement was based on the semi-implicit method. This numerical treatment was successfully applied and the numerical tests show the effectiveness of this approach. This approach decreases the interpolation calculation to obtain not-solved-variables at cell or face. Only the diffusion terms require the interpolation, which is thought to be of minor importance.

NOMENCLATURE

A	[m^2]	area
D	[m^2/s]	general diffusion coefficient or mass diffusion coefficient of gas species
$\hat{\mathbf{d}}_f$	[m]	directional normal vector for face f
$\mathbf{d}_{LR}$	[m]	distance vector from point $\mathbf{x}_L$ to $\mathbf{x}_R$
E_ϕ^w	[W/m^3]	wall heat transfer to field ϕ not including phase change
F_ϕ^w	[N·sec/m^4]	wall drag coefficient between wall and field
$\mathbf{f}_{LR}$	[m]	distance vector connecting left cell center to right cell center across face f
G_i	[kg/m^3·sec]	mass source of species i per unit volume and time
$\mathbf{g}$	[m/s^2]	gravity vector
$H_{gli\leftrightarrow g}$	[W/m^{5}K]	gas-liquid-interface to gas heat transfer coefficient per volume
$H_{gli\leftrightarrow l}$	[W/m^{5}K]	gas-liquid-interface to liquid heat transfer coefficient per volume
$H_{dgi\leftrightarrow g}$	[W/m^{5}K]	gas-drop-interface to gas heat transfer coefficient per volume
$H_{dgi\leftrightarrow d}$	[W/m^{5}K]	gas-drop-interface to drop heat transfer coefficient per volume
h_ϕ	[J/kg]	specific enthalpy of field
h_ϕ^*	[J/kg]	modified specific enthalpy of field
k	[W/m·K]	thermal conductivity
$\mathbf{M}$	[N/m^3]	generalized drag
p	[Pa]	pressure
T	[K]	temperature
t	[sec]	time
U	[J/kg]	specific internal energy
V	[m^3]	volume
V_ϕ	[m/sec]	normal velocity of phase ϕ on face f
$\mathbf{x}$	[m]	location
Y_i	[-]	mass fraction of species i, $\left(=\rho_i/\rho_g\right)$

Special characters

α	[-]	void fraction or local concentration
Γ	[kg/m^3·sec]	mass volumetric production rate
γ_A	[-]	area porosity

γ_v	[-]	volume porosity
ρ	[kg/m^3]	density
Φ	[W/m^3]	energy dissipation
μ	[kg/m·sec]	viscosity

Subscripts

d	drop region or dispersed drop field
deent	de-entrainment or deposition
dgi	drop-gas interface
dli	drop-liquid interface
ent	entrainment
g	gas field
gdi	gas-drop interface
gli	gas-liquid interface
l	continuous liquid field
ldi	liquid- drop interface
lgi	liquid-gas interface
n	all noncondensable gases including air and hydrogen, normal direction
R	remote
S	cell or control volume surface
S′	another cell or control volume surface
ϕ	phase or field index

Superscripts

CD		bulk condensation
EV		bulk evaporation
s		saturated
t		turbulence
w		wall or solid surface

INTRODUCTION

Differently from laboratory and academic environments, industrial application in computational fluid dynamics (CFD deals with the domain of complicated shape. Through the long experiences in the assessment of complex geometry, unstructured grids of arbitrary shaped mesh such as tetrahedron rather than a hexahedron has been found to be less man-hour consuming than the generation of structured grids. Unstructured grids also give the merits of easy refinement of meshes for the interesting region. Together with the advancement of computational capacity, the unstructured grids have become more popular, even though the structured grid is still used for the more exact calculation in academic research for simple geometry domain.

In the process of differencing the governing equations, finite volume method (FVM) is usually adopted, because it can easily conserve the fluid properties. Since the FVM is a kind of finite element method (FEM), it requires an integration domain, i.e. a numerical control volume. FVM is applied on two grid systems; staggered grid and collocated grid. In the staggered grid system scalar variables such as pressure, temperature, and so on are located at the cell centre, and the vector variables such as velocity are located in cell face. Thus, for the implementation of FVM the staggered control volume (or mesh) for momentum equation should be additionally defined, as shown in Figure 1. As shown in Figure 1, the staggered control volumes should be independently defined for each coordinates, for example, x-directional staggered control volume should be defined for x-directional velocity component, and y-directional staggered control volume should be defined for y-directional velocity component in Cartesian coordinate. In the collocated grid system all the variables, regardless that they are scalar variables or vector variables, are located in the cell centre.

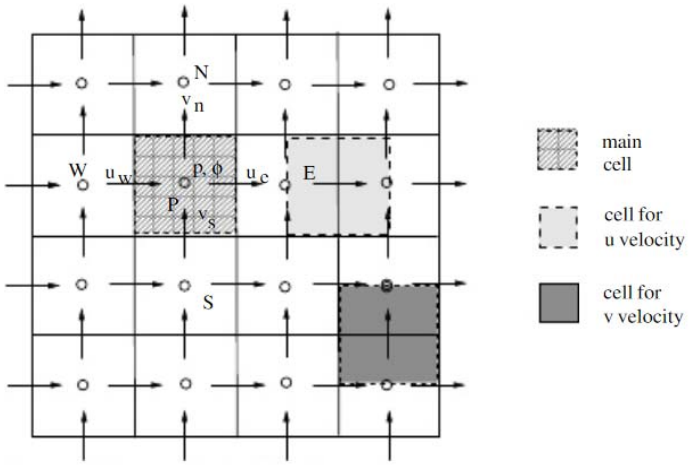


Figure 1 Numerical control volume for momentum equation in staggered grid system

The merit of the staggered grid system is that it can avoid the unrealistic check board type pressure distribution and it can easily conserve the convective properties through the faces because the velocities are defined at the faces. However in spite of such merits the staggered grid system is not generally adopted in 3-dimensional complex geometry because of the difficulties in the generation of staggered control volume in arbitrary mesh shapes such as tetrahedral mesh. So, commercial computational fluid dynamics codes usually adopt the collocated grid system together with unstructured grid system for the analysis of complicated domain.

