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Steam Explosion Simulation Code JASMINE v.3 User's Guide: Revised for Code Version 3.3c

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A steam explosion is defined as a phenomenon that occurs when a hot liquid comes into contact with a low-temperature cold liquid with volatile properties. The rapid transfer of heat from the hot liquid to the cold liquid results in a chain reaction of the explosive vaporization of the cold liquid and fine fragmentation of the hot liquid. The explosive vaporization of the cold liquid initiates the propagation of shock waves in the cold liquid. The expansion of the hot and cold liquid mixture exerts mechanical forces on the surrounding structures. In severe accidents of light water reactors, the molten core (melt) is displaced into the coolant water, resulting in fuel-coolant interactions (FCIs). The explosive FCI, referred to as a steam explosion, has been identified as a significant safety assessment issue as it can compromise the integrity of the primary containment vessel. The JASMINE code is an analytical tool developed to evaluate the mechanical forces imposed by steam explosions in nuclear reactors. It performs numerical simulations of steam explosions in a mechanistic manner. The present report describes modeling concepts, basic equations, numerical solutions, and example simulations, as well as instructions for input preparation, code execution, and the use of supporting tools for practical purpose. The present report is the updated version of the "Steam Explosion Simulation Code JASMINE v.3 User's Guide, JAEA-Data/Code 2008-014". The present report was compiled and updated based on the latest version of the code, JASMINE 3.3c, with corrections for minor errors of the distributed code JASMINE 3.3b, and conformance to recently widely used compilers on UNIX-like environments such as the GNU compiler. The numerical simulations described in the present report were obtained using the latest version JASMINE 3.3c. The latest parameter adjustment method for a model parameter proposed by the previous study is employed to conduct the numerical simulations.

Keywords: Light Water Reactor, Severe Accident, Safety Assessment, Numerical Simulation, JASMINE

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水蒸気爆発解析コード JASMINE v.3 取扱説明書:改訂版 コードバージョン 3.3c

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水蒸気爆発では、揮発性を有する低温の液体に高温の液体が接触した場合に高温の液体から 低温の液体への急激な熱伝達により、高温の液体の細粒化と低温の液体の爆発的な相変化が連 鎖的に発生する。爆発的な相変化により発生する衝撃波は低温の液体の内部を伝播する。衝撃 波の伝播に伴い高温の液体と低温の液体の混合物が膨張することにより、周囲に存在する構造 体に機械的な負荷を与える可能性がある。軽水炉のシビアアクシデントでは、原子炉格納容器 へ移行した溶融炉心(溶融物)と冷却水との相互作用に起因して発生する水蒸気爆発が原子炉 格納容器の健全性に対する脅威となることが想定される。このことから、水蒸気爆発の発生が 周囲に存在する構造体へ与える機械的な負荷を評価することが安全評価の観点から重要となる。 原子力機構では、実際の原子炉にて発生した水蒸気爆発が周囲に存在する構造体へ与える機械 的な負荷を評価することを目的として JASMINE コードを開発した。機構論的な手法を取り入 れることにより、JASMINE コードは水蒸気爆発を数値解析上で取り扱うことができる。本書 は JASMINE コードに採用されている基礎方程式、数値解法及び数値解析例を記載した取扱説 明書である。本書に記載した数値解析例を参照することにより、JASMINE コードによる数値 解析で得られた結果を検証できるように配慮した。入力条件の作成方法、コードの実行手順及 び補助ツールの使用方法を記載することにより、JASMINE コードを用いた数値解析を実践で きるよう配慮した。本書は「水蒸気爆発解析コード JASMINE v.3 ユーザーズガイド (JAEA-Data/Code 2008-014)」の改訂版である。公開されている JASMINE 3.3b の軽微な不具合の修正 に加えて、UNIX 系システムで広く使用されている GNU コンパイラー等に適合するための修正 を施した最新版を JASMINE 3.3c とした。改訂版は、新規に公開される JASMINE 3.3c による 数値解析の結果に基づき作成されているために、掲載されている数値解析の結果を再現できる。 数値解析の実施に際しては、既存研究により提案されている調整係数の決定方法を採用した。

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1. Introduction

1.1 Background

A steam explosion is defined as a phenomenon that occurs when a high-temperature (hot) liquid comes into contact with a low-temperature (cold) liquid with volatile properties. In a steam explosion, the rapid transfer of heat from the hot liquid to the cold liquid results in a chain reaction of the explosive vaporization of the cold liquid and the fine fragmentation of the hot liquid. The explosive vaporization of the cold liquid then initiates the propagation of shock waves in the cold liquid. The expansion of the hot and cold liquid mixture exerts mechanical forces on the surrounding structures. A steam explosion is a thermodynamic process whereby the internal energy of a hot liquid is converted into the kinetic energy of a cold liquid.

In severe accidents of a light water reactor, the molten core (melt) is displaced from the reactor pressure vessel (RPV) into the coolant water, resulting in fuel-coolant interactions (FCIs). The FCIs encompass both the explosive and mild interactions. The explosive FCI, which is referred to as a steam explosion, has been identified as a significant safety assessment issue due to the potential for mechanical forces imposed by the steam explosion to compromise the integrity of the primary containment vessel of a light water reactor in severe accidents.

In order to evaluate the mechanical forces that will be imposed by the steam explosion that is anticipated to occur in the actual reactors, an analytical approach is generally or typically employed. The analytical approach allows for the extrapolation of the knowledge that has been obtained from the experiments conducted under the simulated conditions to the prototypical conditions expected in the actual reactors. In order to develop the analytical tool in a mechanistic manner, it is necessary to provide a comprehensive description of the physical phenomena associated with the entire steam explosion process. A steam explosion progresses through distinct stages^(1, 2) as illustrated in Fig. 1.1.



Fig. 1.1 A schematic of the stages in steam explosions: (a) premixing stage, (b) triggering stage, (c) propagation stage, and (d) expansion stage.

1. Premixing Stage:

The melt particles, which have been detached from the melt (coarse break-up), disperse and mix with the coolant water in a thermally insulated state by a vapor film around the melt particle [see Fig. 1.1 (a)]. The premixing stage is a process that occurs over a timescale of 0.1 to several seconds.

2. Triggering Stage:

The destabilization of the vapor film at the local level results in direct contact between the melt particle and the coolant water [see Fig. 1.1 (b)]. The rapid transfer of heat from the melt particle to the coolant water results in an explosive vaporization of the coolant water.

3. Propagation Stage:

The explosive vaporization of the coolant water, in conjunction with the fine fragmentation of the melt particles, initiates a series of events, including the propagation of shock waves (pressure pulses) [see Fig. 1.1 (c)]. The propagation stage is a process that occurs over a timescale of a few milliseconds.

4. Expansion Stage:

The propagation of shock waves results in the expansion of the melt and coolant water mixture [see Fig. 1.1 (d)]. The kinetic energy of the expansion of the hot and cold liquid mixture exerts mechanical forces on the surrounding structures.

Table 1.1 The physical phenomena involved in the premixing and explosion steps, and the specific terminology defined and employed in the present report.

Stage (step) Premixing Explosion					
Specified terminology					
Discontinuous melts droplets (particles) (fine) fragments					
Discontinuous process coarse break-up of a melt jet fragmentation of melt particle	s				
Physical phenomena					
Dominance in process convection by gravity/buoyancy convection driven by shock w	vave				
Scale in time 0.1–10 sec 0.1–10 ms					
Scale in size 1–10 mm 1–100 μm					

Table 1.1 summarizes the physical phenomena involved in the premixing and explosion stages, as well as the definitions of the specific terminology used in the present report. The discontinuous process of the melt is present in both the premixing and explosion stages, as illustrated in Fig. 1.1. Given that the evident disparity exists in the dominant process across the two stages, it is imperative to distinguish and delineate the specific terminology associated with each stage.

The previous studies^(2, 3) proposed the methods for an analytical approach: thermodynamic models that establish the limits of energy conversion efficiency, and multi-dimensional transient thermohydraulic models that simulate the process mechanistically. The present studies⁽⁴⁾ organized the steam explosion process into two specified steps: premixing and explosion, to facilitate the analytical approach. The following descriptions provide an overview of the analytical approach, delineating the methodology employed for each step.

1. Premixing Step:

The melt particles are subjected to a coarse break-up, resulting in dispersion and subsequent mixing with the coolant water. The mixture of melt particles with a certain amount of void is defined as the "premixed melt". It is assumed that the premixed melt will participate in the subsequent explosion step.

2. Explosion Step:

The propagation and expansion stages are treated as a single process. The combination of the explosive vaporization of the coolant water and the fragmentation of the premixed melt particles gives rise to a series of events, namely the propagation and expansion.

The previous experiments⁽⁵⁾ reported an inconsistent triggering event, whereby the triggering event was observed to occur on occasion and not on other occasions, even in the presence of minor uncontrollable alterations to the experimental conditions. It is challenging to predict the occurrence or absence of spontaneous triggering through an analytical approach. In safety assessments, the triggering stage merits particular attention, as the presence or absence of the triggering event has a profound impact on the outcome, either resulting in mechanical forces or in the absence of such mechanical forces. In the triggering stage, the present studies assume that a sufficiently strong trigger is placed to initiate the steam explosion, as the objective of the present studies is to evaluate the mechanical forces imposed by the steam explosion. It should be noted that, even with a sufficiently strong trigger, it is impossible to initiate a steam explosion in reality.

1.2 Outline of Code Structures

Fig. 1.2 depict a schematic of the structures utilized in the JASMINE (JAEA Simulator for Multiphase INteractions and Explosions) code. The latest version of the JASMINE code consists of two distinct modules for the simulation of the melt and coolant water. The melt module is constituted by sub-models for the melt pool, and the melt particle. The melt jet and the melt pool models represent the melt stream falling into the coolant water, and the continuous melt body spreading on the bottom, respectively, in one-dimensional geometries. The melt particle model represents the dispersion of the melt due to the coarse breakup of the melt jet and the settling to the bottom due to gravity, based on the particle group concept within a Lagrangian framework. The coolant water module is composed of a modified version of the ACE3D code, developed at the Japan Atomic Energy Research Institute (JAERI)⁽⁶⁾. The module addresses the multiphase flow and thermo-hydraulics of the coolant water.



Fig. 1.2 A schematic of the structures utilized in the JASMINE code: (a) premixing step, and (b) explosion step. The distinct physical phenomena ate focused and modeled in each step.

The latest version of the JASMINE code employs a two-step simulation of the steam explosion process: the premixing step and the explosion step, as described in the previous section. In the premixing step [see Fig. 1.2 (a)], the JASMINE code simulates solely the premixing stage. In the explosion step [see Fig. 1.2 (b)], the JASMINE code simulates the propagation and expansion stages. The input data utilized for the explosion step are derived from the output data obtained in the premixing step. An artificial trigger is employed to initiate the steam explosion. The melt jet and melt pool are excluded from the premixed melt, which participates in the steam explosion, as indicated by the transparent area surrounded by dotted lines in Fig. 1.2 (b), because the melt jet and melt pool contribute less to the steam explosion due to their smaller surface areas than the melt particles.

1.3 Code Development History

The first version of the JASMINE code was developed in 1995⁽⁷⁾. The first version, designated JASMINE-pre, employed a three-fluid Eulerian model: coolant water comprising steam, and melt, which was utilized to simulate solely the premixing step. The JASMINE-pre was employed in the OECD International Standard Problem No. 39 (ISP-39) exercise, which focused on a large-scale experiment on FCIs (FARO-L-14)⁽⁸⁾. In order to simulate the explosion step, JASMINE-pro^(9, 10) was developed as a standalone code in 2000. The JASMINE-pro employed a five-fluid Eulerian approach, augmented by two additional fields for the fine fragments of the melt in the propagation stage and a small amount of coolant water interacting with the fine fragments.

A substantial modification to the JASMINE code was incorporated in 1997. The second version, designated JASMINE-pre v.2.0, utilized the Lagrangian framework to simulate the dynamics of melt particles. In 2003, the models utilized to simulate the explosion step were incorporated into JASMINE-pre 2.2.¹ The third version, designated JASMINE 3.0, was equipped with the capability to perform both the premixing and explosion steps. The JASMINE 3.0 was utilized in the OECD/SERENA Phase 1^(11, 12). The JASMINE 3.3a was fixed in 2008 in the preparation for the previous report⁽⁴⁾. The JASMINE 3.3b was fixed in 2010 for incorporation into the distribution package. The structures of the JASMINE code remain consistent throughout the code version 3.x. The most recent code release is the code version 3.3c. The updates to JASMINE 3.3b addressed a number of minor issues, reorganized directory structures, and enhanced the supporting tools that are included in the distribution package. The code version 3.3b resulted in operational failure in UNIX-like environments with recently widely used compilers, such as the GNU compiler. The code version 3.3c was modified to be compatible with the GNU compiler on UNIX-like environments in addition to the minor description errors in the code version 3.3b.

1.4 Updates and Current Focuses

The previous report⁽⁴⁾ has been revised to reflect the latest updates to JASMINE 3.3b. The present report supersedes the descriptions based on the simulations with JASMINE 3.3c, rectifies typographical errors, and provides updates to information regarding to the methods for input parameter adjustments, instructions for output processing, and the utilization of supporting tools. The major updates incorporated in the present report are as follows:

1. Program Discrepancy:

The code version (JASMINE 3.3a) employed to prepare the previous report⁽⁴⁾ differed from the one documented within the distribution package (JASMINE 3.3b). The simulations conducted with JASMINE 3.3b exhibited a heightened intensity of the steam explosions relative to those conducted with JASMINE

¹ The previous reports mentioned that "the propagation-related models in JASMINE-pro v.1.1 were merged into JASMINE-pre v.2.2". In fact, only the fundamental concepts were retained, which resulted in JASMINE-pro v.1.1 becoming obsolete.

3.3a. The discrepancy of the code version was attributed to the incorporation of minor corrections. The simulations in the present report were conducted using JASMINE 3.3c. The simulations in the present report can be reproduced using the consistent code version included in the distribution package.

2. Parameter Adjustment:

Moriyama and Furuya⁽¹³⁾ proposed a method for adjusting an input parameter: the fragmentation constant C_{frg} , which influences the intensity of the steam explosion. In order to facilitate the adjustment method, the authors employed time-dependent impulse histories, which were estimated from the different pressure sensors that were situated within the experimental facility. It was highlighted that the adjustment method, which is based on a single value of the kinetic energy obtained from the experiments, may result in an overestimation of the intensity of the steam explosion. The numerical simulations in the present report are based on the fragmentation constant C_{frg} determined by applying the parameter adjustment method proposed by Moriyama and Furuya⁽¹³⁾.

Since the release of JASMINE 3.3b, a number of organizations have undertaken independent modifications to JASMINE 3.3b. At the Secretariat of the Nuclear Regulation Authority (NRA), Hotta et al.⁽¹⁴⁾ utilized JASMINE 3.3b for the analytical exercises in the OECD/SERENA Phase 2. The model was developed particle formation across a range of sizes through the use of random numbers. At Pohang University of Science and Technology (POSTECH), Moriyama and Park^(15, 16) utilized JASMINE 3.3b to examine the influence of input parameters, including the coolant water depth and triggering time, on the intensity of the steam explosion. Morivama and Park⁽¹⁷⁾ enhanced JASMINE 3.3b to simulate the processes of melt-jet breakup and debris formation over an extended period. The models were incorporated to simulate particle formation across a range of sizes though the use of random numbers, and non-local radiation heat transfer from melt particles to coolant water. Moriyama and Park^(18, 19) utilized the modified JASMINE 3.3b to simulate the processes of melt-jet breakup and debris formation in a nuclear reactor. At the Japan Atomic Energy Agency (JAEA), Matsumoto et al.⁽²⁰⁾ incorporated the models to simulate particle formation across a range of sizes thorough the use of random numbers, crust formation with sub/supercritical flow in the spreading of the melt pool, as well as the agglomeration of melt particles at the bottom. The ongoing development of the JASMINE code at JAEA is a work in progress. It should be noted that the aforementioned updates to JASMINE 3.3b at NRA, POSTECH, and JAEA have not been incorporated into JASMINE 3.3c, as the updates fall outside the scope of the present report.

1.5 Remaining Chapters and Appendices

The remaining chapters provide detailed explanations of the modeling concepts, numerical methods, and example simulations. The appendices provide supplementary information regarding modeling concepts and numerical methods, as well as instructions for the JASMINE code and supporting tools. Chapter 2 provides an overview of the modeling concepts, while Chapter 3 delves into the numerical

methods. Chapter 4 presents the example simulations. Chapter 5 concludes the report. Appendices A–D provides supplementary information regarding the modeling concepts and numerical methods. Appendix E delineates the method of input parameter adjustment: the empirical constant C_{frg} , and its influence on the mechanical forces exerted by the steam explosions. Appendices F–H provide instructions for the input/output file contents, and practical program usages.

2. Modeling Concepts

2.1 Framework

The most recent version of the JASMINE code comprises distinct modules for the simulation of melt and coolant water or two-phase flow, as illustrated in Fig. 1.2. The melt module is composed of three sub-models: the melt jet, the melt pool, the melt particle, and the melt fragment. The two-phase flow module employs a cylindrical sector with a sector angle Θ as the simulation domain. The simulation domain of the x-z plane is divided into the finite difference meshes for the two-dimensional simulation of the two-phase flow. The melt jet model utilizes the common area of a single center column within the simulation domain of the two-phase flow for the one-dimensional simulation. The melt pool model utilizes the common area of a single bottom low within the simulation domain of the two-phase flow for the one-dimensional simulation. The melt particle model employs the common area of the simulation domain of the two-phase flow for the two-dimensional simulation area of the simulation domain of the two-phase flow for the two-dimensional simulation framework.

In order to simulate the interaction of the melt with the liquid water and gases (steam and noncondensable gases), it is essential to microplate the effects of the flow regimes into the constitutive models. The flow regimes implemented in the JASMINE code are contingent on the total void fraction α of the two-phase flow, which encompasses both steam and non-condensable gases. The following definitions have been established for the flow regimes:

1. Bubbly Flow Regime:

In the bubbly flow regime, the continuous phase is the liquid water, while the dispersed phase is the gases. The bubbly flow regime is identified when the α of the two-phase flow is less than 0.30.

2. Droplet Flow Regime:

In the droplet flow regime, the continuous phase is the gases, while the dispersed phase is the liquid water. The droplet flow regime is identified when the α of the two-phase flow is more than 0.75.

3. Transition Regime:

In the transition regime, a change in the flow regime occurs between the bubbly flow regime and the droplet flow regime when the α of the two-phase flow falls between 0.30 and 0.75.

As the constitutive models express the single component for the liquid water or gases, the JASMINE code employed a weighting function f_{α} , to average the constitutive models, as shown in Eq. (2.1). Note that the weighting function f_{α} introduces a simple linear interpolation in the transition regime.

$$f_{\alpha} = \begin{cases} 0 & (0 \le \alpha \le 0.30) \\ (\alpha - 0.30)/0.45 & (0.30 \le \alpha \le 0.75). \\ 1 & (0.75 \le \alpha \le 1.00) \end{cases}$$
(2.1)

The component of the two-phase flow or the coolant water, designated X, is expressed in terms of the individual components for the liquid phase X_l and the gas phase X_g . In the present report, the averaging method [Eq. (2.2)] is employed to express the component of the two-phase flow:

$$X = (1 - f_\alpha)X_l + f_\alpha X_q.$$
(2.2)

The weighting function f_{α} is employed to determine the heat flux from the melt pool and melt particles in the convection regime [Eqs. (2.24) and (2.56)], the drag force that acts on the melt particles [Eq. (2.53)], the heat transfer coefficients from the liquid-gas interface to the steam and liquid water of the two-phase flow [Eqs. (2.114) and (2.115)], as well as the interfacial friction between the continuous and dispersed phases of the two-phase flow [Eq. (2.117)].

The symbol f_{α} also denotes the cut-off function to decline the heat flux in the boiling regime [Eqs.(2.35), and (2.36)], radiation heat flux [(2.37)] from the melt pool and melt particles, as well as the rapid mass and heat release rate [Eqs. (2.102) and (2.105)] of the melt fragments, depending of the void fraction of the two-phase flow. The form of the cut-off function f_{α} differs from that of the weighting function f_{α} . The cut-off function is implemented to cut off the boiling heat transfer from the melt pool or melt particles to the gas phases of the two-phase flow, and to achieve the numerical stability in the situation where the liquid phase of the two-phase flow is present in few amounts within the cells.

2.2 Melt Model

2.2.1 Melt Jet

Basic Equations

The melt jet model represents a solution to one-dimensional conservation equations in the vertical direction. Fig. 2.1 (a) depicts a schematic model of the melt jet erosion and the particle formation in the coolant water. Fig. 2.1 (b) depicts the finite volume element used to derive the conservation equations pertaining to the mass, internal energy, and momentum. The basic equations are expressed as Eqs. (2.3) -(2.5) in a non-conservation form. The coordinate z is defined as the positive vertical upward direction from the bottom of the simulation domain depicted in Fig. 2.1. The conservation equations have been derived for the finite volume element, which is represented by the red volume in Fig. 2.1 (b), and are expressed as follows:

$$\frac{\partial A_J \rho_J}{\partial t} + v_J \frac{\partial A_J \rho_J}{\partial z} = -\sqrt{2\Theta A_J} m_e - A_J \rho_J \frac{\partial v_J}{\partial z}, \tag{2.3}$$

$$\frac{\partial e_J}{\partial t} + v_J \frac{\partial e_J}{\partial z} = -\frac{\sqrt{2\Theta A_J}}{\rho_J A_J} q, \qquad \text{and} \qquad (2.4)$$

$$\frac{\partial v_J}{\partial t} + v_J \frac{\partial v_J}{\partial z} = -\frac{1}{\rho_J} \frac{\partial p_a}{\partial z} + K_{fJ} (v_c - v_J) + g, \qquad (2.5)$$

where ρ denotes the density, e denotes the internal energy, and v denotes the velocity. The subscripts J and c denote the melt jet, and the coolant water, respectively. The symbol p_a denotes the ambient pressure exerted by the coolant water. The cross-sectional area of the angular sector A_J indicates the red hatched area in the simulation domain [Fig. 2.1 (b)], and is expressed by $A_J = \Theta D_J^2/8$ using the sector angle of the simulation domain Θ and the diameter of the melt jet D_J .

The m_e denotes the mass flux resulting from the entrainment of the melt particles from the surface of the melt jet, the q denotes the heat flux from the surface of the melt jet to the coolant water, and the K_{fJ} denotes the friction coefficient between the melt jet and the coolant water. Note that the $\sqrt{2\Theta A_J}$ in Eqs. (2.3) and (2.4) means the surface area of the finite volume element. The values of m_e , q, and K_{fJ} in the source terms are specified through the constitutive models.



Fig. 2.1 A coordinate system and schematic of the melt jet model: (b) the melt jet erosion and the particle formation in the coolant water, (a) the finite volume element used to derive the conservation equations.

Constitutive Models

Melt Erosion and Particle Formation

The constitutive model for the entrainment of the melt particles from the surface of the melt jet m_e was derived from the mass conservation of the melt jet, as illustrated in Fig. 2.1 (a). As the melt jet descends within the coolant water, the diameter of the melt jet D_J decreases as a consequence of the

entrainment of the melt particles. The length of the melt jet, at which a coherent column of the melt jet collapses, is referred to as the jet-breakup length, denoted by L_{brk} . The semi-empirical correlations are available for determining L_{brk} . From the mass conservation of the melt jet within the finite volume element, which is illustrated by the volume surrounded by the dotted line in Fig. 2.1 (b), the volume flux resulting from the entrainment rate of the melt particles V_e can be expressed as follows:

$$V_e = \frac{V_J}{\pi D_J} \frac{dA}{dz},\tag{2.6}$$

where V denotes the velocity and D denote diameters. The subscript J denotes the melt jet. The cross-sectional area A indicates the gray area within the finite volume element [Fig. 2.1 (a)], expressed by $A = \pi D_J^2/4$. Eq. (2.6) indicates that the V_e is contingent upon alterations in the configuration of the melt jet or dA/dz. The quantity of the eroded melt jet is equivalent to the quantity of melt particles released into the coolant water.

Based on the assumption that D_J decreases linearly with z, then dD_J/dz becomes a constant value, which is expressed as Eq. (2.7). Consequently, Eq. (2.6) can be rewritten as Eq. (2.8) using Eq. (2.7). Note that D_{Ji} denotes the diameter of the melt jet at the surface of the coolant water:

$$\frac{dD_J}{dz} = \frac{D_{Ji}}{L_{brk}}, \qquad \text{and} \tag{2.7}$$

$$V_e = \frac{V_J}{2} \frac{D_{Ji}}{L_{brk}}.$$
(2.8)

Eq. (2.8) is employed under the deep coolant water condition $L_{brk} < H_{pl}$ (complete melt jet-breakup). A factor $(H_{pl}/L_{brk})^{1/2}$ is applied to Eq. (2.8) under the shallow coolant water condition $L_{brk} > H_{pl}$ (incomplete melt jet-breakup) to account for the upward steam flow surrounding the melt jet⁽²¹⁾.

The correlation proposed in the literature⁽²²⁾ is employed to estimate L_{brk} based on the Bond number Bo_J , which is defined in terms of the melt jet properties [Eq. (2.9)]. The proposed correlation employs a correlation designated as the "Taylor type" correlation⁽²³⁾ [Eq. (2.10)] when $Bo_J \ge 50$, and a correlation proposed by Saito et al.⁽²⁴⁾ [Eq. (2.11)] when $Bo_J < 50$:

$$Bo_J = \frac{\rho_J g D_{Ji}^2}{\sigma_J},\tag{2.9}$$

$$\frac{L_{brk}}{D_{Ji}} = 10 \left(\frac{\rho_J}{\rho_c}\right)^{1/2}, \qquad \text{and} \qquad (2.10)$$

$$\frac{L_{brk}}{D_{Ji}} = 2.1 \left(\frac{\rho_J}{\rho_c}\right)^{1/2} \left(\frac{V_{Ji}}{gD_{Ji}}\right)^{1/2},\tag{2.11}$$

where ρ denotes the density, and σ denotes the surface tension. The subscripts J and c denote the melt jet and the coolant water, respectively. The symbols D_{Ji} denotes the inlet diameter of the melt jet diameter and V_{Ji} denote the inlet velocity of the melt jet.

The mass flux resulting from the entrainment rate of the melt particles m_e from the melt jet surface is defined as follows, employing a constant value C_{ent} specified through the input file:

$$m_e = C_{ent} \rho_J V_e. \tag{2.12}$$

The L_{brk} is equivalent to the estimated value derived from the proposed correlation when $C_{ent} = 1.0$. An increase in C_{ent} results in a reduction on L_{brk} . The velocity components in the x and z directions of the entrained melt particle v_{ex} and v_{ez} can be expressed as follows:

$$v_{ex} = C_{vx}(2V_e), \qquad \text{and} \qquad (2.13)$$

$$v_{ez} = C_{vzwt}v_J + (1 - C_{vzwt})v_c, (2.14)$$

where C_{vx} and C_{vzwt} are adjustable coefficients specified through the input files. The v_J and v_c denotes the velocity of the melt jet and the coolant water in the z-direction, respectively. It is recommended that the values of C_{vx} and C_{vzwt} is set to approximately 5 and 0.5, respectively.

Friction

The friction coefficient K_{fJ} is determined based on the relative flow velocity between the melt jet and the coolant water under the development of the velocity boundary layer around the melt jet:

$$K_{fJ} = C_{fJ} f_J \frac{\rho_c}{\rho_J} \sqrt{\frac{\Theta}{2A_J}} |v_c - v_J|, \qquad (2.15)$$

where C_{fJ} denotes a constant value, f_J denotes the friction factor, ρ denotes the density, v denote the velocity, A_J denote the cross-sectional area of the melt jet, and Θ denotes the sector angle of the melt jet. The subscripts J and c denote the melt jet and the coolant water, respectively. At present, C_{fJ} is set to unity, and f_J is determined by the following equations:

$$f_J = \max(16/Re_d, 0.0791/Re_d^{0.25}), \tag{2.16}$$

$$Re_{d} = \rho_{c} d_{bnd} (v_{J} - v_{c}) / \mu_{c}, \qquad (2.17)$$

$$d_{bnd} = 0.37 z_{bnd} / Re_z^{0.2}, \qquad \text{and} \qquad (2.18)$$

$$Re_{z} = \rho_{c} z_{bnd} (v_{J} - v_{c}) / \mu_{c}, \qquad (2.19)$$

where Re_d denotes the Reynolds number using the thickness of the velocity boundary layer d_{bnd} , and Re_z denotes the Reynolds number using the distance of the melt jet leading edge z_{bnd} from the surface of the coolant water, and μ denotes the kinematic viscosity. Eq. (2.18) is based on the development of a turbulent boundary layer on a horizontal flat plate⁽²⁵⁾. An alternative option to determining K_f is available, whereby the friction factor f_J is determined through the input file:

$$K_{fJ} = f_J \frac{\rho_c}{\rho_J} \sqrt{\frac{\Theta}{2A_J}} |v_c - v_J|.$$
(2.20)

Heat Transfer

The heat transfer from the surface of the melt jet is currently disregarded due to the significantly smaller surface area of the melt jet in comparison to those of the melt pool and the melt particle, which is attributed to the short time period of travel in the coolant water. Consequently, the heat flux q in Eq. (2.4) is set to zero in the latest version in the JASMINE code.

2.2.2 Melt Pool

Basic Equations

The melt pool model represents a solution to one-dimensional conservation equations in the horizontal (radial) direction. The melt jet or melt particle reached the bottom and contributed to the formation of a continuous melt pool. The conservation equations for mass, internal energy, and momentum in a non-conservation form are expressed as Eqs. (2.21)–(2.23). The shallow water approximation is applied for the melt pool model to introduce the conservation equation, utilizing the melt pool height h_P . Note that the coordinate x is defined as the positive horizontal direction from the center of the simulation domain.

$$\frac{\partial(wh_P\rho_P)}{\partial t} + \frac{\partial(wh_P\rho_P)}{\partial x} = wm_s, \qquad (2.21)$$

$$\frac{\partial e_P}{\partial t} + v_P \frac{\partial e_P}{\partial x} = \frac{q}{h_P \rho_P} + \frac{(e_{ms} - e_P) \max(m_s, 0)}{h_P \rho_P}, \qquad \text{and} \qquad (2.22)$$

$$\begin{split} \frac{\partial v_P}{\partial t} + v_P \frac{\partial v_P}{\partial x} &= -\frac{1}{\rho_P} \left[\frac{\partial p_a}{\partial x} + \frac{g}{2} \frac{\partial (h_P \rho_P)}{\partial x} \right] + K_{fP} (v_c - v_P) - K_{fw} v_P \\ &+ \frac{(v_{ms} - v_P) \max(m_s, 0)}{h_P \rho_P}, \end{split}$$
(2.23)

where ρ denotes the density, e denotes the internal energy, and v denotes the velocity. The subscripts P and c denote the melt pool, and the coolant water respectively. The width of the simulation domain or the cell grid is described as $w = x\Theta$. The symbol p_a denote the ambient pressure exerted by the coolant water.

The m_s denotes the mass flux resulting from the merging of the melt jet and melt particle to the melt pool, and the q denotes the heat flux from the surface of the melt pool. The K_{fP} and K_{fw} denote the friction coefficient between the melt pool and coolant water, and between the melt pool and bottom floor, respectively. The values of m_s , q, K_{fP} and K_{fw} in the source terms are specified thorough the application of the constitutive models.

Constitutive Models

Friction

The friction on the surface and bottom of the melt pool is currently disregarded, as the primary object is the heat and mass transfer. The objective of the melt pool model is to incorporate the heat and mass transfer or exchange from the melt jet and melt particles in a manner that is consistent with underlying physical principles. Consequently, the friction coefficients K_{fP} and K_{fw} in Eq. (2.23) are set to zero in the latest version of the JASMINE code.

Heat Transfer

The heat transfer from the surface of the melt pool, including radiation, film boiling, nucleate boiling, and convection, is expressed using a collection of available correlations. In order to represent the boiling heat transfer, the boiling curve is expressed by combining the correlations associated with different boiling regimes, as illustrated in Fig. 2.2. Note that the boiling heat transfer is operational when the surface temperature of the melt pool T_w exceeds the saturation temperature of the coolant water T_{sat} .

1. Convection:

In order to ascertain the heat flux q_{cvf} in the convection regime, a correlation for natural convection over a horizontal plane⁽²⁶⁾ is utilized, which is expressed as follows:

$$q_{cvf} = Nu_{cvf}(\lambda_a/d)(T_w - T_a), \tag{2.24}$$

$$Nu_{cvf} = 0.15 Ra_a^{1/3},$$
 and (2.25)

$$Ra_a = Gr_a Pr_a = \{g\beta(T_w - T_a)d^3\nu_a^2\}Pr_a, \qquad (2.26)$$

where Nu_{cvf} denotes the Nusselt number, λ denotes the thermal conductivity, ν denote the dynamic viscosity, Ra denotes the Rayleigh number, Gr denotes the Grashof number, and Pr denotes the Prandtl number. The subscripts a denotes the ambient water in the liquid l or gas (steam) v phases. The symbol d denotes the spreading distance of a melt pool, which is defined as the distance from the impingement point of the melt jet to the tip of the melt pool. The correlation [Eq. (2.24)] is approximately valid for $Nu_{cvf} = 50 - 1000$.

The heat flux in the convection regime for the liquid and gas components of the coolant water, or q_{cvfl} and q_{cvfg} , is calculated separately, and then combined to determine q_{cvf} , according to the flow regime, or weighting function Eqs. (2.1) and (2.2), which is expressed as $q_{cvf} = (1 - f_{\alpha})q_{cvfl} + f_{\alpha}q_{cvfg}$.



Fig. 2.2 A conceptual framework for boiling heat transfer that encompasses the combined correlations associated with the boiling regimes: convection, nucleate boiling, transition boiling, and film boiling.

