

Is it possible to design universal multi-phase flow analyzer?

Keynote Lecture

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1. Introduction

Transient 3D-multiphase flows consisting of many chemical constituents in nature and technology (Figs. 1 and 2) are the common case of flows. In many technical applications we have to do with particular realization of the multi-phase flows like steady state flows, or single component flows or single phase flows etc.

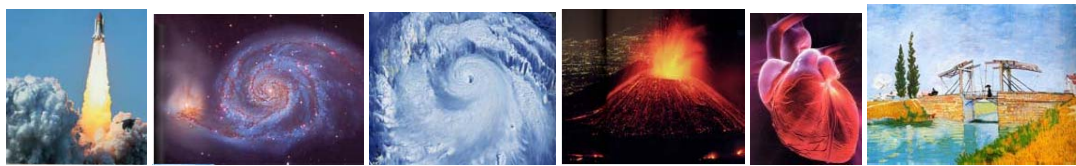


Fig. 1. The fascinating picture of the discovery start, the peace of universe, the tornado, the volcano, the flows in the human heart or even the "pure" water or the sky in the picture of Van Gogh are in fact different forms of multiphase flows

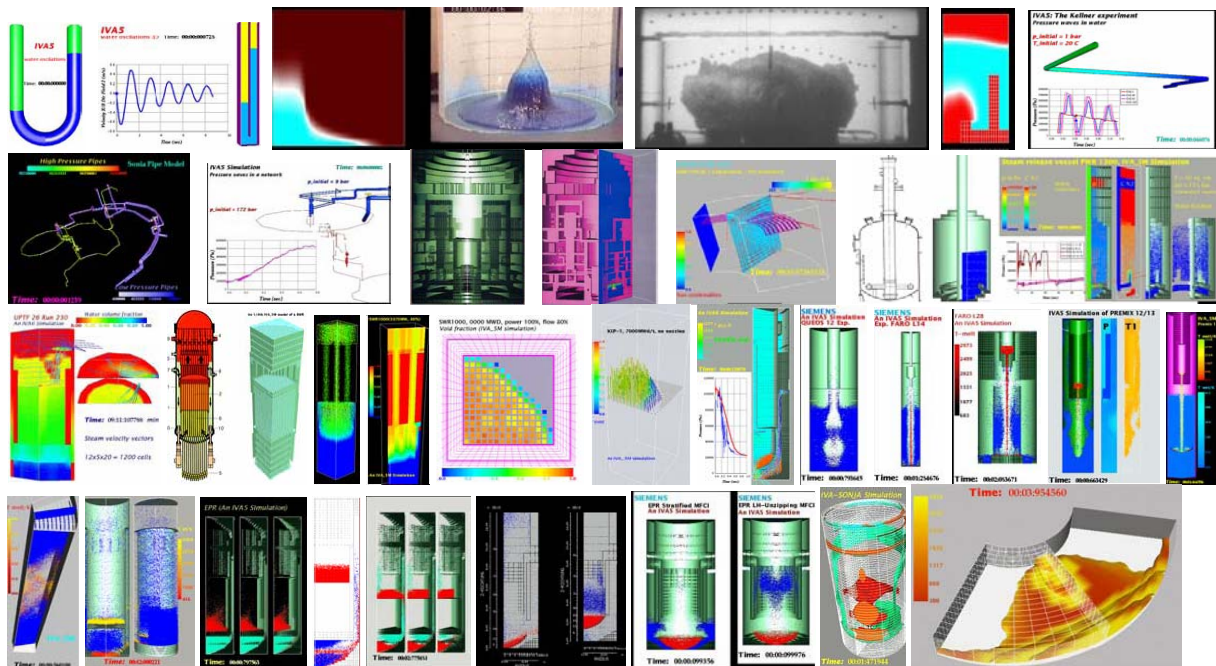


Fig. 2. Examples of multiphase flows in the nuclear technology, see <http://www.herzovision.de/kolev-nikolay/>

Engineers and scientists created hundreds of computer codes for description of more or less specific realizations of multi-phase flows. If one compares the structure of these codes one is astonished by the waste of the human resources for programming repeating model elements like equations of state, friction laws in variety of geometry, heat transfer coefficients, mathematical equation solvers, data handling procedures, graphical environment etc. It is hardly to expect, that the best solution for the specific sub-phenomenon is available in all codes. Looking in other branches of the technology like computer chips production we realize that the revolutionary idea of having common “chips” within complex applications is very far from its practical realization in the computational multi-phase flow dynamics. Following this line of arguments I expressed several times in my publications explicitly or implicitly the idea, that it is possible to create a universal multi-phase flow analyzer in the sense of computer architecture, that is capable to absorb the adequate multi-phase knowledge data base specified in Appendix 1. The subject of this paper is to summarize some of the main ideas, some of them already realized by this author, on the way of creating such computer code architecture, to illustrate how they work, and to make an outlook regarding what are the challenges in the future developments.

We confine deliberately our attention to the solution of the so called local volume and time averaged system of PDE's for a simple reason: Direct numerical resolution of interacting fluids is possible as demonstrated for small scales by many researchers, but for real large scale engineering problems it is still very expensive. I believe that this will remain so for decades.

1. The idea of multiple velocity fields

Field is defined as a part of the flow having its own well defined spatially and temporally evolving boundary to its environment: another field or a wall. Zimanski uses the same definition for phase [7] but we understand phase as a synonym for state of aggregate. A field possesses many attributes. One flow attribute is for instance the velocity. Thermodynamic attributes are the density specific enthalpy, entropy, etc. Transport attributes are e.g. viscosities, conductivities etc. Constituents attributes are for instance the number of the chemical components inside the field, their mass concentration etc. The field is in itself a heterogeneous structure e.g. internal circulation of a drop, boundary layers for thermal and mechanical interactions etc. The field can be represented with its internal averaged properties and boundary layer properties. A complex flow model may then be constructed as consisting of a many fields inside the mixture.

The mixture is characterized by the number of the fields and their volumetric concentrations inside the field. The scale at which the mixture is modeled may be large enough to contain several processes that happen in subscales. This is valid for the time scale as well for the spatial resolution scale. Therefore local volume averaging is necessary to obtain the conservation laws valid on the macro-scale. During the averaging a record is kept for the subscale especially how formally the processes are incorporated in the large scale method. Mathematical consistency is crucial for creating functioning general architecture.

2. Do we have adequate mathematical reflection of the conservation laws based on averaging?

The answer is yes. The system of the partial differential equations reflecting the instantaneous and local conservation of mass, momentum and energy exists since the 19th century. The 20th century generated many ideas about averaging this equation over large scale volume e.g. assembly averaging, statistical averaging etc. Among the mathematical tools for averaging the spatial averaging theorem by Slattery and Whitaker [1-6] together with the Leibnitz rule allows to apply averaging of the instant conservation-equations over a volume. Considering as one special field the structure defining the channel, results in the so called porous body concept [8]. In [9] the fields are considered as consisting of many chemical components allowing molecular diffusion inside them if they are continuous. The next step is the time averaged called also Reynolds averaging of the resulting systems. The resulting system is then what we need to integrate in space and time to describe in averaged the behavior of the field. During the averaging processes a large number of terms originate [9] having particular meaning reflecting the Appendix 1. The elaboration of these terms is a long living task in the science. A useful representation of the state of the art in this field is given in [10].

3. Coexisting fields

Now, we can define the number of the abstract fields which we would like to fill with physical meaning. The maximum number of the fields have to be specified and then the place holders for the interaction terms. The

general approach requires clear physical and mathematical understanding of the structure of these terms. Usually they are strongly non-linear.

4. Geometry definition

We follow the following strategy: We consider the technical systems as a combination of pipe-networks with valves, pumps and other components that may be connected with 3D volumes. That is why our geometry definition contains three elements: (1) pipe network; (2) multiple blocks in boundary fitted coordinates interconnected to each other. In many daily applications (3) a single 3D-block in Cartesian or cylindrical geometry is sufficient and very useful for development purposes. The set of conservation equations required is given in Appendix 2 through 4. The reader will find details of the derivation in [9].

5. Solvers

The system of partial differential equations is usually transferred in a discrete form with a priori specified accuracy of discretization. Designing working solvers for the resulting non-homogeneous algebraic system with variable coefficients is art. The challenge is to design as strong as possible coupling within the different processes within a single step. Some examples that for sure will be improved in the future are given in [9].

6. Summary of the ideas

I deliberately do not go in details in this presentation in order to make the main structure of the analyzer clear:

- (1) The flow is presented as coexisting fields inside the control volume;
- (2) Each field possesses variety of attributes originating from the interaction with the environment and from the mathematical procedure of the averaging;
- (3) The coexisting fields are described by a system of well founded partial differential equations that are local volume- and time-averaged;
- (4) The geometry is a combination of pipe-networks, multiple interconnected volumes that are boundary fitted;
- (6) The solution of discretized form is based on strong coupling of the interactions between the fields.