Such a trend is also similar in the field of multi-dimensional two-phase flow, especially in nuclear system application. Neptune_CFD, in which the six classical transport equations (mass, momentum and energy for both liquid and gas) of the two-phase model, with the same pressure in the two phases, are solved is based on a fully unstructured finite volume meshing, together with a collocated arrangement for all flow variables[1]. CUPID (Component Unstructured Program for Interfacial Dynamics) code, which has been developed by Korea Atomic Energy Research Institute (KAERI), and treats 3-field equations (gas field, continuous liquid field, and dispersed drop field), also adopts the collocated method on an unstructured grid system[2]. SPACE(Safety and Performance Analysis CodE) code, which has been developed by

Korean nuclear industry as a design code of safety analysis for nuclear power plant, treats similar equations to those of CUPID, and is based on collocated method for 3-dimentional part on an unstructured grid system[33]. The other nuclear system codes such as COBRA/TRAC, MARS, and GOTHIC are based on staggered method, but they use the structured grid system[4,5,6].

In spite of favourlessness in industrial application some researchers have been interested in the staggered method. Wenneker et al. proposed new type staggered cell such as the shaded part in Figure 2, whereas in the conventional staggered grid system the staggered cell takes the halves of the neighbouring two scalar cells, as shown in Figure 1. And they applied it successfully to a compressible flow[7].

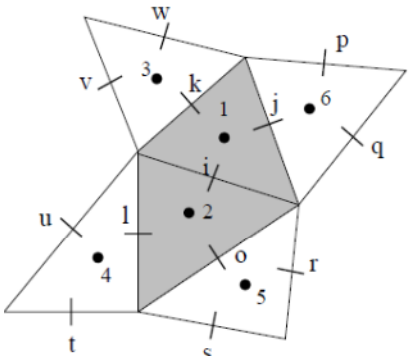


Figure 2 Numerical control volume for momentum equation in staggered grid system proposed by Wenneker et al.[7]

Momentum cell in Figure 2 make it easy to integrate convective terms, because the surfaces of momentum cell are surfaces of scalar cell, at which the velocities are already defined. This paper is a trial to the application of such momentum cell to two-phase flow of two-fluid model, even though compressible flow, which is the domain of Wenneker et al.'s, is far different from two-phase flow which is based on two-fluid model in numerical analysis.

GOVERNING EQUATIONS

Governing equations for the numerical implementation are those of CAP (Containment Analysis Package) which has been developed for the assessment of thermal hydraulic behaviours in containment for the design of nuclear power plant [8]. CAP code plays a role of boundary condition of SPACE which solves the response of RCS (Reactor Coolant System). CAP code is based on 3-field, 2-phase flow model. Gas phase falls to a gas field, and liquid phase to a continuous liquid field or a dispersed drop field. Fluids under consideration are water in the form of gas and liquid, air, and hydrogen. Each field interchanges mass, momentum, and energy, each other. Homogeneous and equilibrium assumptions for gas species are known to be quite valid in many cases. These fluids also exchange momentum and energy with boundary walls. More detailed phenomena in containment are described in reference 8.

Continuity Equation

Continuity equation for each field has the source terms; mass generation from the other fields and general source term.

For gas field which are the mixture of steam, air, and hydrogen.

$$\frac{\partial}{\partial t}\left(\alpha_g\rho_g\right)+\nabla\cdot\left(\alpha_g\rho_g\mathbf{v}_g\right) = -\frac{\frac{p_v}{p}H_{gli\leftrightarrow g}\left(T^s\left(p_v\right)-T_g\right)+H_{gli\leftrightarrow l}\left(T^s\left(p_v\right)-T_l\right)}{\left(h_g^*-h_l^*\right)} - \frac{\frac{p_v}{p}H_{dgi\leftrightarrow g}\left(T^s\left(p_v\right)-T_g\right)+H_{dgi\leftrightarrow d}\left(T^s\left(p_v\right)-T_d\right)}{\left(h_g^*-h_d^*\right)} +\Gamma_g \quad (1)$$

For continuous liquid

$$\frac{\partial}{\partial t}\left(\alpha_l\rho_l\right)+\nabla\cdot\left(\alpha_l\rho_l\mathbf{v}_l\right) = \frac{\frac{p_v}{p}H_{gli\leftrightarrow g}\left(T^s\left(p_v\right)-T_g\right)+H_{gli\leftrightarrow l}\left(T^s\left(p_v\right)-T_l\right)}{\left(h_g^*-h_l^*\right)} -\Gamma_{ent}+\Gamma_{deent}+\Gamma_l \quad (2)$$

For dispersed drop

$$\frac{\partial}{\partial t}\left(\alpha_d\rho_d\right)+\nabla\cdot\left(\alpha_d\rho_d\mathbf{v}_d\right) = \frac{\frac{p_v}{p}H_{dgi\leftrightarrow g}\left(T^s\left(p_v\right)-T_g\right)+H_{dgi\leftrightarrow d}\left(T^s\left(p_v\right)-T_d\right)}{\left(h_g^*-h_d^*\right)} +\Gamma_{ent}-\Gamma_{deent}+\Gamma_d \quad (3)$$

Momentum Equation

The source terms in momentum equation in each field is composed of pressure force, body force (gravity), viscous force, force due to phase change, inter-phase frictional force, wall friction force, virtual mass force, and general momentum source.