2. Nucleate Boiling:

In order to determine the heat flux q_{nbf} in the nucleate boiling regime, a correlation proposed by Kutateladze⁽²⁷⁾ is employed, which is expressed as follows:

$$q_{nbf} = 3.05 \times 10^{-11} \{\lambda_l (T_w - T_{sat})\} P r_l^{7/6} \left\{ \frac{\sigma_l}{g(\rho_l - \rho_v)} \right\}^{2/3} \left(\frac{p_a \rho_l}{\sigma_l \Delta h_{fg} \mu_l \rho_v} \right),$$
(2.27)

where λ denotes the thermal conductivity, Pr denotes the Prandtl number, σ denotes the surface tension, ρ denotes the density, Δh_{fq} denotes the latent heat of evaporation, and μ denotes the

kinematic viscosity. The subscripts l and v denote the coolant water in a liquid and gas (steam) phases, respectively. The symbol p_a denotes the ambient pressure exerted by the coolant water.

3. Critical Heat Flux:

The critical heat flux (CHF) q_{chf} is defined as the heat flux at the point of transition from the nucleate boiling regime to the transition boiling regime. A theoretical formulation proposed by Zuber⁽²⁸⁾ is employed, which is expressed as follows:

$$q_{chf} = 0.131 \frac{\Delta h_{fg} \rho_v}{\{\rho_v^2 / \sigma_l g(\rho_l - \rho_v)\}^{1/4}}.$$
(2.28)

The surface temperature of the melt pool T_{chf} corresponding to q_{chf} is derived by solving Eq. (2.27) when q_{nbf} is equal to q_{chf} . The T_{chf} can be expressed in an analytical form.

4. Film Boiling:

In order to ascertain the heat flux q_{fbf} in the film boiling regime, a correlation proposed by Berenson⁽²⁹⁾ is utilized, which is expressed as follows:

$$q_{fbf} = N u_{fb} (\lambda_{vf} / L) (T_w - T_l), \qquad \text{and} \qquad (2.29)$$

$$Nu_{fbf} = 0.425 \left\{ \frac{g\rho_{vf}(\rho_l - \rho_{vf})L^3/\mu_{vf}^2}{c_{pv}(T_w - T_{sat})/\Delta h_{fg} Pr_{vf}} \right\}^{1/4},$$
(2.30)

where L denote the Laplace length, and $\Delta h'_{fg}$ denotes the modified latent heat of evaporation. The L and $\Delta h'_{fg}$ are defined as follows:

$$L = \sqrt{\sigma_l / g(\rho_l - \rho_{vf})}, \qquad \text{and} \tag{2.31}$$

$$\Delta h'_{fg} = \Delta h_{fg} + 0.5c_{pvf}(T_w - T_{sat}), \tag{2.32}$$

where c_p denotes the specific heat. The subscripts vf denotes the vapor film. The vapor film properties are evaluated based on the film temperature defined as $T_{vf} = 0.5(T_w + T_v)$.

5. Minimum film boiling heat flux:

The minimum film boiling (MFB) heat flux q_{mfb} is defined as the heat flux at which a transition occurs from the transition boiling regime to the film boiling regime. A correlation proposed by Berenson⁽²⁹⁾ is employed, which is expressed as follows:

$$q_{mfb} = 0.09 \frac{\Delta h_{fg} \rho_{vf}}{\{\rho_v^2 / \sigma_l g(\rho_l - \rho_{vf})\}^{1/4} \{(\rho_l - \rho_{vf}) / \rho_{vf}\}^{1/2}}.$$
(2.33)

The temperature of the surface of the melt pool T_{mfb} corresponding to q_{mfb} is derived by solving Eq. (2.29) when q_{fbf} is equal to q_{mfb} . The T_{mfb} can be obtained through the application of the Newton-Raphson Method.

6. Transition Boiling:

The heat flux q_{tbf} in the transition boiling regime is determined through a liner interpolation between the critical heat flux point $(q_{chf} \text{ at } T_{chf})$ and the minimum film boiling point $(q_{mfb} \text{ at } T_{mfb})$ (see Fig. 2.2). The liner interpolation for the heat flux q_{tbf} in the transition boiling regime is standard and frequently used to incorporate the boiling curve into the simulations.

7. Radiation:

In order to ascertain the heat flux q_{rad} for the radiation heat transfer, the Stefan-Boltzmann law is employed, which is expressed as follows:

$$q_{rad} = \epsilon_P \sigma_{SB} (T_w^4 - T_l^4), \tag{2.34}$$

where ϵ_P denotes the emissivity at the surface of the melt pool, and σ_{SB} denotes the Stefan-Boltzmann constant. Note that the liquid water temperature T_l is referred to determine the q_{rad} because the gas (steam) phase is regarded to be transparent with respect to the radiation heat transfer.

It is assumed that the boiling and radiation heat transfer are attenuated by the void formation when the flow regime deviates from the bubbly flow (liquid continuous) regime. Additionally, in order to address the numerical issues, the boiling and radiation heat transfer are terminated or cut off at high void fraction $\alpha > 0.95$. In order to incorporate the void formation, the cut-off functions f_{α} are defined as follows:

Nucleate Boiling:

In the bubbly flow regime, where $\alpha < 0.3$, the value of $f_{\alpha,nb} = 1$. In the high void fraction regime, where $\alpha > 0.5$, the value of $f_{\alpha,nb} = 0$. In the transition regime, the value of $f_{\alpha,nb}$ is determined through a process of linear interpolation.

$$f_{\alpha,nb} = \begin{cases} 1 & (0 \le \alpha \le 0.30) \\ 1 - (\alpha - 0.30)/0.2 & (0.30 \le \alpha \le 0.50). \\ 0 & (0.50 \le \alpha \le 1.00) \end{cases}$$
(2.35)

Film Boiling:

In the bubbly flow regime, where $\alpha < 0.3$, the value of $f_{\alpha,fb} = 1$. In the high void fraction regime, where $\alpha > 0.95$, the value of $f_{\alpha,nb} = 0$. In the transition regime, the value of $f_{\alpha,fb}$ is determined through a process of linear interpolation.

$$f_{\alpha,fb} = \begin{cases} 1 & (0 \le \alpha \le 0.30) \\ \{(0.95 - \alpha)/0.65\}^n & (0.30 \le \alpha \le 0.95). \\ 0 & (0.95 \le \alpha \le 1.00) \end{cases}$$
(2.36)

Radiation:

In the bubbly flow regime, where $\alpha < 0.3$, the value of $f_{\alpha,rd} = 1$. In the high void fraction regime, where $\alpha > 0.95$, the value of $f_{\alpha,rd} = 0$. In the transition regime, the value of $f_{\alpha,rd}$ is determined through a process of linear interpolation.

$$f_{\alpha,rd} = \begin{cases} 1 & (0 \leq \alpha \leq 0.30) \\ \{(0.95 - \alpha)/0.65\}^n & (0.30 \leq \alpha \leq 0.95), \\ 0 & (0.95 \leq \alpha \leq 1.00) \end{cases}$$
(2.37)

where n denotes the value of the arbitrary constant to adjust the attenuation rates for both the film boiling and the radiation heat transfer in the transition regime. The value of n is set to unity.

The heat flux in the film boiling regime is expressed by combining the radiation heat transfer models as proposed by Bromely et al.⁽³⁰⁾ and Liu and Theofanous⁽³¹⁾:

$$q_{fbf} + \frac{7}{8}q_{rad}.$$
 (2.38)

Accordingly, the total heat flux q_{tot} is defined as the sum of the convection, boiling, and radiation heat transfer, and is expressed as follows:

$$q_{tot} = q_{cvf} + q_{bol} + \frac{7}{8}q_{rad},$$
(2.39)

where q_{bol} denotes the boiling heat flux. The boiling heat transfer from the surface of the melt pool is determined based on the following framework.

Convection Regime:

The boiling heat transfer is inoperative or $q_{bol} = 0$ when $T_w < T_{sat}$ within the convection regime. The total heat flux is calculated as $q_{tot} = q_{cvf}$. The radiation heat transfer is also inoperative or $q_{rad} = 0$ in the convection regime.

Nucleate Boiling Regime:

The nucleate boiling heat flux q_{nbf} is applied to q_{bol} when $T_w < T_{chf}$ within the nucleate boiling regime. The total heat flux is calculated as $q_{tot} = q_{cvf} + q_{nbf} + (7/8)q_{rad}$, which includes both the convection and the radiation heat transfer.

Transition Boiling Regime:

The transition boiling heat flux q_{tbf} is applied to q_{bol} when $T_{chf} < T_w < T_{mfb}$ within the transition boiling regime. The total heat flux is calculated as $q_{tot} = q_{cvf} + q_{tbf} + (7/8)q_{rad}$, which includes both the convection and the radiation heat transfer.

Film Boiling Regime:

The film boiling heat flux q_{mbf} is applied to q_{bol} when $T_w > T_{mfb}$ within the film boiling regime. The total heat flux is calculated as $q_{tot} = q_{cvf} + q_{fbf} + (7/8)q_{rad}$, which include both the convection and the radiation heat transfer.

Surface Temperature of Melt Pool

The heat transfer from the surface of the melt pool is dependent upon the surface temperature of the melt pool. Due to the relatively low thermal conductivity of oxide melts, which are typical core melt materials, the surface temperature of the melt pool can be significantly lower than the average temperature. In order to lower the surface temperature of the melt pool, a simple model is employed which assumes a quadratic temperature profile across the melt pool height h_P (see Appendix B). The surface temperature T_{sf} is expressed as follows:

$$T_{sf} = \frac{T_{av} + T_c \frac{h_P H}{6\lambda_P}}{1 + \frac{h_P H}{6\lambda_P}},$$
(2.40)

where T_{av} denotes the average temperature of the melt pool, T_c denotes the temperature of the coolant water, λ_P denotes the thermal conductivity of the melt pool, and H denotes the heat transfer coefficient at the surface of the melt pool. As the simple model is quite coarse, it is essential to confirm that the relation of $T_c \leq T_{sf} \leq T_{av}$ is maintained. If an anomalous value being observed, the value of T_{sf} is set to $0.5(T_{av} + T_c)$ in lieu of the value of T_{sf} estimated from the simple model.

Merging of Melt Jet and Particles into Melt Pool

Upon on the arrival of leading edge of the melt jet at the bottom of the simulation domain, the mass and energy of the melt jet are merged into the melt pool at the central node or cell. The momentum of the melt jet is incarnated into the melt pool through the addition of the stagnant impulse resulting from the impingement of the melt jet on the central node or cell of the simulation domain.

Solidification of Melt Pool

The solidification of the melt pool is evaluated based on the average temperature of the entirety of the melt pool. If the average temperature of the entire body of the melt pool is less than the melting point, the melt pool is considered to be in a solid state or the solid pool. The velocity of the melt pool is set to zero throughout the entirety of the melt pool.

2.2.3 Melt Particle

Basic Equations

The concept of the "group particle" facilitates the practical application of the JASMINE code to large systems, such as plant-scale simulations, where the number of the melt particles may exceed the limits of direct simulation. The grouped particle is scalable in accordance with the available computational resources, whereby an appropriate selection of particle group sizes is made in order to ensure the most efficient use of computational power.

A single "particle group" is defined as a set of n_p melt particles, which are assumed to possess uniform properties within a finite size of $2r_x$ and $2r_z$ on the x-z plane [see Fig. 1.2 (a)]. The finite size of particle groups is advantageous for the uninterrupted transfer of volume, force, and heat sources associated with the melt particles between the two-phase flow cells. If a particle group is assumed to be a point, the source terms for the two-phase flow model would abruptly transition from one cell to another, which could potentially give rise to the numerical issues. For the sake of simplicity, other attributes of the particle group, such as, realistic shape, rotation, and diffusive features, have been excluded from consideration. The conservation of mass and energy for a single melt particle within a particle groups are expressed as follows:

$$\frac{\partial \boldsymbol{v}_p}{\partial t} = \boldsymbol{g} - \frac{\nabla p_a}{\rho_p} + \frac{\boldsymbol{F}_{hy}}{m_p},\tag{2.41}$$

$$\frac{\partial \boldsymbol{x}_p}{\partial t} = \boldsymbol{v}_p, \qquad \text{and} \qquad (2.42)$$

$$\frac{\partial e_p}{\partial t} = -\frac{q}{m_p},\tag{2.43}$$

where v denotes the velocity (v_x, v_z) , x denotes the position (x, z), m denotes the mass, and e denotes the internal energy. The subscript p denotes the melt particle. Noted that m_p is defined as the total mass of the melt particles contained in a particle group, and e_p is defined as the internal energy per unit mass, rather than per unit particle.

The F_{hy} denotes the drag force resulting from hydrodynamic interactions, and the q denotes the heat flux from the surface of the melt particles. The values of F_{hy} and q in the source terms are specified thorough the application of the constitutive models.

Particle Groups Release

As the melt particles are released from the surface of the melt jet, the related variables from each cell of the melt jet at each time step are provided to those of the melt particles. The related variables are the properties of the melt particles, including mass, temperature, diameter, and velocity. The release of a particle group from each cell of the melt jet at each time step results in an excessive number of particle groups. The mass or number of particle groups in a single time step at a specific cell is negligible.

To address the issue of disparate discretization forms within the Eulerian and Lagrangian frameworks, the JASMINE code has introduced the concept of a "pre-particle group" as a buffer, as illustrated in Fig. 2.3. The melt particles that released immediately upon on the surface of the melt jet are temporarily stored in pre-particle groups.



Fig. 2.3 A conceptual framework for the particle group releases from the surface pf the melt jet: the geometrical relationship between the pre-particle groups and the real-particle groups.

The pre-particle groups are released as "real particle groups" when they have reached a sufficient level of mass or particle number, as determined by the relevant criteria. Each pre-particle group is attached to each cell of the melt jet, with a vertical size equivalent to that of the cell of the melt jet or $2r_z = \Delta z_J$. The horizontal size of the pre-particle group $2r_x$ increases in proportion to the mass or number of melt particles as one moves outward. The pre-particle groups are able to exchange momentum and energy with the coolant water until they are released as the real-particle groups. In a state where the total mass of a pre-particle group is greater than zero, the criteria for particle group release are met when one of the following conditions is satisfied:

1. Number of Particles:

If the number of melt particles within a pre-particle group N_p exceeds the specified criterion N_{pcr} through the input file, the pre-particle group is released into the simulation domain.

2. Particle Group Size:

If the half of a pre-particle group in the x-direction r_x exceeds the criterion r_{xcr} , the pre-particle group is released. The r_{xcr} is defined as $\Delta x_{min}/4$, where Δx_{min} denotes the minimum cell size in the x-direction of the simulation domain.

3. Edge Position:

If the edge position of a pre-particle group in the x-direction $x_p + r_x$ exceeds the boundary of the central cell, the pre-particle group is released within the simulation domain.

4. Elapsed Time:

The elapsed time of a pre-particle group since released as the pre-particle group exceeds the specified time step N_{hist} through the input file, the pre-particle group is released within the simulation domain.

In accordance with the release of a pre-particle group, the velocity of the entrained melt jet, as defined by Eq. (2.13), is transferred to the velocity component in the *x*-direction of a real-particle group:

$$m_e v_{ex} = m_p v_{px}.\tag{2.44}$$

If "prmpa_ivxran=1," is specified through the input file, the following multiplier is applied to v_{xp} ,

$$f_r = 0.02 + 0.98\phi_r, \tag{2.45}$$

where ϕ_r denotes a normalized random number distributed uniformly between 0 and 1. The stochastic function f_r serves as a trial model for articulating the stochastic nature of the initial velocity of melt particles released through turbulence surrounding the melt jet.

Interactions between Particle Groups

It is imperative to establish a set of rules in order to prevent the occurrence of physically unreasonable situations that could arise from the interactions between particle groups or between a particle group and a boundary. The interactions between the particle groups include the process of the bounce, the merge, and the passing each other or no interactions.

1. Bounce:

A bounce is defined as occurring when the sum of the volume fractions of melt particles in two particle groups in contact $\alpha_A + \alpha_B$ exceeds the packing limit α_{pack} . In order for the velocity of the particle groups to be updated due to the bounce process, the particle groups need to satisfy the following criteria.

The state of overlapping or separation: if $r_{x,A} + r_{x,B} < dx$ or $r_{z,A} + r_{z,B} < dz$, the particle groups are deemed to be in a state of separation Fig. 2.4, The process is continued if the particle groups are in the state of overlapping.



Fig. 2.4 Schematics to judge the state of overlapping or separation of the particle groups: (a) in a state of separation, and (b) in a state of overlapping.

The degree of overlap in each direction: if $O_x = r_{x,A} + r_{x,B} - dx < O_z = r_{z,A} + r_{z,B} - dz$, the degree of overlap in the *x*-direction is deemed significant [Fig. 2.5 (a)], while if $O_x > O_z$, the degree of overlap in the *z*-direction is deemed significant [Fig. 2.5 (b)]. The process is continued if the degree of overlap is significant.

The direction of movement on approaching or receding: if $x_{p,A} - x_{p,B} < 0$ and $v_{p,A} - v_{p,B} > 0$, the particle groups are approaching [Fig. 2.6 (a)], while if $x_A - x_B < 0$ and $v_{p,A} - v_{p,B} < 0$, the particle groups are rescinding [Fig. 2.6 (b)]. Note that the judgment is made in the direction where the degree of overlapping is significant. The process is continued if the particle groups are approaching.



Fig. 2.5 Schematics to judge the degree of overlapping of the particle groups in each direction: (a) significant overlapping in the x-direction, and (b) significant overlapping in the z-direction.



Fig. 2.6 Schematics for the relationship between the signs of the difference in central positions and velocities to judge the approaching or receding of the particle groups.

Table 2.1 lists the relationship between the signs of the difference in central positions and velocities, which can be used to judge the approaching or receding of the particle groups. The velocity of the particle groups is updated when the requisite criteria have been satisfied. When the degree of overlap of the particle groups is determined based on the second criterion or the degree of overlap in each direction, the velocity component in the direction of the greater degree of overlap is updated according to the following equations:

$$\boldsymbol{v}_{p,cnt} = \frac{m_{p,A} \boldsymbol{v}_{p,A} + m_{p,B} \boldsymbol{v}_{p,B}}{m_{p,A} + m_{p,B}},$$
(2.46)

$$\boldsymbol{v}_{p,A}' - \boldsymbol{v}_{p,cnt} = -C_{damppar}(\boldsymbol{v}_{p,A} - \boldsymbol{v}_{p,cnt}), \qquad \text{and} \qquad (2.47)$$

$$\boldsymbol{v}_{p,B}' - \boldsymbol{v}_{p,cnt} = -C_{damppar}(\boldsymbol{v}_{p,B} - \boldsymbol{v}_{p,cnt}), \qquad (2.48)$$

where $v_{p,cnt}$ denotes the velocity vector of the center of gravity between particle groups, $v_{p,A}$ denotes the velocity vector of particle group A, $v_{p,B}$ denotes the velocity vector of particle group B, $m_{p,A}$ denotes the total mass of particle group A, $m_{p,B}$ denotes the total mass of particle group B, and $C_{damppar}$ denotes a damping factor that is specified through the input file.

Table 2.1 Relationship between the sings of the difference in central positions and velocities, which can be used to judge the approaching or receding of the particle groups.

	$oldsymbol{x}_{p,A} - oldsymbol{x}_{p,B}$	$oldsymbol{v}_{p,A} - oldsymbol{v}_{p,B}$	Movement
	+	+	Receding
<u>C</u> iana	+	_	Approaching
Signs	_	+	Approaching
	_	_	Receding

The relationship between the velocity of the particle groups and the damping factor is introduced based on the definition of the damping factor, as expressed in Eq.(2.49).

$$v'_{p,A} - v'_{p,B} = -C_{damppar}(v_{p,A} - v_{p,B}).$$
 (2.49)

The value of $v_{p,cnr}$ remains constant prior to and subsequent to the bounce process between the particle groups, as the sum of the momentum is in a state of equilibrium or zero. The momentum equations for the particle groups both prior to and subsequent to the bounce process, are described as follows:

$$m_{p,A}(v_{p,A} - v_{p,cnt}) = m_{p,B}(v_{p,B} - v_{p,cnt}), \qquad \text{and} \qquad (2.50)$$

$$m_{p,A}(v'_{p,A} - v_{p,cnt}) = m_{p,B}(v'_{p,B} - v_{p,cnt}).$$
(2.51)

In order to introduce Eqs. (2.47) or (2.48), it is necessary to eliminate the velocity of either of the particle groups in Eq. (2.49) using Eqs. (2.50) or (2.51).

$$\begin{aligned} (\boldsymbol{v}_{p,A}^{'} - \boldsymbol{v}_{p,cnt}^{'}) &- (\boldsymbol{v}_{p,B}^{'} - \boldsymbol{v}_{p,cnt}^{'}) \\ &= -C_{dampar} \{ (\boldsymbol{v}_{p,A} - \boldsymbol{v}_{p,cnt}^{'}) - (\boldsymbol{v}_{p,B} - \boldsymbol{v}_{p,cnt}^{'}) \}. \end{aligned}$$
(2.52)

The elimination of $(v'_{p,B} - v_{p,cnt})$ and $(v_{p,B} - v_{p,cnt})$ from Eq. (2.52), results in the derivation of Eq. (2.47) for example.

2. Merge:

A merge is defined occurring when the sum of the volume fractions of melt particles in two particle groups in contact $\alpha_A + \alpha_B$ falls below the packing limit α_{pack} . In order for the properties of the particle groups to be updated due to the merge process, the particle groups need to satisfy the following criteria.

The state of overlapping or separation, which is analogous to that employed to ascertain the bounce process (Fig. 2.4). A greater degree of overlapping of the particle groups, exceeding 20%, is necessary for the process to be continued.

The overall size of the overlapping the particle groups: if $r_{x,A} + r_{x,B} + dx < \Delta x_{min}$ and $r_{z,A} + r_{z,B} + dz < \Delta z_{min}$, the particle groups are deemed sufficiently close to each other. The symbols Δx_{min} and Δz_{min} denote the minimum size of grid width in each direction.

The difference in the properties of the particle groups: if the relative deviations of total mass, average temperature, and velocity between the particle groups are less than the threshold specified through the input file, the properties are deemed sufficiently close to each other. Once the requisite criteria have been met, the particle groups are merged into a single particle group. The two particle groups are merged into a single entity, designated by the smaller group number. The remaining group number is then to be absent. In the event that a new particle group is generated, the absent group number is not reused.

3. No Interference:

The two particle groups will operate independently or simply pass through each other without any interference when they do not satisfy the requisite criteria for the bounce or merge process.

Interaction Between Particle Groups and Boundaries

1. Complete Bounce:

At the central boundary, the particle groups undergo a deflection and subsequent return to the simulation domain in the complete bounce process. If the center position of the particle group x_p exceeded the boundary position x_{min} , the x_p is repositioned to $x_p = x_{min}$ at the central boundary in the x-direction, as illustrated in Fig. 2.7 (a). The direction of the velocity component in the x-direction is reversed while the magnitude of the velocity remains unaltered with a damping factor $C_{dampwall} = 1.0$.

2. Damped Bounce:

At the upper boundary in the z-direction or lateral boundary in the x-direction, the particle groups undergo a deflection and subsequent return to the simulation domain in the damped bounce process. If the center position of the particle group x_p exceeded the boundary position x_{max} , the x_p is repositioned $x_p = x_{max}$ at the lateral or outer boundary in the x-direction, as illustrated in Fig. 2.7 (b) for example. The direction of the velocity component in the x-direction is reversed while the magnitude of the velocity is reduced with a damping factor $C_{dampwall} = 0.1$.


Fig. 2.7 Schematics of the bounce back processes between the particle groups and boundaries: (a) complete bounce at the central boundary, and (b) damped bounce at outer boundary in the x-direction.



Fig. 2.8 Schematics of the stuck process between the particle group and boundaries: (a) stuck process on the solid pool, and (b) stuck process on the bottom surface.

3. Merge or Stuck:

At the bottom boundary of the simulation domain, the particle groups merge into the melt pool when the melt pool and melt particles are in a molten state. It is necessary for the melt pool depth h_P to be greater than both the threshold Δz_{min} and the melt particle diameter D_p for the merge process. The average or surface temperature is employed to ascertain whether the melt particles and melt pool are in a molten state, which can be specified through the input file. Note that the mass and energy of the particle groups are added to the melt pool while the momentum is not included during the merge process in the latest version of the JASMINE code.

The particle group piles up (stuck) on the solid pool or the bottom surface, and forms a debris bed when they do not satisfy the criteria for the merge process. If a particle group joins in the debris bed, the particle group is vertically collapsed when the volume fraction of the melt particles α is larger than the packing limit α_{lim} . The height of the particle group becomes equal to the particle size, $D_p/2$ or packing limit $r_z(\alpha_{pack}/\alpha)$. The center position of the particle group z_p is adjusted so that the particle groups is set on the solid melt surface or bottom surface, as illustrated in Fig. 2.8.

Constitutive Models

Drag Force

A correlation for a rigid sphere subjected to flow⁽³²⁾ is employed to determine the drag force F_{hy} that acts on the melt particles, which is expressed as follows:

$$\mathbf{F}_{hy} = -C_{fp} f \frac{\pi}{4} D_p^2 \frac{1}{2} \rho_p |\mathbf{v}_r| \mathbf{v}_r,$$
(2.53)

$$f = \max(24/Re_p, 18.5/Re_p^{0.6}, 0.44), \qquad \text{and} \tag{2.54}$$

$$Re_p = \rho_p D_p |\boldsymbol{v}_r| / \mu_a, \tag{2.55}$$

where C_{fp} denotes a correction parameter that accounts for the deformation and irregular shapes of melt particles, v_r denotes the relative velocity between the melt particle and the coolant water in liquid or gas phases, ρ denote the density, and μ denote the kinematic viscosity. The subscript *a* denotes the ambient water in the liquid *l* or gas (steam) *v* phases.

The drag force for the liquid and gas components of the coolant water, or F_{hyl} and F_{hyg} , is calculated separately, and then combined to determine F_{hy} , according to the flow regime or weighting function Eqs. (2.1) and (2.2), which is expressed as $F_{hy} = (1 - f_{\alpha})F_{hyl} + f_{\alpha}F_{hyg}$.

Heat Transfer

The heat transfer from the surface of melt particles, including radiation, film boiling, nucleate boiling, and convection, is expressed using a collection of available correlations around a rigid sphere. In the case of boiling heat transfer, the boiling curve is expressed by combining the correlations associated with different boiling regimes, as illustrated in Fig. 2.2. Note that boiling heat transfer is operational when the surface temperature of the melt particle T_w exceeds the saturation temperature of the coolant water T_{sat} .

1. Convection:

In order to ascertain the heat flux in the convection regime q_{cvp} , a correlation for forced convection around a rigid sphere⁽³³⁾ is utilized, which is expressed as follows:

$$q_{cvp} = N u_{cvp} (\lambda_a / D_p) (T_w - T_a), \qquad (2.56)$$

$$Nu_{cvp} = 2 + 0.6 Ra_p^{1/2} Pr_a^{1/3}, \qquad \text{and} \qquad (2.57)$$

$$Ra_p = \rho_p D_p |\boldsymbol{v}_r| / \mu_a, \tag{2.58}$$

where Nu_{cvp} denotes the Nusselt number, λ denotes the thermal conductivity, D denotes the diameter, Ra denotes the Rayleigh number, Gr denotes the Grashof number, Pr denotes the Prandtl number, $|v_r|$ denotes the absolute value of the relative velocity between the melt particle and the coolant water in liquid or gas phases, ρ denote the density, and μ denote the kinematic viscosity. The subscripts a denotes the ambient water in the liquid l or gas (steam) v phases, and p denotes the melt particle.

The heat flux in the convection regime is calculated for the liquid and gas components of the coolant water separately, and then combined according to the flow regime based on the weighting function Eqs. (2.1) and (2.2). Note that the convection heat transfer is cut off at a high void fraction ($\alpha > 0.90$), which differs from the convection heat transfer utilized in the melt pool.

2. Nucleate Boiling:

In order to ascertain the heat flux q_{nbp} in the nucleate boiling regime, a correlation proposed by Kutateladze⁽²⁷⁾ is utilized, which is expressed as Eq. (2.27).

3. Critical Heat Flux:

The critical heat flux (CHF) q_{chf} is defined as the heat flux at the point of transition from the nucleate boiling regime to the transition boiling regime. A theoretical formulation proposed by Zuber⁽²⁸⁾ is employed, which is expressed as Eq.(2.28). The surface temperature of the melt particle T_{chf} corresponding to q_{chf} is derived by solving Eq. (2.27) when q_{nbp} is equal to q_{chf} . The T_{chf} can be expressed in an analytical form, as employed in the melt pool.

4. Film Boiling:

In order to ascertain the heat flux q_{fbp} in the film boiling regime, a correlation proposed by Liu and Theofanous⁽³¹⁾ is utilized, which is expressed as follows:

$$q_{fbp} = N u_{fbp} (\lambda_{vf} / D_p) (T_w - T_l),$$
(2.59)

$$Nu_{fbp} = \{Nu_p^5 + (F_f Nu_f)^5\}^{1/5},$$
(2.60)

$$F_f = 1 - 0.2 / \left\{ 1 + (Fr_l^{1/2} - 1) \right\}, \tag{2.61}$$

$$Fr_l = |\boldsymbol{v}_{rl}|^2 / gD_p, \tag{2.62}$$

$$Nu_{f} = Nu_{s} + 0.072 Re_{l}^{0.77} Pr_{l}^{1/2}(\mu_{l}/\mu_{vf})(Sc'/Sp'), \qquad (2.63)$$

$$Nu_s = 0.5Re_l^{1/2}(\mu_l/\mu_{vf})(KR^4/Sp')^{1/4},$$
(2.64)

$$Re_l = \rho_l D_p |\boldsymbol{v}_{rl}| / \mu_l, \tag{2.65}$$

$$Nu_p/(1+2/Nu_p) = kc(Ar/Sp')^{1/4}Mc^{1/4},$$
(2.66)

$$Mc = E^{3} / \{ (1 + ESp' Pr_{l})(RPr_{l}Sp')^{2} \},$$
(2.67)

$$E = (A + CB^{1/2})^{1/3} + (A - CB^{1/2})^{1/3} + (1/3)Sc',$$
(2.68)

$$A = (1/27)Sc'^{3} + (1/3)R^{2}Sp'Pr_{l}Sc' + (1/4)R^{2}Sp'^{2}Pr_{l}^{2},$$
(2.69)

$$B = -(4/27)Sc'^{2} + (2/3)Sp'Pr_{l}Sc' - (32/27)R^{2}Sp'^{2}Pr_{l} + (1/4)Sp'^{2}Pr_{l}^{2} + (2/27)Sc'^{3}/R^{2},$$
(2.70)

$$C = (1/2)R^2 Sp' Pr_l, (2.71)$$

$$K = \rho_l / \rho_{vf}, \tag{2.72}$$

$$R = (\mu_{vf} \rho_{vf} / \mu_l \rho_l)^{1/2}, \tag{2.73}$$

$$Ar = g(\rho_l - \rho_{vf}) D_p^3(\mu_{vf}^2 / \rho_{vf}),$$
(2.74)

$$D' = D_p / \{\sigma_l / g(\rho_l - \rho_{vf})\}^{1/2},$$
(2.75)

$$Sc' = c_{pl}\Delta T_{sub} / \Delta h'_{fg} Pr_l, \qquad (2.76)$$

$$Sp' = c_{pvf} \Delta T_{sup} / \Delta h'_{fg} Pr_{vf}, \qquad (2.77)$$

$$\Delta h'_{fg} = \Delta h_{fg} + 0.5c_{pvf}\Delta T_{sup}, \qquad \text{and} \qquad (2.78)$$

$$kc = \begin{cases} 0.5/D'^{1/4} & (D' \le 0.14) \\ 0.86/(1+0.28D') & (0.14 \le D' \le 1.25) \\ 2.4D'/(1+3.0D') & (1.25 \le D' \le 6.6) \\ 0.47D'^{1/4} & (6.6 \le D') \end{cases}$$
(2.79)

where $|v_{rl}|$ denotes the absolute value of the relative velocity between the melt particle and the liquid water. The liquid water temperature T_l is employed in the superheat term, that is, $(T_w - T_l)$, in lieu of the saturation temperature, as this is more favorable for numerical stability. The subscripts vf denotes the vapor film. Note that the physical properties of the vapor film are evaluated using the film temperature, which is defined as $T_{vf} = 0.5(T_w + T_v)$.

In the original correlation, the effect of void fraction α is directly incorporated into the Nu_s . In the latest version of the JASMINE code, the effect of α is incorporated by multiplying the cutoff function f_{α} [Eq. (2.36)] by the film boiling heat flux q_{fbp} . The calculated values of q_{fbp} obtained using the approach demonstrate a high degree of agreement with those obtained from the original correlation.

5. Minimum Film Boiling Heat Flux:

The minimum film boiling (MFB) temperature T_{mfb} is defined as the temperature at which a transition occurs from the transition boiling regime to the film boiling regime. A correlation proposed by Kondo et al.⁽³⁴⁾ is employed, which is expressed as follows:

$$T_{mfb} = T_{sat} + C\left(\frac{27}{32}T_{cr} - T_{sat}\right) + \left(\frac{\lambda_l}{\lambda_{vf}}\right)\frac{Nu_c\Delta T_{sub}}{D_p/\delta_{min} + Nu_r},$$
(2.80)

where C denotes the constant value of 0.6, T_{cr} denotes the critical temperature of the coolant water, and δ_{min} denotes the minimum limit of the vapor film thickness, practically 0.1 mm. The Nu_c denotes the Nusselt number for convection around the vapor film that envelops the melt particle, which is provided by Eq. (2.57).

The Nusselt number for radiation Nu_r is derived in accordance with the Stefan-Boltzmann law, Eq. (2.34), and with due consideration of the condition $T_{mfb} \gg T_l$:

$$Nu_r = \epsilon_P \sigma_{SB} T^3_{mfb} (D_p / \lambda_{vf}), \qquad (2.81)$$

where ϵ_P denotes the emissivity at the surface of the melt particle, and σ_{SB} denotes the Stefan-Boltzmann constant. The heat flux of the surface of the melt particle q_{mfb} corresponding to T_{mfb} is derived by solving Eq. (2.59) when T_w is equal to T_{mfb} .

6. Transition Boiling:

The heat flux q_{tbp} in the transition boiling regime is determined through a liner interpolation between the critical heat flux point $(q_{chf} \text{ at } T_{chf})$ and the minimum film boiling point $(q_{mfb} \text{ at } T_{mfb})$ (see Fig. 2.2).