7. Is there any chance to overcome the complexity and design algorithms that are of practical use?

Yes. We will give here one example based on three multi-component velocity fields in porous structure that may change its geometry in time. The foundations of the computer code IVA [9, 10] allows applications of this multi-phase flow analyzer for mathematical simulation of variety of processes. From two-phase gas-plasma multi-component hydrogen detonation in pipe-network with dissociation of the gases, Fig. 3, through condensation water-steam shock waves in complex pipe networks, Fig. 4, gas solution and dissolution in liquids, dissolved gas release from water in pipe network and gas-slug formation and transport, Fig. 5, diesel injection problems, Fig. 6, particles sedimentation in water, Fig. 7, turbulent mixing and transport in a NPP sump, Fig. 8, termite injection by high pressure steam-hydrogen mixture into air environment, melt-water interaction in postulated SWR 1000 severe accidents, alumina melt jet dropped into a subcooled water, urania melt jet dropped in water, Fig. 9, void formation in existing-, Fig. 10, or future boiling water reactors, Fig. 11, all this demonstrates the capability of single model architecture to handle different material systems, different intensities of interactions, large variety of the spatial and temporal scales of the simulated processes.

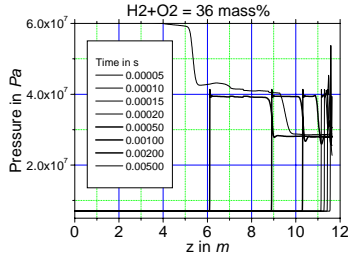


Fig. 3. Pressure as a function of the distance for different times after the ignition [11] p. 432

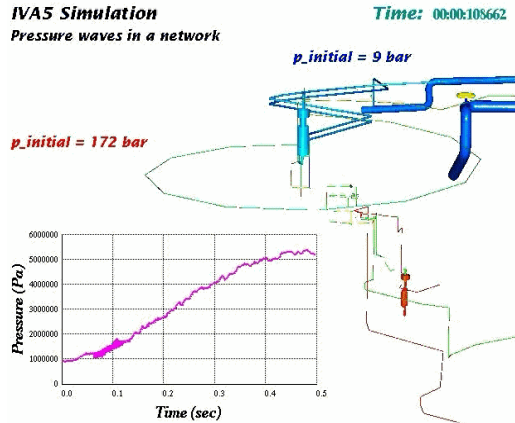


Fig. 4. Tube ruptures into a main recirculation pump seal water heat exchanger

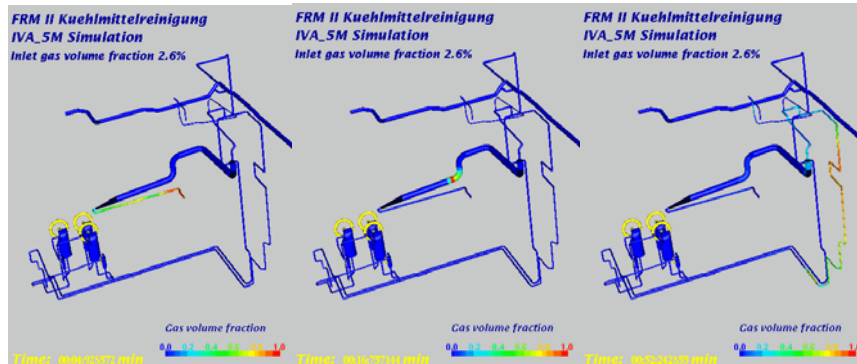


Fig. 5. Gas release from water in pipe network – gas slug formation and transport

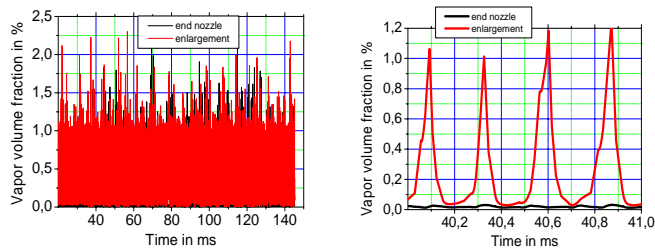


Fig. 6. Diesel vapor volume fraction at the end of 300µm diesel injection nozzle and at the enlargement immediately after the nozzle. The collapses damage the surface

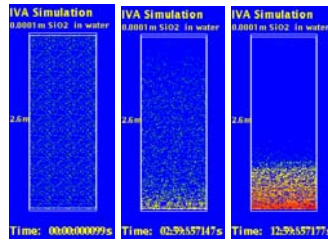


Fig. 7. Sedimentation of 100µm-sand particles (SiO_2). a) Initial state of 10% volume fraction of initially homogeneously distributed in 2.6m deep water pool; b) after 3min; c) 13min

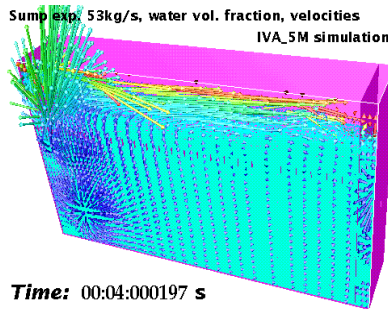


Fig. 8. Free fall of two phase jet into the left end of a water reservoir causing sloshing and mixing. Vortex burst and reflection at the wall

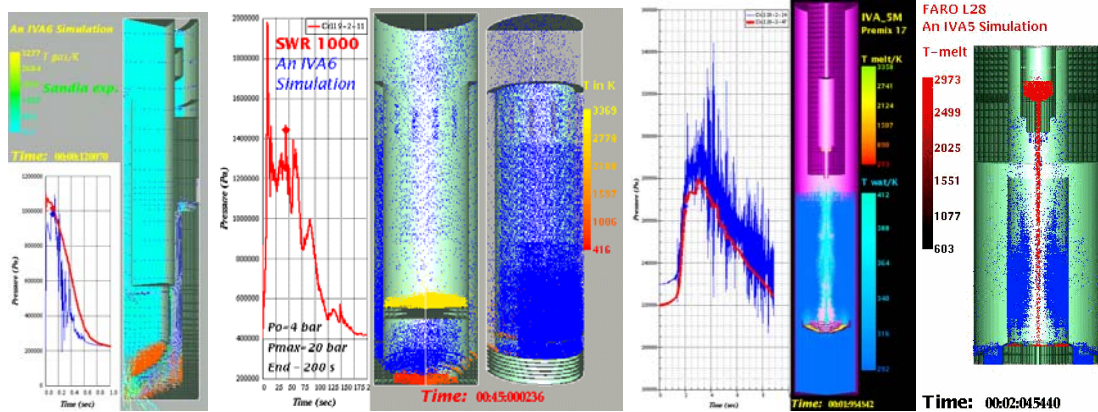


Fig. 9. a) Termitic injection by high pressure steam-hydrogen mixture into air environment; b) Melt-water interaction in postulated SWR 1000 severe accidents; c) Alumina melt jet dropped into a subcooled water; d) Urania melt jet dropped in water

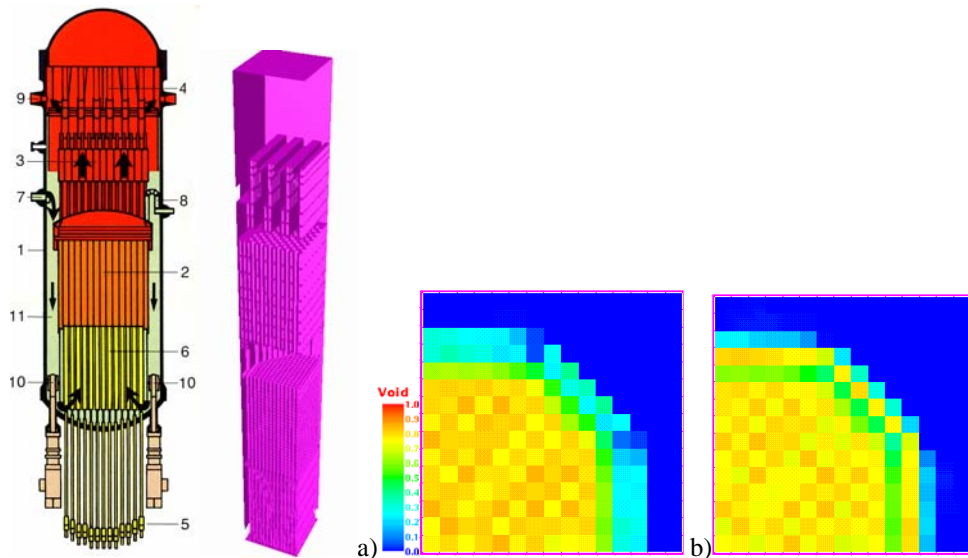


Fig. 10. Void at the exit of a core of BWR for the case (a) without additional nozzles and (b) with nozzles

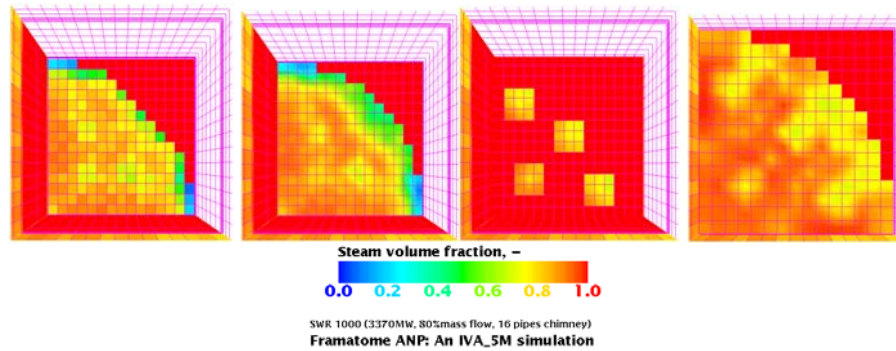


Fig. 11. Void fraction at different elevation inside a SWR 1000, case studies for different geometry

In any case, if stepping to new application, verification with set of particular data is mandatory, for elaboration of the achievable prediction accuracy, experience for the integration of the conservation equations under the particular initial and boundary conditions etc.