For gas field

$$\alpha_g\rho_g\frac{\partial\mathbf{v}_g}{\partial t}+\alpha_g\rho_g\mathbf{v}_g\cdot\nabla\otimes\mathbf{v}_g = -\alpha_g\nabla p+\alpha_g\rho_g\mathbf{g}+\nabla\cdot\left(\alpha_g\left(\mu_g+\mu_g^t\right)\nabla\otimes\mathbf{v}_g\right) +\Gamma_{lg}^{EV}\left(\mathbf{v}_l-\mathbf{v}_g\right)+\Gamma_{dg}^{EV}\left(\mathbf{v}_d-\mathbf{v}_g\right)-\mathbf{v}_g\Gamma_g +\left[F_{gl}\left(\mathbf{v}_l-\mathbf{v}_g\right)+F_{gd}\left(\mathbf{v}_d-\mathbf{v}_g\right)\right]-F_g^w\mathbf{v}_g \quad (4)$$

$$+\left[C_{gl}^{VM}\alpha_g\alpha_l\rho_{gl}\frac{\partial}{\partial t}\left(\mathbf{v}_l-\mathbf{v}_g\right)+C_{gd}^{VM}\alpha_g\alpha_d\rho_{dg}\frac{\partial}{\partial t}\left(\mathbf{v}_d-\mathbf{v}_g\right)\right]$$
$$+\mathbf{M}_g$$

For continuous liquid

$$\begin{aligned}&\alpha_l\rho_l\frac{\partial\mathbf{v}_l}{\partial t}+\alpha_l\rho_l\mathbf{v}_l\cdot\nabla\otimes\mathbf{v}_l\\&=-\alpha_l\nabla p+\alpha_l\rho_l\mathbf{g}+\nabla\cdot\left(\alpha_l\left(\mu_l+\mu_l^t\right)\nabla\otimes\mathbf{v}_l\right)\\&+\Gamma_{gl}^{CD}\left(\mathbf{v}_g-\mathbf{v}_l\right)+\Gamma_{deent}\left(\mathbf{v}_d-\mathbf{v}_l\right)-\mathbf{v}_l\Gamma_l\\&+\left[F_{lg}\left(\mathbf{v}_g-\mathbf{v}_l\right)+F_{ld}\left(\mathbf{v}_d-\mathbf{v}_l\right)-F_l^w\mathbf{v}_l\right]\\&+\left[C_{gl}^{VM}\alpha_g\alpha_l\rho_{gl}\frac{\partial}{\partial t}\left(\mathbf{v}_g-\mathbf{v}_l\right)\right]+\mathbf{M}_l\end{aligned}\quad(5)$$

For dispersed drop

$$\begin{aligned}&\alpha_d\rho_d\frac{\partial\mathbf{v}_d}{\partial t}+\alpha_d\rho_d\mathbf{v}_d\cdot\nabla\otimes\mathbf{v}_d\\&=-\alpha_d\nabla p+\alpha_d\rho_d\mathbf{g}+\nabla\cdot\left(\alpha_d\left(\mu_d+\mu_d^t\right)\nabla\otimes\mathbf{v}_d\right)\\&+\Gamma_{dg}^{CD}\left(\mathbf{v}_g-\mathbf{v}_d\right)+\Gamma_{ent}\left(\mathbf{v}_l-\mathbf{v}_d\right)-\mathbf{v}_d\Gamma_d\\&+\left[F_{dg}\left(\mathbf{v}_g-\mathbf{v}_d\right)+F_{ld}\left(\mathbf{v}_l-\mathbf{v}_d\right)\right]-F_d^w\mathbf{v}_d\\&+\left[C_{gd}^{VM}\alpha_g\alpha_d\rho_{dg}\frac{\partial}{\partial t}\left(\mathbf{v}_g-\mathbf{v}_d\right)\right]+\mathbf{M}_d\end{aligned}\quad(6)$$