7. Radiation:

In order to ascertain the heat flux q_{rad} for the radiation heat transfer, the Stefan-Boltzmann law is utilized, which is expressed as Eq. (2.34). The total heat flux q_{tot} in the film boiling regime is expressed by combining the film boiling heat transfer and the radiation heat transfer, as shown in Eq. (2.38).

The latest version of the JASMINE code postulates that boiling and radiation heat transfer are attenuated or reduced by the effects of void formation when the flow regime deviates from the bubbly flow (liquid continuous) regime. In order to address the numerical issues, the boiling and radiation heat transfer are cut off or terminated at a high void fraction ($\alpha > 0.95$). The weighting functions f_{α} are identical to those defined for the melt pool, Eqs. (2.35)–(2.37), with the exception that the power n is set to 0.3 for the film boiling, in order to align with the correlation proposed by Liu and Theofanous⁽³¹⁾. The value of n for the radiation can be specified through the input file, as the radiation from the melt particles has a significant impact due to large surface areas. It is challenging to determine the value of n with precision within the confines of a simplified model. It should be tuned based on careful considerations, though the recommended value is specified through the input file. The boiling heat transfer of the surface of the met particles and the total heat flux are determined based on the same methodologies as those employed for the melt pool.

As the particle groups descend and settle on the bottom floor, forming a debris bed, they undergo a vertical collapse. In such instances, the heat transfer from the particle group is degraded due to a reduction in contact with the coolant water and a reduction in radiation emission. The simulation of heat transfer degradation is achieved by introducing a reduction factor to the heat transfer coefficient. The reduction factor is specified through the input file, and is typically set to approximately 0.1. In the event that the collapsed particle groups comprise a greater number of a single particle layer, a reduction factor $D_p/2r_z$ is applied to the heat transfer coefficient. This results in a further reduction in the heat transfer for the particle groups comprising a greater number of a single particle layers.

Secondary Breakup of a Melt Particle

The secondary breakup of a melt particle is modeled based on the total breakup time τ_{brk} , and the maximum stable size of a liquid droplet D_{smx} . The values are estimated using the correlation proposed by Pilch and Erdman⁽³⁵⁾,

$$D_{smx} = \frac{We_{cr}\sigma_d}{\rho_c v_0^2} \left(1 - \frac{v^*}{v_0}\right)^{-2},$$
(2.82)

$$\tau_{brk} = \tau^* \frac{D_0}{v_0 \epsilon^{0.5}},\tag{2.83}$$

$$v^* = v_0 \epsilon^{0.5} \left(\frac{0.75 C_d \tau^*}{1 + 0.75 C_d \epsilon^{0.5} \tau^*} \right), \tag{2.84}$$

$$\tau^* = \begin{cases} 6(We - 12)^{-1/4} & (12 \le We < 18) \\ 2.45(We - 12)^{1/4} & (18 \le We < 45) \\ 14.1(We - 12)^{-1/4} & (45 \le We < 351) \\ 0.766(We - 12)^{1/4} & (351 \le We < 2670) \\ 5.5 & (2670 \le We) \end{cases}$$
 and (2.85)

$$C_{d} = \begin{cases} 5.6 & (Re < 4 \times 10^{4}) \\ 3.3 & (4 \times 10^{4} \le Re < 10^{5}), \\ 1.4 & (10^{5} \le Re) \end{cases}$$
(2.86)

where C_d denotes the friction factor, v_0 denotes the original or initial relative velocity between the droplet and the continuous fluid, D_0 denotes the original or initial droplet diameter, Re denotes the Reynolds number, We denotes the Weber number, We_{cr} denotes the critical Weber number, τ^* denotes the non-dimensional breakup time, v^* denotes the relative velocity decrease during the secondary breakup, and ϵ denotes the density ratio.

The non-dimensional values are defined as follows: $Re = \rho_c v_0 D_0 / \mu_c$, $We = \rho_c v_0^2 D_0 / \sigma_d$, and $\epsilon = \rho_c / \rho_d$. The symbols ρ denotes the density, μ denotes the kinematic viscosity, and σ denotes the surface tension. The physical properties of the continuous fluid are defined as follows: $\rho_c = \rho_g + (1 - \alpha)\rho_l$ and $\mu_c = 1/\{\alpha/\mu_g + (1 - \alpha)/\mu_l\}$. The subscripts d, g and l denote the droplet, gas phase, and liquid phase of the continuous fluid, respectively. The decrease rate in the melt particle diameter is evaluated using the following expression:

$$\frac{dD_p}{dt} = \frac{D_{med} - D_p}{t_{brk}}.$$
(2.87)

The mass media diameter of the melt particle after the secondary breakup D_{med} is assumed to be equal to the half of the maximum stable diameter $D_{med} = D_{smx}/2$. Note that the relative velocity v_0 is determined using the coolant water or continuous fluid velocity v_c , which is defined as $v_c = \{\alpha \rho_g \mu_g + (1-\alpha)\rho_l \mu_l\}/\rho_c$.

In accordance with the original interpretation of the correlation proposed by Pilch and Erdman⁽³⁵⁾, the v_0 should be that preceding the onset of the breakup process. However, due to the inherent difficulty in identifying the precise onset and conclusion of the breakup process for each individual droplet (particle group) within the current framework, the relative velocity at the commencement of each time step is utilized in order to ascertain the decrease rate dD_p/dt for that specific time step. The secondary breakup model is operational when the particle groups are in a molten state.

It is not recommended to employ the secondary breakup model for practical applications, such as the safety assessment, due to its susceptibility to the two-phase flow velocity, which can manifest as unstable characteristics in simulations. The secondary breakup model may result in the formation of smaller melt particles than anticipated, which can have a considerable impact on the heat transfer, void formation, and the overall phenomena. It is therefore recommended that the secondary breakup model be deactivated and a parameter study be conducted on the specified melt particle size.

Surface Temperature of a Melt Particle

The surface temperature of a melt particle is of great consequence with regard to the heat transfer and the breakup of the melt particle. Due to the relatively low thermal conductivity of oxide melts, which are typical core melt materials, the surface temperature of the melt particle can be significantly lower than the average temperature.

The modelling of the temperature distribution within a melt particle with the formation of a solid layer at the surface represents a significant challenge, even when a temperature profile with the melt particle is assumed or provided. A simple approach was utilized, wherein a quadratic temperature profile was postulated within the melt particle across the melt particle radius R, and the discrepancy between the surface and average temperature was quantified in accordance with the time elapsed since the particle formation. In accordance with the assumption (see Appendix A), the evolution of the thermal boundary layer thickness δ within a melt particle can be expressed as follows:

$$\delta \left\{ 1 - \frac{3}{4} \left(\frac{\delta}{R} \right) + \frac{1}{5} \left(\frac{\delta}{R} \right)^2 \right\} d\delta = 3\kappa dt,$$
(2.88)

where κ denotes the thermal diffusion coefficient of the melt particle. At the first step in numerical integration following the release or formation of the melt particle, the value of δ is determined through the application of a first-order approximation,

$$\delta = \sqrt{6\kappa\Delta t}.\tag{2.89}$$

The numerical integration of Eq. (2.88) yields the updated value of δ . The discrepancy between the surface temperature T_{sf} and the average temperature T_{av} is evaluated using the following expression:

$$T_{av} - T_{sf} = \frac{\delta q}{2\lambda} \left\{ F_{\delta} = \frac{\delta}{R} - \frac{1}{2} \left(\frac{\delta}{R}\right)^2 + \frac{1}{10} \left(\frac{\delta}{R}\right)^3 \right\},\tag{2.90}$$

where q denotes the heat flux at the surface of the melt particle determined by the constitutive models for the heat transfer, and λ denotes the thermal conductivity.

The latest version of the JASMINE code does not account for the phase change or crust formation on the surface of the melt particle. The approach is effective until the surface temperature reaches the melting point. Once the surface temperature exceeds the melting point, a discrepancy will inevitably arise between the predicted outcome and the actual situation regarding to the surface temperature. To dissipate the discrepancy, the equilibrium temperature during the phase change is represented using the physical properties model. The specific heat is a function of the melt temperature. The additional heat absorbed or dissipated between T_{sol} and T_{liq} , caused by the artificial peak of the specific heat, is modelled to replicate that caused by the latent heat due to the phase change.

2.2.4 Melt Fragment

Basic Equations

The explosion step is modeled based on the fundamental concepts or assumptions in physics that extend the melt particle model. When the melt particles are subjected to a shock wave, namely an intensive relative velocity of the surrounding coolant water, the surface of the melt particle is subjected to a hydrodynamic force, resulting in the production of melt fragments. The melt fragments exhibit a micrometer-order size and an extremely rapid heat release, which vaporizes the coolant water at a sufficient rate to support high pressure and propel the shock wave. The heat release rate is primarily dependent on the mass fragmentation rate.

An additional component of the melt model, designated as the "fragment group," is attached to the particle group for the purpose of implementing the aforementioned concept (Fig. 1.2). A fragment group is defined as a swarm of fine fragments generated from a particle group. The mass of the fragments is separated from that of the "mother" particle group as a result of the action of the hydrodynamic interaction. The principle of mass conservation is expressed by the following equation:

$$\frac{dm_p}{dt} = -m_f, \qquad \text{and} \tag{2.91}$$

$$\frac{dM_f}{dt} = n_p m_f, \tag{2.92}$$

where m_p denotes the mass of a single melt particle within the particle group, n_p denotes the number of melt particles within the particle group, and M_f denotes the mass of fragments within the fragment group. The mass fragmentation rate for a single melt particle m_f is determined by a constitutive model.

The process of the heat transfer is constrained to the heat conduction within the melt fragment. It is supposed that the heat transfer coefficient outside the melt fragment is quite large. The reliability of any steady-state heat transfer coefficient is questionable in the context of a highly transient situation or the explosion step. For a given heat release rate per unit the mass of melt fragments q_f , the principle of energy conservation is expressed as follows:

$$\frac{de_f}{dt} = e_p \frac{n_p m_f}{M_f} - q_f, \tag{2.93}$$

where e_p denotes the specific internal energy of melt particles, and e_f denotes the specific internal energy of melt fragments. The specific internal energy of the mother melt particles remains unaltered throughout the explosion step.

The size of the melt fragment d_{frg} is provided as a constant value in the input file. If the heat release time of the melt fragment is comparable to the numerical time step, the size has a minimal impact on the outcome. No kinetic or momentum equation is solved for the melt fragments. In the absence of a kinetic or momentum equation for the melt fragment, the fragment group is simply assumed to accompany the mother particle group. The primary function of the melt fragments is rapid heat release; thus, the kinetic aspect is therefore not considered to be of importance.

Given that the fundamental process involved in the melt components in the explosion step is the generation of the melt fragments and the rapid heat release from them, it is not necessary to maintain the components of the melt jet and the melt pool. At the inception of an explosion simulation, the melt jet and melt pool are re-cast into particle groups with equivalent surface area and volume. In general, the melt jet and melt pool display a lower surface-to-volume ratio than the melt particles, which consequently contribute only a relatively minor amount to the overall heat release during the explosion step.

Constitutive Models

Melt Fragmentation Rate

The mass fragmentation rate m_f (kg/s) for a single melt particle, which is required in Eq. (2.91), is determined by the following equations:

$$m_f = C_{frg} \frac{1}{t_b^*} \frac{\pi}{6} D_p^2 v_r (\rho_c \rho_p)^{1/2},$$
(2.94)

$$t_b^* = \begin{cases} 1 & : \text{Carachalios et al.}^{(36)} \text{ or} \\ 13.7/Bo^{1/4} & : \text{Yuen et al.}^{(37)}, \end{cases}$$
(2.95)

$$Bo = \frac{3}{16} \frac{C_D \rho_c D_p v_r^2}{\sigma_p},$$
 (2.96)

where t_b^* denotes the non-dimensional time for fragmentation⁽³⁵⁾, D denotes the diameter, v_r denotes the relative velocity between the melt particle and the coolant water, ρ denotes the density, and σ denotes the surface tension. The subscripts p and c denote the melt particle and coolant water, respectively.

The drag coefficient $C_D = 0.44$ in the Newton regime is employed⁽³²⁾. The fragmentation rate C_{frg} is an empirical constant that is adjusted. Eq. (2.94) illustrates a fundamental principle: a single melt

particle with a volume of $(\pi/6)D_p^3$ is fragmented over a characteristic time period of fragmentation t_b . The relationship between t_b and t_b^* for the conversion of Eq. (2.94) to the form utilizing t_b^* :

$$t_b = t_b^* \sqrt{\frac{\rho_p}{\rho_c}} \frac{D_p}{v_r}.$$
(2.97)

The model proposed by Carachalios et al.⁽³⁶⁾ offers a constant value for the t_b^* , whereas the model proposed by Yuen et al.⁽³⁷⁾ incorporates the impact of the Bond number *Bo* [Eq. (2.97)]. The coolant density ρ_c and the relative velocity v_r can be evaluated in a number of ways. The *Bo* number is calculated using the mean density and velocity for the gas and liquid phases, or two-phase flow mixture, as defined below:

$$\rho_c = \rho_g + (1 - \alpha)\rho_l, \tag{2.98}$$

$$\boldsymbol{v_c} = \frac{\{\alpha \rho_g \boldsymbol{v_g} + (1 - \alpha) \rho_l \boldsymbol{v_l}\}}{\rho_c}, \qquad \text{and} \qquad (2.99)$$

$$v_r = |\boldsymbol{v}_p - \boldsymbol{v}_c|. \tag{2.100}$$

The *Bo* number is included with the power of 1/4 in t_b^* , and thus the variables included in the *Bo* number exert a relatively weak impact on the simulations. In contrast, the variables included in \dot{m}_f exert a more pronounced influence and are provided with greater precision by the following options. The first option is to utilize the density and velocity in the liquid phase, expressed follows:

$$\rho_c = \rho_l, \qquad \text{and} \qquad v_r = |\boldsymbol{v}_p - \boldsymbol{v}_l|, \tag{2.101}$$

and the \dot{m}_{f} is attenuated with the cut-off function defined by the following equation:

$$f_{\alpha,frg} = \begin{cases} 1 & (0 \le \alpha \le 0.30) \\ (0.75 - \alpha)/0.45 & (0.30 \le \alpha \le 0.75). \\ 0 & (0.75 \le \alpha \le 1.00) \end{cases}$$
(2.102)

The second option is to utilize the density and velocity in the liquid phase, as defined in Eq. (2.101), and to incorporate the attenuation factor $(1 - \alpha)$ into the \dot{m}_f . The final option is to utilize only the mean density and velocity, as described in Eqs. (2.98)–(2.100).

The implementation of the melt fragment model requires the introduction of an additional parameter $\tau_{fraglife}$, which defines the time period during which the fragmentation remains active following the

passage of the shock wave front due to the triggering. The melt fragment model has been tested with the KROTOS experiment⁽³⁸⁾, and it has been demonstrated that the JASMINE code accurately reproduces the pressure pulses and kinetic energy observed in KROTOS the experiment with $C_{frg} \sim 0.35$, based on the model proposed by Carachalios et al.⁽³⁶⁾ with $\tau_{triglife} \sim 1$ ms.

Rapid Heat Release from a Melt Fragment

The rapid heat release rate \dot{q}_f (J/kg) for a single melt particle, which is required in Eq. (2.93), is determined by the following equations:

$$\dot{q}_{f} = C_{qf} \frac{f_{rel}}{t_{rel}} (E_{ini} - E_{low}),$$
 and (2.103)

$$t_{rel} = \frac{1}{4} \frac{d_{frg}^2}{\kappa_f} \tau_f, \tag{2.104}$$

where E_{ini} and E_{low} denote the internal energy of melt fragments at the initial high and the final low temperatures, respectively. The symbol κ_f denotes the thermal diffusion coefficient of melt fragments. The initial high and the final low temperatures are set to be the melt particles and the coolant water temperatures, respectively. Eq. (2.103) indicates that the fraction f_{rel} of heat possessed by the melt fragment is released over a time period t_{rel} . The t_{rel} is derived from the τ_f as described in Appendix A.2. The analysis of the transient heat conduction within a rigid sphere yielded the constant values: $f_{rel} = 0.632$ and $\tau_f = 0.046$ (see Appendix A.2). The C_{qf} is an empirical constant that is adjusted.

The cut-off function that pertains to the void formation of the coolant water is defined as the following equation:

$$f_{\alpha} = (1 - \alpha)^{0.2}. \tag{2.105}$$

The f_{α} is applied Eq. (2.103) to circumvent the potential numerical issues that may arise from the deposition of a considerable quantity of heat into a single cell with a limited supply of the coolant water.

In accordance with the typical properties of the oxide melt ($\kappa_f \sim 1.0 \times 10^{-6} \text{ m}^2/\text{s}$) and the size of the melt fragment $d_{frg} \sim 10 \text{ }\mu\text{m}$, the τ_{fel} is estimated to be in the order of microseconds. The value of τ_{fel} is comparable to the numerical time steps employed in explosion steps. Accordingly, the instantaneous heat release from the melt fragment, which is the principal concept of the melt fragment model, can be regarded as a valid assumption. In addition, the value of d_{frg} has a negligible impact on the simulations, provided that it is a sufficiently small within the range of $d_{frg} \sim 10 \mu \text{m}$.

2.3 Two-Phase Flow Model

2.3.1 Basic Equations

Extensions for Steam Explosion Simulations

The two-phase flow code ACE3D, developed by Ohnuki et al.⁽⁶⁾, which solves a two-fluid model for steam-water or air-water systems, has been extended to include the following models for the steam explosion simulations.

- 1. A model of the non-fluid volume has been being incorporated into the two-phase flow cells in order to accommodate the melt components.
- 2. A model of the momentum and heat exchange process between the melt components and the twophase flow has been being incorporated.
- 3. A model of the non-condensable gas components has been incorporated in order to facilitate the management of the highly subcooled (non-condensable gas-rich) conditions.

The two-phase flow model encompasses the steam, water, and non-condensable gas components. The mass and energy equations are solved separately for each component, whereas the momentum equations are solved for the liquid (coolant water) and gases (gas mixture). The model assumes mechanical equilibrium among the gases, which means that no unbalanced forces act on any part of the system (single gas component) or on the system as a whole (whole gas phase).

Volume Fractions for Multi Fluid Modeling Approach

In accordance with the conventional multi-fluid modeling approach, the conservation equations are expressed in terms of the volume fraction of each component. The relationship between the volume fractions, α_s : steam, α_a ($a = a_1, a_2, \dots, a_{ng}$), non-condensable gases, α_l : water, and α : total void fraction, is defined by the following equations:

$$\alpha = \alpha_s + \sum_{a=1}^{a_{ng}} \alpha_a, \qquad \text{and} \qquad (2.106)$$

$$\alpha_l = 1 - \alpha. \tag{2.107}$$

The application of the multi-fluid modeling approach necessitates a departure from the actual physical state of the system, wherein the constituent gases are in mixed together, occupying the total gas volume and having a partial pressure. From the perspective of mass accounting or conservation, the mass of each gas component is considered to be equivalent between the multi-fluid modeling approach and the actual physical state of the system, provided that the ideal gas assumption is valid.

The volume fraction of the two-phase flow, which encompasses both the liquid and gas phases, is defined in accordance with the fluid volume within cells, with the melt volume subsequently subtracted. In the following sections, the fluid volume (m^3) will be denoted by V.

Conservation Equations

The mass and energy equations of the fluid components for steam, liquid water, and non-condensable gases are described as follows:

$$\begin{split} \frac{\partial}{\partial t} (V \alpha_k \rho_k) + \nabla \cdot (V \alpha_k \rho_k \boldsymbol{v}_k) &= \Gamma_k, \quad \text{and} \\ \frac{\partial}{\partial t} (V \alpha_k \rho_k e_k) + \nabla \cdot (V \alpha_k \rho_k e_k \boldsymbol{v}_k) &= -pV \left[\frac{\partial \alpha_k}{\partial t} + \nabla \cdot (\alpha_k \boldsymbol{v}_k) \right] \\ &+ q_{ik} + q_{mk} + q_{wk} + \sum_{j \neq k} q_{jk} + \Gamma_k h_k, \end{split}$$
(2.108)

where ρ denotes the density, *e* denote the internal energy, *p* denote the pressure, and *v* denotes the velocity. The suffix *k* denotes either fluid component *s* (steam), *l* (liquid water), or *a* (non-condensable gases). The symbol Γ_k denotes the phase change rate within a single cell, q_{ik} , denotes the heat input from the liquid-gas interface, q_{mk} denotes the heat input from the melt components, q_{wk} denotes the heat input from the walls, and q_{jk} denotes the heat input from other components.

The momentum equation of the fluid in the states of liquid and gases is described as follows:

$$\begin{aligned} \frac{\partial \boldsymbol{v}_{k}}{\partial t} + \boldsymbol{v}_{k} \cdot \nabla \boldsymbol{v}_{k} &= -\frac{1}{\rho_{k}} \nabla p - [K_{ik}(\boldsymbol{v}_{k} - \boldsymbol{v}_{i})]_{i \neq k} \\ &- \frac{\Gamma_{k}^{+}}{V \alpha_{k} \rho_{k}} (\boldsymbol{v}_{k} - \boldsymbol{v}_{i})_{i \neq k} + \frac{F_{mk}}{V \alpha_{k} \rho_{k}} + g. \end{aligned}$$
(2.110)

The suffix k denotes either the fluid phase l (liquid water) or g (gas). Note that the gas phase encompasses the steam and non-condensable gases. The symbols K_{ik} and F_{mk} denotes the interfacial friction coefficient and the body force exerted by the melt components, respectively. The phase change rate Γ_k^+ is equal to Γ_k when $\Gamma_k \ge 0$, and otherwise is equal to zero.

2.3.2 Constitutive Models

Phase Equilibrium: Non-Condensable Gases

In the multi-fluid modeling approach, each gas (steam and non-condensable gases) component occupies a certain or specific volume fraction α_k ($k = s, a_1, a_2, \dots, a_{ng}$), and is compressed by the

total pressure p. In physical reality, the gas components are mixed together, extending to the total void fraction α , resulting in a lower density, corresponding to the partial pressures p_k ($k = s, a_1, a_2, \cdots, a_{ng}$). The discrepancy between the modeled and physical reality is inconsequential with regard to the mass of gas components, provided that the gases can be treated as uniformly mixed ideal gases. The multi-fluid modeling approach offers the advantage of straightforward and simple coding, which is a natural extension of the two-fluid model in the original ACE3D code.

The saturation temperature of the coolant water is evaluated at the "pseudo-partial pressure" of steam, as defined by the following equation:

$$p_s = p \frac{\alpha_s}{\alpha}.$$
(2.111)

The saturation temperature is a function of both α_s and α , as well as p. The density and internal energy of steam are evaluated at the pseudo-partial pressure. Subsequently, the density is converted to the value at the total pressure by means of the following equation:

$$\rho_s(p) = \frac{p}{p_s} \rho_s(p_s). \tag{2.112}$$

Phase Change Rates: Evaporation and Condensation

The phase change rates between the steam and liquid water within a single cell (kg/s) Γ_s and Γ_l are provided by the following expression:

$$\Gamma_{s} = -\Gamma_{l} = \frac{-(q_{is} + q_{il}) + q_{int}}{h_{s} - h_{l}},$$
(2.113)

$$q_{is} = A_i h_{is} (T_{sat} - T_s),$$
 and (2.114)

$$q_{il} = A_i h_{il} (T_{sat} - T_l), (2.115)$$

where q_{is} and q_{il} denotes the heat transfer rates from the liquid-gas interface to the steam and liquid water, q_{int} denotes the heat transferred to the liquid-gas interface from the melt components, h_{is} and h_{il} denotes the interfacial heat transfer coefficients for the steam and liquid water, A_i denotes the interface area between the liquid and gas phases within a single cell. The saturation temperature T_{sat} is calculated based on the pseudo-partial pressure p_s .

Friction and Heat Transfer

The interface exchange terms are derived from the dispersed flow model, in which either the liquid or gas phase is regarded as a continuous phase, while the other is regarded as a dispersed phase depending on the void fraction. The corresponding regime is selected according to the void fraction α : the bubbly flow regime, the droplet flow regime, and the transition regime. The interpolation method for the transition regime, $0.3 < \alpha < 0.75$, is defined as follows using the weighting function f_{α} , as defined in Eq. (2.1):

$$X = (1 - f_{\alpha})X_b + f_{\alpha}X_d.$$
 (2.116)

1. Friction Coefficient

The interfacial friction coefficient between the continuous and dispersed phases K_{ik} is employed for the two-phase flow simulations. The K_{ik} is ascertained based on the correlations utilized in the TRAC-PF1 code⁽³⁹⁾, expressed as following expressions:

$$K_{ik} = \frac{3}{4} \frac{\alpha_d C_d \rho_c}{d_d} \frac{|\boldsymbol{v}_k - \boldsymbol{v}_i|}{\alpha_k \rho_k},\tag{2.117}$$

$$C_{d} = \begin{cases} 240 & (Re_{d} < 0.1031) \\ 24(1 + 0.15Re_{d}^{0.687})/Re_{d} & (0.1031 \le Re_{d} < 989), \\ 0.44 & (989 \le Re_{d}) \end{cases}$$
(2.118)

$$Re_d = \frac{\rho_c d_d |\boldsymbol{v}_r|}{\mu_c}, \qquad \text{and} \qquad (2.119)$$

$$d_d = \frac{W e_{cr} \sigma}{\rho_c |\boldsymbol{v}_r|^2},\tag{2.120}$$

where C_d denotes the friction factor, Re denotes the Reynolds number, d denotes the characteristic phase size, $|v_r|$ denotes the relative velocity between the phases, and σ denotes the surface tension. The subscripts c and d denotes the continuous and dispersed phases, respectively. The critical Weber number We_{cr} is set at 7.5 for bubbles and 4.0 for droplets, respectively. The $|v_r|$ is evaluated through two distinct methodologies: the first entails the direct application of the relative velocity $|v_k - v_i|$, while the second entails the force balance of the buoyancy and drag forces acting on a single bubble or droplet in a steady state at a terminal velocity, as described by the following equation:

$$\frac{\pi}{6}d_d^3(\rho_l - \rho_g)g = C_d \frac{\pi}{4}d_d^2 \frac{1}{2}\rho_c |\boldsymbol{v}_r|^2.$$
(2.121)

In practice, the latter option is employed in order to circumvent the potential issues that may arise due to numerical (as opposed to physical) disturbance in the relative velocities.

The $K_{ik,b}$ and $K_{ik,d}$ for the bubbly and droplet flow regimes are determined, according to Eq. (2.117). The values of d_d , which are included in the K_{ib} and K_{id} , vary depending on the flow regime. Consequently, the K_{ik} is expressed as follows: $K_{ik} = K_{ik,b}$ for the bubbly flow regime, $K_{ik} = (1 - f_\alpha)K_{ik,b} + f_\alpha K_{ik,d}$ for the transition regime, and $K_{ik} = K_{ik,d}$ for the droplet flow regime. The K_{ik} for the transition regime is expressed in the form of Eq. (2.116).

2. Heat Transfer Coefficient

The interfacial heat transfer coefficients between the liquid-gas interface and the liquid water or gas components h_{il} and h_{ig} are employed for the two-phase flow simulations. The h_{il} and h_{ig} are ascertained based on the correlations utilized in the TRAC-PF1 code⁽³⁹⁾, as expressed follows:

For the bubbly flow regime at a liquid phase:

$$h_{il} = 0.02\rho_l c_{pl} |v_l - v_q|.$$
(2.122)

For the bubbly flow regime at a gas phase:

$$h_{ig} = 200 \frac{\lambda_g}{d_d}.$$
(2.123)

For the droplet flow regime at a liquid phase:

$$h_{il} = 0.02\rho_l c_{pl} |\boldsymbol{v}_{\circ}|, \qquad \text{ and } \tag{2.124}$$

$$|\boldsymbol{v}_{\circ}| = \min\left\{0.5\frac{\mu_{g}}{\mu_{g} + \mu_{l}}|\boldsymbol{v}_{l} - \boldsymbol{v}_{g}|, \ 1.4\left(\frac{\sigma}{d_{d}\rho_{l}}\right)^{1/2}\right\}.$$
(2.125)

For the droplet flow regime at a gas phase:

$$h_{ig} = \left(2 + 0.74 R e_d^{1/2}\right) \frac{\lambda_g}{d_d},$$
 and (2.126)

$$Re_d = \frac{\rho_g d_d |\boldsymbol{v}_l - \boldsymbol{v}_g|}{\mu_g}.$$
(2.127)

The dispersed phase size d_d is determined by the identical method employed for the friction coefficient K_{ik} , Eqs. (2.120) and (2.121). Once the d_d has been determined, the interface area of the liquid-gas interface within a single cell can be calculated using the following equation:

$$A_i = \frac{6V\alpha_d}{d_d}.$$
(2.128)

The $h_{il,b}$ and $h_{ig,b}$ for the bubbly flow regime are determined, according to Eqs (2.122) and (2.123). The $h_{il,d}$ and $h_{ig,d}$ for the droplet flow regime are determined according to Eqs (2.124) and (2.126). Then, the $A_{i,b}$ and $A_{i,d}$ for the bubbly and droplet flow regimes are also employed, according to Eq. (2.128), to determine the h_{il} and h_{ig} .

Consequently, the h_{il} and h_{ig} are expressed as follows: $h_{il}A_i = h_{il,b}A_{i,b}$ and $h_{ig}A_i = h_{ig,b}A_{i,b}$ for the bubbly flow regime, $h_{il}A_i = 1 - f_{\alpha} h_{il,b}A_{i,b} + f_{\alpha}h_{il,d}A_{i,d}$ and $h_{ig}A_i = 1 - f_{\alpha} h_{ig,b}A_{i,b} + f_{\alpha}h_{ig,d}A_{i,d}$ for the transition regime, and $h_{il}A_i = h_{il,d}A_{i,d}$ and $h_{ig}A_i = h_{ig,d}A_{i,d}$ for the droplet flow regime. The $h_{il}A_i$ and $h_{ig}A_i$ for the transition regime are expressed in the form of Eq. (2.116).

Thermal Equilibration of Gas Components

The application of specific heat transfer coefficients has been proven to be a more effective approach to achieve thermal equilibrium of gas components within a specific time period than the application of heat transfer coefficients derived from the approach based on the geometrical configurations such as the contact areas of bubbles or droplets as Eqs. (2.122)–(2.128). The approach for applying the specific heat transfer coefficients is utilized to regulate or promote the heat transfer between the steam and non-condensable gases, ensuring a consistent or identical temperature across both gas components. The heat transfer rate R_{sa} (W/K) is provided by the following equation:

$$R_{sa} = \frac{V(\alpha \rho c_p)_m}{\tau_{rsa}},$$
(2.129)

where the subscript m denotes the one of two components: the steam or non-condensable gases, which exhibit the smaller heat capacity. The temperature with smaller heat capacity approaches the temperature of the counterpart .The heat in the one component $V(\alpha \rho c_p)_m$ is dissipated to the other component over a specific time period τ_{rsa} per 1 K temperature difference. The R_{sa} is multiplied by the temperature difference $T_s - T_{nc}$ and treated as the heat transfer speed (W).

Steam Diffusion in a Gas Component

An auxiliary diffusion model is employed to replicate the diffusion of steam in the gas phase. The absence of a diffusion term between gas components in the conservation equation Eqs. (2.108)–(2.110)

allows for the possibility of physically implausible gaps in steam condensation within the gas phase, which could result in a sudden shift in the saturation temperature of steam or a loss of numerical stability. The objective of the diffusion model is not to create gaps in steam concentration by enhancing the intermixing of gas components. The diffusion of steam in opposition to a mixture of non-condensable gases is represented by the following equation:

$$\frac{\partial (V\alpha_s \rho_s)}{\partial t} + \nabla \cdot (V \boldsymbol{j}_s) = 0, \qquad (2.130)$$

where j_s denotes the mass flux resulting from the diffusion of steam. The subscript s denotes the steam. The j_s is obtained from the following equation:

$$\boldsymbol{j}_{s} = -\left(\frac{c_{g}^{2}}{\rho_{g}}\right) M_{s} M_{nc} \mathcal{D} \nabla\left(\frac{\alpha_{s}}{\alpha}\right), \tag{2.131}$$

where c_g denotes the total molar concentration of the mixture of the gas phase, ρ_g denotes the total mass concentration of the mixture of the gas phase, M_s denotes the molecular weight of the steam, M_{nc} denotes the average molecular weight of the non-condensable gases, and \mathcal{D} denotes the diffusion coefficient. The concentrations and the average molecular weight are defined by the following equation:

$$c_g = \frac{1}{\alpha} \left(\frac{\alpha_s \rho_s}{M_s} + \sum \frac{\alpha_a \rho_a}{M_a} \right), \tag{2.132}$$

$$\rho_g = \frac{1}{\alpha} \left(\alpha_s \rho_s + \sum \alpha_a \rho_a \right), \qquad \text{and} \qquad (2.133)$$

$$M_{nc} = \frac{\sum \alpha_a M_a}{\alpha - \alpha_s},\tag{2.134}$$

where the subscript a denotes the non-condensable gas components: $a = a_1, a_2, \dots, a_{ng}$. The value of \mathcal{D} is set to a large range of 0.01 to 0.1 m²/s in order to ensure the efficacy of the diffusion model.

The auxiliary diffusion model is solved independently of the conservation equations. Prior to solving the conservation equations, the volume fraction of steam α_s in each cell is modified in accordance with Eqs. (2.130) and (2.131). Subsequently, the non-condensable gases are transferred in order to compensate for the steam volume in each cell, thereby maintaining the consistency in the total pressure and total gas volume. The correction of the non-condensable gas volume fraction is calculated in accordance with the following equations:

$$\frac{\partial (V\alpha_a \rho_a)}{\partial t} + \nabla \cdot (V \boldsymbol{j}_a) = 0, \qquad \text{and} \qquad (2.135)$$

$$\boldsymbol{j}_a = -\boldsymbol{j}_s \frac{\rho_a}{\rho_s} \frac{\alpha_a}{\alpha - \alpha_s}.$$
(2.136)

where j_a denotes the mass flux resulting from the diffusion of steam. The subscript s denotes the steam.