We deliberately do not talk about validation and verification procedures here. The reader will find large number of comparison of the prediction of IVA computer code with experimental data in the CD attached to [9].

Conclusions

- 1) Computational analysis of multi-phase flows in the practice requires special computer code architecture that is not trivially derivable from the single phase fluid mechanics and thermodynamics;
- 2) Universal code architecture follows rigorously the analytical procedure of gaining the local volume- and time- averaged conservation equations reflecting elements like fields, their attributes, their interfacial exchange terms etc.
- 3) The coupling between the non-linear equations with variable coefficients in the system is designed as close as possible within a single analytical step.
- 4) Such approach allows the best single model of a particular process or mathematical manipulation procedure to be multiply used by all different applications.
- 5) Such approach unifies the efforts of teams in using components with prescribed interfaces derived from the basic derivation of the conservation equations. So with the time the data base behind the analyzer will grow and be exchangeable;
- 6) Graphical visualization of the processes is crucial not only for the development but later also for understanding better the processes simulated.

Appendix 1 Knowledge data base required to design a universal multi-phase flow analyzer

1. Technical thermodynamics; simple and multi-component systems, equations of state;
2. Behavior meta-stable liquids;
3. Heat and mass transfer in single- and complex multi-phase systems;
4. Fluid mechanics;
5. Review of the world literature in particular fields of multi-phase flows and processes associated with them;
6. Multiphase flows; transient; one-, two and three-dimensional; in simple geometry; in complicated geometry;
7. Interaction of multiphase flows with technical structures; evaporation; condensation; spontaneous evaporation; spontaneous condensation; cavitation; flow instabilities; flow induced vibrations; starting of steam generators; computation of forces caused by fluid transients;
8. Design of components, apparatus and facilities based on mathematical modeling of complex thermal processes including complicated multi-phase flows;
9. Pressure and concentration waves in pipes, complex pipe systems, complex three dimensional equipment;
10. Analysis of explosive fluid-fluid interactions, melt-water interactions; steam explosion in nuclear facilities, in metallurgical facilities, in manufacturing, in space technology, in combustion motors; hydrogen deflagration and detonation, powder combustion and powder detonation; detonation of meta-stable fluids;
11. Numerical methods for analysis of complex flow processes;

12. Design of complex computer codes for simulation of the system behavior of coupled components in single-, two-, and multi-phase flow region;
13. Computing: numerical methods for integration of systems of ordinary and partial differential equations;
14. Uncertainty analysis of computational methods;
15. Nuclear technology: developing and applying of mathematical methods for description and simulation of the physics of thermo-hydraulic processes in the reactor, primary-, secondary, and tertiary circuit, in the containment in normal operation, in transients and by severe accidents with catastrophic consequences;
16. Quality assurance of complicated thermo-hydraulic computations;
17. Quality assurance of developments of code systems for modeling of complex thermodynamic processes;
18. Education of specialists in all of the above fields, courses, consultations

Appendix 2: Summary of the local volume- and time-averaged conservation equations for 1D-networks

Mass conservation equation for each field:

$$\frac{\partial}{\partial \tau} (\alpha_l \rho_l \gamma_v) + \frac{\partial}{\partial z} (\alpha_l \rho_l w_l \gamma_z) = \gamma_v \sum_{m=1}^{l_{\max}, w} (\mu_{ml} - \mu_{lm}). \quad (A1.1)$$

Mass conservation equation for each species inside the velocity field:

$$\frac{\partial}{\partial \tau} (\alpha_l \rho_l C_{il} \gamma_v) + \frac{\partial}{\partial z} \left[\alpha_l \rho_l \left(w_l C_{il} - D_{il}^* \frac{\partial C_{il}}{\partial z} \right) \gamma_z \right] = \gamma_v \sum_{m=1}^{l_{\max}, w} (\mu_{iml} - \mu_{ilm}) \quad (A1.2)$$

for $\alpha_l \geq 0$, $i = 1, i_{\max}$, or alternatively

$$\alpha_l \rho_l \left(\gamma_v \frac{\partial C_{il}}{\partial \tau} + w_l \gamma_z \frac{\partial C_{il}}{\partial z} \right) - \frac{\partial}{\partial z} \left[\alpha_l \rho_l \left(D_{il}^* \frac{\partial C_{il}}{\partial z} \right) \gamma_z \right] = \gamma_v (\mu_{il} - C_{il} \mu_l). \quad (A1.3)$$

Particle number density equation for each field:

$$\frac{\partial}{\partial \tau} (n_l \gamma_v) + \frac{\partial}{\partial z} \left[\left(w_l n_l - \frac{v_l'}{Sc_l'} \frac{\partial n_l}{\partial z} \right) \gamma_z \right] = \gamma_v (\dot{n}_{l,kin} - \dot{n}_{l,coal} + \dot{n}_{l,sp}) \quad \text{for } \alpha_l \geq 0. \quad (A1.4)$$

Momentum equation for each field:

$$\begin{aligned} & \alpha_l \rho_l \gamma_v \frac{\partial w_l}{\partial \tau} + \alpha_l^e \rho_l \gamma_z \frac{1}{2} \frac{\partial w_l^2}{\partial z} - \frac{\partial}{\partial z} \left(\alpha_l^e \rho_l \nu_l^* \gamma_z \frac{\partial w_l}{\partial z} \right) + \alpha_l^e \gamma_z \frac{\partial p_l}{\partial z} - \Delta p_m^{w\sigma^*} \frac{\partial \gamma_z}{\partial z} + f_{l\alpha} + \gamma_v \alpha_l \rho_l g \cos \varphi \\ & - \gamma_v \left\{ \sum_{\substack{m=1 \\ m \neq l}}^3 \left[\bar{c}_{ml}^{vm} \left(\frac{\partial \Delta w_{ml}}{\partial \tau} + w_l \frac{\partial \Delta w_{ml}}{\partial z} \right) \right] - \rho_l \bar{c}_{lw}^{vm} \frac{\partial w_l}{\partial \tau} \right\} \\ & = \gamma_v \left\{ \sum_{\substack{m=1 \\ m \neq l}}^3 \left[\bar{c}_{ml}^d |\Delta w_{ml}| \cdot \Delta w_{ml} + \mu_{ml} (w_m - w_l) \right] + \bar{c}_{lw}^d |w_l| w_l \right\} \\ & \quad \left. + \mu_{wl} (w_{wl} - w_l) - \mu_{lw} (w_{lw} - w_l) \right\}. \end{aligned} \quad (A1.5)$$

Here φ is the polar angle between the flow direction and the upwards directed vertical.

The entropy equation:

$$\begin{aligned}
& \rho_l \left(\alpha_l \gamma_v \frac{\partial s_l}{\partial \tau} + \alpha_l^e w_l \gamma_z \frac{\partial s_l}{\partial z} \right) - \frac{1}{T_l} \frac{\partial}{\partial z} \left[\left(\alpha_l^e \lambda_l^* \frac{\partial T_l}{\partial z} \right) \gamma_z \right] \\
& - \frac{\partial}{\partial z} \left\{ \alpha_l^e \rho_l \left[\sum_{i=2}^{i_{\max}} (s_{il} - s_{il}) D_{il}^* \frac{\partial C_{il}}{\partial z} \right] \gamma_z \right\} \\
& = \gamma_v \left[\frac{1}{T_l} D T_l^N + \sum_{i=1}^{i_{\max}} \mu_{il} (s_{il} - s_i) \right] \text{ for } \alpha_l \geq 0,
\end{aligned} \tag{A1.6}$$