Energy Equation

The source terms in energy equation in each field is composed of

For gas field

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\alpha_g\rho_gU_g\right)+\nabla\cdot\left(\alpha_g\rho_gU_g\mathbf{v}_g\right)\\&=-p\frac{\partial\alpha_g}{\partial t}-p\nabla\cdot\left(\alpha_g\mathbf{v}_g\right)\\&+\nabla\cdot\left(\alpha_g\left(k_g\nabla T_g+k_g^t\nabla T_g\right)\right)+\Phi_g\\&+\left[-\frac{h_l^*}{\left(h_g^*-h_l^*\right)}\frac{p_v}{p}H_{gli\leftrightarrow g}\left(T^s\left(p_v\right)-T_g\right)\right.\\&-\frac{h_g^*}{\left(h_g^*-h_l^*\right)}H_{gli\leftrightarrow l}\left(T^s\left(p_v\right)-T_l\right)\\&\left.+\frac{p_n}{p}H_{l\leftrightarrow n}\left(T_l-T_g\right)\right]\\&+\left[-\frac{h_d^*}{\left(h_g^*-h_d^*\right)}\frac{p_v}{p}H_{dgi\leftrightarrow g}\left(T^s\left(p_v\right)-T_g\right)\right.\\&-\frac{h_g^*}{\left(h_g^*-h_d^*\right)}H_{dgi\leftrightarrow d}\left(T^s\left(p_v\right)-T_d\right)\\&\left.+\frac{p_n}{p}H_{d\leftrightarrow n}\left(T_d-T_g\right)\right]\\&+E_g^w+E_g\end{aligned}\quad(7)$$

For continuous liquid

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\alpha_l\rho_lU_l\right)+\nabla\cdot\left(\alpha_l\rho_lU_l\mathbf{v}_l\right)\\&=-p\frac{\partial\alpha_l}{\partial t}-p\nabla\cdot\left(\alpha_l\mathbf{v}_l\right)\\&+\nabla\cdot\left(\alpha_l\left(k_l\nabla T_l+k_l^t\nabla T_l\right)\right)+\Phi_l\\&+\left[\frac{h_l^*}{\left(h_g^*-h_l^*\right)}\frac{p_v}{p}H_{gli\leftrightarrow g}\left(T^s\left(p_v\right)-T_g\right)\right.\\&+\frac{h_g^*}{\left(h_g^*-h_l^*\right)}H_{gli\leftrightarrow l}\left(T^s\left(p_v\right)-T_l\right)\\&\left.+\frac{p_n}{p}H_{n\leftrightarrow l}\left(T_g-T_l\right)\right]\\&+\left[-h_l\Gamma_{ent}+h_d\Gamma_{deent}\right]+E_l^w+E_l\end{aligned}\quad(8)$$

For dispersed drop

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\alpha_d\rho_dU_d\right)+\nabla\cdot\left(\alpha_d\rho_dU_d\mathbf{v}_d\right)\\&=-p\frac{\partial\alpha_d}{\partial t}-p\nabla\cdot\left(\alpha_d\mathbf{v}_d\right)\\&+\nabla\cdot\left(\alpha_d\left(k_d\nabla T_d+k_d^t\nabla T_d\right)\right)+\Phi_d\\&+\left[\frac{h_d^*}{\left(h_g^*-h_d^*\right)}\frac{p_v}{p}H_{dgi\leftrightarrow g}\left(T^s\left(p_v\right)-T_g\right)\right.\\&+\frac{h_g^*}{\left(h_g^*-h_d^*\right)}H_{dgi\leftrightarrow d}\left(T^s\left(p_v\right)-T_d\right)\\&\left.+\frac{p_n}{p}H_{n\leftrightarrow d}\left(T_g-T_d\right)\right]\end{aligned}\quad(9)$$

Gas Motion Equation

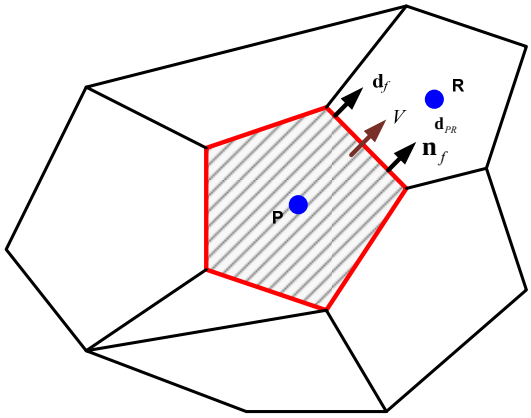
Gas motion equation describes the convection and diffusion of each gas species. The source terms are composed of diffusion term and general source term.

$$\frac{\partial\left(\alpha_g \rho_g Y_i\right)}{\partial t} + \nabla\cdot\left(\alpha_g \rho_g \mathbf{v}_g Y_i\right) = \nabla\cdot\left(\alpha_g D_i \rho_g \nabla Y_i\right) + G_i \quad (10)$$

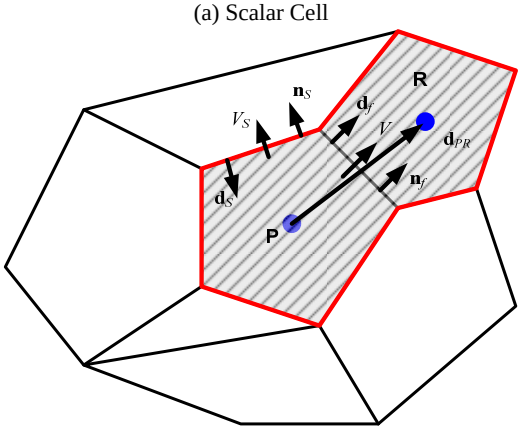
For the subscript *i*, 1 means steam, 2 air, and 3 hydrogen. And for the mixture of noncondensable gas, air and hydrogen, *n* is used. In the numerical process in this study the noncondensable gas mixture equation of subscript *n* is used

GRID SYSTEM

The staggered grid system is considered in this study. Conceptual figuration of grid is shown in Figure 3.