Heat Exchange with Melt Components

Prior to the two-phase flow simulation, the melt simulation is conducted in the latest version of the JASMINE code. The melt simulation furnishes the information regarding the melt volume, the external force, and the heat transfer within each cell, which are then utilized by the two-phase flow simulation.

The fluid volume V within each cell is determined based on the information regarding the melt volume provided by the melt simulation. The mass and energy equations utilized in the two-phase flow simulation incorporate a term representing the rate of change in volume dV/dt. The values of both new and old time steps are employed in order to estimate dV/dt.

The external force exerted by the melt components within each cell is distributed into the liquid water, steam, and non-condensable gas in a manner that ensures an uniform acceleration across all components. The approach to distribute the external force is not exact from a physical standpoint, but it is a simple and numerically stable approach that produces the physically reasonable simulation outcomes.

The heat released from the melt components within each cell is distributed into the liquid water, steam, and non-condensable gas, as well as the liquid-gas interface. The heat deposited on the liquid-gas interface is utilized for the evaporation. The simple approach to distribute the heat is described as follows:

Case 1: Absence of Melt Components within a Cell

The heat transfer between the liquid water and gas components becomes dominant in the absence of melt components within a cell (Fig. 2.9). The heat deposited at the liquid-gas interface is utilized for the evaporation of the liquid water or condensation of the steam, respectively, in accordance with Eq. (2.113).

Case 2: Presence of Melt Components within a Cell at Premixing Steps

1. Principle Situation [Fig. 2.10 (a)]

A part of the heat released from the melt components $Q_{melt} F_{hint}$ is deposited at the liquid-gas interface, and is utilized for the evaporation. It is recommended that a fraction of the heat employed for the evaporation be set at $F_{hint} \sim 0.02$ for reasonable simulations of the experiments. The remaining heat $Q_{melt} (1 - F_{hint})$ is distributed to the liquid water, steam, and non-condensable gas in a manner that ensures an uniform temperature increase across all components. The heat transfer between the liquid-gas interface and the liquid water or gas is suppressed using the factors $f_{higkill}$ and $f_{hilkill}$ in order that the heat transfer from the melt components to the liquid-gas interface becomes dominant.

2. Situation in Saturated Water Temperature [Fig. 2.10 (b)]

Once the coolant water temperature reaches the saturation temperature T_{sat} , the heat released from the melt components $Q_{melt} (1 - F_{hint})$, which is typically distributed to the bulk water, is instead distributed to the liquid-gas interface.

3. Situation in Absence of Liquid Water [Fig. 2.10 (c)]

In the absence of the bulk water or latent heat for the evaporation, the heat released from the melt components $Q_{melt} F_{hint}$, which is typically distributed to the liquid-gas interface, is instead distributed to the steam and non-condensable gas components.



Fig. 2.9 A schematic of heat distribution within a single cell in the absence of melt components: the heat is transferred between the liquid-gas interface and the liquid water or gases (steam and non-condensable gases).

Case 3: Presence of Melt Components within a Cell at Explosion Steps

A part of the heat released from the melt fragments $Q_{melt} K_{ev}$ is deposited at the liquid-gas interface, and it is utilized for the evaporation (Fig. 2.11). It is recommended that a fraction of the heat employed for the evaporation, a heat release partition, be set at $K_{ev} \sim 0.7$ for reasonable simulations of the experiments. The remaining heat released $Q_{melt} (1 - K_{ev})$ is distributed to exclusively the liquid water and steam. The heat transfer between the liquid-gas interface and the liquid water or gas components is principally suspended: $h_{ig} = h_{il} = 0$ unless the physical conditions become unstable, such as superheated water or supercooled steam, or an extremely high gas temperature.

The heat released by the melt components within a cell is distributed to the liquid water, steam, and non-condensable gas in a manner that ensures a uniform temperature increase across all components. The approach to distribute the heat is not exact from a physical standpoint, but it is a simple and numerically stable approach that produces physically reasonable simulation outcomes.



Fig. 2.10 A schematic of heat distribution within a single cell in the presence of melt components at premixing steps: (a) basic situation, (b) saturated water temperature, and (c) absent of bulk water.



Fig. 2.11 A schematic of heat distribution with in a single cell in the presence of melt components at explosion steps: the heat transfer at liquid-gas interfaces is suspended unless the physical conditions become unstable, such as superheated water or supercooled steam, or an extremely high gas temperature.

3. Numerical Methods

3.1 Coupling of Melt and Two-Phase Flow Modules

The latest version of the JASMINE code incorporates independent modules for the simulation of both the melt and the coolant water. The two-phase flow module is utilized for the coolant water simulation. The coupling of the melt and two-phase modules is explicit in time, as illustrated in Fig. 3.1.

The melt module is called at the beginning of a new time step, and refers the two-phase flow variables in the previous time step obtained from the two-phase flow module. The two-phase flow variables are interpolated to the cells where the melt jet, and melt pool, and the melt particles are present. The melt sub-models (melt jet, melt particle, and melt pool) sequentially calculate the information for the exchange variables among the melt sub-models: the melt jet outflow to the melt pool, the melt-jet break up to the melt particles, and the melt particles merging to the melt pool. The exchange variables from the melt module, specifically melt volume, heat transfer, and external force, are aggregated for the two-phase flow cells and returned to the two-phase flow module for updating to the subsequent new time step.

Time step	Two-phase flow module	Melt module		
		Melt jet	Melt particles	Melt pool
t	densities, velocities, pressure, temperature, volume fractions	(interpolation)	(interpolation)	(interpolation)
		(calc.) out flow to melt pool — melt particle formation velocity, temperature, volume,	(calc.) merging to melt pool - velocity, temperature, volume, positions	velocity, temperature, volume
	(calc.) ←		→ (cell average/sum) ↔	
$t + \Delta t$	densities, velocities, pressure, temperature, volume fractions			

Fig. 3.1 A schematic depicts the coupling method of the melt and two-phase modules: the coupling of the melt and two-phase modules is achieved explicitly in time.

3.2 Numerical Methods for Melt Module

Fig. 3.2 illustrates the configuration of the simulation domain. The numerical grids utilized for the twophase flow module on the x-z plane are commonly employed as the numerical grids for the melt jet and melt pool modules. As the numerical grids for the melt jet module, the one-dimensional grids in the zdirection for the two-phase flow module are employed. As the numerical grids for the melt pool module, the one-dimensional grids in the x-direction for the two-phase flow module are employed.



Fig. 3.2 A schematic of the simulation domain that describes the numerical grids for the melt jet, melt pool, and two-phase modules. The numerical grids utilized for the two-phase flow module on the x-z plane are commonly employed as the numerical grids for the melt jet and melt pool modules.

3.2.1 Melt Jet

Discretization and Numerical Schemes

A two-phase flow cell is subdivided into the melt jet cells with N_{sub} , thereby facilitating the attainment of a higher resolution than that of the two-phase flow cell. Fig. 3.3 provides a schematic illustration of the numerical grids utilized for the melt jet module. As a consequence of utilizing the staggered grid, the scalar variables are defined at the cell centers, whereas the vector variables are defined at the cell boundaries.

The conservation equations Eqs. (2.3)–(2.5) are calculated by the Cubic-Interpolated Pseudo particle (CIP) method, which is a high-resolution numerical scheme⁽⁴⁰⁾. In conceptual terms, there is no numerical diffusion resulting from the finite differences of the advection terms. The CIP method is a simultaneous solution to the conservation equations for the variables and the derivatives. The general form of the conservation equations is expressed by the following set of equations:



Fig. 3.3 The numerical grids utilized for the melt jet module. The scalar variables are defined at the cell centers, whereas the vector variable is defined at the cell boundaries due to the staggered grid. The cell boundary indices "i-1/2," "i+1/2," and "i+3/2" are practically denoted by "i," "i+1," and "i+2" within the code description, respectively.

$$\frac{\partial f}{\partial t} + v_J \frac{\partial f}{\partial t} = G,$$
 and (3.1)

$$\frac{\partial f'}{\partial t} + v_J \frac{\partial f'}{\partial t} = G' - v'_J \frac{\partial f'}{\partial t}, \qquad (3.2)$$

where f denotes the conservation variable for advection, and G denotes the source term. Based on the conservation equations Eqs. (2.3)–(2.5), the f and G for the melt jet module are expressed as the following expressions. The indices "i" or "i+1/2" are employed to indicate the position of the variable definition. The cell center is represented by "i," while the two ends or the cell boundaries are represented by "i-1/2" and "i+1/2," respectively:

$$f_{i} = A_{J}\rho_{J}|_{i}, \qquad \text{and}$$

$$G_{i} = -\sqrt{2\Theta A_{J}}m_{e}|_{i} - A_{J}\rho_{J}|_{i}\frac{\partial v_{J}}{\partial z}\Big|_{i}, \qquad (3.3)$$
for mass.

$$f_i = e_{J,i},$$
 and
 $G_i = -\sqrt{\frac{2\Theta}{A_J} \frac{q}{\rho_J}}\Big|_i,$ (3.4)
for energy.

 $f_{i+1/2} = v_{J,i+1/2},$

$$G_{i+1/2} = -\frac{1}{\rho_J} \frac{\partial p_a}{\partial z} \Big|_{i+1/2} + K_f (v_c - v_J) \Big|_{i+1/2} + g_{i+1/2}, \qquad (3.5)$$

and

The manner in which the variable definition is positioned differs between the velocity (cell centers) and the other variables (cell boundaries). It is essential to employ an interpolation scheme for the velocity to the cell centers in order to calculate the conservation equations for mass and energy. The interpolation scheme is of third-order precision due to the fact that the scheme employs the derivative values. The interpolation of the velocity and derivative are defined by the following expressions:

$$\begin{aligned} v_{J,i} &= \frac{\left(v_{J,i+1/2} + v_{J,i-1/2}\right)}{2} & \text{and} & (3.6) \\ & -\frac{\left(z_{i+1/2} - z_{i-1/2}\right)}{8} \left(v'_{J,i+1/2} - v'_{J,i-1/2}\right), \\ \frac{\partial v_J}{\partial z}\Big|_i &= \frac{3}{2\left(z_{i+1/2} - z_{i-1/2}\right)} \left(v_{J,i+1/2} - v_{J,i-1/2}\right) \\ & -\frac{\left(v'_{J,i+1/2} + v'_{J,i-1/2}\right)}{4}. \end{aligned}$$

In order to derive Eq. (3.6) and (3.7), the Taylor expansions of $v_{J,i+1/2}$ and $v_{J,i-1/2}$ around the cell center "i" are employed using $\Delta z = (z_{i+1/2} - z_{i-1/2})/2$:

$$v_{J,i+1/2} \simeq v_{J,i} + \frac{\partial v_J}{\partial z}\Big|_i \Delta z + \frac{1}{2} \frac{\partial^2 v_J}{\partial z^2}\Big|_i \Delta z^2 + \frac{1}{6} \frac{\partial^3 v_J}{\partial z^3}\Big|_i \Delta z^3,$$
(3.8)

$$v_{J,i-1/2} \simeq v_{J,i} - \frac{\partial v_J}{\partial z}\Big|_i \Delta z + \frac{1}{2} \frac{\partial^2 v_J}{\partial z^2}\Big|_i \Delta z^2 - \frac{1}{6} \frac{\partial^3 v_J}{\partial z^3}\Big|_i \Delta z^3,$$
(3.9)

$$v'_{J,i+1/2} \cong v'_{J,i} + \frac{\partial v'_J}{\partial z}\Big|_i \Delta z + \frac{1}{2} \frac{\partial^2 v'_J}{\partial z^2}\Big|_i \Delta z^2, \quad \text{and}$$
(3.10)

$$v'_{J,i-1/2} \cong v'_{J,i} - \frac{\partial v'_J}{\partial z}\Big|_i \Delta z + \frac{1}{2} \frac{\partial^2 v'_J}{\partial z^2}\Big|_i \Delta z^2,$$
(3.11)

From Eqs. (3.8)–(3.11), Eqs. (3.12) and (3.13) can be obtained. The interpolation scheme for the velocity to the cell center, or Eq. (3.6) can be derived by substituting Eq. (3.12) into Eq. (3.13),

$$v_{J,i+1/2} + v_{J,i-1/2} = 2v_{J,i} + \frac{\partial^2 v_J}{\partial z^2} \Big|_i \Delta z^2, \qquad \text{and} \tag{3.12}$$

$$v'_{J,i+1/2} - v'_{J,i-1/2} = 2 \frac{\partial^2 v_J}{\partial z^2} \Big|_i \Delta z.$$
 (3.13)

From Eqs. (3.8)–(3.11), Eqs. (3.14) and (3.15) can be obtained. The interpolation scheme for the velocity gradient to the cell center, or Eq. (3.7) can be derived by substituting Eq. (3.14) into Eq. (3.15),

$$v_{J,i+1/2} - v_{J,i-1/2} = 2v'_{J,i}\Delta z + \frac{1}{3} \frac{\partial^2 v'_J}{\partial z^2}\Big|_i \Delta z^3$$
 and (3.14)

$$v'_{J,i+1/2} + v'_{J,i-1/2} = 2v'_{J,i} + \frac{\partial^2 v'_J}{\partial z^2} \Big|_i \Delta z^2.$$
(3.15)

Similarly, the interpolation scheme for the pressure gradient or derivative to the cell boundaries is requisite component for the calculation of the conservation equations for momentum. The pressure gradient is defined by the following expression:

$$\frac{1}{\rho_J} \frac{\partial p_a}{\partial z} \Big|_{i+1/2} = \frac{2}{\rho_{i+1} - \rho_i} \frac{p_{a,i+1} - p_{a,i}}{z_{i+1} - z_i}.$$
(3.16)

The spatial derivative of pressure is determined by a simple first-order difference of two-points, and the density is determined by the average of the two-points.

The CIP method employs a two-step approach to solving the conservation equations: advection and non-advection (source term) phases. The advection phase is solved to obtain the intermediate variables f^* using the CIP1 scheme from the conservation variables f_n in the old time step "n". Subsequently, the non-advection (source term) phase is solved using the ordinary finite difference scheme to obtained the updated conservation variables f_{n+1} in the new time step "n+1".

Boundary Conditions

The boundary conditions are defined at the "njmax+1" cell for the jet inlet boundary, and the "njmin-1" cell for the outlet boundary for the melt pool module (see Fig. 3.3). The boundary cells serve as glue lines for receiving the variables from the input files or passing the variables to the melt pool module. Inlet Boundary:

The values of v_{Jin} , D_{Jin} , and T_{Jin} are specified through the input file. Note that the value of v_{Jin} is passed to the cell boundary designated as "njmax+1/2", while the values of D_{Jin} , and T_{Jin} are passed to the cell center designated as "njmax+1/2", while the staggered grid. The values for the conservation variables A_{Jin} and e_{Jin} are calculated from the values of D_{Jin} and T_{Jin} , respectively.

Outlet Boundary:

The cell boundary designated as "njmin-1/2" corresponds to the floor bottom. In order to determine the values at the "njmin-1" cell, a simple linear interpolation is employed. The $v_{J,njmin-3/2}$ is calculated from the velocities at the cell boundary designated as "njmin-1/2". The values of the mass and internal energy $f_{njmin-1}$ are calculated from the values of the mass and internal energy at the cell center designated as "njmin-1/2."

The evaluation of the outflow mass at the boundary of the melt jet outlet necessitates a high degree of accuracy, given that a significant portion of the melt jet mass is transferred to the melt jet pool through the boundary. The accuracy directly impacts on the total mass conservation. As the melt pool increases, the height of the boundary between the melt jet and the melt pool h_{mlevel} becomes different from the floor. In order to calculate the mass and internal energy at h_{mlevel} , cubic interpolation is employed:

$$f(z') = az'^3 + bz'^2 + cz' + d.$$
(3.17)

The interpolation function f(z') is expressed in a coordinate system with the origin at z' = 0, which is corresponds to the mid-value of the cell centers directly above and below the h_{mlev} . If the cell centers directly above and below h_{mlev} are denoted as z_{mlev} and z_{mlev-1} , the mid-value of the cell centers or the origin of the coordinate system z' = 0 is expressed as follows:

$$z = \frac{1}{2}(z_{mlev} + z_{mlev-1}), \tag{3.18}$$

and the distance from z' = 0 to $z = z_{mlev}$ or z_{mlev-1} can be expressed as follows:

$$\Delta z' = \frac{1}{2}(z_{mlev} - z_{mlev-1}). \tag{3.19}$$

The constants of f(z') can be determined from the values of the function and its derivative at $z' = \pm \Delta z'$. The velocity at h_{mlevel} is calculated from the velocity at the cell boundary designated as "njmin-1/2" through a simple linear interpolation.

If $h_{mlev} = 0$, the boundary between the melt jet and the melt pool remains the floor or the cell boundary designated as "njmin-1/2." The interpolation function f(z') is employed to determine the mass and internal energy at the floor or the cell boundary designated as "njmin-1/2." The cell-centered variables at the "njmin-1" and "njmin" are interpolated to the cell boundary designated as "njmin-1/2" with the third-order accuracy, as expressed by the following equation:

$$f_{njmin-1/2} = \frac{1}{2} (f_{njmin} + f_{njmin-1}) + \frac{\Delta z'}{4} (f'_{njmin} - f'_{njmin-1}), \qquad \text{where,} \qquad (3.20)$$

$$\Delta z' = \frac{1}{2} (z_{njmin} - z_{njmin-1}).$$
(3.21)

The values of v_{Jout} , D_{Jout} , and T_{Jout} are determined by averaging the interpolated values at the new and old time steps, and subsequently transferred to the melt jet pool.

3.2.2 Melt Pool

Discretization and Numerical Schemes

A two-phase flow cell is utilized for a melt pool cell. Fig. 3.3 provides a schematic illustration of the numerical grids employed for the melt pool module. In order for a conventional upwind scheme with a staggered grid to be effective, it is necessary to define the scalar variables at the cell centers and the vector variables at the cell boundaries.

In order to calculate the conservation equations Eqs. (2.21)–(2.23), the SIMPLE method⁽⁴¹⁾ is employed as the numerical scheme. The conservation equations for mass and momentum are initially calculated by the SIMPLE method, which is employed for the purpose of updating the values of the mass and velocity. Subsequently, the conservation equation for the energy is calculated. The conservation equations in the discrete form are expressed by the following equations:

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} = -\frac{1}{x_{i+1/2} - x_{i-1/2}} \left(\tilde{f}_{i+1/2}^{n+1} v_{P,i+1/2}^{n+1} - \tilde{f}_{i-1/2}^{n+1} v_{P,i-1/2}^{n+1} \right) + w m_s|_i,$$
(3.22)

$$\begin{aligned} \frac{e_{P,i}^{n+1} - e_{P,i}^{n}}{\Delta t} &= -\left(\max(\tilde{v}_{P,i}^{n+1}, 0) \frac{e_{P,i}^{n+1} - e_{P,i-1}^{n+1}}{x_{i} - x_{i-1}} + \min(\tilde{v}_{P,i}^{n+1}, 0) \frac{e_{P,i+1}^{n+1} - e_{P,i}^{n+1}}{x_{i+1} - x_{i}} \right) \\ &+ \frac{q}{h_{p}\rho_{P}} \bigg|_{i} + \frac{(e_{ms} - e_{P}^{n+1}) \max(m_{s}, 0)}{h_{p}\rho_{P}} \bigg|_{i}, \end{aligned}$$
(3.23)

$$\begin{split} & \frac{v_{P,i+1/2}^{n+1} - v_{P,i-1/2}^{n}}{\Delta t} \\ = -\left(\max\left(v_{P,i+1/2}^{n+1}, 0\right) \frac{v_{P,i+1/2}^{n+1} - v_{P,i-1/2}^{n+1}}{x_{i+1/2} - x_{i-1/2}} + \min\left(v_{P,i+1/2}^{n+1}, 0\right) \frac{v_{P,i+3/2}^{n+1} - v_{P,i+1/2}^{n+1}}{x_{i+3/2} - x_{i+1/2}} \right) \\ & - \frac{1}{\rho_{P,i+1/2}} \left[\frac{p_{a,i+1} - p_{a,i}}{x_{i+1} - x_{i}} + \frac{g}{2} \frac{(h_{p}\rho_{p})_{i+1} - (h_{p}\rho_{p})_{i}}{x_{i+1} - x_{i}} \right] \\ & + K_{fa}(v_{c} - v_{P})|_{i+1/2} - K_{fw}v_{P}|_{i+1/2} + \frac{(v_{ms} - v_{P}^{n})\max(m_{s}, 0)}{h_{P}\rho_{P}} \Big|_{i+1/2}, \end{split}$$
(3.24)

where f denotes the conservation variable and \tilde{f} denotes the conservation variable interpolated with respect to the cell boundaries. The conservation variable is defined as $f = wh_P \rho_P$ and the interpolated conservation variable is simply defined as $\tilde{f}_{i+1/2} = (f_{i+1} + f_i)/2$. Similarly, the symbol \tilde{v} denotes the velocity interpolated with respect to the cell centers. The interpolated velocity is simply defined as $\tilde{v}_i = (v_{i+1/2} + v_{i-1/2})/2$.



Fig. 3.4 The numerical grids utilized for the melt pool module. The scalar variables are defined at the cell centers, whereas the vector variable is defined at the cell boundaries due to the staggered grid. The cell boundary indices "i-1/2," "i+1/2," and "i+3/2" are practically denoted by "i," "i+1," and "i+2" within the code description, respectively.

The SIMPLE method⁽⁴¹⁾ typically entails a convergence calculation with respect to the pressure. However, due to the utilization of the shallow water equation in the melt pool model, the conservation variable f is employed in lieu of the pressure. In the conservation equation for momentum, the terms representing momentum change due to friction and phase change are excluded from the calculation.

Upon reaching the inlet of the melt pool, the melt jet causes a sudden increase in both the mass and velocity of the melt pool, which results in the numerical instability. In order to circumvent the issue, an artificial viscosity term⁽⁴²⁾ is incorporated into the right-hand side of the momentum equation, which is expressed as follows:

$$\frac{\mu_a}{\rho_P} \frac{\partial^2 v_P}{\partial x^2},\tag{3.25}$$

where $\,\mu_a\,$ denotes the artificial viscosity, which is defined as follows:

$$\frac{\mu_a}{\rho_P} = \begin{cases} b_0 \Delta x_0^{-2} \left| \frac{\partial v_P}{\partial x} \right| & \text{if } \frac{\partial v_P}{\partial x} v_P < 0, \text{or} \\ 0 & \text{otherwise.} \end{cases}$$
(3.26)

In the JASMINE code, it is recommended that the value of the constant $b_0 \sim 10$ for the melt pool in order for the stable calculation. In the event that the artificial viscosity term is not equal to zero, the discretized form of the acritical viscosity term is provided as follows:

$$\begin{split} & \frac{\mu_a}{\rho_P} \frac{\partial^2 v_P}{\partial x^2} \Big|_{i+1/2} \\ &= b_0^2 \left. x_{i+1} - x_i \right. \left| \frac{\partial v_P}{\partial x} \right|_{DW} \left(\frac{v_{P,i+3/2}^{n+1} - v_{P,i+1/2}^{n+1}}{x_{i+3/2} - x_{i+1/2}} - \frac{v_{P,i+1/2}^{n+1} - v_{P,i-1/2}^{n+1}}{x_{i+1/2} - x_{i-1/2}} \right), \end{split}$$
(3.27)

where the subscript DW denotes the downwind finite difference, which is provided by the following expression:

$$\left| \frac{\partial v_P}{\partial x} \right|_{DW} = \begin{cases} \left| \frac{v_{P,i+3/2}^{n+1} - v_{P,i+1/2}^{n+1}}{x_{i+3/2} - x_{i+1/2}} \right| & \text{if } v_{P,i+1/2}^n < 0, \text{or} \\ \left| \frac{v_{P,i+1/2}^{n+1} - v_{P,i-1/2}^{n+1}}{x_{i+1/2} - x_{i-1/2}} \right| & \text{otherwise.} \end{cases}$$

$$(3.28)$$

Boundary Conditions

The boundary conditions are defined at the positions of the inner and outer ends of the melt pool (see Fig. 3.4). The mirror condition is applied to both the inner and outer ends of the melt pool as the boundary condition. The cell boundary variable is fixed at $v_P = 0$ at the "npmin-1/2" and "npmax+1/2" points. The cell-centered variables h_P and e_P at the "npmin-1" and "npmax+1" points are determined in accordance with the simple conservation approach, which is expressed as follows:

$$f_{npmin-1} = f_{npmin} \frac{w_{npmin-1}}{w_{npmin}}, \qquad \text{and} \qquad (3.29)$$

$$f_{npmax+1} = f_{npmax} \frac{w_{npmax+1}}{w_{npmax}}.$$
(3.30)

Given that the mirror condition has been implemented, the cell-centered variables h_P and e_P are simply identical between the cell centers. Eq. (3.29) and (3.30) are derived based on the relation of $h_{P,npmin-1} = h_{P,npmin}$ for example.

The pressure p_{Jout} , which is exerted by the melt-jet impingement at the outlet of the melt jet, is added to the ambient pressure p_a at the inlet of the melt pool or "npmin" cell. The p_{Jout} drives the melt pool flow in the x direction, and is expressed as follows:

$$p_{Jout} = \frac{1}{2} \frac{\rho_J v_{Jout}^2 D_{Jout}^2}{4x_1^2},$$
(3.31)

where ρ denotes the density, v denotes the velocity, D denotes the diameter, and x_1 denote the cell size at the inlet of the melt pool. The subscript J denotes the melt jet. The internal energy e_P at the inlet of the melt pool is calculated from the T_{Jout} .

3.2.3 Melt Particle

Discretization and Numerical Schemes

The conservation of mass and energy conservations for a particle group is calculated by a simple explicit scheme for time advancement.

$$\frac{\boldsymbol{v}_p^{n+1} - \boldsymbol{v}_p^n}{\Delta t} = \boldsymbol{g} - \frac{\nabla p_a}{\rho_p} + \frac{\boldsymbol{F}_{hy}}{m_p},\tag{3.32}$$

$$\frac{\boldsymbol{x}_p^{n+1} - \boldsymbol{x}_p^n}{\Delta t} = \boldsymbol{v}_p^{n+1}, \qquad \text{and} \qquad (3.33)$$

$$\frac{e_p^{n+1} - e_p^n}{\Delta t} = -\frac{q}{m_p},\tag{3.34}$$

where v denotes the velocity (v_x, v_z) , x denotes the position (x, z), and p_a denotes the ambient pressure exerted by the coolant water. The subscript p denotes the melt particle. The symbol F_{hy} denotes the drag force resulting from hydrodynamic interactions, and q denotes the heat flux from the surface of the melt particle, respectively.

In order to evaluate of the values of ∇p_a , F_{hy} , and q, it is necessary to interpolate the two-phase flow variables to the position of the particle groups. The indices "i" and "k" of the two-phase flow cells, in which the particle groups exists, are determined using the bisection algorithm. At the outset of the calculation of the melt particles, the two-phase flow variables at the cell where the melt particles exist are interpolated. The melt volume, the force, and the heat transferred to the two-phase flow are summed and stored for each two-phase flow cell, and then passed to the calculation of the two-phase flow.

3.2.4 Melt Fragment

Discretization and Numerical Schemes

The conservation of mass and energy conservations for a fragment group is calculated by a simple explicit scheme for time advancement, which is applied in the same manner to the particle group.

$$\frac{m_p^{n+1} - m_p^n}{\Delta t} = -m_f,\tag{3.35}$$

$$\frac{M_p^{n+1} - M_p^n}{\Delta t} = n_p m_f, \qquad \text{and} \tag{3.36}$$

$$\frac{e_f^{n+1} - e_f^n}{\Delta t} = e_p \frac{n_p m_f}{M_f} - q_f,$$
(3.37)

where m_p denotes the mass of a single melt particle in the particle group, n_p denotes the number of melt particles within the particle group, and M_f denotes the mass of fragments within the fragment group. The symbols m_f denotes the mass fragmentation rate for a single melt particle, and q_f denotes the heat release rate per unit the mass of melt fragments, respectively.

In order to evaluate the values of m_f , and q_f , it is necessary to interpolate the two-phase flow variables to the position of the fragment groups. The indices "i" and "k" of the two-phase flow cells, in which the fragment groups exist, are determined using the bisection algorithm. At the outset of the calculation of the melt fragments, the two-phase flow variables are interpolated. The melt volume, the force, and the heat transferred to the two-phase flow are summed and stored for each two-phase flow cell, and subsequently passed to the calculation of the two-phase flow.

3.3 Numerical Methods for Two-Phase Flow Module

3.3.1 Overview

Fig. 3.5 illustrates a schematic of the numerical grids utilized for the two-phase flow model. The ACE3D code was originally developed for the two-phase flow simulations and is capable of solving the basic equations derived for the Cartesian or cylindrical coordinates in three dimensions. The JASMINE code, however, employs the ACE3D code in a restricted manner, utilizing it only in the cylindrical coordinate system in two dimensions. The basic equations for the cylindrical coordinate system in three dimensions are presented in the following sections. The numerical solutions are obtained through the application of a conventional finite-difference method, specifically a semi-implicit scheme for time advancement, a staggered mesh, and an upwind scheme for spatial discretization. The number of $10 + 2n_q$ discretized basic equations are solved in order to determine the independent variables.

Mass: steam, steam+liquid water, and non-condensable gases $(2 + n_a)$

Energy: steam, steam+liquid water, and non-condensable gases $(2 + n_q)$

Momentum: gas (steam+non-condensable gases), and liquid water (2 phases \times 3 directions= 6)

The independent variables are the total pressure, the $2 + n_g$ temperatures, the $1 + n_g$ volume fractions (from which the volume fraction of liquid water can be derived from the others), and the 3 velocity components for 2 phases, resulting in a total of $10 + 2n_g$ variables.



Fig. 3.5 The numerical grids utilized for the two-phase flow model. The scalar variables are defined at the cell centers, whereas the vector variable is defined at the cell boundaries due to the staggered grid. The cell boundary indices "i-1/2," "i+1/2," and "i+3/2" are practically denoted by "i," "i+1," and "i+2" within the code description, respectively.

The mass and energy equations for the liquid water and steam mixture are included to ensure that at least one of the two equations remain significant when either the liquid water or steam is absent. In constructing the innermost system equation set, a variable conversion $T \rightarrow \alpha T$ is performed, which is solved by matrix inversion and Newton iteration, to handle singularity for absent components.

The velocities at the new time step can be expressed in terms of the pressures in adjacent cells by transforming the momentum equations. The utilization of these expressions serves to eliminate the velocities from the mass and energy equations. The mass and energy equations are linearized with respect to the variance of the independent variables, specifically, pressure, volume fractions of steam and non-condensable gases, and temperature of all the components. Consequently, a system of linear equations for Newton-Raphson iteration is derived. A specific subset of the pressure equations, which exclusively incorporates the pressure at adjacent cells, is selected from the system of linear equations. In order to solve the system of linear equations, it is first necessary to obtain the pressure correction through the pressure equation. The remaining variables are corrected by substituting the obtained pressure correction into the remaining equations in the system of linear equations. The iteration process is repeated until the residual is sufficiently reduced, at which point the variables, with the exception of those pertaining to velocity at the new time step, are obtained. The momentum equations are employed in order to calculate the velocity from the pressure.

3.3.2 Discretization Scheme

The suffixes *i*, *j*, and *k* are employed to indicate the coordinate in the x/r, y/θ , and *z* directions, respectively. The absence of the suffixes signifies that the equations or variables are defined at the original location: the cell-centered variable $p_{i,j,k} \rightarrow p$, and the cell boundary variable $u_{i+1/2,j,k} \rightarrow u$. The subscript *m* denotes a fluid component either *s* (steam), *l* (liquid water), or *a* (non-condensable gases) in the conservation equations for the mass and energy equations, while denotes a fluid component either *g* (gas mixture), or *l* (liquid water) in the conservation equation for the momentum. The superscripts "n" denotes the old time step and "n+1" denotes the new time step. The notation $\langle x \rangle u$ indicates that the variable *x* is utilized at the upwind side of the location where the velocity *u* is defined: in case of $u_{i+1/2} > 0$, $\langle x \rangle u = x_i u_{i+1/2}$.