Alternatively, the temperature equation is used instead of the entropy equation for the gas field:

$$\begin{aligned}
& \rho_l c_{pl} \left(\alpha_l \gamma_v \frac{\partial T_l}{\partial \tau} + \alpha_l^e w_l \gamma_z \frac{\partial T_l}{\partial z} \right) - \left[1 - \rho_l \left(\frac{\partial h_l}{\partial p} \right)_{T_l, \text{all } C's} \right] \left(\alpha_l \gamma_v \frac{\partial p}{\partial \tau} + \alpha_l^e w_l \gamma_z \frac{\partial p}{\partial z} \right) \\
& - \frac{\partial}{\partial z} \left[\left(\alpha_l^e \lambda_l^* \frac{\partial T_l}{\partial z} \right) \gamma_z \right] + T_l \sum_{i=2}^{i_{\max}} \Delta s_{il}^{np} \frac{\partial}{\partial z} \left[\left(\alpha_l^e \rho_l D_{il}^* \frac{\partial C_{il}}{\partial z} \right) \gamma_z \right] \\
& = \gamma_v \left[D T_l^N - T_l \sum_{i=2}^{i_{\max}} \Delta s_{il}^{np} (\mu_{il} - C_{il} \mu_l) \right].
\end{aligned} \tag{A1.7}$$

The volume conservation equation is used instead of the one field mass conservation equation:

$$\frac{\gamma_v}{\rho a^2} \frac{\partial p}{\partial \tau} + \gamma_z \left(\sum_{l=1}^{l_{\max}} \frac{\alpha_l w_l}{\rho_l a_l^2} \right) \frac{\partial p}{\partial z} + \frac{\partial}{\partial z} \left(\sum_{l=1}^{l_{\max}} \alpha_l w_l \gamma_z \right) = \sum_{l=1}^{l_{\max}} D \alpha_l - \frac{\partial \gamma_v}{\partial \tau}, \tag{A1.8}$$

where

$$D \alpha_l = \frac{1}{\rho_l} \left\{ \gamma_v \mu_l - \frac{1}{\rho_l} \left[\frac{\partial \rho_l}{\partial s_l} \overline{D s_l^N} + \sum_{i=2}^{i_{\max}} \frac{\partial \rho_l}{\partial C_{il}} \overline{D C_{il}^N} \right] \right\} \tag{A1.9}$$

and

$$\overline{D C_{il}^N} = \frac{\partial}{\partial z} \left[\alpha_l^e \rho_l \left(D_{il}^* \frac{\partial C_{il}}{\partial z} \right) \gamma_z \right] + \gamma_v (\mu_{il} - C_{il} \mu_l), \tag{A1.10}$$

$$\begin{aligned}
\overline{D s_l^N} &= \frac{1}{T_l} \frac{\partial}{\partial z} \left[\left(\alpha_l^e \lambda_l^* \frac{\partial T_l}{\partial z} \right) \gamma_z \right] + \frac{\partial}{\partial z} \left\{ \alpha_l^e \rho_l \left[\sum_{i=2}^{i_{\max}} (s_{il} - s_{il}) D_{il}^* \frac{\partial C_{il}}{\partial z} \right] \gamma_z \right\} \\
&+ \gamma_v \left[\frac{1}{T_l} D T_l^N + \sum_{i=1}^{i_{\max}} \mu_{il} (s_{il} - s_i) \right].
\end{aligned} \tag{A1.11}$$

Remember that a is the *sonic velocity* in a homogeneous multi-phase mixture defined as

$$\frac{1}{\rho a^2} = \sum_{l=1}^3 \frac{\alpha_l}{\rho_l a_l^2} = \frac{1}{p} \sum_{l=1}^3 \frac{\alpha_l}{\kappa_l} = \frac{1}{\kappa p}, \tag{A1.12}$$

and

$$\rho = \sum_{l=1}^3 \alpha_l \rho_l \tag{A1.13}$$

is the mixture density.

Appendix 3: Summary of the local volume- and time-averaged conservation equations for 3D-single block

Mass conservation equation for each field:

$$\frac{\partial}{\partial \tau} (\alpha_l \rho_l \gamma_v) + \nabla \cdot (\alpha_l \rho_l \mathbf{V}_l \gamma) = \gamma_v \mu_l \quad (\text{A2.1})$$

Mass conservation equation for each species inside the velocity field:

$$\alpha_l \rho_l \left[\gamma_v \frac{\partial C_{il}}{\partial \tau} + (\mathbf{V}_l \gamma \nabla) C_{il} \right] - \nabla \cdot (\alpha_l \rho_l D_{il}^* \gamma \nabla C_{il}) + \gamma_v \mu_l^+ C_{il} = \gamma_v D C_{il} \quad (\text{A2.1})$$

Particle number density equation for each field:

$$\frac{\partial}{\partial \tau} (n_l \gamma_v) + \nabla \cdot (n_l \mathbf{V}_l \gamma) = \gamma_v (\dot{n}_{kin} - \dot{n}_{col} + \dot{n}_{isp}) \quad \text{for } \alpha_l > 0, \quad (\text{A2.3})$$

Momentum equation for each field:

$$\begin{aligned} & \frac{\partial}{\partial \tau} (\alpha_l \rho_l \mathbf{V}_l \gamma_v) + \nabla \cdot [(\alpha_l \rho_l \mathbf{V}_l \mathbf{V}_l + \bar{\tau}_l) \gamma] + \alpha_l \gamma \nabla p + (\alpha_l \rho_l \mathbf{g} + \mathbf{f}_l) \gamma_v \\ & = \gamma_v \left[\mu_{wl} \mathbf{V}_{wl} - \mu_{lw} \mathbf{V}_{lw} + \sum_{m=1}^{l_{\max}} (\mu_{ml} \mathbf{V}_m - \mu_{lm} \mathbf{V}_l) \right], \end{aligned} \quad (\text{A2.4})$$

The entropy equation:

$$\alpha_l \rho_l \left[\gamma_v \frac{\partial s_l}{\partial \tau} + (\mathbf{V}_l \gamma \nabla) s_l \right] - \frac{1}{T_l} \nabla \cdot (\alpha_l^e \lambda_l^* \gamma \nabla T) + \gamma_v \mu_l^+ s_l = \gamma_v D s_l \quad \text{for } l = 2, 3 \quad (\text{A2.6})$$

Alternatively, the temperature equation is used instead of the entropy equation for the gas field:

$$\begin{aligned} & \rho_l c_{pl} \left[\alpha_l \gamma_v \frac{\partial T_l}{\partial \tau} + (\alpha_l^e \mathbf{V}_l \gamma \cdot \nabla) T_l \right] - \nabla \cdot (\alpha_l^e \lambda_l^* \gamma \nabla T) \\ & - \left[1 - \rho_l \left(\frac{\partial h_l}{\partial p} \right)_{T_l, \text{all } C_s} \right] \left[\alpha_l \gamma_v \frac{\partial p}{\partial \tau} + (\alpha_l^e \mathbf{V}_l \gamma \cdot \nabla) p \right] + T_l \sum_{i=2}^{i_{\max}} \Delta s_{il}^{np} \nabla (\alpha_l^e \rho_l D_{il}^* \gamma \nabla C_{il}) \\ & = \gamma_v \left[D T_l^N - T_l \sum_{i=2}^{i_{\max}} \Delta s_{il}^{np} (\mu_{il} - C_{il} \mu_l) \right], \quad \text{for } l = 1, \end{aligned} \quad (\text{A2.7})$$

The volume conservation equation is used instead of the one field mass conservation equation:

$$\frac{\gamma_v}{\rho a^2} \frac{\partial p}{\partial \tau} + \sum_{i=1}^{i_{\max}} \frac{\alpha_i}{\rho_i a_i^2} (\mathbf{V}_i \gamma \cdot \nabla) p + \nabla \cdot \sum_{i=1}^{i_{\max}} (\alpha_i \mathbf{V}_i \gamma) = \sum_{i=1}^{i_{\max}} D \alpha_i - \frac{\partial \gamma_v}{\partial \tau}, \quad (\text{A2.8})$$

where

$$\overline{DC_{il}^N} = \nabla \left(\alpha_l \rho_l D_{il}^* \gamma \nabla C_{il} \right) + \gamma_v \left(\mu_{il} - C_{il} \mu_l \right), \quad (\text{A2.9})$$

$$\begin{aligned} \overline{DS_l^N} &= \frac{1}{T_l} \nabla \cdot \left(\alpha_l^e \lambda_l^* \gamma \nabla T_l \right) + \nabla \cdot \left\{ \alpha_l^e \rho_l \gamma \left[\sum_{i=1}^{i_{\max}} s_{il} D_{il}^* \nabla C_{il} \right] \right\} \\ &+ \gamma_v \left[\frac{1}{T_l} DT_l^N + \sum_{i=1}^{i_{\max}} \mu_{il} (s_{il} - s_l) \right], \end{aligned} \quad (\text{A2.10})$$

For description of the multi-phase turbulence k - ε models for each velocity field are used:

$$\begin{aligned} \alpha_l \rho_l \left(\gamma_v \frac{\partial k_l}{\partial \tau} + \mathbf{V}_l \gamma \cdot \nabla k_l \right) - \nabla \cdot \left[\alpha_l \rho_l v_l^k \gamma \nabla k_l \right] + \mu_l k_l &= P_{k,ul} + \alpha_l \rho_l \left(v_l \overline{P_{kl}} + \gamma_v G_{kl} \right) \\ &+ \alpha_l \rho_l \frac{c_{\eta l}}{\text{Pr}_{kl}^t} \overline{P_{kl}} \frac{k_l^2}{\varepsilon_l} - \alpha_l \rho_l \gamma_v \varepsilon_l, \end{aligned} \quad (\text{A2.11})$$

where

$$v_l^k = v_l + \frac{v_l^t}{\text{Pr}_{kl}^t}, \quad (\text{A2.12})$$

$$P_{k,ul} = \gamma_v \left[\mu_{wl} k_{wl} - \mu_{lw} k_l + \sum_{m=1}^{l_{\max}} \left(\mu_{ml} k_{ml}^* - \mu_{lm} k_l \right) \right], \quad (\text{A2.13})$$

k_{wl} is the kinetic energy of turbulent pulsation introduced with the external mass source μ_{wl} , k_{ml}^* is the kinetic energy of turbulent pulsation introduced with the mass source coming from the neighboring velocity field.