(a) Scalar Cell



(b) Momentum Cell

Figure 3 Grid system for numerical implementation

For the implementation of differencing the equations over the numerical cell several geometrical vector should be defined. The centroid of the scalar cell is calculated as

$$\mathbf{x}_{centroid} = \frac{1}{N}\sum_{i=1}^{n}\mathbf{x}_i \quad (11)$$

$\mathbf{x}_i$ is each vertex of the cell. Each face, *f*, of the scalar cell has the normal directional vector, $\hat{\mathbf{d}}_f$, which implies the unique direction of the face. It is set during the generation of the mesh and never changed in the process of numerical implementation. On the normal directional vector velocity, *V*, is defined.

$$\mathbf{v} \equiv V\hat{\mathbf{d}}_f \quad (12)$$

Thus, the velocity vector is perpendicular to the face *f*. *V* has the positive sign if the direction is same to $\hat{\mathbf{d}}_f$, and negative if sign if the direction is inverse to $\hat{\mathbf{d}}_f$.

And outward normal vector, $\mathbf{n}_f$, should be defined temporally. The word 'temporally' means that the sign of $\mathbf{n}_f$ changes when the neighbouring cell are under implementation. Using this outward normal vector in- and out-flow can be identified;

$$\begin{aligned}
&\text{if } V \geq 0, \text{ and } \hat{\mathbf{d}}_f\cdot\mathbf{n}_f \geq 0, \text{ then } F \equiv AV\left(\hat{\mathbf{d}}_f\cdot\mathbf{n}_f\right) \geq 0 : \textit{Outflow}\\
&\text{if } V \geq 0, \text{ and } \hat{\mathbf{d}}_f\cdot\mathbf{n}_f < 0, \text{ then } F \equiv AV\left(\hat{\mathbf{d}}_f\cdot\mathbf{n}_f\right) < 0 : \textit{Inflow}\\
&\text{if } V < 0, \text{ and } \hat{\mathbf{d}}_f\cdot\mathbf{n}_f \geq 0, \text{ then } F \equiv AV\left(\hat{\mathbf{d}}_f\cdot\mathbf{n}_f\right) < 0 : \textit{Inflow}\\
&\text{if } V < 0, \text{ and } \hat{\mathbf{d}}_f\cdot\mathbf{n}_f < 0, \text{ then } F \equiv AV\left(\hat{\mathbf{d}}_f\cdot\mathbf{n}_f\right) \geq 0 : \textit{Outflow}
\end{aligned} \quad (13)$$

Connection vector $\mathbf{d}_{PR}$ or $\mathbf{d}_{f,PR}$ is required in order to indicate the information of connection from the centroid of the cell *P* of interest to the centroid of the cell *R* or remote neighbour, which has the attribute of

$$\mathbf{d}_{PR}\cdot\hat{\mathbf{d}}_f > 0 \quad (14)$$

IMPLEMENTATION OF FINITE VOLUME METHOD

Primitive unknown variables in this implementation are summarised in Table 1. For gas mass fraction the noncondensable gas mixture is solved firstly, and then the mass fractions of individual gas are solved in order.

Table 1 Primitive unknown variables

	Variables	No. of Variables
Field Volume Fraction	α_g, α_l	2
Pressure	p	1
Velocity	$u_g, v_g, w_g,$ $u_l, v_l, w_l,$ u_d, v_d, w_d	9
Specific Internal Energy	U_g, U_l, U_d	3
Gas Mass Fraction	Y_{air}, Y_{H_2}	2
Total	-	17

Porosity method was introduced in order to make a larger cell for stable calculation[9]. Some noticeable integration results are presented here.

Through the FVM (Finite Volume Method) the convective term in continuity equation of field ϕ is developed to be

$$\frac{1}{\delta t}\int_{t^{(n)}}^{t^{(n+1)}}\int_{CV} H(\mathbf{x})\nabla\cdot\left(\alpha_\phi\rho_\phi\mathbf{v}_\phi\right)dvdt = \sum_S\left(\tilde{\alpha}_\phi^{(n)}\tilde{\rho}_\phi^{(n)}F_\phi^{(n+1)}\right)_S \quad (15)$$

, where

$$F_{\phi,S}^{(n+1)} \equiv \gamma_{A,S}A_S\mathbf{v}_{\phi,S}^{(n+1)}\cdot\mathbf{n}_S = \gamma_{A,S}A_S V_{\phi,S}^{(n+1)}\left(\mathbf{n}_S\cdot\mathbf{d}_S\right) \quad (16)$$

Upwind scheme was used in the above formulation and the symbol ~ means the upstream property.

Then, convective term in momentum equation becomes through the integration over the momentum cell in Figure 3.

$$\frac{1}{\delta t}\int_{t^{(n)}}^{t^{(n+1)}}\int_{CV} H(\mathbf{x})\alpha_\phi\rho_\phi\mathbf{v}_\phi\cdot\nabla\otimes\mathbf{v}_\phi\,dvdt = \sum_S\left\{\left(\tilde{\alpha}_\phi^{(n)}\tilde{\rho}_\phi^{(n)}V_\phi^{(n)}\right)_S F_{\phi,S}^{(n)}\mathbf{d}_S\right\} - V_{\phi,f}^{(n)}\mathbf{d}_f\sum_S\left(\tilde{\alpha}_\phi^{(n)}\tilde{\rho}_\phi^{(n)}\right)_S F_{\phi,S}^{(n)} \quad (17)$$