The mass equation at the cell (i, j, k):

$$\begin{split} M_{m} &= V\{(\alpha_{m}\rho_{m})^{n+1} - (\alpha_{m}\rho_{m})^{n}\} + \Delta t \frac{dV}{dt} (\alpha_{m}\rho_{m})^{n} \\ &+ \Delta t V \frac{\langle \alpha_{m}\rho_{m} \rangle_{i+1/2,j,k}^{n} u_{m,i+1/2,j,k}^{n+1} - \langle \alpha_{m}\rho_{m} \rangle_{i-1/2,j,k}^{n} u_{m,i-1/2,j,k}^{n+1} \\ &+ \Delta t V \frac{\langle \alpha_{m}\rho_{m} \rangle_{i,j+1/2,k}^{n} v_{m,i,j+1/2,k}^{n+1} - \langle \alpha_{m}\rho_{m} \rangle_{i,j-1/2,k}^{n} v_{m,i,j-1/2,k}^{n+1} \\ &+ \Delta t V \frac{\langle \alpha_{m}\rho_{m} \rangle_{i,j,k+1/2}^{n} w_{m,i,j,k+1/2}^{n+1} - \langle \alpha_{m}\rho_{m} \rangle_{i,j,k-1/2}^{n} w_{m,i,j,k-1/2}^{n+1} \\ &+ \Delta t V \frac{\langle \alpha_{m}\rho_{m} \rangle_{i,j,k+1/2}^{n} w_{m,i,j,k+1/2}^{n+1} - \langle \alpha_{m}\rho_{m} \rangle_{i,j,k-1/2}^{n} w_{m,i,j,k-1/2}^{n+1} \\ &- \Delta t \Gamma_{m}^{n+1} = 0. \end{split}$$

$$(3.38)$$

The energy equation at the cell (i, j, k):

$$\begin{split} E_{m} &= V\{(\alpha_{m}\rho_{m}e_{m})^{n+1} - (\alpha_{m}\rho_{m}e_{m})^{n}\} + \Delta t \frac{dV}{dt} (\alpha_{m}\rho_{m}e_{m})^{n} \\ &+ \Delta t V \frac{\langle \alpha_{m}\rho_{m}e_{m} \rangle_{i+1/2,j,k}^{n} u_{m,i+1/2,j,k}^{n+1} - \langle \alpha_{m}\rho_{m}e_{m} \rangle_{i-1/2,j,k}^{n} u_{m,i-1/2,j,k}^{n+1} \\ &+ \Delta t V \frac{\langle \alpha_{m}\rho_{m}e_{m} \rangle_{i,j+1/2,k}^{n} v_{m,i,j+1/2,k}^{n+1} - \langle \alpha_{m}\rho_{m}e_{m} \rangle_{i,j-1/2,k}^{n} v_{m,i,j-1/2,k}^{n+1} \\ &+ \Delta t V \frac{\langle \alpha_{m}\rho_{m}e_{m} \rangle_{i,j,k+1/2}^{n} u_{m,i,j,k+1/2}^{n+1} - \langle \alpha_{m}\rho_{m}e_{m} \rangle_{i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n+1} \\ &+ \Delta t V \frac{\langle \alpha_{m}\rho_{m}e_{m} \rangle_{i,j,k+1/2}^{n} u_{m,i,j,k+1/2}^{n+1} - \langle \alpha_{m}\rho_{m}e_{m} \rangle_{i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n+1} \\ &+ \Delta t V p \left[\frac{\alpha_{m}^{n+1} - \alpha_{m}^{n}}{\Delta t} \\ &+ \frac{\langle \alpha_{m} \rangle_{i+1/2,j,k}^{n} u_{m,i+1/2,j,k}^{n+1} - \langle \alpha_{m} \rangle_{i-1/2,j,k}^{n} u_{m,i-1/2,j,k}^{n+1} \\ &+ \frac{\langle \alpha_{m} \rangle_{i,j+1/2,k}^{n} v_{m,i,j+1/2,k}^{n+1} - \langle \alpha_{m} \rangle_{i,j-1/2,k}^{n} v_{m,i,j-1/2,k}^{n+1} \\ &+ \frac{\langle \alpha_{m} \rangle_{i,j,k+1/2}^{n} u_{m,i,j,k+1/2}^{n+1} - \langle \alpha_{m} \rangle_{i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n+1} \\ &+ \frac{\langle \alpha_{m} \rangle_{i,j,k+1/2}^{n} u_{m,i,j,k+1/2}^{n+1} - \langle \alpha_{m} \rangle_{i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n+1} \\ &+ \frac{\langle \alpha_{m} \rangle_{i,j,k+1/2}^{n} u_{m,i,j,k+1/2}^{n+1} - \langle \alpha_{m} \rangle_{i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n+1} \\ &+ \frac{\langle \alpha_{m} \rangle_{i,j,k+1/2}^{n} u_{m,i,j,k+1/2}^{n+1} - \langle \alpha_{m} \rangle_{i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n+1} \\ &+ \frac{\langle \alpha_{m} \rangle_{i,j,k+1/2}^{n} u_{m,i,j,k+1/2}^{n+1} - \langle \alpha_{m} \rangle_{i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n+1} \\ &+ \frac{\langle \alpha_{m} \rangle_{i,j,k+1/2}^{n} u_{m,i,j,k+1/2}^{n+1} - \langle \alpha_{m} \rangle_{i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n+1} \\ &+ \frac{\langle \alpha_{m} \rangle_{i,j,k+1/2}^{n} u_{m,i,j,k+1/2}^{n} - \langle \alpha_{m} \rangle_{i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n} \\ &+ \frac{\langle \alpha_{m} \rangle_{i,j,k+1/2}^{n} u_{m,i,j,k+1/2}^{n} - \langle \alpha_{m} \rangle_{i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n} \\ &+ \frac{\langle \alpha_{m} \rangle_{i,j,k+1/2}^{n} u_{m,i,j,k+1/2}^{n} - \langle \alpha_{m} \rangle_{i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n} \\ &+ \frac{\langle \alpha_{m} \rangle_{i,j,k+1/2}^{n} u_{m,i,j,k+1/2}^{n} - \langle \alpha_{m} \rangle_{i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n} u_{m,i,j,k-1/2}^{n} \\ &+ \frac{\langle \alpha_{m} \rangle_{i,j,k+1}^{n} + u_{m,k}^{n} + u_{m,k}^{n} + u_{m,k}$$

The momentum equation at the (i + 1/2, j, k) cell in the x-direction:

$$\frac{u_m^{n+1} - u_m^n}{\Delta t} + u_m^n \left\langle \frac{\partial u_m}{\partial x} \right\rangle_{i+1/2,j,k}^n + v_m^n \left\langle \frac{\partial v_m}{\partial y} \right\rangle_{i+1/2,j,k}^n + w_m^n \left\langle \frac{\partial w_m}{\partial z} \right\rangle_{i+1/2,j,k}^n + \frac{1}{\rho_m} \frac{p_{i+1}^{n+1} - p_i^{n+1}}{x_{i+1} - x_i} + \left(K_{im} + \frac{\Gamma_m^+}{V\alpha_m\rho_m} \right) (u_m^{n+1} - u_i^n)_{j \neq m} + \frac{F_{mk}}{V\alpha_m\rho_m} - g_x = 0.$$
(3.40)

The momentum equations are simultaneous equations of u_l and u_g . By solving the momentum equations analytically, the equations for u_l and u_g in the new time step in terms of the pressure p at the new time step can be obtained as follows:

$$u_{g,i+1/2}^{n+1} = C_{gx,i+1/2} + D_{gx,i+1/2}(p_{i+1}^{n+1} - p_i^n), \qquad \text{and} \qquad (3.41)$$

$$u_{l,i+1/2}^{n+1} = C_{lx,i+1/2} + D_{lx,i+1/2}(p_{i+1}^{n+1} - p_i^n),$$
(3.42)
where C_{gx} , D_{gx} , C_{lx} , and D_{lx} denote constants that include only the variables from the old time step. Similarly, the velocities of the liquid and gas phases in the new times step in terms of the pressure at the new time step can be obtained as follows:

$$v_{g,j+1/2}^{n+1} = C_{gy,j+1/2} + D_{gy,j+1/2} (p_{j+1}^{n+1} - p_j^n),$$
(3.43)

$$v_{l,j+1/2}^{n+1} = C_{ly,j+1/2} + D_{ly,j+1/2} (p_{j+1}^{n+1} - p_j^n),$$
(3.44)

$$w_{g,k+1/2}^{n+1} = C_{gz,k+1/2} + D_{gz,k+1/2}(p_{k+1}^{n+1} - p_k^n), \qquad \text{and} \qquad (3.45)$$

$$w_{l,k+1/2}^{n+1} = C_{lz,k+1/2} + D_{lz,k+1/2}(p_{k+1}^{n+1} - p_k^n).$$
(3.46)

These equations are incorporated into the mass and energy equations in order to eliminate the velocities in the new time step. Once the velocities have been eliminated, Eqs. (3.37) and (3.38) are expressed in the following form:

$$\begin{split} M_m \big(p^{n+1}, p^{n+1}_{ahj}, \alpha^{n+1}_m, T^{n+1}_m \big) \\ &= V(\alpha_m \rho_m)^{n+1} + \Delta t \frac{dV}{dt} (\alpha_m \rho_m)^n + V \sum_{adj} \widetilde{m}_{m,adj} (p^{n+1}_{adj} - p^{n+1}) \\ &- V \widetilde{M}_m - \Delta t \Gamma^{n+1}_m = 0. \end{split}$$
(3.47)

$$\begin{split} E_m(p^{n+1}, p^{n+1}_{ahj}, \alpha^{n+1}_m, T^{n+1}_m) \\ &= V(\alpha_m \rho_m e_m)^{n+1} + \Delta t \frac{dV}{dt} (\alpha_m \rho_m e_m)^n \\ &+ V \sum_{adj} (\tilde{e}^{(1)}{}_{m,adj} + \tilde{e}^{(2)}{}_{m,adj} p^{n+1}) (p^{n+1}_{adj} - p^{n+1}) + V p^{n+1} \alpha^{n+1}_m \\ &+ V p^{n+1} \widetilde{D}_m - \Delta t (q^{n+1}_{im} + \Gamma^{n+1}_m h^{n+1}_m) - \Delta t \sum_{j \neq m} q^{n+1}_{jm} \\ &- V \widetilde{E}_m + \nabla \cdot q^{\prime\prime} \Delta t = 0. \end{split}$$
(3.48)

The suffixes adj denotes the adjacent cells, m denotes the components either s (steam), l (liquid water), or a (non-condensable gases). The symbols $\widetilde{m}_{m,adj}$, \widetilde{M}_m , $\tilde{e}^{(n)}_{m,adj}$, \widetilde{D}_m and \tilde{E}_m denote constants that include only the variables from the old time step, derived from the advection terms.

The summation of $\widetilde{m}_{m,adj}(p_{adj}^{n+1}-p^{n+1})$ in the second term of the right-hand side of the mass equation Eq. (3.47) is expanded as follows:

$$\begin{split} &\sum_{adj} \widetilde{m}_{m,adj} (p_{adj}^{n+1} - p^{n+1}) \\ &= \frac{\Delta t}{x_{i+1/2} - x_{i-1/2}} D_{mx,i+1/2} \langle \alpha_m \rho_m \rangle_{i+1/2} (p_{i+1}^{n+1} - p^{n+1}) \\ &+ \frac{\Delta t}{x_{i+1/2} - x_{i-1/2}} D_{mx,i-1/2} \langle \alpha_m \rho_m \rangle_{i-1/2} (p_{i-1}^{n+1} - p^{n+1}) \\ &+ \frac{\Delta t}{y_{j+1/2} - y_{j-1/2}} D_{my,j+1/2} \langle \alpha_m \rho_m \rangle_{j+1/2} (p_{j+1}^{n+1} - p^{n+1}) \\ &+ \frac{\Delta t}{y_{j+1/2} - y_{j-1/2}} D_{my,j-1/2} \langle \alpha_m \rho_m \rangle_{j-1/2} (p_{j-1}^{n+1} - p^{n+1}) \\ &+ \frac{\Delta t}{z_{k+1/2} - z_{k-1/2}} D_{mz,k+1/2} \langle \alpha_m \rho_m \rangle_{k+1/2} (p_{k+1}^{n+1} - p^{n+1}) \\ &+ \frac{\Delta t}{z_{k+1/2} - z_{k-1/2}} D_{my,k-1/2} \langle \alpha_m \rho_m \rangle_{k-1/2} (p_{k-1}^{n+1} - p^{n+1}). \end{split}$$

The constant $\,\widetilde{M}_m\,$ is expressed as follows:

$$\begin{split} \widetilde{M}_{m} &= \alpha_{m}\rho_{m} + \Delta t \frac{\langle \alpha_{m}\rho_{m} \rangle_{i+1/2} C_{mx,i+1/2} - \langle \alpha_{m}\rho_{m} \rangle_{i-1/2} C_{mx,i-1/2}}{x_{i+1/2} - x_{i-1/2}} \\ &+ \Delta t \frac{\langle \alpha_{m}\rho_{m} \rangle_{j+1/2} C_{my,j+1/2} - \langle \alpha_{m}\rho_{m} \rangle_{j-1/2} C_{my,j-1/2}}{y_{j+1/2} - y_{j-1/2}} \\ &+ \Delta t \frac{\langle \alpha_{m}\rho_{m} \rangle_{k+1/2} C_{mz,k+1/2} - \langle \alpha_{m}\rho_{m} \rangle_{k-1/2} C_{mz,k-1/2}}{z_{k+1/2} - z_{k-1/2}}. \end{split}$$
(3.50)

The constant $\,\widetilde{D}_m\,$ and $\,\widetilde{E}_m\,$ are expressed as follows:

$$\begin{split} \widetilde{D}_{m} &= -\alpha_{m} + \Delta t \frac{\langle \alpha_{m} \rangle_{i+1/2} C_{mx,i+1/2} - \langle \alpha_{m} \rangle_{i-1/2} C_{mx,i-1/2}}{x_{i+1/2} - x_{i-1/2}} \\ &+ \Delta t \frac{\langle \alpha_{m} \rangle_{j+1/2} C_{my,j+1/2} - \langle \alpha_{m} \rangle_{j-1/2} C_{my,j-1/2}}{y_{j+1/2} - y_{j-1/2}} \\ &+ \Delta t \frac{\langle \alpha_{m} \rangle_{k+1/2} C_{mz,k+1/2} - \langle \alpha_{m} \rangle_{k-1/2} C_{mz,k-1/2}}{z_{k+1/2} - z_{k-1/2}}, \end{split}$$
 and (3.51)

$$\begin{split} \tilde{E}_{m} &= \alpha_{m}\rho_{m}e_{m} + \Delta t q_{melt,m}/V \\ &+ \Delta t \frac{\langle \alpha_{m}\rho_{m}e_{m} \rangle_{i+1/2}C_{mx,i+1/2} - \langle \alpha_{m}\rho_{m}e_{m} \rangle_{i-1/2}C_{mx,i-1/2}}{x_{i+1/2} - x_{i-1/2}} \\ &+ \Delta t \frac{\langle \alpha_{m}\rho_{m}e_{m} \rangle_{j+1/2}C_{my,j+1/2} - \langle \alpha_{m}\rho_{m}e_{m} \rangle_{j-1/2}C_{my,j-1/2}}{y_{j+1/2} - y_{j-1/2}} \\ &+ \Delta t \frac{\langle \alpha_{m}\rho_{m}e_{m} \rangle_{k+1/2}C_{mz,k+1/2} - \langle \alpha_{m}\rho_{m}e_{m} \rangle_{k-1/2}C_{mz,k-1/2}}{z_{k+1/2} - z_{k-1/2}}. \end{split}$$
(3.52)

The summation of $(\tilde{e}^{(1)}_{m,adj} + \tilde{e}^{(2)}_{m,adj}p^{n+1})(p^{n+1}_{adj} - p^{n+1})$ in the second term of the right-hand side of the energy equation Eq. (3.48) is expanded as follows:

$$\begin{split} &\sum_{adj} \left(\tilde{e}^{(1)}_{m,adj} + \tilde{e}^{(2)}_{m,adj} p^{n+1} \right) \left(p^{n+1}_{adj} - p^{n+1} \right) \\ &= \frac{\Delta t}{x_{i+1/2} - x_{i-1/2}} D_{mx,i+1/2} \left(\langle \alpha_m \rho_m e_m \rangle_{i+1/2} + \langle \alpha_m \rangle_{i+1/2} p^{n+1} \right) \left(p^{n+1}_{i+1} - p^{n+1} \right) \\ &+ \frac{\Delta t}{x_{i+1/2} - x_{i-1/2}} D_{mx,i-1/2} \left(\langle \alpha_m \rho_m e_m \rangle_{i-1/2} + \langle \alpha_m \rangle_{i-1/2} p^{n+1} \right) \left(p^{n+1}_{i-1} - p^{n+1} \right) \\ &+ \frac{\Delta t}{y_{j+1/2} - y_{j-1/2}} D_{my,j+1/2} \left(\langle \alpha_m \rho_m e_m \rangle_{j+1/2} + \langle \alpha_m \rangle_{j+1/2} p^{n+1} \right) \left(p^{n+1}_{j+1} - p^{n+1} \right) \\ &+ \frac{\Delta t}{y_{j+1/2} - y_{j-1/2}} D_{my,j-1/2} \left(\langle \alpha_m \rho_m e_m \rangle_{j-1/2} + \langle \alpha_m \rangle_{j-1/2} p^{n+1} \right) \left(p^{n+1}_{j-1} - p^{n+1} \right) \\ &+ \frac{\Delta t}{z_{k+1/2} - z_{k-1/2}} D_{mz,k+1/2} \left(\langle \alpha_m \rho_m e_m \rangle_{k+1/2} + \langle \alpha_m \rangle_{k+1/2} p^{n+1} \right) \left(p^{n+1}_{k+1} - p^{n+1} \right) \\ &+ \frac{\Delta t}{z_{k+1/2} - z_{k-1/2}} D_{my,k-1/2} \left(\langle \alpha_m \rho_m e_m \rangle_{k-1/2} + \langle \alpha_m \rangle_{k-1/2} p^{n+1} \right) \left(p^{n+1}_{k-1} - p^{n+1} \right). \end{split}$$

The mass and energy equations incorporate the unknown variables: the pressure, volume fractions, and temperature at the local cell (i, j, k), as well as the pressure at the adjacent cells $(i \pm 1, j \pm 1, k \pm 1)$. The mass and energy equations at the local cell are connected to those of at the adjacent cells only through the pressure, which is in linear dependence. The dependence on the variables within the local cell is non-linear due to the phase change term and the physical properties. The mass and energy equations are solved using the Newton–Raphson method, which is described in detail in the subsequent section.

3.3.3 Boundary Conditions

Cell Boundary Variables

The boundary conditions for the cell boundary variable or velocity are delineated. The expressions are provided at the cell (i, 1, 1) for illustrative purposes (see Fig. 3.5). The velocity of the two-phase flow in the normal direction is defined on the wall surface or boundary of the simulation domain. The velocity is determined using Eqs. (3.41)–(3.46).

1. Fill Boundary:

The fill boundary condition is utilized to represent the inlet condition, wherein the velocity is specified at the boundary of the simulation domain as $w_{i,1,1/2} = w_{in}$. The fill boundary is achieved through the application of $C_{mz,1/2} = w_{in}$ and $D_{mz,1/2} = 0$ for the liquid or gas component.

2. Break Boundary:

The break boundary condition is utilized to represent the outlet condition, wherein the pressure is specified at the boundary cell as $p_{i,1,0} = p_{in}$ in the exterior of the simulation domain. The velocity $w_{i,1,1/2}$ can be derived by solving the solutions of the momentum equation.

The velocity of two-phase flow in the tangential direction cannot be defined just on the wall boundary or surface. The velocity at the boundary cell $u_{i+1/2,1,0}$ in the exterior of the simulation domain is specified in terms of the velocity at $u_{i+1/2,1,1}$ in order to specify the boundary conditions.

3. Slip Boundary:

The slip boundary condition is utilized to achieve the condition of zero-shear force at the boundary of the simulation domain. The slip boundary is achieved through the differentiation of the tangential velocity in the normal direction, resulting in $\partial u/\partial z = 0$ or $u_{i+1/2,1,0} = u_{i+1/2,1,1}$.

4. Non-Slip Boundary:

The non-slip boundary is utilized to achieve the condition wherein the tangential velocity is set to be zero at the boundary of the simulation domain. The non-slip boundary in the *x*-direction is achieved through the following relations, for example:

$$u_{i+1/2,1,1/2} \simeq \frac{(z_{1/2} - z_{-1/2})u_{i+1/2,1,0} + (z_{3/2} - z_{1/2})u_{i+1/2,1,1}}{(z_{1/2} - z_{-1/2}) + (z_{3/2} - z_{1/2})};$$
(3.54)

therefore,
$$u_{i+1/2,1,0} = -\frac{(z_{1/2} - z_{-1/2})}{(z_{3/2} - z_{1/2})} u_{i+1/2,1,1}$$
 (3.55)

Cell-Centered Variables

The boundary conditions for the cell-centered variables, including pressure, volume fractions, and temperatures are described. The variables should be specified at the boundary cell in the outside of the simulation domain in order to determine the velocity at the boundary in the fill and break boundaries.

3.3.4 Newton–Raphson Method

General Description

The discretized equations employed in the two-phase flow simulations constitute a set of non-linear equations. The i-th non-linear equation among the n non-linear equations is expressed as follows:

$$F_i(x_1, x_2, \cdots, x_n) = 0, \tag{3.56}$$

where $i = 1, \dots, n$. The solutions can be identified through an iterative process, beginning with the initial value x_i^0 and modifying x_i^k using δx_i^k ,

$$x_i^{k+1} = x_i^k + \delta x_i^k, \tag{3.57}$$

where k denotes the number of iterations. In order to derive the correction values δx_i , it is necessary to focus on the residual errors of F_i in the k-th iteration,

$$\delta F_i^k = F_i^{k+1} - F_i^k. \tag{3.58}$$

Since the purpose of the iteration is $F_i^{k+1} = 0$, or

$$\delta F_i^k = -F_i^k. \tag{3.59}$$

Conversely, the residual errors of F_i^k are approximated using the Taylor expansion:

$$\delta F_i^k \simeq \frac{\partial F_i^k}{\partial x_1^k} \delta x_1^k + \frac{\partial F_i^k}{\partial x_2^k} \delta x_2^k + \dots + \frac{\partial F_i^k}{\partial x_n^k} \delta x_n^k.$$
(3.60)

Eqs. (3.59) and (3.60) provide a set of the non-linear equations for correcting the values of x_i^k ,

$$J\delta x^k = -F^k, \qquad \text{or} \qquad (3.61)$$

$$J\begin{pmatrix} \delta x_1^k\\ \delta x_2^k\\ \vdots\\ \delta x_n^k \end{pmatrix} = -\begin{pmatrix} F_1^k\\ F_2^k\\ \vdots\\ F_n^k \end{pmatrix},$$
(3.62)

where J denotes Jacobian matrix. The components of the Jacobian matrix, or $J_{ij} = \partial F_i / \delta x_j$, in the k-th iteration are expressed as follows:

$$\boldsymbol{J} = \begin{pmatrix} \partial F_1^k / \delta x_1^k & \partial F_1^k / \delta x_2^k & \cdots & \partial F_1^k / \delta x_n^k \\ \partial F_2^k / \delta x_1^k & \partial F_2^k / \delta x_2^k & \cdots & \partial F_2^k / \delta x_n^k \\ \vdots & \vdots & & \vdots \\ \partial F_n / \delta x_1 & \partial F_n^k / \delta x_2^k & \cdots & \partial F_n^k / \delta x_n^k \end{pmatrix}.$$
(3.63)

In order to obtain δx_i^k , it is necessary to solve the simultaneous equation Eq. (3.62) in a single iteration process. The iteration process is continued until the residual errors δF_i^k have been sufficiently reduced to zero, or until the solutions have been reached.

Practical Application

The Newton-Raphson method is applied for the solution of the mass and energy equations, whereas an alternative method is applied for the solution of the momentum equation. The equations for the correction of a local cell i, j, k are provided as below:

$$\boldsymbol{J}\begin{pmatrix} \delta p \\ \delta \alpha_{s} \\ \delta \beta_{s} \\ \delta \beta_{s} \\ \delta \beta_{l} \\ \delta \alpha_{a_{1}} \\ \vdots \\ \delta \alpha_{a_{n_{g}}} \\ \delta \beta_{a_{n_{g}}} \end{pmatrix} = -\begin{pmatrix} M_{sl} \\ M_{s} \\ E_{s} \\ E_{s} \\ M_{a_{1}} \\ E_{a_{1}} \\ \vdots \\ M_{a_{n_{g}}} \\ B_{a_{n_{g}}} \end{pmatrix} - \sum_{adj} \begin{pmatrix} \partial M_{sl}/\partial p_{adj} \\ \partial M_{s}/\partial p_{adj} \\ \partial E_{s}/\partial p_{adj} \\ \partial M_{a_{1}}/\partial p_{adj} \\ \partial E_{a_{1}}/\partial p_{adj} \\ \partial E_{a_{n_{g}}}/\partial p_{adj} \\ \partial E_{a_{n_{g}}}/\partial p_{adj} \end{pmatrix} \delta p_{adj},$$
(3.64)

where the suffix sl denotes the sum of the equations for the steam and liquid water, which can be expressed as $M_{sl} = M_s + M_l$, and $E_{sl} = E_s + E_l$. The variable transformation $\beta_m \equiv \alpha_m T_m$ is employed as an independent variable in lieu of T_m in order to circumvent the numerical issues associated with the lack of components when $\alpha_m = 0$. The Jacobian matrix J is a matrix of partial derivatives of the variables in the first term on the right-hand side with respect to the variables: p, α_s , β_s , β_l , α_{a_1} , β_{a_1} , \cdots , $\alpha_{a_{ng}}$ and $\beta_{a_{ng}}$.

The pressures in adjacent cells are excluded from the Jacobian matrix and are instead solved separately, along with all other pressures within the system or simulation domain. By matrix inversion, Eq. (3.64) is transformed into

$$\begin{pmatrix} \delta p \\ \delta \alpha_s \\ \delta \beta_s \\ \delta \beta_s \\ \delta \beta_l \\ \delta \alpha_{a_1} \\ \vdots \\ \delta \alpha_{a_n} \\ \delta \beta_{a_1} \\ \vdots \\ \delta \alpha_{a_ng} \\ \delta \beta_{a_ng} \end{pmatrix} = -\mathbf{J}^{-1} \begin{pmatrix} M_{sl} \\ M_s \\ E_s \\ E_s \\ B_{sl} \\ M_{a_1} \\ E_{a_1} \\ \vdots \\ M_{a_ng} \\ E_{a_ng} \end{pmatrix} - \mathbf{J}^{-1} \sum_{adj} \begin{pmatrix} \partial M_{sl}/\partial p_{adj} \\ \partial M_s/\partial p_{adj} \\ \partial E_s/\partial p_{adj} \\ \partial M_{a_1}/\partial p_{adj} \\ \partial E_{a_1}/\partial p_{adj} \\ \vdots \\ \partial M_{a_ng}/\partial p_{adj} \\ \partial E_{a_ng}/\partial p_{adj} \end{pmatrix} \delta p_{adj},$$
(3.65)

which can be written as follows:

$$\begin{pmatrix} \delta p \\ \delta \alpha_{s} \\ \delta \beta_{s} \\ \delta \beta_{s} \\ \delta \beta_{l} \\ \delta \alpha_{a_{1}} \\ \delta \beta_{a_{1}} \\ \vdots \\ \delta \alpha_{a_{ng}} \\ \delta \beta_{a_{ng}} \end{pmatrix} = - \begin{pmatrix} f_{1} \\ f_{2} \\ f_{3} \\ f_{4} \\ f_{5} \\ f_{6} \\ \vdots \\ f_{4+2ng-1} \\ f_{4+2ng} \end{pmatrix} - \sum_{adj} \begin{pmatrix} g_{1} \\ g_{2} \\ g_{3} \\ g_{4} \\ g_{5} \\ g_{6} \\ \vdots \\ g_{4+2ng-1} \\ g_{4+2ng} \end{pmatrix} \delta p_{adj}.$$
(3.66)

The first line in Eq. (3.66)

$$\delta p = -f_1 - \sum_{adj} g_1 \,\delta p_{adj} \tag{3.67}$$

encompasses only the pressures of the local cell and adjacent cells. The equation can be solved as a system-wide pressure equation. Once the requisite correction values for all pressures within the system or simulation domain have been obtained via Eq. (3.67), the correction values for other variables are obtained cell by cell through the application of the remaining lines in Eq. (3.66).

3.3.5 Organization of the Pressure Equations

The pressure equation Eq. (3.67) incorporates the pressures in the local cell (i, j, k) and six adjacent cells. To facilitate the solution of the system-wide set of equations, it is advantageous to employ a one-dimensional index (one-dimensional array), which is defined as follows:

$$m(i,j,k) = i + n_x(j-1) + n_x n_y(k-1),$$
(3.68)

where n_x and n_y denote the number of cells in the x and y directions, respectively. The matrix for the system-wide pressure equations is transformed into a multi-band coarse matrix of $n_x n_y n_z$ dimensions, comprising seven non-zero bands. The non-zero elements are located on the diagonal (i, j, k), on both sides of the diagonal $(i \pm 1, j, k)$, and at the distances of n_x $(i, j \pm 1, k)$ and $n_x n_y$ $(i, j, k \pm 1)$ from the diagonal. The mapping scheme outlined in Eq. (3.68) is advantageous when the number of the cells in the z direction is greater than those in the x and y directions. The pressure equation is solved using the ILU-BCG (incomplete LU decomposition BiConjugate Gradient) method⁽⁴³⁾.

3.3.6 Elements of the Jacobian Matrix

The Mass and Energy Equations

The mass and energy equations, along with the associated derivatives for the Jacobian matrix, is provided in this section. The derivatives are expressed in terms of the original independent variables p, α_m , and T_m . Subsequently, a variable transformation is presented as a means of circumventing numerical issues associated with temperatures of missing components.

Mass (steam):

$$M_s = V(\alpha_s \rho_s)^{n+1} + \Delta t \frac{dV}{dt} (\alpha_s \rho_s)^n$$
(3.69)

$$+ V \sum_{adj} \widetilde{m}_{s,adj} (p_{adj}^{n+1} - p^{n+1}) - V \widetilde{M}_s - \Delta t \Gamma_s^{n+1}$$

$$\frac{\partial M_s}{\partial p} = V \alpha_s \frac{\partial \rho_s}{\partial p} - \Delta t \frac{\partial \Gamma_s}{\partial p} - V \sum_{adj} \widetilde{m}_{s,adj}$$
(3.70)

$$\frac{\partial M_s}{\partial \alpha_s} = V \rho_s - \Delta t \frac{\partial \Gamma_s}{\partial \alpha_s} \tag{3.71}$$

$$\frac{\partial M_s}{\partial T_s} = V \alpha_s \frac{\partial \rho_s}{\partial T_s} - \Delta t \frac{\partial \Gamma_s}{\partial T_s}$$
(3.72)

$$\frac{\partial M_s}{\partial T_l} = -\Delta t \frac{\partial \Gamma_s}{\partial T_l} \tag{3.73}$$

$$\frac{\partial M_s}{\partial \alpha_a} = -\Delta t \frac{\partial \Gamma_s}{\partial \alpha_a} \tag{3.74}$$

$$\frac{\partial M_s}{\partial T_a} = 0 \tag{3.75}$$

Mass (steam+liquid water):

$$M_{sl} = V(\alpha_s \rho_s + \alpha_l \rho_l)^{n+1} + \Delta t \frac{dV}{dt} (\alpha_s \rho_s + \alpha_l \rho_l)^n$$

$$+ V \sum_{l=1}^{\infty} (\widetilde{\alpha}_s - \lambda_l \widetilde{\alpha}_s - \lambda_l (\alpha_s \rho_s + \alpha_l \rho_l)^n$$
(3.76)

$$+ v \sum_{adj} (m_{s,adj} + m_{l,adj}) (p_{adj} - p^{-1}) - v (M_s + M_l)$$

$$\frac{\partial M_{sl}}{\partial p} = V\left(\alpha_s \frac{\partial \rho_s}{\partial p} + \alpha_l \frac{\partial \rho_l}{\partial p}\right) - V\sum_{adj} (\widetilde{m}_{s,adj} + \widetilde{m}_{l,adj})$$
(3.77)

$$\frac{\partial M_{sl}}{\partial \alpha_s} = V(\rho_s - \rho_l) \tag{3.78}$$

$$\frac{\partial M_{sl}}{\partial T_s} = V \alpha_s \frac{\partial \rho_s}{\partial T_s} \tag{3.79}$$

$$\frac{\partial M_{sl}}{\partial T_l} = V \alpha_l \frac{\partial \rho_l}{\partial T_l} \tag{3.80}$$

$$\frac{\partial M_{sl}}{\partial \alpha_a} = -V\rho_l \tag{3.81}$$

$$\frac{\partial M_{sl}}{\partial T_a} = 0 \tag{3.82}$$

Mass (non-condensable gases):

$$M_a = V(\alpha_a \rho_a)^{n+1} + \Delta t \frac{dV}{dt} (\alpha_a \rho_a)^n$$
(3.83)

$$+ V \sum_{adj} (\widetilde{m}_{a,adj}) (p_{adj}^{n+1} - p^{n+1}) - V \widetilde{M}_a$$

$$\frac{\partial M_a}{\partial p} = V \alpha_a \frac{\partial \rho_a}{\partial p} - V \sum_{adj} \widetilde{m}_{a,adj}$$
(3.84)

$$\frac{\partial M_a}{\partial \alpha_s} = 0 \tag{3.85}$$

$$\frac{\partial M_a}{\partial T_s} = 0 \tag{3.86}$$

$$\frac{\partial M_a}{\partial T_l} = 0 \tag{3.87}$$

$$\frac{\partial M_a}{\partial \alpha_a} = V \rho_a \tag{3.88}$$

$$\frac{\partial M_a}{\partial T_a} = V \alpha_a \frac{\partial \rho_a}{\partial T_a} \tag{3.89}$$

Energy (steam):

$$\begin{split} E_{s} &= V(\alpha_{s}\rho_{s}e_{s})^{n+1} + V\sum_{adj} (\tilde{e}^{(1)}{}_{s,adj} + \tilde{e}^{(2)}{}_{s,adj}p^{n+1})(p^{n+1}_{adj} - p^{n+1}) \\ &+ Vp^{n+1}\alpha^{n+1}_{s} + Vp^{n+1}\widetilde{D}_{s} - \Delta t(q^{n+1}_{is} + \Gamma^{n+1}_{s}h^{n+1}_{s}) + \Delta t\sum_{a} q^{n+1}_{sa} \\ &- V\tilde{E}_{s} + (\alpha_{s}\rho_{s}e_{s})^{n}\Delta t\frac{dV}{dt} \end{split}$$
(3.90)

$$\begin{split} \frac{\partial E_s}{\partial p} &= V \alpha_s \left(\frac{\partial \rho_s}{\partial p} e_s + \rho_s \frac{\partial e_s}{\partial p} \right) - V \sum_{adj} \{ \tilde{e}^{(1)}{}_{s,adj} + \tilde{e}^{(2)}{}_{s,adj} (2p - p_{adj}) \} \\ &+ V \alpha_s + V \widetilde{D}_s - \Delta t \left(\frac{\partial q_{is}}{\partial p} + \frac{\partial \Gamma_s}{\partial p} h_s + \Gamma_s \frac{\partial h_s}{\partial p} \right) \end{split}$$
(3.91)

$$\frac{\partial E_s}{\partial \alpha_s} = V \rho_s e_s + V p - \Delta t \left(\frac{\partial q_{is}}{\partial \alpha_s} + \frac{\partial \Gamma_s}{\partial \alpha_s} h_s \right)$$
(3.92)

$$\frac{\partial E_s}{\partial T_s} = V\alpha_s \left(\frac{\partial \rho_s}{\partial T_s}e_s + \rho_s \frac{\partial e_s}{\partial T_s}\right) - \Delta t \left(\frac{\partial q_{is}}{\partial T_s} + \frac{\partial \Gamma_s}{\partial T_s}h_s + \Gamma_s \frac{\partial h_s}{\partial T_s}\right) + \Delta t \sum_a R_{sa}$$
(3.93)

$$\frac{\partial E_s}{\partial T_l} = -\Delta t \frac{\partial \Gamma_s}{\partial T_l} h_s \tag{3.94}$$

$$\frac{\partial E_s}{\partial \alpha_a} = -\Delta t \left(\frac{\partial q_{is}}{\partial \alpha_a} + \frac{\partial \Gamma_s}{\partial \alpha_a} h_s \right)$$
(3.95)

$$\frac{\partial E_s}{\partial T_a} = -\Delta t R_{sa} \tag{3.96}$$

The heat flux between the steam and the non-condensable gas is expressed as $q_{sa} = R_{sa}(T_s - T_a)$, where R_{sa} denotes the heat transfer coefficient between the steam and the non-condensable gas. Given that the non-condensable gas is comprised of multiple components, the heat exchange terms are expressed using a summation sign. The q_{is} , which is referenced in Eq. (2.113), denotes the heat flux from the twophase interface to the steam. The steam is typically high temperature than the two-phase flow interface (saturation temperature), which results in heat absorption at the two-phase flow interface and subsequent evaporation. The enthalpy introduced into the steam by the newly formed steam resulting from evaporation at the two-phase flow interface is designated as $\Gamma_s h_s$. The q_{is} and $\Gamma_s h_s$ have different meanings. Note that when E_s is differentiated by T_a , no summation sign is added, as the differentiation is focused on a single component of non-condensable gas.