The equation for the *rate of dissipation of the kinetic energy of isotropic turbulent pulsation* is used in analogy with the derivation for single-phase flows *intuitive*, without strong proof in non-conservative form

$$\begin{aligned} \alpha_l \rho_l \left(\gamma_v \frac{\partial \varepsilon_l}{\partial \tau} + \mathbf{V}_l \gamma \cdot \nabla \varepsilon_l \right) - \nabla \cdot \left[\alpha_l \rho_l v_l^\varepsilon \gamma \nabla \varepsilon_l \right] + \mu_l \varepsilon_l &= \alpha_l \rho_l \frac{\varepsilon_l}{\kappa_l} \left(c_{\varepsilon 1} v_l \overline{P_{kl}} + c_{\varepsilon 3} \gamma_v G_{kl} \right) \\ &+ \alpha_l \rho_l \frac{c_{\eta l}}{\text{Pr}_{\varepsilon l}^t} \overline{P_{kl}} k_l - \alpha_l \rho_l \gamma_v c_{\varepsilon 2} \frac{\varepsilon_l^2}{\kappa_l}, \end{aligned} \quad (\text{A2.14})$$

where

$$v_l^\varepsilon = v_l + \frac{v_l^t}{\text{Pr}_{\varepsilon l}^t}, \quad (\text{A2.15})$$

$$S_{\varepsilon l} = c_{\varepsilon 1} P_{kl} + c_{\varepsilon 3} \gamma_v G_{kl}, \quad (\text{A2.16})$$

$$S_{kl} = P_{kl} + \gamma_v G_{kl}, \quad (\text{A2.17})$$

is a source term of turbulent kinetic energy consisting of

- a term proportional to the *direct dissipation of the kinetic energy* in the velocity field (for the derivation of this term)

$$\begin{aligned} \gamma_v \frac{\alpha_l}{\alpha_l^e} \frac{P_{kl}}{v_l} &= 2 \left\{ \gamma_r \left(\frac{\partial u_l}{\partial r} \right)^2 + \gamma_\theta \left[\frac{1}{r^\kappa} \left(\frac{\partial v_l}{\partial \theta} + \kappa u_l \right) \right]^2 + \gamma_z \left(\frac{\partial w_l}{\partial z} \right)^2 \right\} \\ &+ \left[\frac{\partial v_l}{\partial r} + \frac{1}{r^\kappa} \left(\frac{\partial u_l}{\partial \theta} - \kappa v_l \right) \right] \left[\gamma_r \frac{\partial v_l}{\partial r} + \gamma_\theta \frac{1}{r^\kappa} \left(\frac{\partial u_l}{\partial \theta} - \kappa v_l \right) \right] \end{aligned}$$

$$\begin{aligned}
& + \left[\frac{\partial w_l}{\partial r} + \frac{\partial u_l}{\partial z} \right] \left[\gamma_r \frac{\partial w_l}{\partial r} + \gamma_z \frac{\partial u_l}{\partial z} \right] \\
& + \left[\frac{1}{r^\kappa} \frac{\partial w_l}{\partial \theta} + \frac{\partial v_l}{\partial z} \right] \left[\gamma_\theta \frac{1}{r^\kappa} \frac{\partial w_l}{\partial \theta} + \gamma_z \frac{\partial v_l}{\partial z} \right] \\
& - \frac{2}{3} \left[\frac{\partial u_l}{\partial r} + \frac{1}{r^\kappa} \left(\frac{\partial v_l}{\partial \theta} + \kappa u_l \right) + \frac{\partial w_l}{\partial z} \right] \left[\gamma_r \frac{\partial u_l}{\partial r} + \gamma_\theta \frac{1}{r^\kappa} \left(\frac{\partial v_l}{\partial \theta} + \kappa u_l \right) + \gamma_z \frac{\partial w_l}{\partial z} \right]
\end{aligned} \tag{A2.18}$$

- a term taking into account the *change of the density* of the continuous velocity field

$$G_k = \frac{v^\varepsilon}{\rho \sigma_t} \left(g_r \frac{\partial \rho}{\partial r} + g_\theta \frac{1}{r^\kappa} \frac{\partial \rho}{\partial \theta} + g_z \frac{\partial \rho}{\partial z} \right). \tag{A2.20}$$

Appendix 4: Summary of the local volume- and time-averaged conservation equations for 3D-multiple blocks in boundary fitted coordinates

Mass conservation equation for each field:

$$\frac{\partial}{\partial \tau} (\alpha_l \rho_l \gamma_v \sqrt{g}) + \frac{\partial}{\partial \xi^k} (\alpha_l \rho_l \gamma_k \sqrt{g} \bar{V}_l^k) = \gamma_v \sqrt{g} \mu_l. \tag{A3.1}$$

where $\bar{V}_l^k = \mathbf{a}^k \cdot (\mathbf{V}_l - \mathbf{V}_{cs})$ is the contravariant field relative velocity vector components. It is perpendicular to the coordinate surface defined by $\xi^i = const$.

Mass conservation equation for each species inside the velocity field:

$$\alpha_l \rho_l \sqrt{g} \left(\gamma_v \frac{\partial C_{il}}{\partial \tau} + \sum_{k=1}^3 \gamma_k \bar{V}_l^k \frac{\partial C_{il}}{\partial \xi^k} \right) - \sum_{m=1}^3 \frac{\partial}{\partial \xi^m} \left[\alpha_l \rho_l \sqrt{g} \gamma_m D_{il}^* \left(\sum_{k=1}^3 g^{mk} \frac{\partial C_{il}}{\partial \xi^k} \right) \right] = \gamma_v \sqrt{g} (\mu_{il} - \mu_l C_{il}). \tag{A3.2}$$

Particle number density equation for each field:

$$\frac{\partial}{\partial \tau} (n_l \sqrt{g} \gamma_v) + \sum_{m=1}^3 \frac{\partial}{\partial \xi^m} \left\{ \sqrt{g} \gamma_m \left[n_l \bar{V}_l^m - \frac{v_l^i}{S c^i} \left(\sum_{k=1}^3 g^{mk} \frac{\partial n_l}{\partial \xi^k} \right) \right] \right\} = \gamma_v \sqrt{g} (\dot{n}_{l,kin} - \dot{n}_{l,coal} + \dot{n}_{l,sp}). \tag{A3.3}$$

Momentum equation for each field:

The flux notation of the x -component of the momentum equation is

$$\begin{aligned}
& \sqrt{g} \left[\alpha_l \rho_l \gamma_v \frac{\partial u_l}{\partial \tau} + \left(\sum_{k=1}^3 \gamma_k \mathbf{a}^k \frac{\partial u_l}{\partial \xi^k} \right) \cdot \mathbf{G}_l \right] + \sum_{k=1}^3 \frac{\partial}{\partial \xi^k} \left(\gamma_k \sqrt{g} \mathbf{a}^k \cdot \mathbf{F}_l^u \right) + \sqrt{g} \alpha_l \left(\sum_{k=1}^3 a^{k1} \gamma_k \frac{\partial p}{\partial \xi^k} \right) \\
& - \sqrt{g} \gamma_v \left[\sum_{\substack{m=1 \\ m \neq l}}^3 \bar{c}_{ml}^d |\Delta \mathbf{V}_{ml}| \Delta u_{ml} - \bar{c}_{wl}^d |\Delta \mathbf{V}_{wl}| \Delta u_{wl} \right] - \gamma_v \sqrt{g} \sum_{\substack{m=1 \\ m \neq l}}^{l_{max}} \bar{c}_{ml}^L \left[(\mathbf{V}_l - \mathbf{V}_m) \times \left(\sum_{k=1}^3 \mathbf{a}^k \times \frac{\partial \mathbf{V}_m}{\partial \xi^k} \right) \right]_x \\
& - \gamma_v \sqrt{g} \bar{c}_{wl}^L \left[(\mathbf{V}_l - \mathbf{V}_{cs}) \times \left(\sum_{k=1}^3 \mathbf{a}^k \times \frac{\partial \mathbf{V}_{cs}}{\partial \xi^k} \right) \right]_x - \gamma_v \sqrt{g} \sum_{\substack{m=1 \\ m \neq l}}^3 \bar{c}_{ml}^{vm} \left[\frac{\partial \Delta u_{ml}}{\partial \tau} + \sum_{k=1}^3 \mathbf{a}^k \cdot (\mathbf{V}_l - \mathbf{V}_{cs}) \frac{\partial \Delta u_{ml}}{\partial \xi^k} \right]
\end{aligned}$$