Pressure term in momentum equation is differenced to be

$$\frac{1}{\delta t}\int_{CV}\int_{t^{(n)}}^{t^{(n+1)}} -H(\mathbf{x})\alpha_\phi\nabla p\,dtdv = -\gamma_{v,f}V_f\hat{\alpha}_{\phi,f}^{(n)}\nabla p_f \quad (18)$$

, where ∇p_f is not still known, but multiplying $\mathbf{d}_{f,LR}$ make the calculation easy

$$-\gamma_{v,f}V_f\hat{\alpha}_{\phi,f}^{(n)}\nabla p_f\cdot\mathbf{d}_{f,LR} = -\gamma_{v,f}V_f\hat{\alpha}_{\phi,f}^{(n)}\left(p_R - p_L\right) \quad (19)$$

Viscosity term in momentum equation

$$\frac{1}{\delta t}\int_{CV}\int_{t^{(n)}}^{t^{(n+1)}} H(\mathbf{x})\nabla\cdot\left[\alpha_\phi\left(\mu_\phi+\mu_\phi^t\right)\nabla\otimes\mathbf{v}_\phi\right]dtdv = \sum_S\left[\alpha_{\phi,S}^{(n)}\left(\mu_{\phi,S}^{(n)}+\mu_{\phi,S}^{t,(n)}\right)\cdot\left\{\left(\mathbf{n}_S\cdot\mathbf{d}_S\right)\left(\sum_{S'}\left(\frac{A_{S'}V_\phi^{(n)}\mathbf{d}_{S'}}{V_{S'}}\right)\right)\right\}\left(\gamma_{A,S}A_S\right)\right] \quad (20)$$

For the final arrangement of momentum equations the face directional vector, $\mathbf{d}_{f,LR}$, should be multiplied.

Conduction term in energy equation can be treated as followings;

$$\frac{1}{\delta t}\int_{CV}\int_{t^{(n)}}^{t^{(n+1)}} H(\mathbf{x})\nabla\cdot\left(\alpha_\phi\left(k_\phi\nabla T_\phi + k_\phi^t\nabla T_\phi\right)\right)dtdv$$

$$= \sum_S\left[\hat{\alpha}_{\phi,S}^{(n)}\left(\hat{k}_\phi+\hat{k}_\phi^t\right)_S^{(n)}\cdot\left\{\frac{\left(T_{\phi,R}^{(n)}-T_{\phi,P}^{(n)}\right)_S A_S}{\mathbf{d}_{S,PR}\cdot\mathbf{n}_S}+\left(\overline{\nabla T_{\phi,S}^{(n)}}\cdot\mathbf{n}_S\right)A_S-\frac{\left(\overline{\nabla T_{\phi,S}^{(n)}}\cdot\mathbf{d}_{S,PR}\right)}{\mathbf{d}_{S,PR}\cdot\mathbf{n}_S}\right\}\cdot\gamma_{A,S}A_S\right] \quad (21)$$

$\left(T_{g,R}^{(n)}-T_{g,P}^{(n)}\right)_S$ means the temperature difference between the cell P and R, which are the neighbouring cells around surface S. $\overline{\nabla T_{g,S}^{(n)}}$ is the distance-weighted-average of the temperature gradient at the cell centre. Distance means the distance from the surface S and each cell centre. The temperature gradient at the cell centre can be obtained by Green-Gauss theorem.

$$\nabla T_{\phi,P}^{(n)} = \frac{1}{V_P}\sum_{S'}T_{\phi,S'}^{(n)}\mathbf{n}_{S'}A_{S'} \quad (22)$$

$T_{\phi,S'}^{(n)}$ is the temperature at surface S', and calculated from averaging the neighbouring cell temperature by weight the distance from the surface S' to the cell centre.

The other terms are easily integrated without difficulties. As shown in the above development the interpolation approach is used usually in diffusion term. So the diffusion terms may include some errors. Reviewing the computational code of two-phase flow the diffusion terms in source terms have been frequently omitted [2,3,5]. So the accuracy of the interpolation for diffusion term is thought to be minor.

TIME ADVANCEMENT

Differencing method for time was based on semi-implicit method. Thus, momentum equations are explicitly treated, and then the pressure field is calculated from continuity equations and energy equations. This method is especially referred to as ICE (Implicit Continuous Eulerian) [10].

Unknowns of the new time step should be linearized based on the old time step variables and the thermodynamic relations. Detailed formulations are described in reference 8.

Difference equations of momentum equations are arranged in the form of

$$\begin{bmatrix} m_{gg} & m_{gl} & m_{gd} \\ m_{lg} & m_{ll} & m_{ld} \\ m_{dg} & m_{dl} & m_{dd} \end{bmatrix}\begin{bmatrix} V_g^{(n+1)} \\ V_l^{(n+1)} \\ V_d^{(n+1)} \end{bmatrix} = \begin{bmatrix} s_g \\ s_l \\ s_d \end{bmatrix} - \begin{bmatrix} V_{\alpha,g} \\ V_{\alpha,l} \\ V_{\alpha,d} \end{bmatrix}\left(p_R^{(n+1)} - p_L^{(n+1)}\right) \quad (23)$$