Energy (steam+liquid water):

$$\begin{split} E_{sl} &= V(\alpha_{s}\rho_{s}e_{s} + \alpha_{l}\rho_{l}e_{l})^{n+1} + (\alpha_{s}\rho_{s}e_{s} + \alpha_{l}\rho_{l}e_{l})^{n}\Delta t\frac{dV}{dt} - V(\tilde{E}_{s} + \tilde{E}_{l}) \\ &+ V\sum_{adj} (\tilde{e}^{(1)}{}_{s,adj} + \tilde{e}^{(1)}{}_{l,adj} + \tilde{e}^{(2)}{}_{s,adj}p^{n+1} + \tilde{e}^{(2)}{}_{l,adj}p^{n+1})(p^{n+1}_{adj} - p^{n+1}) \\ &+ Vp^{n+1}(\alpha_{s} + \alpha_{l})^{n+1} + Vp^{n+1}(\widetilde{D}_{s} + \widetilde{D}_{l}) + \Delta t\sum_{a} q^{n+1}_{sa} + \Delta t\sum_{a} q^{n+1}_{la} \\ &- \Delta tq_{int} \end{split}$$
(3.97)

$$\begin{split} \frac{\partial E_{sl}}{\partial p} &= V \left\{ \alpha_s \left(\frac{\partial \rho_s}{\partial p} e_s + \rho_s \frac{\partial e_s}{\partial p} \right) + \alpha_l \left(\frac{\partial \rho_l}{\partial p} e_l + \rho_l \frac{\partial e_l}{\partial p} \right) \right\} \\ &- V \sum_{adj} \{ \tilde{e}^{(1)}{}_{s,adj} + \tilde{e}^{(1)}{}_{l,adj} + (\tilde{e}^{(2)}{}_{s,adj} + \tilde{e}^{(2)}{}_{s,adj})(2p - p_{adj}) \} \\ &+ V(\alpha_s + \alpha_l) + V \Big(\widetilde{D}_s + \widetilde{D}_l \Big) \end{split}$$
(3.98)

$$\frac{\partial E_{sl}}{\partial \alpha_s} = V(\rho_s e_s - \rho_l e_l) \tag{3.99}$$

$$\frac{\partial E_{sl}}{\partial T_s} = V\alpha_s \left(\frac{\partial \rho_s}{\partial T_s} e_s + \rho_s \frac{\partial e_s}{\partial T_s}\right) + \Delta t \sum_a R_{sa}$$
(3.100)

$$\frac{\partial E_{sl}}{\partial T_l} = V \alpha_l \left(\frac{\partial \rho_l}{\partial T_l} e_l + \rho_l \frac{\partial e_l}{\partial T_l} \right) + \Delta t \sum_a R_{la}$$
(3.101)

$$\frac{\partial E_{sl}}{\partial \alpha_a} = -V\rho_l e_l - Vp \tag{3.102}$$

$$\frac{\partial E_{sl}}{\partial T_a} = -\Delta t R_{sa} - \Delta t R_{la} \tag{3.103}$$

The heat flux between the liquid water and the non-condensable gas is expressed as $q_{la} = R_{la}(T_l - T_a)$, where R_{la} denotes the heat transfer coefficient between the liquid water and the non-condensable gas. Since the E_{sl} [Eq. (3.97)] is an equation in which the right-hand side of the original equation [Eq. (2.109)] is transferred to the left-hand side, the heat input is expressed with a negative sign. The q_{int} , which is also referenced in Eq. (2.113), denotes the heat flux (heat input) from the melt components (outside the system) directly to the two-phase interface for the evaporation process, resulting in a negative sign in the E_{sl} . The q_{is} and q_{il} , which are also referenced in Eq. (2.113), denote the heat flux from the two-phase interface to the steam and the liquid water, respectively. The two-phase flow interface experiences exothermic or endothermic as a consequence of the phase change, yet the resulting phase retains energy: thus the q_{is} and q_{il} do not appear in the E_{sl} or in the steam and liquid water system. Note that when E_s and E_l are differentiated by T_a , no summation sign is added, as the differentiations are focused on a single component of non-condensable gas.

Energy (non-condensable gases):

$$\begin{split} E_{a} &= V(\alpha_{a}\rho_{a}e_{a})^{n+1} + \Delta t \frac{dV}{dt} (\alpha_{a}\rho_{a}e_{a})^{n} \\ &+ V \sum_{adj} (\tilde{e}^{(1)}{}_{a,adj} + \tilde{e}^{(2)}{}_{a,adj}p^{n+1}) (p^{n+1}_{adj} - p^{n+1}) + V p^{n+1} \alpha^{n+1}_{a} \\ &+ V p^{n+1} \widetilde{D}_{a} - \Delta t q^{n+1}_{sa} - \Delta t q^{n+1}_{la} - V \widetilde{E}_{a} \end{split}$$
(3.104)

$$\begin{aligned} \frac{\partial E_a}{\partial p} &= V \alpha_a \left(\frac{\partial \rho_a}{\partial p} e_a + \rho_a \frac{\partial e_a}{\partial p} \right) - V \sum_{adj} \{ \tilde{e}^{(1)}{}_{a,adj} + \tilde{e}^{(2)}{}_{a,adj} (2p - p_{adj}) \} \\ &+ V \alpha_a + V \widetilde{D}_a \end{aligned}$$
(3.105)

$$\frac{\partial E_a}{\partial \alpha_s} = 0 \tag{3.106}$$

$$\frac{\partial E_a}{\partial T_s} = -\Delta t R_{sa} \tag{3.107}$$

$$\frac{\partial E_a}{\partial T_l} = -\Delta t R_{la} \tag{3.108}$$

$$\frac{\partial E_a}{\partial \alpha_a} = V \rho_a e_a - V p \tag{3.109}$$

$$\frac{\partial E_a}{\partial T_a} = V \alpha_a \left(\frac{\partial \rho_a}{\partial T_a} e_a + \rho_a \frac{\partial e_a}{\partial T_a} \right) + \Delta t R_{sa} + \Delta t R_{la}$$
(3.110)

Note that since Eq. (3.104)–(3.110) are related to a single non-condensable gas component, no summation sign is added to the differentiations.

The Phase Change and Heat Transfer Terms

The phase change term (evaporation and condensation) provided by Eq. (2.113) is dependent upon the temperature of steam and liquid water, as well as the pressure and volume fractions through the saturation temperature at the steam partial pressure. The derivatives of Γ_s and q_{is} with respect to the original independent variables p, α_m , and T_m , for the Jacobian matrix, are provided below.

$$\frac{\partial \Gamma_s}{\partial p} = -A_i \frac{h_{is} + h_{il}}{h_s - h_l} \frac{\partial T_{sat}}{\partial p_s} \frac{\partial p_s}{\partial p} - A_i \frac{\Gamma_s}{h_s - h_l} \left(\frac{\partial h_s}{\partial p} - \frac{\partial h_l}{\partial p}\right)$$
(3.111)

$$\frac{\partial \Gamma_s}{\partial \alpha_s} = -A_i \frac{h_{is} + h_{il}}{h_s - h_l} \frac{\partial T_{sat}}{\partial p_s} \frac{\partial p_s}{\partial \alpha_s}$$
(3.112)

$$\frac{\partial \Gamma_s}{\partial T_s} = A_i \frac{h_{is}}{h_s - h_l} - A_i \frac{\Gamma_s}{h_s - h_l} \frac{\partial h_s}{\partial T_s}$$
(3.113)

$$\frac{\partial \Gamma_s}{\partial T_l} = A_i \frac{h_{il}}{h_s - h_l} + A_i \frac{\Gamma_s}{h_s - h_l} \frac{\partial h_l}{\partial T_l}$$
(3.114)

$$\frac{\partial \Gamma_s}{\partial \alpha_a} = -A_i \frac{h_{is} + h_{il}}{h_s - h_l} \frac{\partial T_{sat}}{\partial p_s} \frac{\partial p_s}{\partial \alpha_a}$$
(3.115)

$$\frac{\partial q_{is}}{\partial p} = A_i h_{is} \frac{\partial T_{sat}}{\partial p_s} \frac{\partial p_s}{\partial p}$$
(3.116)

$$\frac{\partial q_{is}}{\partial \alpha_s} = A_i h_{is} \frac{\partial T_{sat}}{\partial p_s} \frac{\partial p_s}{\partial \alpha_s}$$
(3.117)

$$\frac{\partial q_{is}}{\partial T_s} = -A_i h_{is} \tag{3.118}$$

$$\frac{\partial q_{is}}{\partial \alpha_a} = A_i h_{is} \frac{\partial T_{sat}}{\partial p_s} \frac{\partial p_s}{\partial \alpha_a}$$
(3.119)

The derivatives of the pseudo-partial pressure of steam Eq. (2.111) are provided below.

$$\frac{\partial p_s}{\partial p} = \frac{\alpha_s}{\alpha} \tag{3.120}$$

$$\frac{\partial p_s}{\partial \alpha_s} = p \frac{\alpha - \alpha_s}{\alpha^2} \tag{3.121}$$

$$\frac{\partial p_s}{\partial \alpha_a} = -p \frac{\alpha_s}{\alpha^2} \tag{3.122}$$

Variable Transformation

In order to circumvent the singularity that results from the absence of requisite components, a variable transformation $T_m \rightarrow \alpha_m T_m$ is implemented prior to the construction of the Jacobian matrix. The variable transformation is expressed as follows:

$$f(p, \alpha_s, T_s, T_l, \alpha_a, T_a) \to f(P, A_s, \beta_s, \beta_l, A_a, \beta_a), \tag{3.123}$$

where the new set of the independent variables are defined as follows:

$$P = p, \tag{3.124}$$

$$A_s = \alpha_s, \tag{3.125}$$

$$\beta_s = \alpha_s T_s, \tag{3.126}$$

$$\beta_l = \alpha_l T_l, \tag{3.127}$$

$$A_a = \alpha_a,$$
 and (3.128)

$$\beta_a = \alpha_a T_a. \tag{3.129}$$

The relationship between the partial derivatives are provided as follows:

$$\frac{\partial f}{\partial P} = \frac{\partial f}{\partial p},\tag{3.130}$$

$$\frac{\partial f}{\partial A_s} = \frac{\partial f}{\partial \alpha_s} - \frac{\partial f}{\partial T_s} \frac{T_s}{\alpha_s} + \frac{\partial f}{\partial T_l} \frac{T_l}{\alpha_l},\tag{3.131}$$

$$\frac{\partial f}{\partial \beta_s} = \frac{\partial f}{\partial T_s} \frac{1}{\alpha_s},\tag{3.132}$$

$$\frac{\partial f}{\partial \beta_l} = \frac{\partial f}{\partial T_l} \frac{1}{\alpha_l},\tag{3.133}$$

$$\frac{\partial f}{\partial A_a} = \frac{\partial f}{\partial \alpha_a} + \frac{\partial f}{\partial T_l} \frac{T_l}{\alpha_l} + \frac{\partial f}{\partial T_a} \frac{T_a}{\alpha_a}, \qquad \text{and} \qquad (3.134)$$

$$\frac{\partial f}{\partial \beta_a} = \frac{\partial f}{\partial T_a} \frac{1}{\alpha_a}.$$
(3.135)

The elements of the Jacobian matrix, expressed in terms of the transformed variables $P, A_s, \beta_s, \beta_l, A_a$ and β_a are presented below. The corresponding matrix variable names in the code are also indicated for convenience.

Mass (steam): (ipos=4+2*iigas-1)

-cc(2,7)

$$M_{s} = V(\alpha_{s}\rho_{s})^{n+1} + \Delta t \frac{dV}{dt} (\alpha_{s}\rho_{s})^{n}$$

$$(3.136)$$

$$+ V \sum_{adj} \widetilde{m}_{s,adj} (p_{adj}^{n+1} - p^{n+1}) - V \widetilde{M}_s - \Delta t \Gamma_s^{n+1}$$

aa(2,1)
$$\frac{\partial M_s}{\partial P} = V \alpha_s \frac{\partial \rho_s}{\partial p} - \Delta t \frac{\partial \Gamma_s}{\partial p} - V \sum_{adj} \widetilde{m}_{s,adj}$$
(3.137)

aa(2,2)
$$\frac{\partial M_s}{\partial A_s} = V \rho_s - \Delta t \frac{\partial \Gamma_s}{\partial \alpha_s} - X_1 T_s + X_2 T_l$$
 (3.138)

aa(2,3)
$$\frac{\partial M_s}{\partial \beta_s} = V \alpha_s \frac{\partial \rho_s}{\partial T_s} - \Delta t \frac{\partial \Gamma_s}{\partial T_s} \equiv X_1$$
 (3.139)

aa(2,4)
$$\frac{\partial M_s}{\partial \beta_l} = -\Delta t \frac{\partial \Gamma_s}{\partial T_l} \equiv X_2$$
 (3.140)

aa(2, ipos)
$$\frac{\partial M_s}{\partial A_a} = -\Delta t \frac{\partial \Gamma_s}{\partial \alpha_a} + X_2 T_l$$
 (3.141)

aa(2,ipos+1)
$$\frac{\partial M_s}{\partial \beta_a} = 0$$
 (3.142)

Mass (steam+liquid water): (ipos=4+2*iigas-1)

$$M_{sl} = V(\alpha_s \rho_s + \alpha_l \rho_l)^{n+1} + \Delta t \frac{dV}{dt} (\alpha_s \rho_s + \alpha_l \rho_l)^n$$
(3.143)

-cc(1,7)

$$+V\sum_{adj} (\widetilde{m}_{s,adj} + \widetilde{m}_{l,adj}) (p_{adj}^{n+1} - p^{n+1}) - V \left(\widetilde{M}_s + \widetilde{M}_l\right)$$

aa(1,1)
$$\frac{\partial M_{sl}}{\partial P} = V\left(\alpha_s \frac{\partial \rho_s}{\partial p} + \alpha_l \frac{\partial \rho_l}{\partial p}\right) - V \sum_{adj} (\widetilde{m}_{s,adj} + \widetilde{m}_{l,adj})$$
(3.144)

aa(1,2)
$$\frac{\partial M_{sl}}{\partial A_s} = V(\rho_s - \rho_l) - X_1 T_s + X_2 T_l$$
(3.145)

aa(1,3)
$$\frac{\partial M_{sl}}{\partial \beta_s} = V \frac{\partial \rho_s}{\partial T_s} \equiv X_1$$
 (3.146)

aa(1,4)
$$\frac{\partial M_{sl}}{\partial \beta_l} = V \frac{\partial \rho_l}{\partial T_l} \equiv X_2$$
 (3.147)

aa(1,ipos)
$$\frac{\partial M_{sl}}{\partial A_a} = -V\rho_l + X_2 T_l$$
 (3.148)

aa(1,ipos+1)
$$\frac{\partial M_{sl}}{\partial \beta_a} = 0$$
 (3.149)

Mass (non-condensable gases): (ipos=4+2*iigas-1)

$$M_a = V(\alpha_a \rho_a)^{n+1} + V \sum_{adj} \widetilde{m}_{a,adj} (p_{adj}^{n+1} - p^{n+1})$$

$$(3.150)$$

-cc(ipos,7)

$$+(\alpha_a\rho_a)^n\Delta t\frac{dV}{dt}-V\widetilde{M}_a$$

aa(ipos,1)
$$\frac{\partial M_a}{\partial P} = V \alpha_a \frac{\partial \rho_a}{\partial p} - V \sum_{adj} \widetilde{m}_{a,adj}$$
 (3.151)

aa(ipos,2)
$$\frac{\partial M_a}{\partial A_s} = 0$$
 (3.152)

aa(ipos,3)
$$\frac{\partial M_a}{\partial \beta_s} = 0$$
 (3.153)

aa(ipos,4)
$$\frac{\partial M_a}{\partial \beta_l} = 0$$
 (3.154)

aa(ipos,ipos)
$$\frac{\partial M_a}{\partial A_a} = V \rho_a - X_1 T_a$$
 (3.155)

aa(ipos,ipos+1)
$$\frac{\partial M_a}{\partial \beta_a} = V \alpha_a \frac{\partial \rho_a}{\partial T_a} \equiv X_1$$
 (3.156)

Energy (steam): (ipos=4+2*iigas-1)

 $-V\tilde{E}_s+(\alpha_s\rho_s e_s)^n\Delta t\frac{dV}{dt}$

$$\begin{split} E_s &= V(\alpha_s \rho_s e_s)^{n+1} + V \sum_{adj} (\tilde{e}^{(1)}{}_{s,adj} + \tilde{e}^{(2)}{}_{s,adj} p^{n+1}) (p^{n+1}_{adj} - p^{n+1}) \\ &+ V p^{n+1} \alpha^{n+1}_s + V p^{n+1} \widetilde{D}_s - \Delta t (q^{n+1}_{is} + \Gamma^{n+1}_s h^{n+1}_s) + \Delta t \sum_a q^{n+1}_{sa} \end{split}$$
(3.157)

-cc(3,7)

$$\frac{\partial E_s}{\partial p} = V \alpha_s \left(\frac{\partial \rho_s}{\partial p} e_s + \rho_s \frac{\partial e_s}{\partial p} \right)$$

$$-V \sum_{adj} \{ \tilde{e}^{(1)}{}_{s,adj} + \tilde{e}^{(2)}{}_{s,adj} (2p - p_{adj}) \} + V \alpha_s + V \widetilde{D}_s$$

$$(3.158)$$

aa(3,2)
$$\frac{\partial E_s}{\partial \alpha_s} = V \rho_s e_s + V p - \Delta t \left(\frac{\partial q_{is}}{\partial \alpha_s} + \frac{\partial \Gamma_s}{\partial \alpha_s} h_s \right) - X_1 T_s + X_2 T_l$$
(3.159)

$$\frac{\partial E_s}{\partial T_s} = V \left(\frac{\partial \rho_s}{\partial T_s} e_s + \rho_s \frac{\partial e_s}{\partial T_s} \right) - \frac{\Delta t}{\alpha_s} \left(\frac{\partial q_{is}}{\partial T_s} + \frac{\partial \Gamma_s}{\partial T_s} h_s + \Gamma_s \frac{\partial h_s}{\partial T_s} \right)$$
(3.160)

aa(3,3)

$$+\frac{\Delta t}{\alpha_s} \sum_a R_{sa} \equiv X_1$$

aa(3,4)
$$\frac{\partial E_s}{\partial \beta_l} = -\Delta t \frac{\partial \Gamma_s}{\partial T_l} h_s \equiv X_2$$
 (3.161)

aa(3,ipos)
$$\frac{\partial E_s}{\partial A_a} = -\Delta t \left(\frac{\partial q_{is}}{\partial \alpha_a} + \frac{\partial \Gamma_s}{\partial \alpha_a} h_s \right) + X_2 T_l - X_3 T_a$$
 (3.162)

aa(3, ipos+1)
$$\frac{\partial E_s}{\partial \beta_a} = -\frac{\Delta t}{\alpha_a} R_{sa} \equiv X_3$$
 (3.163)

Energy (steam+liquid water): (ipos=4+2*iigas-1)

$$E_{sl} = V(\alpha_{s}\rho_{s}e_{s} + \alpha_{l}\rho_{l}e_{l})^{n+1} + \Delta t \frac{dV}{dt}(\alpha_{s}\rho_{s}e_{s} + \alpha_{l}\rho_{l}e_{l})^{n} - V(\tilde{E}_{s} + \tilde{E}_{l})$$

$$+V\sum_{adj}(\tilde{e}^{(1)}{}_{s,adj} + \tilde{e}^{(1)}{}_{l,adj} + \tilde{e}^{(2)}{}_{s,adj}p^{n+1} + \tilde{e}^{(2)}{}_{l,adj}p^{n+1})(p^{n+1}_{adj} - p^{n+1})$$

$$+Vp^{n+1}(\alpha_{s} + \alpha_{l})^{n+1} + Vp^{n+1}(\tilde{D}_{s} + \tilde{D}_{l}) + \Delta t\sum_{a}q^{n+1}_{sa} + \Delta t\sum_{a}q^{n+1}_{la}$$

$$-\Delta tq_{int}$$
(3.164)

$$\frac{\partial E_{sl}}{\partial P} = V \left\{ \alpha_s \left(\frac{\partial \rho_s}{\partial p} e_s + \rho_s \frac{\partial e_s}{\partial p} \right) + \alpha_l \left(\frac{\partial \rho_l}{\partial p} e_l + \rho_l \frac{\partial e_l}{\partial p} \right) \right\}$$

$$aa(4,1) \quad -V \sum_{adj} \left\{ \tilde{e}^{(1)}{}_{s,adj} + \tilde{e}^{(1)}{}_{l,adj} + \left(\tilde{e}^{(2)}{}_{s,adj} + \tilde{e}^{(2)}{}_{s,adj} \right) (2p - p_{adj}) \right\}$$

$$+V(\alpha_s + \alpha_l) + V \left(\widetilde{D}_s + \widetilde{D}_l \right)$$

$$\partial E \qquad (3.165)$$

aa(4,2)
$$\frac{\partial E_{sl}}{\partial A_s} = V(\rho_s e_s - \rho_l e_l) - X_1 T_s + X_2 T_l$$
(3.166)

aa(4,3)
$$\frac{\partial E_{sl}}{\partial \beta_s} = V\left(\frac{\partial \rho_s}{\partial T_s}e_s + \rho_s\frac{\partial e_s}{\partial T_s}\right) + \frac{\Delta t}{\alpha_s}\sum_a R_{sa} \equiv X_1$$
 (3.167)

aa(4,4)
$$\frac{\partial E_{sl}}{\partial \beta_l} = V\left(\frac{\partial \rho_l}{\partial T_l}e_l + \rho_l\frac{\partial e_l}{\partial T_l}\right) + \frac{\Delta t}{\alpha_l}\sum_a R_{la} \equiv X_2$$
 (3.168)

aa(4, ipos)
$$\frac{\partial E_{sl}}{\partial A_a} = -V\rho_l e_l - Vp + X_2 T_l - X_3 T_a$$
(3.169)

aa(4,ipos+1)
$$\frac{\partial E_{sl}}{\partial \beta_a} = -\frac{\Delta t}{\alpha_s} R_{sa} - \frac{\Delta t}{\alpha_l} R_{la} \equiv X_3$$
 (3.170)

Energy (non-condensable gases): (ipos=4+2*iigas)*

$$E_{a} = V(\alpha_{a}\rho_{a}e_{a})^{n+1} + V\sum_{adj} (\tilde{e}^{(1)}{}_{a,adj} + \tilde{e}^{(2)}{}_{a,adj}p^{n+1})(p^{n+1}_{adj} - p^{n+1}) + Vp^{n+1}\alpha^{n+1}_{a} + Vp^{n+1}\widetilde{D}_{a} - \Delta tq^{n+1}_{sa} - \Delta tq^{n+1}_{la}$$

$$V\tilde{E} + (\alpha_{a}, \alpha_{a})^{n}\Delta t \frac{dV}{dV}$$
(3.171)

-cc(ipos,7)

$$-V\tilde{E}_{a} + (\alpha_{a}\rho_{a}e_{a})^{n}\Delta t \frac{dV}{dt}$$

$$\frac{\partial E_{a}}{\partial P} = V\alpha_{a} \left(\frac{\partial\rho_{a}}{\partial p}e_{a} + \rho_{a}\frac{\partial e_{a}}{\partial p}\right)$$

$$-V\sum_{adj} \{\tilde{e}^{(1)}{}_{a,adj} + \tilde{e}^{(2)}{}_{a,adj}(2p - p_{adj})\} + V\alpha_{a} + V\widetilde{D}_{a}$$
(3.172)

aa(ipos,1

aa(ipos,2)
$$\frac{\partial E_a}{\partial A_s} = -X_1 T_s + X_2 T_l$$
 (3.173)

aa(ipos,3)
$$\frac{\partial E_a}{\partial \beta_s} = -\frac{\Delta t}{\alpha_a} R_{sa} \equiv X_1$$
 (3.174)

aa(ipos,4)
$$\frac{\partial E_a}{\partial \beta_l} = -\frac{\Delta t}{\alpha_a} R_{la} \equiv X_2$$
 (3.175)

aa(ipos,ipos-1)
$$\frac{\partial E_a}{\partial A_a} = V \rho_a e_a - V p + X_2 T_l - X_3 T_a$$
(3.176)

aa(ipos,ipos)
$$\frac{\partial E_a}{\partial \beta_a} = V \left(\frac{\partial \rho_a}{\partial T_a} e_a + \rho_a \frac{\partial e_a}{\partial T_a} \right) + \frac{\Delta t}{\alpha_a} R_{sa} + \frac{\Delta t}{\alpha_a} R_{la} \equiv X_3$$
 (3.177)

*ipos here differs from others

4. Example Simulations

4.1 Simulations for Model Verifications

The simulations for model verification were conducted for the models included in the JASMINE code. The verification of the conservation laws, and the reproduction of the physical phenomena expressed by the analytical solutions serve to confirm the accuracy and quality of the JASMINE code.

4.1.1 Melt Jet and Melt Pool

The simulations were conducted to examine the free-fall of the melt jet in the gas phase, and the subsequent spreading of the melt pool at the bottom surface. The transient profiles and the conservation of mass from the melt jet to the melt pool were verified through the simulations. The leading edges of the melt jet are compared with both the theoretical solution based on the simple mass conservation principle and the numerical solution obtained using the conventional upwind scheme.

Simulation Conditions

Fig. 4.1 depicts the simulation domain employed for the verification of the melt jet and melt pool models. The simulation domain is axisymmetric about the central axis indicated by "C.L." The figure indicates the location of the melt jet injection, and the cell grids.



Fig. 4.1 A schematic of the simulation domain employed for the verification of the melt jet and melt pool models. The simulation domain is enclosed and filled with a gas (steam).

A single melt jet with an initial diameter of 90 mm and an initial velocity of 0.5 m/s at the inlet flows into a closed chamber with a radius of 0.2 m and a height of 1 m, which is filled with a gas (steam). The chamber is free of any non-condensable gases ("ngas=0"). The melt jet is subject to the effects of gravitational acceleration. The pressure within the camber is set at 0.1 MPa. Given that the inlet velocity of the melt jet is relatively low, it can be reasonably assumed that the resistance from the gas phase is insignificant. The chamber is discretized into 0.1 m cells in the vertical direction, with each vertical cell subdivided into finer cells for the purpose of the melt jet simulations.

The simulations were conducted in accordance with following cases: the base case, the "dz" case, and the "dt" case. In the base case, the cell size of the melt jet was set at 20 mm ($n_{sub} = 5$), with the maximum time step set at 1 ms. The "dz" case employed a reduced melt jet cell size of 5 mm ($n_{sub} = 20$), and the "dt" case employed a reduced maximum time step of 0.1 ms.

Simulation Results

Figs.4.2–4.4 illustrate the transient profiles of melt jet and melt pool simulations, obtained in the base case, the "dz" case, and the "dt" case, respectively. The images provide clear confirmation of the trailing of the melt jet, the impact of the melt jet at the bottom surface, and the spreading of the melt pool at the bottom surface.



Fig. 4.2 A series of snapshots of the transient profiles of the melt jet and melt pool simulations, obtained in the base case: dz = 20 mm, and dt = 1 ms.



Fig. 4.3 A series of snapshots of the transient profiles of the melt jet and melt pool simulations, obtained in the "dz" case: dz = 5 mm, and dt = 1 ms.



Fig. 4.4 A series of snapshots of the transient profiles of the melt jet and melt pool simulations, obtained in the "dt" case: dz = 20 mm, and dt = 0.1 msec.

At t = 0.1 sec, the melt jet, indicated by the green line, was trailing into the chamber in all cases. At t = 0.2 sec, a satellite droplet was dislodged from the tip of the melt jet in the base and "dt" cases. In contrast, no satellite droplet was detached from the tip of the melt jet at t = 0.2 sec in the "dz" case with fine grids. Subsequently, the impact of the melt jet at the bottom surface, the resulting melt pool, indicated by the green line, exhibited a spread at the bottom surface at t = 0.4 - 1.4 sec in all cases.



Fig. 4.5 The profiles of melt jet obtained from the CIP method, which are compared with those obtained from the numerical solution of the finite difference method (FDM) using the conventional upwind scheme, and the theoretical solution based on the simple mass conservation: (a) t = 0.3 sec, and (b) t = 1.0 sec.

Fig. 4.5 illustrates the profiles of the melt jet at t = 0.3 and 1.0 sec, respectively, obtained from the simulation using the CIP method. The profiles of the melt jet obtained from the numerical solution of the finite difference method (FDM) using the conventional upwind scheme, as well as the theoretical solution based on the simple mass conservation, are indicated in the figures.

Fig. 4.6 illustrates a schematic for deriving the theoretical solution for the melt jet profile. The theoretical solution is derived based on a coordinate system with the vertical downward direction z'. In the JASMINE code, the melt jet is fed over a specified time interval Δt , with the diameter increasing gradually in accordance with a specific rate, thereby ensuring stable the melt jet injection. The simulations utilized a time interval of $\Delta t = 0.005$ sec, from the start of the melt jet injection to the end of the melt jet reaching the inlet diameter. The position of z' = a indicates the point at t = 0.3 sec, where the melt jet begins to enter the inlet. The position of z' = b indicates the point at t = 0.3 sec, where the melt jet reaches the inlet diameter.



Fig. 4.6 A schematic of the melt jet profile and the coordinate system at t = 0.3 sec, which is employed to introduce the theoretical solution based on the simple mass conservation.

In the interval $0 \le z' \le b$, the radius of the melt jet $r_j(z')$ is determined based on the simple mass conservation, which can be expressed as follows:

$$r_j(z') = (V_{ji}/V_j(z'))^{1/2} r_{ji},$$
(4.1)

where V_{ji} denotes the inlet velocity of the melt jet, $V_j(z')$ denotes the velocity of the melt jet, and r_{ji} denotes the inlet radius of the melt jet. The velocity of the melt jet is determined by the free-fall curve:

$$V_j(z') = (V_{ji}^2 + 2gz')^{1/2}.$$
(4.2)

In the interval $b \le z' \le a$, the radius of the melt jet $r_j(z')$ is determined through the application of a liner interpolation, expressed as follows:

$$r_{j}(z') = \frac{z'-a}{b-a}r_{j}(b),$$
(4.3)

The positions of z' = a and b are determined by the free-fall curve:

$$z' = V_{ji}t + \frac{1}{2}gt^2, (4.4)$$

where t denotes the time from the start of the melt jet injection. The position of z' = a is derived when t = 0.3 sec, and the position of z' = a is derived when t = 0.3 - 0.005 sec.

As illustrated in Fig. 4.5, the profiles of the melt jet obtained from the base case exhibited a reasonable degree of agreement with the theoretical solution. The profiles obtained from the numerical solution of the FDM using the conventional upwind scheme were unable to simulate a sharp profile at the edge of the melt jet due to the effects of the numerical diffusion. The profiles obtained from the "dz" case with fine grids exhibited superior agreement with the theoretical solution in comparison to those obtained from the base case. The profiles obtained from the "dt" case with a smaller time step exhibited characteristics that were nearly identical to those obtained from the base case.

Fig. 4.7 depicts the comparison between the leading edge position of the melt jet obtained from the simulations using the CIP method and the analytical solution or free-fall curve, as expressed by Eq. (4.4). The leading edge obtained from the base case initially exceeded the analytical solution up to around t = 0.2 sec, but then exhibited regression, aligning with the analytical solution. The leading edge obtained from the "dz" case with fine grids exhibited superior agreement with the analytical solution. The leading edge obtained from the "dz" case with a smaller time step initially exceeded the analytical solution up to around t = 0.2 sec, but then exhibited regression, aligning with the analytical solution.

The regression of the leading edge is a consequence of the satellite droplet being identified as the leading edge of the melt jet within the JASMINE code. Once the diameter of the satellite droplet is sufficiently diminished in comparison to the inlet diameter of the melt jet, it is no longer identified as the leading edge, and the subsequent melt jet is tracked. While the leading edge position obtained from the simulation is influenced by the criteria utilized to identify the presence of a melt jet with the grids, the position of the leading edge remains aligned with the trajectory of the free-fall curve.



Fig. 4.7 The comparison of the leading edge position of the melt jet obtained from the simulations conducted using the CIP method with that obtained from the analytical solution or the free-fall curve.

Fig. 4.8 illustrates the mass transfer from the melt jet to the melt pool during the impact of the melt jet and the subsequent spreading of the melt pool at the bottom surface in the base case. The figure demonstrates the superior mass conservation between the melt jet and the melt pool models. The total melt mass error thorough the simulation was less than 0.2%.



Fig. 4.8 The mass transfer from the melt jet to the melt pool during the impact of the melt jet and the subsequent spreading of the melt pool at the bottom surface in the base case.