$$-\gamma_v \sqrt{g} \bar{c}_{wl}^{vm} \left[\frac{\partial \Delta u_{csl}}{\partial \tau} + \sum_{k=1}^3 \mathbf{a}^k \cdot (\mathbf{V}_l - \mathbf{V}_{cs}) \frac{\partial \Delta u_{csl}}{\partial \xi^k} \right] = \gamma_v \sqrt{g} \left[-\alpha_l \rho_l g_x + \sum_{m=1}^{3,w} [\mu_{ml} (u_m - u_l)] + \mu_{lw} (u_{lw} - u_l) \right], \quad (\text{A3.4})$$

where

$$\mathbf{F}_l^u = \mathbf{F}_l^{uv} + \mathbf{F}_l^{uvb} + \mathbf{F}_l^{uvT}, \quad (\text{A3.5})$$

is the diffusion momentum flux in the x -direction with components

$$\mathbf{F}_l^{uv} = -\alpha_l \rho_l v_l^* \left(\sum_{k=1}^3 \mathbf{a}^k \frac{\partial u_l}{\partial \xi^k} \right), \quad \mathbf{F}_l^{uvb} = \alpha_l^e \rho_l v_l^* \frac{2}{3} (\nabla \cdot \mathbf{V}_l) \mathbf{i}, \quad \mathbf{F}_l^{uvT} = -\alpha_l^e \rho_l v_l^* \frac{\partial \mathbf{V}_l}{\partial x}. \quad (\text{A3.6-8})$$

The flux notation of the y -component of the momentum equation is

$$\begin{aligned} & \sqrt{g} \left[\alpha_l \rho_l \gamma_v \frac{\partial v_l}{\partial \tau} + \left(\sum_{k=1}^3 \gamma_k \mathbf{a}^k \frac{\partial v_l}{\partial \xi^k} \right) \cdot \mathbf{G}_l \right] + \sum_{k=1}^3 \frac{\partial}{\partial \xi^k} \left(\gamma_k \sqrt{g} \mathbf{a}^k \cdot \mathbf{F}_l^v \right) + \sqrt{g} \alpha_l \left(\sum_{k=1}^3 a^{k2} \gamma_k \frac{\partial p}{\partial \xi^k} \right) \\ & - \sqrt{g} \gamma_v \left[\sum_{\substack{m=1 \\ m \neq l}}^3 \bar{c}_{ml}^d |\Delta \mathbf{V}_{ml}| \Delta v_{ml} - \bar{c}_{wl}^d |\Delta \mathbf{V}_{wl}| \Delta v_{wl} \right] - \gamma_v \sqrt{g} \sum_{\substack{m=1 \\ m \neq l}}^{l_{\max}} \bar{c}_{ml}^L \left[(\mathbf{V}_l - \mathbf{V}_m) \times \left(\sum_{k=1}^3 \mathbf{a}^k \times \frac{\partial \mathbf{V}_m}{\partial \xi^k} \right) \right]_y \\ & - \gamma_v \sqrt{g} \bar{c}_{wl}^L \left[(\mathbf{V}_l - \mathbf{V}_{cs}) \times \left(\sum_{k=1}^3 \mathbf{a}^k \times \frac{\partial \mathbf{V}_{cs}}{\partial \xi^k} \right) \right]_y - \gamma_v \sqrt{g} \sum_{\substack{m=1 \\ m \neq l}}^3 \bar{c}_{ml}^{vm} \left[\frac{\partial \Delta v_{ml}}{\partial \tau} + \sum_{k=1}^3 \mathbf{a}^k \cdot (\mathbf{V}_l - \mathbf{V}_{cs}) \frac{\partial \Delta v_{ml}}{\partial \xi^k} \right] \\ & - \gamma_v \sqrt{g} \bar{c}_{wl}^{vm} \left[\frac{\partial \Delta v_{csl}}{\partial \tau} + \sum_{k=1}^3 \mathbf{a}^k \cdot (\mathbf{V}_l - \mathbf{V}_{cs}) \frac{\partial \Delta v_{csl}}{\partial \xi^k} \right] = \gamma_v \sqrt{g} \left[-\alpha_l \rho_l g_y + \sum_{m=1}^{3,w} [\mu_{ml} (v_m - v_l)] + \mu_{lw} (v_{lw} - v_l) \right], \quad (\text{A3.9}) \end{aligned}$$

where

$$\mathbf{F}_l^v = \mathbf{F}_l^{vv} + \mathbf{F}_l^{vvb} + \mathbf{F}_l^{vvT} \quad (\text{A3.10})$$

is the diffusion momentum flux in the y -direction with components

$$\mathbf{F}_l^{vv} = -\alpha_l \rho_l v_l^* \left(\sum_{k=1}^3 \mathbf{a}^k \frac{\partial v_l}{\partial \xi^k} \right), \quad \mathbf{F}_l^{vvb} = \alpha_l^e \rho_l v_l^* \frac{2}{3} (\nabla \cdot \mathbf{V}_l) \mathbf{j}, \quad \mathbf{F}_l^{vvT} = -\alpha_l^e \rho_l v_l^* \frac{\partial \mathbf{V}_l}{\partial y}. \quad (\text{A3.11-13})$$

The flux notation of the z -component of the momentum equation is

$$\begin{aligned} & \sqrt{g} \left[\alpha_l \rho_l \gamma_v \frac{\partial w_l}{\partial \tau} + \left(\sum_{k=1}^3 \gamma_k \mathbf{a}^k \frac{\partial w_l}{\partial \xi^k} \right) \cdot \mathbf{G}_l \right] + \sum_{k=1}^3 \frac{\partial}{\partial \xi^k} \left(\gamma_k \sqrt{g} \mathbf{a}^k \cdot \mathbf{F}_l^w \right) + \sqrt{g} \alpha_l \left(\sum_{k=1}^3 a^{k3} \gamma_k \frac{\partial p}{\partial \xi^k} \right) \\ & - \sqrt{g} \gamma_v \left[\sum_{\substack{m=1 \\ m \neq l}}^3 \bar{c}_{ml}^d |\Delta \mathbf{V}_{ml}| \Delta w_{ml} - \bar{c}_{wl}^d |\Delta \mathbf{V}_{wl}| \Delta w_{wl} \right] - \gamma_v \sqrt{g} \sum_{\substack{m=1 \\ m \neq l}}^{l_{\max}} \bar{c}_{ml}^L \left[(\mathbf{V}_l - \mathbf{V}_m) \times \left(\sum_{k=1}^3 \mathbf{a}^k \times \frac{\partial \mathbf{V}_m}{\partial \xi^k} \right) \right]_z \\ & - \gamma_v \sqrt{g} \bar{c}_{wl}^L \left[(\mathbf{V}_l - \mathbf{V}_{cs}) \times \left(\sum_{k=1}^3 \mathbf{a}^k \times \frac{\partial \mathbf{V}_{cs}}{\partial \xi^k} \right) \right]_z - \gamma_v \sqrt{g} \sum_{\substack{m=1 \\ m \neq l}}^3 \bar{c}_{ml}^{vm} \left[\frac{\partial \Delta w_{ml}}{\partial \tau} + \sum_{k=1}^3 \mathbf{a}^k \cdot (\mathbf{V}_l - \mathbf{V}_{cs}) \frac{\partial \Delta w_{ml}}{\partial \xi^k} \right] \\ & - \gamma_v \sqrt{g} \bar{c}_{wl}^{vm} \left[\frac{\partial \Delta w_{csl}}{\partial \tau} + \sum_{k=1}^3 \mathbf{a}^k \cdot (\mathbf{V}_l - \mathbf{V}_{cs}) \frac{\partial \Delta w_{csl}}{\partial \xi^k} \right] = \gamma_v \sqrt{g} \left[-\alpha_l \rho_l g_z + \sum_{m=1}^{3,w} [\mu_{ml} (w_m - w_l)] + \mu_{lw} (w_{lw} - w_l) \right], \quad (\text{A3.14}) \end{aligned}$$

where

$$\mathbf{F}_l^w = \mathbf{F}_l^{wv} + \mathbf{F}_l^{wvb} + \mathbf{F}_l^{wvT} \quad (\text{A3.15})$$

is the diffusion momentum flux in the z -direction with components

$$\mathbf{F}_l^{wv} = -\alpha_l \rho_l \nu_l^* \left(\sum_{k=1}^3 \mathbf{a}^k \frac{\partial w_l}{\partial \xi^k} \right), \quad \mathbf{F}_l^{wvb} = \alpha_l^e \rho_l \nu_l^* \frac{2}{3} (\nabla \cdot \mathbf{V}_l) \mathbf{k}, \quad \mathbf{F}_l^{wvT} = -\alpha_l^e \rho_l \nu_l^* \frac{\partial \mathbf{V}_l}{\partial z}. \quad (\text{A3.16-18})$$