Replacing the pressure at time step (n+1) by at (n), the velocities become intermediate values, and are expressed using

superscript * instead of (n+1). Then above equation changes to be the form of

$$\begin{bmatrix} V_g^* \\ V_l^* \\ V_d^* \end{bmatrix} = \begin{bmatrix} H_g \\ H_l \\ H_d \end{bmatrix} - \begin{bmatrix} A_{\alpha,g} \\ A_{\alpha,l} \\ A_{\alpha,d} \end{bmatrix} \left(p_R^{(n)} - p_L^{(n)} \right) \quad (24)$$

And the velocity correction can be define as like;

$$\begin{bmatrix} V_g' \\ V_l' \\ V_d' \end{bmatrix} \equiv \begin{bmatrix} V_g^{(n+1)} \\ V_l^{(n+1)} \\ V_d^{(n+1)} \end{bmatrix} - \begin{bmatrix} V_g^* \\ V_l^* \\ V_d^* \end{bmatrix} = - \begin{bmatrix} A_{\alpha,g} \\ A_{\alpha,l} \\ A_{\alpha,d} \end{bmatrix} \left(\delta p_R - \delta p_L \right) \quad (25)$$

Using this equation the flow quantity in equation (16) can be expressed in terms of old time step values.

$$F_{\phi,f}^{(n+1)} = F_{\phi,f}^* - \gamma_{A,f} A_f A_{\alpha,\phi} \left(\delta p_R - \delta p_L \right) \left(\mathbf{n}_f \cdot \hat{\mathbf{d}}_f \right) \quad (26)$$

This equation means that the flow in new time step is expressed in terms of intermediate flow and pressure difference driven flow.

All the scalar equations are arranged to be

$$\begin{bmatrix} a_{11} & \cdots & a_{17} \\ & & \\ \vdots & \ddots & \vdots \\ & & \\ a_{71} & \cdots & a_{77} \end{bmatrix} \begin{bmatrix} \delta Y_n \\ \delta U_g \\ \delta U_l \\ \delta U_d \\ \delta \alpha_g \\ \delta \alpha_l \\ \delta p \end{bmatrix} = \begin{bmatrix} \hat{b}_1 \\ \hat{b}_2 \\ \hat{b}_3 \\ \hat{b}_4 \\ \hat{b}_5 \\ \hat{b}_6 \\ \hat{b}_7 \end{bmatrix} + \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{bmatrix} \quad (27)$$

Further simpler form is

$$\mathbf{A}\mathbf{x} = \hat{\mathbf{b}} + \mathbf{f}^* + \mathbf{p}' \quad (28)$$

$$\mathbf{x} = \begin{bmatrix} \delta Y_n & \delta U_g & \delta U_l & \delta U_d & \delta \alpha_g & \delta \alpha_l & \delta p \end{bmatrix}^T \quad (29)$$

$$\hat{\mathbf{b}} = \begin{bmatrix} \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \hat{b}_4 & \hat{b}_5 & \hat{b}_6 & \hat{b}_7 \end{bmatrix}^T \quad (30)$$

$$\mathbf{f}^* + \mathbf{p}' = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{bmatrix} = \begin{bmatrix} f_1^* \\ f_2^* \\ f_3^* \\ f_4^* \\ f_5^* \\ f_6^* \\ f_7^* \end{bmatrix} + \begin{bmatrix} c_{1,P}\delta p_P + \sum_S c_{1,S}\delta p_R \\ c_{2,P}\delta p_P + \sum_S c_{2,S}\delta p_R \\ c_{3,P}\delta p_P + \sum_S c_{3,S}\delta p_R \\ c_{4,P}\delta p_P + \sum_S c_{4,S}\delta p_R \\ c_{5,P}\delta p_P + \sum_S c_{5,S}\delta p_R \\ c_{6,P}\delta p_P + \sum_S c_{6,S}\delta p_R \\ c_{7,P}\delta p_P + \sum_S c_{7,S}\delta p_R \end{bmatrix} \quad (31)$$

Introducing $\mathbf{b} \equiv \hat{\mathbf{b}} + \mathbf{f}^*$ the equation (28) becomes

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b} + \mathbf{A}^{-1}\mathbf{p}' = \mathbf{A}^{-1}\mathbf{b} + \left[\mathbf{A}^{-1}\mathbf{p}'_P \delta p_P + \mathbf{A}^{-1} \sum_S \mathbf{p}'_S \delta p_R \right] \quad (32)$$

Simpler form of this equation is

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b} + \left[\left(\mathbf{c}_P \delta p_P \right) + \sum_S \left(\mathbf{c}_S \delta p_R \right) \right] \quad (33)$$

The last row of the matrix in equation (33) is for the pressure correction. That is,

$$\delta p_P = \left[\mathbf{A}^{-1}\mathbf{b} \right]_7 + \left[\left[\left(\mathbf{c}_P \right)_7 \delta p_P \right] + \sum_S \left[\left(\mathbf{c}_S \right)_7 \delta p_R \right] \right] \quad (34)$$

This is reduced to

$$\left[\left\{ 1 - \left(\mathbf{c}_P \right)_7 \right\} \delta p_P \right] - \sum_S \left[\left(\mathbf{c}_S \right)_7 \delta p_R \right] = \left[\mathbf{A}^{-1}\mathbf{b} \right]_7 \quad (35)$$