4.1.2 Melt Particles and Melt Pool

The simulations were conducted to examine on the free fall of the melt particles, and subsequent merging into the melt pool, or stacking at the bottom surface. The transient profiles, leading positions of the melt particles, and mass conservation from the melt particles to the melt pool were verified through the simulations.

Simulation Conditions

Fig. 4.9 depicts the simulation domain employed for the verification of the melt particles and melt pool models. The simulation domain is axisymmetric about the central axis denoted by "C.L.". The figure indicates the initial location of the particle groups, and the cell grids.

The particle groups with constant radial and vertical spacing are initially distributed in the upper part of a closed chamber with a radius of 0.2 m and a height of 1 m, which is filled with a gas (steam). The chamber is free of any non-condensable gases ("ngas=0"). The diameter of the melt particles within each particle groups is 1 mm, and the number of the melt particles in each particle group is specified so that the particle volume fraction is 0.2. The initial vertical velocity of the particle groups is set to zero and subjected to the gravitational acceleration. The pressure within the camber is set at 0.1 MPa. Given that the velocity of the melt particles is relatively low, it can be reasonably assumed that the resistance from the gas phase is insignificant. The chamber is discretized into 0.1 m cells in the vertical direction.



Fig. 4.9 A schematic of the simulation domain employed for the verification of the melt particles and melt pool models. The simulation domain is enclosed and filled with a gas (steam).

The simulations were conducted in accordance with the following cases: the base case, the "dt" case, the "solid" case, and the "solid-rand" case. In the base case, the melt particles in a molten state with zero velocity in the x-direction were fed, with the maximum time step set at 1 ms. The "dt" case employed a reduced maximum time step of 0.1 ms, the "solid" case introduced the melt particles in a solid state, and the "solid-rand" case introduced the melt particles in a solid state, and the "solid-rand" case introduced the melt particles in a solid state with an initial velocity in the in the x-direction. The initial velocity was randomly specified within the range of $-0.2 < v_{px} < 0.2$ m/s.

Simulation Results

Figs. 4.10–4.12 illustrate the transient profiles of melt jet particles and melt pool simulations, obtained in the base case, the "solid" case, and the "solid-rand" case, respectively. The typical positions of the melt particles are indicated as the center position of the particle groups. The images provide clear visual confirmation of the trailing of the melt particles, the falling of the melt particles at the bottom surface, and subsequent merging to the melt pool at the bottom surface.



Fig. 4.10 A series of snapshots of the transient profiles of the melt particles and melt pool simulations, obtained in the base case: melt particles in molten state with $v_{px} = 0$ m/s, and dt = 1 ms.



Fig. 4.11 A series of snapshots of the transient profiles of the melt particles and melt pool simulations, obtained in the "solid" case: melt particles in a solid state with $v_{px} = 0$ m/s, and dt = 1 ms.



Fig. 4.12 A series of snapshots of the transient profiles of the melt particles and melt pool simulations, obtained in the "solid-rand" case: melt particles in a solid state with $-0.2 < v_{px} < 0.2$ m/s, and dt = 1 ms.

At t = 0.2 sec, the melt or solid particles, indicated by the red circles, were descend into the chamber in all cases. At t = 0.4 - 0.6 sec, the melt particles were merged into the melt pool, as indicated by the green line, in the base case. In contrast, the solid particles accumulated at the bottom surface in the "solid" case and the "solid-rand" case. In the "solid-rand" case, the initial horizontal velocities of the melt particles were randomized, resulting in a different trend from that obtained in the "solid" case.



Fig. 4.13 The comparison of the leading edge position of the melt particles obtained from the simulations with that obtained from the analytical solution or the free-fall curve.

Fig. 4.13 depicts the comparison between the leading edge position of the melt particles obtained from the simulations and the analytical solution or free-fall curve, as expressed by Eq. (4.4). The leading edge obtained from all cases exhibited superior agreement with the analytical solution.



Fig. 4.14 The mass transfer from the melt particles to the melt pool during the fall of the melt particles and the subsequent merging to the melt pool at the bottom surface in the base case.

Fig. 4.14 illustrates that the mass transfer from the melt particles to the melt pool in the base case. The figure demonstrates the superior mass conservation between the melt particles and the melt pool models. The total melt mass error thorough the simulation was less than 0.01%.

4.1.3 Two-Phase Flow: Pressure Propagation

The simulations were conducted to examine the pressure propagation in the two-phase flow. The dependence of the pressure propagation on the void fraction of the two-phase flow was verified through the simulations in both a nearly one-dimensional and two-dimensional geometries.

Simulation Conditions: One Dimension

Fig. 4.15 (a) depicts the simulation domain in the one-dimensional geometry. The simulation domain is axisymmetric about the central axis indicated by "C.L." The figure indicates the initial liquid water level, the cover gas (air) component and the liquid water levels at which the pressure histories were detected. The simulation domain is a nearly one-dimensional cylindrical chamber with a radius of 0.2 m and a height of 2.5 m, filled with liquid water to a level of 2.05 m. A specified quantity of high-pressure compressed gas (air) is positioned at cells, with a void fraction of 0.5 and a pressure of 0.12 MPa at the bottom center in the simulation domain for the trigger. The initial system pressure is set at 0.1 MPa.

The velocity of pressure propagation was estimated by tracing the wave front of the pressure propagation in the simulations. The analytical solution for the comparison is derived under the assumption of the two-phase flow in the homogeneous bubbly flow, which can be expressed as follows:

$$\frac{c_{hom} \alpha}{c_g} = \left\{ \alpha^2 + \alpha \ 1 - \alpha \ \frac{\rho_l}{\rho_g} + \left(1 - \alpha^2 + \alpha \ 1 - \alpha \ \frac{\rho_g}{\rho_l} \right) \left(\frac{c_g}{c_l} \right)^2 \right\}^{-1/2},\tag{4.5}$$

where c denotes the sonic velocity, ρ denotes the density, and α denotes the void fraction. The subscript g and l denotes the gas and liquid phases of the two-phase flow, respectively. The c_{hom} denotes the sonic velocity in the homogeneous bubbly flow. Eq. (4.5) is derived under on the assumption that the components of the two-phase flow exhibit no slip and that no mass transfer occurs between the two-phases⁽⁴⁴⁾. The sonic velocities in the gas and liquid phases are calculated as follows: $c_g = 343$ m/s is the sonic velocity of an ideal gas (air), and $c_l = 1,488$ m/s is the sonic velocity of liquid water.



Fig. 4.15 A schematic of the simulation domain employed for the verification of the pressure propagation in the two-phase flow: (a) one-dimensional geometry, and (b) two-dimensional geometry.

Simulation Results in One Dimension

Figs.4.16–4.18 illustrate the pressure histories at the liquid water heights of 0.475 m, 0.975 m, and 1.95 m, respectively. In the figures, the red lines indicate the pressure histories with void fraction $\alpha = 10^{-5}$, the green lines indicate the pressure histories with $\alpha = 10^{-3}$, and the blue lines indicate the pressure histories with $\alpha = 10^{-1}$. The front of the pressure propagation was defined as point at which the pressure pulse reached the halfway of the first peak. The figures demonstrate that the pressure propagation was delayed in proportion to the void fraction, and that the pressure pulses underwent a rapid attenuation when $\alpha = 10^{-1}$.



Fig. 4.16 The pressure histories at the liquid water heights of 0.475 m: the red lines indicate the pressure histories with void fraction $\alpha = 10^{-5}$, the green lines indicate the pressure histories with $\alpha = 10^{-3}$, and the blue lines indicate the pressure histories with $\alpha = 10^{-1}$.



Fig. 4.17 The pressure histories at the liquid water heights of 0.975 m: the red lines indicate the pressure histories with void fraction $\alpha = 10^{-5}$, the green lines indicate the pressure histories with $\alpha = 10^{-3}$, and the blue lines indicate the pressure histories with $\alpha = 10^{-1}$.



Fig. 4.18 The pressure histories at the liquid water heights of 1.95 m: the red lines indicate the pressure histories with void fraction $\alpha = 10^{-5}$, the green lines indicate the pressure histories with $\alpha = 10^{-3}$, and the blue lines indicate the pressure histories with $\alpha = 10^{-1}$.



Fig. 4.19 The relationship between the pressure propagation velocity and the void fraction of the twophase flow: the pressure propagation velocity is compared with the analytical solution.

The velocity of the pressure propagation was estimated from the arrival of the pressure propagation, and plotted against the theoretical solution [Eq. (4.5)] in Fig. 4.19. The estimated velocity of the pressure propagation from the simulations demonstrated concordance with that derived from the analytical solution for $\alpha = 10^{-5}$ and 10^{-3} . The velocity of the pressure propagation obtained from the simulations was found to exceed that obtained from the analytical solution for $\alpha = 10^{-1}$. The assumption of homogeneous bubbly flow for the analytical solution is considered invalid for $\alpha = 10^{-1}$. The non-uniformity of the void fraction resulted in selective propagation in the liquid phase, whereby the pressure propagated with greater ease.

Simulation Conditions in Two Dimension

Fig. 4.15 (b) depicts the simulation domain in the two-dimensional geometry. The simulation domain is axisymmetric about the central axis indicated by "C.L." The figure indicates the initial liquid water level, the cover gas (air) component, and the liquid water levels at which the pressure histories were detected. The simulation domain is a two-dimensional cylindrical chamber with a radius of 1 m and a height of 2 m, filled with liquid water to a level of 1.78 m. A specified quantity of high-pressure compressed gas (air) is positioned at cells, with a void fraction of 0.5 and a pressure of 1 MPa at the bottom center in the simulation domain for the trigger. The initial system or ambient pressure is set at 0.1 MPa. The initial void fraction is set at $\alpha = 10^{-4}$.



Fig. 4.20 A series of snapshots for the pressure distribution obtained from the simulation in twodimensional geometry, which demonstrated the spherical propagation of the pressure pulse.

Simulation Results in Two Dimension

Fig. 4.20 shows the pressure distribution obtained from the simulation. The pressure pulse propagated spherically from the trigger location and was reflected off the side walls. The two-dimensional wave of the pressure pulse was adequately captured or reproduced by the two-phase flow simulation.

4.2 Simulations of Premixing Experiments

The simulations of the premixing experiments were conducted to validate the associated models with the adjusted parameters in the JASMINE code. The empirical parameters were utilized in the associated models to process premixing simulations. The FARO experiments conducted at the EU JRC Ispra^(45, 46) were employed for validation purposes.

4.2.1 Simulation Conditions

In the FARO experiments, approximately 100 kg of corium (a mixture of UO_2 and ZrO_2) was injected into the coolant water. The FARO-L14, L28, and L31 were employed for the purposes of validation due to the varied parameters, including coolant water subcooling, cover gas pressure, and initial melt jet diameter. The experimental results for the pressure histories and the swelling of the coolant water level due to steam generation during the melt-jet breakup, as well as the particle size distribution of the recovered debris, are available for validation purposes.

Table 4.1 enumerates the simulation conditions, including the melt injection, coolant water, initial and boundary conditions, as well as the parameter specifications. Fig. 4.21 depicts the simulation domains employed to simulate the FARO experiments. The simulation domains are axisymmetric about the central axis indicated by "C.L.". The vessel wall is represented by the solid lines. The figure indicates the melt jet injection location, and the initial coolant water level.

4.2.2 Parameter Specifications

In order to validate the premixing simulations, the associated models and parameters were adjusted to reproduce the melt jet and melt particle dynamics observed in the experiments. The empirical correlation for estimating the jet-breakup length L_{brk} with the entrainment parameter C_{ent} was adjusted to align with the observed L_{brk} in the experiments. The empirical correlation, called Taylor type⁽²³⁾, was selected for the FARO experiments. The diameter of the melt particles D_p in the simulations was specified based on the mass median diameter obtained from the experiments. The simulation results obtained with the selected models and adjusted parameters were compared with the experimental results.

The values of N_{pcr} and N_{hist} employed in the present report are smaller in comparison to those utilized in the previous report⁽⁴⁾. The N_{pcr} denotes the maximum number of particle groups that can be stored in the buffers or "pre-groups" prior to the release as "real-groups". The N_{hist} denotes the

maximum time duration for particle groups that can be stored in the buffers or "pre-groups" prior to the release as "real-groups". The smaller N_{pcr} and N_{hist} values indicate that the particle groups are more likely to be released into the simulation domain. The growth in computational power has facilitated the simulation of a significant number of the particle groups released into the simulation domain.

		L14	L28	L31
Melt	Material	Corium ^{a)}		
	Release mass (kg)	125	175	92
	Temperature (K)	3,073	3,053	2,990
	Release diameter (mm)	92	44	48
	Free fall height (m)	0.985	0.83	0.72
Coolant water	Temperature (Subcooling) (K)	537 (1)	424 (1)	291 (104)
	Depth (m)	2.05	1.44	1.45
	Vessel diameter (m)		0.71	
Cover gas	Material	Steam		Argon
	Pressure (MPa)	5.0	0.51	0.22
	Volume (m ³)	1.26	3.53	3.49
Premixing	Swelling water levels (m)	~1.4	~0.6	~0.3
results	Pressure peaks (MPa)	2.5	1.2	0.04
	Lump debris (kg)	20 (16%)	77 (44%)	0
	Mass median diameter (mm)	5.0	3.0	3.3
Simulation	Maximum time step (ms)		~0.5	
conditions	Melt jet inlet velocity (m/s)	3.0	~3	~2.7
	Melt jet flow duration (sec)	0.8	5.2	2.5
	Melt particle diameter (mm)	5.0 3.0		
	Model: jet-breakup length ^{b)}	Taylor		
	$C_{ent}^{ \mathbf{b})}$	1		
	Model: surface temp. drop	Active		
	$N_{pcr}^{\ \ \mathrm{c}}$	200		
	$N_{hist}^{\rm c)}$	200		
	$F_{htint}{}^{\mathrm{d}}$	0.02		

Table 4.1 The simulation conditions of the FARO-L14, L28, and L31 experiments employed to validate the premixing simulations.

a) UO₂ (80wt%)-ZrO₂ (20wt%), and $T_{sol}/T_{liq} = 2,830/2,850$ K.

b) See, 2.2.1.

c) See, 2.2.3.

d) See, 2.3.2.



Fig. 4.21 A schematic of the simulation domain employed to validate the premixing simulations for the FARO experiments: (a) L-14, and (b) L28 and L31.

4.2.3 Premixing Simulations

Figs. 4.22 and 4.23 illustrate the comparison of the pressure histories and the swelling of the coolant water levels between the simulations and the experiments for the FARO experiments. The figures demonstrate that the pressure histories and the swelling of the coolant water level exhibited agreement between the simulations and the experiments. In conditions of low cover gas pressure (L28 and L31), the pressure histories were found to be underestimated while the swelling of the coolant water levels were found to be overestimated. The steam bubbles generated in the premixing zone could escape at a faster rate in reality than in simulations, particularly in conditions of low cover gas pressure. It would appear that a significant amount of effort is required to enhance the constitutive models for two-phase flow in order to overcome the limitation observed in the premixing simulations.

Fig. 4.24 indicates the comparison of the mass fractions of continuous melt or lump debris observed at the bottom of the experimental facilities. The lump debris can be formed by the direct arrival of a coherent melt jet, or by the merging of separated melt particles. The simulations are unable to reproduce the experiments. As a consequence of the inability to simulate the debris bed formation, the current version of the JASMINE code is unsuitable for the evaluation of the long-term coolability.


Fig. 4.22 A comparison of the pressure histories between the simulation and the experiments with regards to the FARO L14, L28, and L31: "sim." denotes the simulation results, and "exp." denotes the experimental results.



Fig. 4.23 A comparison of swelling of the coolant water levels between the simulation and the experiments with regards to the FARO L14, L28, and L31: "sim." denotes the simulation results, and "exp." denotes the experimental results.



Fig. 4.24 A comparison of mass fractions of the lump debris between the simulation and the experiments with regards to the FARO L14, L28, and L31: "sim." denotes the simulation results, and "exp." denotes the experimental results.

4.3 Simulations of Explosion Experiments

The simulations of the explosion experiments were conducted to validate the associated models with the adjusted parameters in the JASMINE code. The empirical parameters were utilized in associated models to process the explosion simulations. The KROTOS and FARO experiments conducted at the EU JRC Ispra^(47, 48) were employed for validation purposes.

4.3.1 Simulation Conditions

In the KROTOS experiments, several kilograms of alumina or corium (a mixture of UO₂ and ZrO₂) were injected into the coolant water, and a steam explosion was triggered by a pressure pulse using the release of argon. The KROTOS-44, 42, and 37 experiments were employed for the purposes of validation due to the different melt (alumina or corium) injection under similar experimental conditions. In the FARO experiments, approximately 100 kg of corium was injected into the coolant water, and a steam explosion was triggered by a pressure pulses using a detonator. The FARO-L33 experiment is employed for the purposes of validation for a large scale experiment.

Table 4.2 enumerates the simulation conditions, including the melt injection, coolant water, initial and boundary conditions, trigger conditions, as well as the parameter specifications. In the KROTOS-44 experiment, helium was utilized as the cover gas within the test section, whereas argon was employed as the trigger⁽⁴⁷⁾. For the sake of simplicity, helium was employed as the trigger in the simulation, although

argon is typically preferred. In the KROTOS-44 experiment of the near-saturated condition, the principal component of the cover gas was identified as steam in the simulation. In the simulation of the FARO-L33 experiments, air was employed as the trigger, although argon is typically preferred. Fig. 4.25 depicts the simulation domains employed to simulate the experiments. The simulation domains are axisymmetric about the central axis indicated by "C.L.". The vessel wall is represented by the solid lines. The figure indicates the melt jet injection location, the initial coolant water level, and the trigger location. In addition, the figure indicates the correlation between the coolant water levels to which the pressure histories were referenced for comparison in the experiments and the simulations.

4.3.2 Parameter Specifications

The simulation of the steam explosion is processed in two steps: premixing and explosion. In the premixing step, the associated models and empirical parameters were adjusted to reproduce observed dynamics of the melt jet and particle in the experiments. The empirical correlation for estimating the jet-breakup length L_{brk} with the entrainment parameter C_{ent} was adjusted to align with the observed L_{brk} in the experiment under the conditions similar to a NO steam explosion. The empirical correlation proposed by Saito et al.⁽²⁴⁾ was selected for the KROTOS experiments due to the transient nature of the melt delivery⁽⁴⁷⁾, and the empirical correlation, called Taylor type⁽²³⁾, was selected for the FARO experiment. The diameter of the melt particles D_p in the simulations was determined in a same manner as employed in the premixing simulations.

The premixing simulation is deemed to be an accurate representation of the experiments if the total void fraction at the moment of the trigger in the simulation is in consistent with that observed in the experiments. The premixing simulation was utilized as the initial conditions for the explosion simulation. The explosion simulations employed an identical set of the empirical parameters for the fragmentation model: $C_{frg} = 0.25$, $d_{frg} = 50$ µm, $t_{triglife} = 1$ ms, and $K_{ev} = 0.7$, respectively. The JASMINE code is designed on the premise that an identical set of the empirical parameters for the fragmentation model will yield reasonable explosion simulations, given that the premixing simulations are reasonable.

The empirical parameters for the explosion simulations were first adjusted to reproduce the pressure histories and the size distributions of the melt fragments produced by the steam explosion, as observed in the KROTOS-42 experiment⁽⁴⁾. The adjusted value of the fine fragmentation rate $C_{frg} = 0.35$, based on the KROTOS-44 experiments, resulted in an explosion simulation that underestimated the impulse observed in the FARO-L33 experiment. The simulation suggests that the attenuation effect of the corium was well reproduced. Moriyama and Furuya⁽¹³⁾ readjusted the C_{frg} based on the impulse estimated from the pressure histories at different vertical locations between the experiments and the simulations for the KROTOS-44 and the FARO-L33 experiments. The value of $C_{frg} = 0.25$ was determined in order to prevent significant underestimation or overestimation of the impulses.

		K44	K42	K37	L33	
Melt	Material	Alumina ^{a)}		Cor	Corium ^{b)}	
	Release mass (kg)	1.50	1.54	3.22	100	
	Temperature (K)	2,673	2,465	3,018	3,070	
	Release diameter (mm)		30		48	
	Free fall height (m)		0.44		0.77	
Coolant water	Temperature (Subcooling) (K)	363 (10)	293 (80)	296 (77)	294 (124)	
	Depth (m)		1.105		1.62	
	Vessel radius (m)		0.20		0.71	
Cover gas	Material	Steam		Argon		
	Pressure (MPa)		0.10		0.41	
	Volume (m ³)		0.290		3.496	
Premixing	Swelling water levels (cm)	12	3	30	9	
results	Jet-breakup length (m)	~0.3 ~0.8 ~1.1		~1.1		
Explosion	Pressure peaks (PPs) (MPa)	~50	~50	N/A ^{c)}	~6	
results	Half height width of PPs (ms)	~1.5	~1	N/A ^{c)}	~3	
	Debris < 0.106 mm (%)	47	31	1.4	$\sim 8^{d)}$	
Simulation	Maximum time step (µs)	~2 (explosion steps)				
conditions	Melt jet inlet velocity (m/s)		3.0		~2.9	
	Melt jet flow duration (sec)	0.270	0.255	0.191	2.55	
	Melt particle diameter (mm)	1	0	2	3	
	Model: jet-breakup length ^{e)}		Saito		Taylor	
	C_{ent}	2	.5	1.6	1	
	Model: surface temp. drop		Act	tive		
	$N_{pcr}^{}^{}$ f)		100		200	
	N_{hist} ^{f)}		100		200	
	Trigger pressure (MPa)		14.8		35	
	Trigger volume (cm ³)		15		29	
	Trigger time (sec)	0	.9	0.5	1.12	
	$C_{frg}^{\ \ \mathbf{g})}$	0.25				
	$d_{frg}^{\hspace{0.1cm}\mathrm{g}}(\mu\mathrm{m})$	50				
	$t_{triglife}{}^{g)}$ (ms)	1.0				
	p_{trig}^{g} (MPa)		0.2		0.5	
	Fragmentation criterion	$T_{av} \geq T_{melt}$				
	$K_{ev}^{\ \ \mathrm{h})}$		0.7			

Table 4.2 The simulation conditions of the KROTOS-37, 42, 44 and the FARO-L33 experiments employed to the explosion simulations ("K#" denotes numbers of the KROTOS experiments).

a) $T_{melt} = 2,300$ K. b) UO₂ (80wt%)-ZrO₂ (20wt%), and $T_{sol}/T_{liq} = 2,830/2,850$ K.

c) Reportedly "no steam explosion occurrence"⁽⁴⁸⁾.

d) Extrapolated value from the size distribution of fragments⁽⁴⁹⁾. The ratio to the melt mass in the system at trigger time is ~ 40 kg, i.e., ~ 20%.

e) See, 2.2.1. f) See, 2.2.3. g) See, 2.2.4. h) See, 2.3.2.



Fig. 4.25 A schematic of the simulation domain employed to validate the explosion simulations for the KROTOS and FARO experiments: (a) K44, K42 and K47, and (b) L31.

4.3.3 Premixing Simulations

Fig. 4.26 illustrates the differences in the masses of alumina and corium derived from the premixing simulations conducted for the KROTOS experiments. In the figure, the red line represents the total melt mass, the green line represents the melt mass in a molten state, and the blue line represents the premixed melt mass, respectively. From Fig. 4.26 (a), the melt remained in a molten state throughout the simulation, and a considerable quantity of steam did not envelop the melt in the KROTOS-42 experiments. The majority of the melt is capable of participating in the steam explosion. From Fig. 4.26 (b), the majority of the melt was in a solid state, and the steam enveloped the melt in a highly voided state at the moment of the trigger. Only a limited quantity of the melt is capable of participating in the steam explosion.



Fig. 4.26 The differences in the masses of alumina and corium derived from the premixing simulations conducted for the KROTOS experiments: (a) K42, and (b) K37.

The differences in the physical properties and the initial melt temperature resulted in the differences in the premixing simulations. In terms of physical properties, alumina exhibits a lower melting point, a lower density, and a higher latent heat than corium. In terms of initial melt temperature, the experiment with alumina (KROTOS-42) was conducted at a lower initial melt temperature than the experiment conducted with corium (KROTOS-37). The experiment with alumina resulted in the formation of larger melt particles, and a longer solidification time compared to the experiment with corium. The heat transfer from alumina to the coolant water is slower than that of corium due to the lower initial melt temperature and the smaller surface area per volume of the melt. The simulations provide an explanation for the well-known experimental observation that corium does not tend to cause strong steam explosions⁽⁵⁰⁾.

4.3.4 Trigger Specifications

A specific volume of high-pressure compressed gas was applied to a single cell situated in the lower central position of the simulation domains. The trigger employed in the KROTOS experiments, which utilized a gas chamber, was replicated using argon. The simulations were conducted under the identical triggering conditions that employed in the experiments: V = 15 cm³, p = 14.8 MPa, and $pV \sim 220$ J. The detonator employed in the FARO experiment was replicated using air. The simulation specified the equivalent volume (V = 29 cm³) for the equivalent triggering condition based on the measured pressure pulse (p = 35 MPa) and the energy released from the detonator ($pV \sim 1$ kJ).

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Fig. 4.27 illustrates the propagation of the pressure pulse in the coolant water for the FARO-L33 experiment. As indicated in the legend, the distances in the figure represent the distances from the bottom of the simulation domain. The objective of the simulation was to ascertain whether the pressure pulse observed in the experiment, which was caused by the detonator, could be replicated by the placement of the high-pressure compressed gas. The initial equilibrium condition with hydrostatic pressure was established through a premixing simulation of 0.1 sec without the melt jet injection. Subsequently, the trigger was applied to an explosion simulation. As the distances from the bottom of the simulation domain decreases, the pressure pulse reaches the peak at an increasingly faster rate. The pressure pulse of approximately 7 MPa with a time duration of 2 ms at 490 mm propagates from 715 mm to 1,390 mm. The propagation of pressure pulses obtained in the simulation replicates that observed in experiments⁽⁵¹⁾.



Fig. 4.27 A propagation of the pressure pulse in the coolant water for the FARO-L33 experiment without the melt jet injection to verify the replication of the pressure propagation using the detonator.

4.3.5 Explosion Simulations

Figs. 4.28 and 4.29 illustrate the comparisons between the simulations and experiments regarding to the pressure histories at different vertical locations for the KROTOS-44 and 42 experiments. In the figures, the red lines indicate the pressure histories observed in the experiments, and the green lines indicate the pressure histories obtained in the simulations, respectively. The K1-K5 in the legends correspond to different vertical measurement locations (see Fig. 4.25). In the KROTOS-44 experiment, the pressure pulse obtained in the simulation precedes and exhibits a smaller value compared to that in the experiments measured near the bottom (e.g. K1 and K2 in Fig. 4.28). In the KROTOS-42 experiment, the pressure pulse obtained in the simulation delays and exhibits a larger value compared to that in the experiments measured near the surface (e.g. K4 and K5 in Fig. 4.29). The simulations of the KROTOS-44 and 42 experiments replicated the overall trends observed in the experiments, with the adjusted parameters.



Fig. 4.28 A comparison of the simulation and experiment regarding to the pressure histories at different vertical locations in the KROTOS-44 (alumina, and saturated condition): the K1-K5 in the legends correspond to different vertical measurement locations.



Fig. 4.29 A comparison of the simulation and experiment regarding to the pressure histories at different vertical locations in the KROTOS-42 (alumina, and subcooled condition): the K1-K5 in the legends correspond to different vertical measurement locations.

Fig. 4.30 illustrates the pressure pulses obtained from the simulation for the KROTOS-37 experiment. No energetic steam explosion was observed in the course of the experiment⁽⁴⁷⁾. In the simulation, the pressure pulse induced by the trigger exhibits an escalation in the vicinity of the bottom, from K1 to K2, while exhibiting a decay near the surface of the coolant water, from K4 to K5. The simulation indicates that the pressure pulse did not escalate and propagate for the KROTOS-37 experiment, thereby supporting the conclusion that no energetic steam explosion occurred during the experiment.



Fig. 4.30 A propagation of pressure pulse in the coolant water KROTOS-37 experiment: the K1-K5 in the legends correspond to different vertical measurement locations.

Fig. 4.31 illustrates the comparisons between the simulation and experiments regarding to the pressure histories at different vertical locations for the FARO-L33 experiment. The pressure pulse obtained in the simulations exhibits a rapid rise and a slow decay in comparison to that observed in the experiments measured near the surface of the coolant water (e.g. at z = 490 mm and 1645 mm in Fig. 4.31). The simulation replicates the overall trends observed in the experiments, with the adjusted parameters.

Fig. 4.32 illustrates the comparisons between the simulations and experiments regarding to the kinetic energy of the coolant water for the KROTOS experiments. The simulations for the KROTOS-42 and 44 experiments yielded comparable values for the kinetic energy, approximately 0.11 MJ, whereas the experiments reported 0.109 MJ and 0.153 MJ, respectively. As illustrated in Fig. E.5 in Appendix E, the reported value of the kinetic energy (see "EXP.reported") in the KROTOS-44 experiment could be an overestimation. As the kinetic energy estimated from the impulses measured in the experiment (see "EXP.K0-K3") predominantly exhibits values below 0.1 MJ, the simulations appear to be reasonable. The simulation for the KROTOS-37 experiment indicated a markedly low value of the kinetic energy, which aligns with the observation that no energetic steam explosion occurred in the experiment.



Fig. 4.31 A comparison of the simulation and experiment regarding to the pressure histories at different vertical locations in the FARO-L33 (corium, and subcooled condition):



Fig. 4.32 A comparison between the simulations and experiments regarding to the kinetic energy of the coolant water for the KROTOS experiments.

Fig. 4.33 shows the comparisons between the simulation and experiment regarding to the kinetic energy of the coolant water for the FARO experiment. The simulation for the FARO-L33 experiment replicated with the experiments⁽⁵²⁾.



Fig. 4.33 A comparison between the simulations and experiments regarding to the kinetic energy of the coolant water for the FARO-L33 experiment.

Fig. 4.34 illustrates the comparison between the simulations and experiments regarding the mass fraction of fine fragments produced by steam explosions in the KROTOS experiments. Note that a precise comparison is not feasible due to discrepancies in the classification of debris size. In the simulations, the size of fine fragments is represented by a uniform size as $d_{frg} = 50$ µm. In the experiments, the size of

fine fragments is defined as the debris with a size less than 0.106 mm. The mass fractions of fine fragments obtained in the simulation were lower, yet exhibited close values to those obtained in the experiment. Fig. 4.35 shows the comparison between the simulation and experiment regarding the mass fraction of fine fragments produced by steam explosion in the FARO experiment. The mass fraction of fine fragments obtained in the simulation was lower, yet exhibited a similarity to that observed in the experiment.



Fig. 4.34 A comparison between the simulations and experiments regarding to the mass fractions of the fine fragments produced by the steam explosions for the KROTOS experiments: the fine fragments collected from the test section subsequent to the overall process of the experiment.



Fig. 4.35 A comparison between the simulations and experiments regarding to the mass fractions of the fine fragments produced by the steam explosions for the FARO experiments: the fine fragments collected from the test section subsequent to the overall process of the experiment.

4.4 Simulations of an Actual Reactor

The premixing and explosion simulation for a typical pressurized water reactor (PWR) is presented as an illustrative example of the capabilities of the JASMINE code. The simulations demonstrate the practical applications of the JASMINE code to an actual reactor. The simulation assumes that the steam explosion occurs in a reactor cavity or ex-vessel configuration.

4.4.1 Simulation Conditions

Table 4.3 enumerates the simulation conditions, including the melt injection, coolant water, initial and boundary conditions, trigger conditions, as well as the parameter specifications. Fig. 4.36 depicts the simulation domain for a reactor cavity of a typical or representative PWR. The simulation domain is axisymmetric about the central axis indicated by "C.L.". The lower head of the RPV is represented by the solid line, and the actual structure is represented by a curved dotted line. The figure indicates the melt jet injection location, the coolant water level, and the trigger location.

4.4.2 Parameter Specifications

The premixing simulation utilized the empirical correlation proposed by Saito et al.⁽²⁴⁾ with $C_{ent} = 1$ for estimating the jet-breakup length L_{brk} . The values of $N_{pcr} = 2,000$ and $N_{hist} = 500$ utilized in the present report are smaller in comparison to the values of $N_{pcr} = 5,000$ and $N_{hist} = 1,000$ in the previous report⁽⁴⁾. The explosion simulation employed the identical set of the empirical parameters for the fragmentation model: $C_{frg} = 0.25$, $d_{frg} = 50 \ \mu m$, $t_{triglife} = 1 \ ms$, and $K_{ev} = 0.7$.

4.4.3 Premixing Simulations

Fig. 4.37 presents snapshots of the melt and coolant water dynamics obtained from the premixing simulation. In the figure, the time t indicates the time elapsed since the execution of the premixing simulation. The green lines represent the melt jet and melt pool, the red circles represent the melt particles in a molten state, as well as the black circles represent the melt particles in a solid state (solid particles). The dark blue cells represent a liquid phase and the yellow cells represent a gas phase of the coolant water. The scale bar indicates the correlation between the cell colors and the void fraction within the cells.

The melt jet was released from the RPV and entered the coolant water from t = 0.2 - 0.5 sec. The melt jet reached the bottom, and the melt pool had begun to spread from t = 1.0 - 2.0 sec. Some of the melt particles underwent a phase change, resulting in the formation of solid particles. The solid particles moved with the upward steam flow to the vicinity of the RPV in approximately 2.0 sec. The penetration of the melt jet and the formation of large steam pockets impede the contact between the coolant water and the melts. The steam or void is then expelled, allowing the coolant water to reestablish contact with the melts.