The entropy equation:

$$\begin{aligned} & \alpha_l \rho_l \sqrt{g} \left(\gamma_v \frac{\partial s_l}{\partial \tau} + \sum_{k=1}^3 \gamma_k \bar{V}_l^k \frac{\partial s_l}{\partial \xi^k} \right) - \sum_{m=1}^3 \frac{\partial}{\partial \xi^m} \left\{ \alpha_l \rho_l \sqrt{g} \gamma_m \sum_{i=2}^{i_{\max}} \left[(s_{il} - s_{il}) D_{il}^* \left(\sum_{k=1}^3 g^{mk} \frac{\partial C_{il}}{\partial \xi^k} \right) \right] \right\} \\ & - \frac{1}{T_l} \sum_{m=1}^3 \frac{\partial}{\partial \xi^m} \left[\alpha_l^e \lambda_l^* \sqrt{g} \gamma_m \left(\sum_{k=1}^3 g^{mk} \frac{\partial T_l}{\partial \xi^k} \right) \right] = \gamma_v \sqrt{g} \left[\frac{1}{T_l} DT_l^N + \sum_{i=1}^{i_{\max}} \mu_{il} (s_{il} - s_l) \right]. \end{aligned} \quad (\text{A3.19})$$

Alternatively, the temperature equation is used instead of the entropy equation for the gas field:

$$\begin{aligned} & \sqrt{g} \alpha_l \rho_l c_{pl} \left(\gamma_v \frac{\partial T_l}{\partial \tau} + \sum_{k=1}^3 \gamma_k \bar{V}_l^k \frac{\partial T_l}{\partial \xi^k} \right) - \alpha_l \sqrt{g} \left[1 - \rho_l \left(\frac{\partial h_l}{\partial p} \right)_{T_l, \text{all } C's} \right] \left(\gamma_v \frac{\partial p_l}{\partial \tau} + \sum_{k=1}^3 \gamma_k \bar{V}_l^k \frac{\partial p_l}{\partial \xi^k} \right) \\ & + T_l \sum_{i=2}^{i_{\max}} \left\{ \Delta s_{il}^{np} \left(\sum_{m=1}^3 \frac{\partial}{\partial \xi^m} \left[\alpha_l \rho_l \sqrt{g} \gamma_m D_{il}^* \left(\sum_{k=1}^3 g^{mk} \frac{\partial C_{il}}{\partial \xi^k} \right) \right] \right) \right\} - \sum_{m=1}^3 \frac{\partial}{\partial \xi^m} \left[\alpha_l \lambda_l^* \sqrt{g} \gamma_m \left(\sum_{k=1}^3 g^{mk} \frac{\partial T_l}{\partial \xi^k} \right) \right] \\ & = \gamma_v \sqrt{g} \left[DT_l^N - T_l \sum_{i=2}^{i_{\max}} \Delta s_{il}^{np} (\mu_{il} - C_{il} \mu_l) \right]. \end{aligned} \quad (\text{A3.20})$$

The volume conservation equation is used instead of the one field mass conservation equation:

$$\begin{aligned} & \gamma_v \sqrt{g} \frac{1}{\rho a^2} \frac{\partial p}{\partial \tau} + \sqrt{g} \sum_{l=1}^{l_{\max}} \frac{\alpha_l}{\rho_l a_l^2} \left(\sum_{k=1}^3 \gamma_k \bar{V}_l^k \frac{\partial p}{\partial \xi^k} \right) + \sum_{l=1}^{l_{\max}} \left[\sum_{k=1}^3 \frac{\partial}{\partial \xi^k} (\alpha_l \gamma_k \sqrt{g} \bar{V}_l^k) \right] \\ & = \sqrt{g} \sum_{i=1}^{i_{\max}} \frac{1}{\rho_i} \left[\gamma_v \mu_i - \frac{1}{\rho_i} \left(\frac{\partial \rho_i}{\partial s_i} D s_i^N + \sum_{i=2}^{i_{\max}} \frac{\partial \rho_i}{\partial C_{il}} D C_{il}^N \right) \right] - \frac{\partial}{\partial \tau} (\gamma_v \sqrt{g}). \end{aligned} \quad (\text{A3.21})$$

For description of the multi-phase turbulence k - ε models for each velocity field are used:

$$\begin{aligned} & \alpha_l \rho_l \sqrt{g} \left(\gamma_v \frac{\partial k_l}{\partial \tau} + \sum_{k=1}^3 \gamma_k \bar{V}_l^k \frac{\partial k_l}{\partial \xi^k} \right) - \sum_{m=1}^3 \frac{\partial}{\partial \xi^m} \left[\alpha_l \rho_l \nu_l^k \sqrt{g} \gamma_m \left(\sum_{k=1}^3 g^{mk} \frac{\partial k_l}{\partial \xi^k} \right) \right] \\ & + \mu_l k_l \sqrt{g} = \sqrt{g} \left[P_{k_{il}} + \alpha_l \rho_l (v_l \bar{P}_{kl} + \gamma_v G_{kl}) + \alpha_l \rho_l \frac{c_{\eta l}}{\text{Pr}_{kl}^i} \bar{P}_{kl} \frac{k_l^2}{\varepsilon_l} - \alpha_l \rho_l \gamma_v \varepsilon_l \right]. \end{aligned} \quad (\text{A3.22})$$

$$\begin{aligned} & \alpha_l \rho_l \sqrt{g} \left(\gamma_v \frac{\partial \varepsilon_l}{\partial \tau} + \sum_{k=1}^3 \gamma_k \bar{V}_l^k \frac{\partial \varepsilon_l}{\partial \xi^k} \right) - \sum_{m=1}^3 \frac{\partial}{\partial \xi^m} \left[\alpha_l \rho_l \nu_l^k \sqrt{g} \gamma_m \left(\sum_{k=1}^3 g^{mk} \frac{\partial \varepsilon_l}{\partial \xi^k} \right) \right] \\ & + \mu_l \varepsilon_l \sqrt{g} = \sqrt{g} \left[\alpha_l \rho_l \frac{\varepsilon_l}{\kappa_l} (c_{\varepsilon 1} v_l \bar{P}_{kl} + c_{\varepsilon 3} \gamma_v G_{kl}) + \alpha_l \rho_l \frac{c_{\eta l}}{\text{Pr}_{\varepsilon l}^i} \bar{P}_{kl} k_l - \alpha_l \rho_l \gamma_v c_{\varepsilon 2} \frac{\varepsilon_l^2}{\kappa_l} \right]. \end{aligned} \quad (\text{A3.23})$$

NOMENCLATURE

Latin

a	speed of sound, m/s
C_{il}	mass concentration of the inert component i in the velocity field l
c	coefficients, <i>dimensionless</i>
C_m	mass concentration of the component m in the velocity field, <i>dimensionless</i>
C_i	mass concentration of the component i in the velocity field, <i>dimensionless</i>
c_p	specific heat at constant pressure, $J/(kgK)$
c^{vm}	virtual mass force coefficient, <i>dimensionless</i>
c^d	drag force coefficient, <i>dimensionless</i>
c^L	lift force coefficient, <i>dimensionless</i>
D_{il}^l	coefficient of molecular diffusion for species i into the field l , m^2/s
D_{il}^t	coefficient of turbulent diffusion, m^2/s
D_{il}^*	total diffusion coefficient, m^2/s
DC_{il}	right-hand side of the non conservative conservation equation for the inert component, $kg/(sm^3)$
D	diffusivity, m^2/s
d	total differential
E	total energy, J
e	specific internal energy, J/kg
f	force per unit flow volume, N/m^3
f	fraction of entrained melt or water in the detonation theory
g	acceleration due to gravity, m/s^2
H	height, m
h	specific enthalpy, J/kg
h_i	eigen vectors corresponding to each eigen value
I	unit matrix, <i>dimensionless</i>
i	unit vector along the x -axis
J	matrix, <i>Jacobian</i>
j	unit vector along the y -axis
k	unit vector along the k -axis
k	cell number
k	kinetic energy of turbulent pulsation, m^2/s^2
L	length, m
n_{il}	number of the particle from species i per unit flow volume, m^{-3}
n_l	number of particles of field l per unit flow volume, particle number density of the velocity field l , m^{-3}
\dot{n}_{coal}	number of the disappeared particles due to coalescence per unit time and unit volume, m^{-3}
$\dot{n}_{l,kin}$	particle production rate due to nucleation during evaporation or condensation, $1/(m^3s)$
n_{lw}''	number of the activated seeds on unit area of the wall, m^{-2}
\dot{n}_{lh}	number of the nuclei generated by homogeneous nucleation in the donor velocity field per unit time and unit volume of the flow, $1/(m^3s)$
$\dot{n}_{l,dis}$	number of the nuclei generated from dissolved gases in the donor velocity field per unit time and unit volume of the flow, $1/(m^3s)$
$\dot{n}_{l,sp}$	number of particles of the velocity field l arising due to hydrodynamic disintegration per unit time and unit volume of the flow, $1/(m^3s)$
P	probability
P	irreversibly dissipated power from the viscous forces due to deformation of the local volume and time average velocities in the space, W/kg
p_{li}	$l = 1$: partial pressure inside the velocity field l $l = 2,3$: pressure of the velocity field l