Applying above equation for all cell, a system pressure equation is obtained

$$\mathbf{A}'\mathbf{p} = \mathbf{r} \quad (36)$$

$$\mathbf{A}' = \begin{bmatrix} \left(1-(\mathbf{c}_P)_7\right)_1 & \cdots & \cdots & A_{1,i} & \cdots & \cdots & A_{1,N} \\ \vdots & \ddots & & \vdots & & & \vdots \\ \vdots & & \ddots & A_{i-1,i} & & & \vdots \\ A_{i,1} & \cdots & A_{i,i-1} & \left(1-(\mathbf{c}_P)_7\right)_i & A_{i,i+1} & \cdots & A_{i,N} \\ \vdots & & & A_{i+1,i} & \ddots & & \vdots \\ \vdots & & & \vdots & & \ddots & \vdots \\ A_{N,1} & \cdots & \cdots & A_{N,i} & \cdots & \cdots & \left(1-(\mathbf{c}_P)_7\right)_N \end{bmatrix} \quad (37)$$

$$\mathbf{p} = \begin{bmatrix} \delta p_1 & \cdots & \cdots & \delta p_i & \cdots & \cdots & \delta p_N \end{bmatrix}^T \quad (38)$$

$$\mathbf{r} = \begin{bmatrix} \left(\left[\mathbf{A}^{-1}\mathbf{b}\right]_7\right)_1 & \cdots & \cdots & \left(\left[\mathbf{A}^{-1}\mathbf{b}\right]_7\right)_i & \cdots & \cdots & \left(\left[\mathbf{A}^{-1}\mathbf{b}\right]_7\right)_N \end{bmatrix}^T \quad (39)$$

Once the pressure field is obtained the new velocity field is obtained from the velocity correction of equation (25), Known pressure field and velocity field enables to get the other scalar variables easily by solving the equation (27).

Such a numerical analysis results were coded using C++ language and several tests were conducted.

NUMERICAL TESTS

The preliminary calculation was conducted with simple geometry and physical conditions. Figure 4 shows the computational domain used in preliminary calculation.

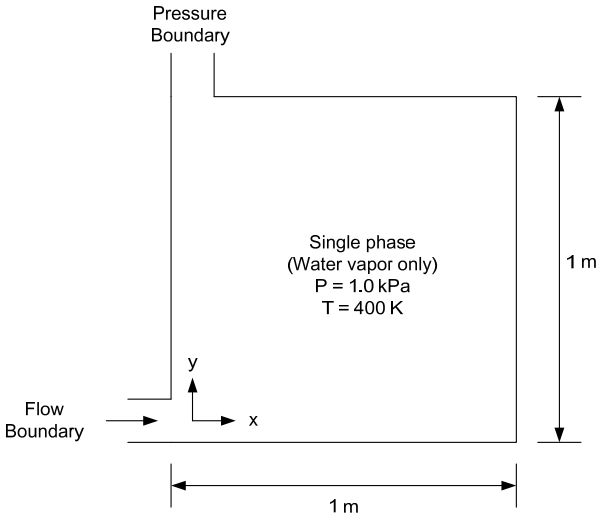


Figure 4 Computational domain

The flow boundary condition with the constant normal velocity of $V_{x,g} = 1.0\,m/s$ is attached on the left-bottom corner and the pressure boundary condition with $P = 1.0e5\,kPa$ on the left-upper. The whole domain is initially filled with the single phase water vapour at $P = 1.0e5\,kPa$ and $T_g = 400\,K$ condition and supplied with same phase through the flow boundary. The 10X10 structured computational meshes were generated. The numerical scheme derived in this study is surely applicable to the unstructured grid though, and the simple structured grid cell was adopted in this preliminary stage for the intuitive inspection approach.

Typical flow pattern of calculation result in the form of vector is shown in Figure 5. The numerical technique applied newly should be carefully examined in various aspect and conditions, i.e. term by term effects, mesh size sensitivities, numerical stabilities etc. Currently, applicability of the numerical technique derived in this study, however, was studied. The further studies on error analysis and comparative analysis with commercial CFD tools are planned. And essential numerical test for unstructured mesh is also to be carried out.

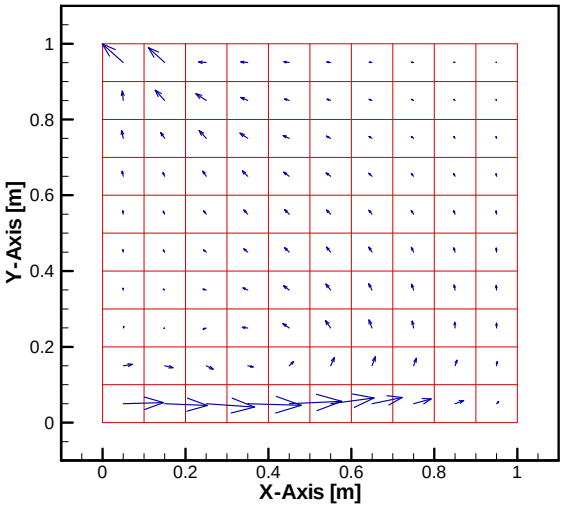


Figure 5 Calculation result (velocity field)

CONCLUSION

This study shows the successful development of numerical analysis method based on staggered grid for arbitrary 3-dimensional mesh shape for two-phase three-field model. The benefit of this method is to minimize the interpolation. The interpolation appears only in diffusion terms. However the diffusion terms in two-phase flow has been considered less important.

The algorithm developed in this study will be used in 3-dimensional module in CAP code, and further verification and validation will be performed.

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