p	pressure, Pa
\dot{q}'''	Thermal power per unit flow volume introduced into the fluid, W / m^3
$\dot{q}_{\sigma l}'''$	$l = 1,2,3$. Thermal power per unit flow volume introduced from the interface into the velocity field l , W / m^3
$\dot{q}_{w\sigma l}'''$	thermal power per unit flow volume introduced from the structure interface into the velocity field l , W / m^3
$\mathbf{r}(x,y,z)$	position vector, m
R	(with indexes) gas constant, $J/(kgK)$
\mathbf{s}	arc length vector, m
S	total entropy, J/K
s	specific entropy, $J/(kgK)$
Sc^t	turbulent <i>Schmidt</i> number, <i>dimensionless</i>
T	temperature, K
T_l	temperature of the velocity field l , K
\mathbf{T}	shear stress tensor, N / m^2
\mathbf{t}	unit tangent vector
\mathbf{U}	dependent variables vector
Vol	control volume, m^3
$Vol^{1/3}$	size of the control volume, m
Vol_l	volume available for the field l inside the control volume, m^3
$\sum_{l=1}^{l_{max}} Vol_l$	volume available for the flow inside the control volume, m^3
\mathbf{V}	instantaneous fluid velocity with components, u, v, w in r, θ , and z direction, m/s
\mathbf{V}_l	time-averaged velocity, m/s
\mathbf{V}_l'	pulsation component of the instantaneous velocity field, m/s
$\Delta \mathbf{V}_{lm}$	$\mathbf{V}_l - \mathbf{V}_m$, velocity difference, disperse phase l , continuous phase m carrying l , m/s
v	specific volume, m^3 / kg
x	mass fraction, <i>dimensionless</i>
y	distance between the bottom of the pipe and the center of mass of the liquid, m
\times	vector product

Greek

α_l	part of $\gamma_v Vol$ available to the velocity field l , local instantaneous volume fraction of the velocity field l , <i>dimensionless</i>
α_{il}	the same as α_l in the case of gas mixtures; in the case of mixtures consisting of liquid and macroscopic solid particles, the part of $\gamma_v Vol$ available to the inert component i of the velocity field l , local instantaneous volume fraction of the inert component i of the velocity field l , <i>dimensionless</i>
γ_v	the part of $dVol$ available for the flow, volumetric porosity, <i>dimensionless</i>
γ	surface permeability, <i>dimensionless</i>
Δ	finite difference
δ	small deviation with respect to given value
δ_l	= 1 for continuous field; = 0 for disperse field, <i>dimensionless</i>
∂	partial differential
ε	dissipation rate for kinetic energy from turbulent fluctuation, irreversibly dissipated power by the viscous forces due to turbulent fluctuations, W / kg
η	dynamic viscosity, $kg/(ms)$
θ	θ -coordinate in the cylindrical or spherical coordinate systems, rad
κ	= 0 for Cartesian coordinates, = 1 for cylindrical coordinates
κ	isentropic exponent
λ	thermal conductivity, $W/(mK)$

μ_l	time average of the local volume-averaged mass transferred into the velocity field l per unit time and unit mixture flow volume, local volume-averaged instantaneous mass source density of the velocity field l , $kg/(m^3s)$
μ_{wl}	mass transport from exterior source into the velocity field l , $kg/(m^3s)$
μ_{il}	time average of the local volume-averaged inert mass from species i transferred into the velocity field l per unit time and unit mixture flow volume, local volume-averaged instantaneous mass source density of the inert component i of the velocity field l , $kg/(m^3s)$
μ_{iml}	time average of the local volume-averaged instantaneous mass source density of the inert component i of the velocity field l due to mass transfer from field m , $kg/(m^3s)$
μ_{ilm}	time average of the local volume-averaged instantaneous mass source density of the inert component i of the velocity field l due to mass transfer from field l into velocity field m , $kg/(m^3s)$
ν	kinematic viscosity, m^2/s
ν_l^t	coefficient of turbulent kinematic viscosity, m^2/s
ξ	angle between $\mathbf{n}_{l\sigma}$ and $\Delta\mathbf{V}_{lm}$, rad
ρ	density, kg/m^3
ρ	instantaneous density, density; without indexes, mixture density, kg/m^3
ρ_l	instantaneous field density, kg/m^3
ρ_{il}	instantaneous inert component density of the velocity field l , kg/m^3
$(\rho w)_{23}$	entrainment mass flow rate, $kg/(m^2s)$
$(\rho w)_{32}$	deposition mass flow rate, $kg/(m^2s)$
σ, σ_{12}	surface tension between phases 1 and 2, N/m
τ	time, s
φ	angle giving the projection of the position of the surface point in the plane normal to $\Delta\mathbf{V}_{lm}$, rad
$\chi_l^{m\sigma}$	the product of the effective heat transfer coefficient and the interfacial area density, $W/(m^3K)$. The subscript l denotes inside the velocity field l . The superscript $m\sigma$ denotes location at the interface σ dividing field m from field l . The superscript is only used if the interfacial heat transfer is associated with mass transfer. If there is heat transfer only, the linearized interaction coefficient is assigned the subscript ml only, indicating the interface at which the heat transfer takes place.

Subscripts

c	continuous
d	disperse
lm	from l to m or l acting on m
w	region "outside of the flow"
e	entrances and exits for control volume Vol
l	velocity field l
i	inert components inside the field l , non-condensable gases in the gas field $l = 1$, or microscopic particles in water in field 2 or 3
i	corresponding to the eigen value λ_i in Chapter 4
M	non-inert component
m	mixture of entrained coolant and entrained melt debris that is in thermal and mechanical equilibrium behind the shock front
ml	from m into l
iml	from im into il
max	maximum number of points
n	inert component
0	at the beginning of the time step
E	entrainment
$coal$	coalescence
sp	splitting, fragmentation
σ	interface

τ	old time level
$\tau + \Delta\tau$	new time level
*	initial
0	reference conditions
p, v, s	at constant p, v, s , respectively
L	left
R	right
1	vapor
2	water
3	melt

Superscripts

'	time fluctuation
d	drag
i	component (either gas or solid particles) of the velocity field
i_{\max}	maximum for the number of the components inside the velocity field
L	lift
$l\sigma$	averaged over the surface of the sphere
m	component
n	normal
n	old iteration
$n+1$	new iteration
t	turbulent, tangential
vm	virtual mass
τ	temporal, instantaneous
$-$	averaging sign

Operators

$\nabla \cdot$	divergence
∇	gradient
∇_n	normal component of the gradient
∇_t	tangential component of the gradient
∇_l	surface gradient operator, $1/m$
∇^2	<i>Laplacian</i>

Nomenclature required for coordinate transformations

(x, y, z) Coordinates of a Cartesian, left oriented coordinate systems (*Euclidean* space). Another notation which is simultaneously used is x_i ($i = 1, 2, 3$): x_1, x_2, x_3 .

(ξ, η, ζ) Coordinates of the curvilinear coordinate system called transformed coordinate system. Another notation which is simultaneously used is ξ^i ($i = 1, 2, 3$): ξ^1, ξ^2, ξ^3 .

\mathbf{V}_{cs} The velocity of the curvilinear coordinates system.

\sqrt{g} *Jacobian* determinant or *Jacobian* of the coordinate transformation $x = f(\xi, \eta, \zeta)$, $y = g(\xi, \eta, \zeta)$, $z = h(\xi, \eta, \zeta)$.

a_{ij} Elements of the *Jacobian* determinant

a^{ij} Elements of the determinant transferring the partial derivatives with respect to the transformed coordinates into partial derivatives with respect to the physical coordinates. The second superscript indicating the Cartesian components of the contravariant vectors.

$(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ Covariant base vectors of the curvilinear coordinate system - tangent vectors to the three curvilinear coordinate lines represented by (ξ, η, ζ) .

$(\mathbf{a}^1, \mathbf{a}^2, \mathbf{a}^3)$ Contravariant base vectors, normal to a coordinate surface on which the coordinates ξ , η and ζ are constant, respectively.

g_{ij} Covariant metric tensor (symmetric).

g^{ij} Contravariant metric tensor (symmetric).

$(\mathbf{e}^1, \mathbf{e}^2, \mathbf{e}^3)$ Unit vectors normal to a coordinate surface on which the coordinates ξ , η and ζ are constant, respectively.

$\mathbf{V}^i = \mathbf{a}^i \cdot \mathbf{V}$, Contravariant components of the vector \mathbf{V} .

$\mathbf{V}_i = \mathbf{a}_i \cdot \mathbf{V}$, Covariant components of the vector \mathbf{V} .

$(\gamma_\xi, \gamma_\eta, \gamma_\zeta)$ Permeabilities of coordinate surfaces on which the coordinates ξ , η and ζ are constant, respectively.

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