		PWR ex-vessel
Melt	Material	Corium ^{a)}
	Release mass (kg)	41,000
	Temperature (K)	2,950
	Release diameter (m)	0.5
	Free fall height (m)	0.9
Coolant water	Temperature (Subcooling) (K)	342 (50)
	Depth (m)	4.0
	Vessel radius (m)	2.75
Cover gas	Material	Air
	Pressure (MPa)	0.2
	Volume (m ³)	15.2
Simulation	Maximum time step (ms)	~0.2 (premixing step)
conditions	Melt jet inlet velocity (m/s)	~5.5
	Melt jet flow duration (sec)	~5.0
	Melt particle diameter (mm)	5
	Model: jet-breakup length ^{b)}	Saito
	C_{ent}	1
	Model: surface temp. drop	Active
	$N_{pcr}^{\ c)}$	2,000
	N _{hist} ^{c)}	500
	Trigger pressure (MPa)	10
	Trigger volume (m ³)	0.1
	Trigger time (sec)	0.70
	$C_{frg}^{d)}$	0.25
	$d_{frg}^{\rm d)}$ (µm)	50
	$t_{triglife}^{d}$ (ms)	1.0
	p_{trig}^{d} (MPa)	5.0
	Fragmentation criterion	$T_{av} \geq T_{melt}$
	$K_{ev}^{e)}$	0.7

Table 4.3 The simulation conditions for premixing and explosion simulation in a reactor cavity or exvessel of a typical PWR.

a) UO₂ (80wt%)-ZrO₂ (20wt%), and $T_{sol}/T_{liq} = 2,830/2,850$ K.

- c) See, 2.2.3.
- d) See, 2.2.4.
- e) See, 2.3.2.

b) See, 2.2.1.



Fig. 4.36 A schematic of the simulation domain employed for the premixing and explosion simulation in a reactor cavity or ex-vessel of a typical PWR.



Fig. 4.37 A series of snapshots of the melt and the coolant water dynamics obtained from the premixing simulation in a reactor cavity or ex-vessel of a typical PWR.

4.4.4 Triggering Specifications

The moment of the trigger was identified through the premixing simulation. The effective melt mass engaged in the steam explosion is defined as the mass that is in a molten state and situated in regions with a moderate void fraction. The mass of the melt jet and the melt particles (exclusive of the melt pool) whose temperature exceeds the melting point, and which are present in the cells where the void fraction is less than 0.75, is defined as the "premixed melt mass."

Fig. 4.38 illustrates the historical evolution of the total melt mass, molten melt mass, and premixed melt mass, as obtained from the premixing simulation. The time t indicates the time elapsed since the execution of the premixing simulation. The molten melt mass exhibited a relatively consistent level of approximately 5300 kg, which is attributable to the equilibrium between the melt penetration, solidification, and merging of the melt particles into the melt pool. The premixed melt mass exhibited oscillation due to the steam or void formation and subsequent escape of steam from the liquid water. The simulation experience with the JASMINE code concluded that the most energetic steam explosion is achieved by applying a trigger at the time when the premixed melt mass reached the first peak. In the present simulation, this occurred approximately 0.7 sec after the execution. The dependence of the steam explosion energetics on various input parameters, including the trigger time, has been investigated with JASMINE 3.3b by Moriyama and Park⁽¹⁶⁾.



Fig. 4.38 A historical evolution of the total melt mass, molten melt mass, and premixed melt mass, as obtained from the premixing simulation in a reactor cavity or ex-vessel of a typical PWR.

A specific volume of high-pressure compressed gas was applied to a single cell situated in the lower central position of the simulation domain. The trigger was simulated using air ($V = 0.1 \text{ m}^3$, p = 10 MPa, and $pV \sim 1 \text{ MJ}$). The volume and pressure of the non-condensable gas (air) were estimated based on the

energy released from the trigger, which was calculated to be $pV \sim 1$ MJ. The strength of the external trigger is typically determined by heuristic rules of thumb, whereby the energy is sufficiently small compared to the kinetic energy induced by the steam explosion, yet strong enough to cause the steam explosion as a computational phenomenon. In this case, the kinetic energy induced by the steam explosion is relatively unaffected by the strength of the external trigger.

4.4.5 Explosion Simulations

Fig. 4.39 depicts the three-dimensional diagrams of the pressure pulse propagation obtained from the explosion simulation. In the figure, the time t indicates the time elapsed since the execution of the explosion simulation. The red grid indicates the boundaries of the cells. The pressure pulse propagates in a radial direction from the cell that initiates the trigger and subsequently propagates in a vertical direction. The pressure pulse is reflected at the bottom of the RPV.



Fig. 4.39 A series of snapshots of the three-dimensional diagrams of the pressure pulse propagation obtained from the explosion simulation in a reactor cavity or ex-vessel of a typical PWR.

Fig. 4.40 illustrates the historical evolution of the kinetic energy of the coolant water induced by the steam explosion. The kinetic energy of the coolant water reached approximately 185 MJ at 14 ms following the trigger. The impulse imparted to the wall structures can be obtained by integrating the pressure pulse with the cells in close proximity to the wall structures. The impulse would be a more useful metric for evaluating the integrity of the wall structures than the kinetic energy^(53, 54).



Fig. 4.40 A historical evolution of the kinetic energy of the coolant water induced by the steam explosion obtained from the explosion simulation in a reactor cavity or ex-vessel of a typical PWR.

5. Conclusions

The JASMINE code is an analytical tool developed for the purpose of evaluating the mechanical forces imposed by steam explosions in nuclear reactors. It performs numerical simulations of steam explosions in a mechanistic manner. The present report presents the fundamentals of the modeling concepts, basic equations, numerical solutions, and example simulations, as well as instructions for input preparation, code execution, and the use of supporting tools for practical applications.

The latest updates to JASMINE 3.3b have addressed a number of minor issues, reorganized directory structures, and enhanced the supporting tools that are included in the distribution package. The current version of the code release is 3.3c. The previous report⁽⁴⁾ has been revised to incorporate with these updates. The present or updated report provides updated information on the method for parameter adjustments, instructions for output processing, and the use of supporting tools. Furthermore, it replaces descriptions based on the simulations with JASMINE 3.3c, corrects typographical errors, and provides a summary of the limitations and problems encountered.

Code-Oriented Purposes

The JASMINE code has been developed with the specific objective of simulating steam explosions. The JASMINE code is not optimally suited for the simulations of debris bed formations and long-term coolability, as it was not designed with these specific purposes in mind.

Modeling Approaches

The formation of void in the coolant water and the solidification of melt particles serve to prevent steam explosions. It is of the importance to maintain observation of the progresses in both the modeling and the experiment in order to identify potential areas for improvement.

The simulations of long-term void fractions may be inaccurate due to the conservative selection of the input parameters adjusted to prevent overestimation of the total void fractions. In order to enhance the accuracy of the simulations, it is advised that three-dimensional simulations be utilized.

The attenuation effects of void fractions on steam explosions or fine fragments are straightforwardly expressed through an attenuation factor, designated as f_{α} . The current modelling approaches have yet to be validated based on the specific experiments at the fundamental level.

The radiative heat transfer is confined to a single cell. In order to enhance the efficacy of the simulations, it is necessary to either deposit or distribute heat to the surrounding cells. The radiative heat transfer can extend beyond a single cell, when the void fraction within the cell is sufficiently large².

²The coolant water absorbs thermal radiation to a depth of several millimeters, whereas the steam is transparent to thermal radiation. The thermal radiation emitted by the melt in a steam-filled cell should propagate to adjacent cells where the coolant water is present.

The potential for steam explosions to occur as a result of an external trigger placed outside of the center of the simulation domain is not addressed, nor, the effects of chemical reactions, such as heat generation and hydrogen generation resulting from the oxidation of metallic components of the melt^(45, 55).

Numerical Solutions

The difference in heat capacity of the coolant water due to the cell sizes gives rise to the simulation whereby the smaller cells attain a higher temperature and form voids at a more rapid rate than in the larger cells in the two-phase flow. This affects the attenuation due to the formation of void, thereby causing numerical issues.

The melt jet model is constrained to the central column of the simulation domain. As a consequence of the numerical issues resulting from excessive lateral expansion, the one-dimensional modelling of the melt jet is unable to accurately represent strong deformation of the leading edge.

Validation Bases

In the case of nuclear reactors with a melt of ~ 10 tons, an extrapolation of two orders of magnitude in the melt mass is made from the validation bases, the FARO experiment with a melt of ~ 100 kg. The unknown scale factors may introduce additional uncertainty into the simulations.

Practical Program Use

A number of distinct property packages are currently available as separate source files for the melt. The alteration of the melt property packages requires the compilation and linking of the source files. If an alternative coolant is utilized in lieu of coolant water, it is imperative to implement substantial code modifications, as the steam table package is inherently constrained by its hard-coded nature.

The majority of the useful information is contained in the binary format output files, namely the plot file for the two-phase flow and the melt dump file for the melt components. While other text format files are superfluous, they may be useful for a rapid assessment of the simulations.

The restart function is only applicable when the melt model is in use. The restart function is advantageous for the purposes of verifying and improving the two-phase flow model for the coolant water when the melt model is not in use (i.e. only the two-phase flow model is in use).

The programming style in FORTRAN 77 is no longer regarded as the optimal approach. In order to enhance the readability, expandability, and maintainability of the program, it is recommended that the latest features of Modern Fortran (Fortran 90 and later) be utilized. It is recommended that the current code be replaced with a modern or contemporary one for future use.

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Appendix A Heat Transfer Models for Melt Particles and Fragments

A.1 Surface Temperature of a Melt Particle

The conceptual framework of the heat transfer model for a single melt particle in the premixing steps is illustrated in Fig. A.1. In order to express the surface temperature of a single melt particle T_{sf} , which is reduced by the heat transfer, the model introduces the temperature profile within the thermal boundary layer. The temperature profile is defined in terms of the boundary layer thickness δ .



Fig. A.1 A schematic of the heat transfer model for a single melt particle in the premixing step: the reduction in surface temperature resulting from the heat transfer from the surface of a melt particle.

The model assumes that a single melt particle with an initial uniform melt temperature T_c is cooled from the surface of the melt particle surface. A quadratic function T(r) is employed to represent the temperature profile within the thermal boundary layer that develops in the radial direction r:

$$T(r) = T_c - \frac{T_c - T_{sf}}{\delta^2} \{r - (R - \delta)\}^2,$$
 (A.1)

where R denotes the radius of the melt particle. Eq. (A.1) can be derived from Eq. (A.2) by applying the boundary conditions $T(R) = T_{sf}$, $T(R - \delta) = T_c$, and dT/dr = 0 at $r = R - \delta$, to determine the coefficients A, B, and C.

$$T(r) = Ar^2 + Br + C. \tag{A.2}$$

In order to ascertain the relationship between the T(r) and the heat transfer from the melt particle, the model introduces the heat loss Q, which is transferred from the boundary layer. If the finite volume of the spherical shell is provided by dV, the finite amount of heat loss dQ is expressed as follows:

$$dQ = c_p (T_c - T) \rho dV, \tag{A.3}$$

where c_p denotes the specific heat of the melt particle. As the finite volume of the spherical shell, in terms of the finite distance in the radial direction dr, is expressed as $dV = 4\pi r^2 dr$, the Q from the boundary layer $(R - \delta \le r \le R)$ is given by the integral:

$$Q = \int_{R-\delta}^{R} 4\pi\rho c_p (T_c - T)r^2 dr.$$
 (A.4)

Upon substituting T(r), as defined in Eq. (A.1), into Eq. (A.4), the following equation is obtained:

$$Q = \frac{4}{3}\pi R^3 \rho c_p (T_c - T_{sf}) \left\{ \frac{\delta}{R} - \frac{1}{2} \left(\frac{\delta}{R} \right)^2 + \frac{1}{10} \left(\frac{\delta}{R} \right)^3 \right\}.$$
(A.5)

The heat flux q at the surface of the melt particle satisfies the continuity relationship and can be expressed as

$$q = -\lambda \left(\frac{dT}{dr}\right)_{r=R},\tag{A.6}$$

where λ denotes the thermal conductivity. Substituting Eq. (A.1) into Eq. (A.6) yields the following equation:

$$q = 2\lambda \frac{T_c - T_{sf}}{\delta}.$$
(A.7)

The total heat flux flowing out of the surface of the melt particle $4\pi R^2$ is equal to the time variation of the heat loss from the surface of the melt particle dQ/dt. Consequently, the following equation is obtained:

$$4\pi R^2 q = \frac{dQ}{dt}.\tag{A.8}$$

The model assumes that the value of q remains constant throughout the period of surface temperature decrease. Based on the assumption of constant q, the T_{sf} and δ are subjected to variation according to Eq. (A.7). The following equation obtained from Eq. (A.7),

$$T_c - T_{sf} = \frac{\delta q}{2\lambda} \tag{A.9}$$

is substituted in Eq. (A.3). Furthermore, differentiating Eq. (A.3) with respect to time yields the following equation:

$$\frac{dQ}{dt} = \frac{4}{3}\pi R^3 \frac{q}{\kappa} \left\{ \frac{\delta}{R} - \frac{3}{4} \left(\frac{\delta}{R} \right)^2 + \frac{1}{5} \left(\frac{\delta}{R} \right)^3 \right\} \frac{d\delta}{dt},\tag{A.10}$$

where $\kappa = \lambda/(\rho c_p)$ denotes the thermal diffusion coefficient. By combining Eqs. (A.8) and (A.10), we derive a differential equation that describes the evolution of the thermal boundary:

$$\delta \left\{ 1 - \frac{3}{4} \left(\frac{\delta}{R} \right) + \frac{1}{5} \left(\frac{\delta}{R} \right)^2 \right\} d\delta = 3\kappa dt.$$
(A.11)

From Eq. (A.11), the boundary layer thickness $\delta(t)$ can be calculated. Subsequently, Eq. (A.9) can be employed to determine the surface temperature $T_{sf}(t)$.

The average temperature of the melt particle T_{av} is defined in accordance with the residual heat in the melt particle, as follows:

$$\frac{4}{3}\pi R^3 \rho c_p T_{av} = \frac{4}{3}\pi R^3 \rho c_p T_c - Q.$$
(A.12)

Eqs. (A.5) and (A.12) yield the following equation:

$$T_c = \frac{T_{av} - F_\delta T_{sf}}{1 - F_\delta},\tag{A.13}$$

where F_{δ} is defined as

$$F_{\delta} = \frac{\delta}{R} - \frac{1}{2} \left(\frac{\delta}{R}\right)^2 + \frac{1}{10} \left(\frac{\delta}{R}\right)^3. \tag{A.14}$$

Eqs. (A.9) and (A.13) yield the following equation:

$$T_{av} - T_{sf} = \frac{\delta q}{2\lambda} (1 - F_{\delta}). \tag{A.15}$$

From Eq. (A.15), the average temperature $T_{av}(t)$ can be determined. Note that the model exclusively addresses the evolution of the thermal boundary layer, rather than the solidification of the surface of the melt particle.

A.2 Rapid Heat Release from a Melt Fragment

The conceptual framework of the heat transfer model for a single melt fragment in the explosion step is depicted in Fig. A.2, which is analogous to that for a single melt particle in the premixing step. However, the model for a melt fragment encompasses the global cooling phase that occurs subsequent to the full development of the thermal boundary layer. Accordingly, the model is constituted of two distinct phases: the boundary layer development phase (Phase I) and the global cooling phase (Phase II).

In Phase I, the model is essentially analogous to that of a single melt particle. The quantity of heat loss Q is expressed in terms of the boundary layer thickness δ . The relationship between the variables is expressed as follows:

$$Q = \frac{4}{3}\pi R^{3}\rho c_{p} (T_{c0} - T_{sf}) \left\{ \frac{\delta}{R} - \frac{1}{2} \left(\frac{\delta}{R} \right)^{2} + \frac{1}{10} \left(\frac{\delta}{R} \right)^{3} \right\}.$$
(A.16)

where T_{c0} denotes the initial melt temperature in Phase I. The temperature profile T(r) within the boundary layer, and the heat flux q at the surface of the melt particle can be expressed as follows:

$$T(r) = T_{c0} - \frac{T_{c0} - T_{sf}}{\delta^2} \{r - (R - \delta)\}^2, \qquad \text{ and} \qquad (A.17)$$

$$q = 2\lambda \frac{T_{c0} - T_{sf}}{\delta}.$$
(A.18)

The model assumes that the T_{sf} remains constant throughout the period of thermal boundary layer development. The assumption of a constant T_{sf} is typically valid for the interfacial heat conduction of two objects in sudden contact.



Fig. A.2 A schematic of the heat transfer model for a single melt fragment in the explosion steps: (a) the boundary layer development phase (Phase I), and (b) the global cooling phase (Phase II), whereby the melt temperature decreases under the fully developed thermal boundary layer.

From the heat balance at the surface of the melt fragment,

$$4\pi R^2 q = \frac{dQ}{dt},\tag{A.19}$$

Eqs. (A.17) and (A.18), the following differential equation that describes the evolution of the thermal boundary is obtained:

$$\delta \left\{ 1 - \frac{\delta}{R} + \frac{3}{10} \left(\frac{\delta}{R}\right)^2 \right\} d\delta = 6\kappa dt.$$
(A.20)

In order to obtain the non-dimensional form, the normalized variables δ , t, and Q are introduced as the following definitions:

$$x = \frac{\delta}{R}, \qquad \tau = \frac{\kappa t}{R^2}, \qquad \text{and} \qquad \beta = \frac{Q}{Q_0},$$
 (A.21)

where Q_0 denotes the retained heat, with $\delta = 0$, at the instant when the melt fragment contacts the coolant water. Once the surface temperature reaches the T_{sf} , the Q_0 is estimated based on T_{sf} using the following equation:

$$Q_0 = \frac{4}{3}\pi R^3 \rho c_p (T_{c0} - T_{sf}). \tag{A.22}$$

The non-dimensional form of Eqs. (A.16) and (A.20) is described as follows:

$$\beta = x \left(1 - \frac{1}{2}x + \frac{1}{10}x^2 \right),$$
 and (A.23)

$$x\left\{1 - x + \frac{3}{10}x^2\right\}dx = 6d\tau,$$
(A.24)

based on the following relationship derived from Eq. (A.21);

$$d\delta = Rdx,$$
 and $dt = \frac{R^2}{\kappa}d\tau.$ (A.25)

The normalized variable x can be obtained through the numerical integration of Eq. (A.24). The initial value $x_0 = \sqrt{12\tau_0}$ for the numerical integration is obtained as the first-order analytical solution of Eq. (A.24), which is derived from the following equation:

$$xdx \cong 6d\tau. \tag{A.26}$$

The changes of the normalized variables are as follows: $x = 0 \rightarrow 1$, $\tau = 0 \rightarrow \tau_1$, and $\beta = 0 \rightarrow \beta_1$. The normalized value of β_1 is calculated from Eq. (A.23) when x = 1, resulting in a value of 3/5. The normalized variable of τ_1 is obtained through the numerical integration, resulting in a value of 0.040.

In Phase II, the melt temperature T_c at the center of the melt fragment decreases from the T_{c0} , while the boundary layer thickness remains fixed at R. The heat loss Q_1 at the end of Phase I (corresponding to β_1) can be expressed as the follows:

$$Q_1 = \frac{4}{5}\pi R^3 \rho c_p (T_{c0} - T_{sf}). \tag{A.27}$$

The retained heat at the outset of Phase II, the $Q_0 - Q_1$ can be expressed as follows:

$$\Delta Q_2(T_{c0}) = \frac{8}{15} \pi R^3 \rho c_p (T_{c0} - T_{sf}).$$
(A.28)

As the temperature of the melt fragment declines from T_{c0} to T_c , the retained heat during Phase II can be expressed as follows:

$$\Delta Q_2(T_c) = \frac{8}{15} \pi R^3 \rho c_p (T_c - T_{sf}).$$
(A.29)

Consequently, the heat loss in the phase II Q_2 can be expressed as follows:

$$Q_2 = \frac{8}{15} \pi R^3 \rho c_p (T_{c0} - T_c), \tag{A.30}$$

Eq. (A.30) can be used to derive the following equation:

$$\frac{dQ_2}{dt} = -\frac{8}{15}\pi R^3 \rho c_p \frac{dT_c}{dt}.$$
(A.31)

Conversely, once the thermal boundary layer has reached the full development, the heat flux q during Phase II $(T_{c0} \rightarrow T_c)$ can be derived from Eq. (A.18):

$$q = 2\lambda \frac{T_c - T_{sf}}{R}.$$
(A.32)

The conjunction of Eq. (A.19) and Eq. (A.32) leads to the following equation:

$$\frac{dQ_2}{dt} = 8\pi R\lambda (T_c - T_{sf}). \tag{A.33}$$

From Eqs.(A.31) and (A.33), the time evolution for the T_c can be obtained as follows:

$$\frac{dT_c}{dt} = -15(T_c - T_{sf})\frac{\kappa}{R^2}dt.$$
(A.34)

Introducing the normalized temperature

$$\theta = \frac{T_c - T_{sf}}{T_{c0} - T_{sf}},$$
(A.35)

the non-dimensional form of Eqs. (A.30) and (A.34) is expressed as follows:

$$\beta = \beta_1 + \frac{2}{5}(1 - \theta),$$
 and (A.36)

$$d\theta = -15\theta d\tau,\tag{A.37}$$

where the relation of $Q_2 = Q - Q_1$ is applied to the Eq. (A.30), where Q denotes the heat loss through Phases I and II. The heat loss through Phases I and II can be expressed in terms of a single consistent normalized value β , as in Eq. (A.36).

The analytical solution of Eq. (A.37) is obtained as follows based on the initial conditions of $\tau = \tau_1$ and $\theta = 1$:

$$\theta = e^{-15(\tau - \tau_1)}.\tag{A.38}$$

The changes in the normalized variables are as follows: $\theta = 1 \rightarrow 0$, $\tau = \tau_1 \rightarrow \infty$, and $\beta = \beta_1 \rightarrow 1$. The non-dimensional time constant for the heat loss from a melt fragment τ_f is defined as the non-dimensional time τ at which the non-dimensional heat loss β equals $1 - e^{-1} \approx 0.632$. The τ_f indicates the transient response time for the heat release, or the required time for the non-dimensional heat loss to reach a value of 0.632. The value of τ_f is approximately 0.046, which is larger than τ_1 .

Appendix B Heat Transfer Models for Melt Pool

B.1 Surface Temperature of a Melt Pool

The conceptual framework of the heat transfer model for a melt pool in the premixing steps is illustrated in Fig. B.1. In order to express the surface temperature of a melt pool T_{sf} , which is reduced by the heat transfer, the model introduces the temperature profile within the within the thermal boundary layer. The temperature profile is defined in terms of the boundary layer thickness δ .



Fig. B.1 A schematic of the heat transfer model for the melt pool in the premixing step: the reduction in surface temperature resulting from the heat transfer from the surface of the melt pool.

The model assumes that a melt pool with an initial uniform melt temperature T_P is cooled from the surface of the melt pool, and that adiabatic conditions prevail between the bottom floor and the melt pool. The bottom temperature of the melt pool is maintained at a constant value T_P . A quadratic function T(z) is utilized to represent the temperature profile within the thermal boundary layer that develops in the inverse of the depth direction z from the surface of the melt pool:

$$T(z) = T_P - \frac{q}{2\lambda\delta}(\delta - z)^2, \tag{B.1}$$

where λ denotes the thermal conductivity of the melt pool. Eq. (B.1). can be derived from Eq. (B.2) by applying the boundary conditions $T(\delta) = T_P$, dT/dz = 0 at $z = \delta$. The heat flux q at the surface of the melt pool, which satisfies the continuity relationship, is expressed as Eq. (B.3).

$$T(z) = Az^2 + Bz + C, \qquad \text{and} \tag{B.2}$$

$$q = \lambda \left(\frac{dT}{dz}\right)_{z=0}.$$
(B.3)
The model assumes that the boundary layer thickness develops up to $\delta = H_p/2$, and thus T(z) can be expressed as follows:

$$T(z) = T_P - \frac{q}{\lambda H_P} \left(\frac{H_P}{2} - z\right)^2. \tag{B.4}$$

The surface temperature of the melt pool T_{sf} can be expressed as the surface temperature of the melt pool at z = 0 in Eq. (B.4):

$$T_{sf} = T_P - \frac{q}{4\lambda} H_P, \tag{B.5}$$

and the average temperature of the melt pool T_{av} within the thermal boundary layer ($0 \le z \le H_p/2$) can be expressed as follows:

$$T_{av} = T_P - \frac{q}{12\lambda} H_P, \tag{B.6}$$

which is based on the following definition for the average temperature over the thermal boundary layer $(0 \le z \le H_p/2)$ within the melt pool:

$$T_{av} = \frac{\int_0^{H_P/2} T(z)}{\int_0^{H_P/2} z \, dz}.$$
(B.7)

The relationship between T_{sf} , T_{av} , and q at the surface of the melt pool yields the following equation:

$$T_{sf} = T_{av} - \frac{q}{6\lambda} H_P$$
, where $q = h(T_{sf} - T_c)$, and (B.8)

$$T_{sf} = \frac{T_{av} + \frac{hH_P}{6\lambda}T_c}{1 + \frac{hH_P}{6\lambda}},\tag{B.9}$$

where h denotes the heat transfer coefficient at the surface of the melt pool and T_c denotes the coolant water temperature, respectively.

Appendix C Overview of CIP Method

C.1 Principal Concept of CIP Method

The CIP (cubic interpolated pseudo particle) method was developed by Yabe and Aoki⁽⁴⁰⁾. The principal concept of the CIP method is the cubic interpolation of the discrete data and the treatment of the advection term through the movement of the profile, in a manner analogous to the approach employed in the Lagrangian approach. The one-dimensional linear hyperbolic equation is described as follows:

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial z} = 0, \tag{C.1}$$

where v denotes the constant advection velocity. In the light of the spatial profile of the function f, and the velocity v at a specific time t, the concept of advection allows us to express the approximate value of the function f at a specific grid z_i , after a short time interval of time Δt , as follows:

$$f(z_i, t + \Delta t) \simeq f(z_i - v\Delta t, t). \tag{C.2}$$

In the CIP method, the function f and the derivative f' between the grid points are expressed using the interpolation function F_i ,

$$f(z_i,t+\Delta t)\simeq F_i(z_i-v\Delta t,t), \qquad \text{ and } \tag{C.3}$$

$$f'(z_i, t + \Delta t) \simeq F'_i(z_i - v\Delta t, t). \tag{C.4}$$

The interpolation function F_i is expressed as follows:

$$F_i(z) = a_i X^3 + b_i X^2 + f'_i X + f_i,$$
(C.5)

where X denote the distance between the grid points $z - z_i$, and z denotes the target grid point for the interpolation. The constants a_i and b_i are determined based on the continuity of f and f' between the grid points.

In the advection equation, the position of the grid points utilized for the interpolation is altered in accordance with the sign or direction of the advection velocity, whereby ensuring the precise calculation along the propagation of information or characteristic curves. In case of $v \le 0$, the grid points for interpolation are defined as $\Delta z = z_{i+1} - z_i > 0$, as the profile propagates from the downstream point "i+1" to the upstream point "i." In case of v > 0, the grid points for interpolation are defined as $\Delta z = z_{i+1} - z_i > 0$, as the profile propagates from the downstream point "i+1" to the upstream point "i." In case of v > 0, the grid points for interpolation are defined as $\Delta z = z_{i+1} - z_i > 0$, as the profile propagates from the downstream point "i+1" to the upstream point "i."

 $z_{i-1} - z_i < 0$, as the profile propagates from the upstream point "i-1" to the downstream "i" point. The indices of the grid points for interpolation are uniformly represented as follows:

$$i_2 = \left\{ \begin{array}{ll} i+1 & \text{if } v \leq 0\\ i-1 & \text{if } v > 0 \end{array} \right. \tag{C.6}$$

The constants a_i and b_i in the F_i are dependent on the direction of the advection velocity or the gird points for interpolation. They are expressed using the local gradient of the function ϕ , as follows:

$$a_i = \frac{-2\phi + f'_{i_2} + f'_i}{\Delta z^2},$$
(C.7)

$$b_i = \frac{3\phi - f_{i_2}' - 2f_i'}{\Delta z}, \qquad \text{and} \tag{C.8}$$

$$\phi = \frac{f_{i_2} - f_i}{\Delta z}.\tag{C.9}$$

In order to calculate the time evolution of f', it is necessary to use the advection equation for f', because the f and the f' between the grid points are extrapolated in the principal concept or nature of the CIP method.

$$\frac{\partial f'}{\partial t} + v \frac{\partial f'}{\partial z} = -f' \frac{\partial v}{\partial z}.$$
(C.10)

In the case of a linear hyperbolic equation with a constant v, the right-hand side of Eq. (C.10) is equal to zero and therefore the identical to the equation represented by Eq. (C.1). Once the profile of the function and the derivative at a specific time t have been provided, the subsequent time evolution of the profile at the subsequent time $t + \Delta t$ can be calculated as follows:

$$f_i^{new} \simeq F_i(z_i - v\Delta t) = a_i \xi^3 + b_i \xi^2 + f_i' \xi + f_i, \qquad \text{and} \qquad (C.11)$$

$$f_i'^{new} \simeq F_i'(z_i - v\Delta t) = 3a_i\xi^2 + 2b_i\xi^2 + f_i'.$$
(C.12)

where $\xi = -v\Delta t$ denotes the distance traversed due to the advection. The target grid point z for interpolation is then expressed as $z_i - v\Delta t = z_i + \xi$.

C.2 Treatments for Steep Profiles: CIP1 Method

A sharp increase or decrease in function f can be discerned at points such as the leading edge of a melt jet, where the profile undergoes an abrupt transition. The principle scheme of the CIP method entails the occurrence of overshooting or undershooting at specific locations, which is a consequence of the intrinsic characteristics of the cubic polynomial interpolation. A simple solution to the unphysical fluctuation, designated the CIP1 method, is presented by Yabe and Aoki⁽⁴⁰⁾.

The CIP1 method assumes that a given grid point is situated at the edge point of the profile, with one side exhibiting a nearly flat surface and the other displaying a pronounced change in slope. The interpolated function profile on the flat side will diverge significantly from the actual profile, resulting in unphysical overshooting or undershooting. In order to prevent the unphysical fluctuation, two different derivatives are employed on the front and back sides of the edge point: a derivative based on the interpolated profile is specified on the flat or back side; instead a derivative, obtained through a finite difference between the two grid points, is specified on the steep or front side.

In order to identify the position of the steep edge, an index n_p is introduced to place a flag on the point at the edge, based on the following criteria:

1. Edge on Front Side:

In case of an edge on the front side of the profile, $n_p = -1$ is specified when the following criteria is satisfied:

$$\frac{|f_i - f_{i-1}|}{|f_{i+1} - f_i|} < \epsilon \qquad \text{and} \qquad \frac{|f_{i-1} - f_{i-2}|}{|f_{i+1} - f_i|} < \epsilon, \tag{C.13}$$

where $|f_i - f_{i-1}|$ denotes the difference between the function values at the upstream grid point "i-1" and the focused grid point "i," and $|f_{i+1} - f_i|$ denotes the difference between the function values at the downstream grid point "i+1" and the focused grid point "i". The ratio indicates the change in function value in the upstream relative to the downstream. The smaller value of the ratio indicate that a flatter profile exists in the upstream direction, and a steep profile exists in the downstream direction.

2. Edge on Back Side:

In case of an edge on the back side of the profile, $n_p = 1$ is specified when the following criteria is satisfied:

$$\frac{|f_{i+1} - f_i|}{|f_i - f_{i-1}|} < \epsilon \qquad \text{and} \qquad \frac{|f_{i+2} - f_{i+1}|}{|f_i - f_{i-1}|} < \epsilon. \tag{C.14}$$

where $|f_{i+1} - f_i|$ denotes the difference between the function values at the downstream grid point "i+1" and the focused grid point "i," and $|f_i - f_{i-1}|$ denotes the difference between the function values at the upstream grid point "i-1" and the focused grid point "i". The ratio indicates the change in function value in downstream to the downstream. The smaller value of the ratio indicate that a flatter profile exists in the downstream direction, and a steep profile exists in the upstream direction.

If either condition is not satisfied or the steep profile does not exist, $n_p = 0$ is specified. The value of a constant ϵ should be small like 0.05. The derivatives on both sides of the focused grid point "i" is denoted as different names as $f'_{i,1}$ for the front side, and $f'_{i,0}$ for back side. The derivatives on both sides are initially set equal to f'_i , and then altered in case of the position of the steep profile.

1. Edge on Front Side:

In case of an edge on the front side of the profile, where $n_p = -1$ is specified, the derivative on the focused grid point "i" is determined using the function values on the side of the flat profile to suppress the fluctuation:

$$f_{i,0}' = \frac{f_i - f_{i-1}}{z_i - z_{i-1}}.$$
(C.15)

2. Edge on Back Side:

In case of an edge on the back side of the profile, $n_p = 1$ is specified, and the derivative is on the focused grid point "i" is determined using the function values on the side of the flat profile to suppress the fluctuation.

$$f_{i,1}' = \frac{f_{i+1} - f_i}{z_{i+1} - z_i}.$$
(C.16)

The indices of the grid points for interpolation, and for the derivatives are uniformly represented as follows:

$$i_2 = \begin{cases} i+1 \\ i-1 \end{cases} \text{ and } i_3 = \begin{cases} 1 & \text{if } v \le 0 \\ 0 & \text{if } v > 0 \end{cases},$$
(C.17)

The constants a_i and b_i in the F_i are dependent on the direction of the advection velocity or the gird points for interpolation. They are expressed using the local gradient of the function ϕ , as follows:

$$a_i = \frac{-2\phi + f'_{i_2,1-i_3} + f'_{i,i_3}}{\Delta z^2},$$
(C.18)

$$b_i = \frac{3\phi - f'_{i_2,1-i_3} - 2f'_{i,i_3}}{\Delta z}, \qquad \text{and} \qquad (C.19)$$

$$\phi = \frac{f_{i_2} - f_i}{\Delta z},\tag{C.20}$$

where, the subsequent time evolution of the profile at the subsequent time $t + \Delta t$ can be calculated as follows:

$$f_{i}^{new} \simeq F_{i}(z_{i} - v\Delta t) = a_{i}\xi^{3} + b_{i}\xi^{2} + f_{i,i_{3}}^{'}\xi + f_{i}, \qquad \text{ and } \qquad (C.21)$$

$$f_i'^{new} \simeq F_i'(z_i - v\Delta t) = 3a_i\xi^2 + 2b_i\xi^2 + f_{i,i_3}'. \tag{C.22}$$

C.3 Non-Liner Equation with Source Term

The conservation equation for mass, momentum and energy of the melt jet module is described in the form of a non-linear hyperbolic equation with a source term,

$$\frac{\partial f}{\partial t} + \frac{\partial (fv)}{\partial z} = g, \tag{C.23}$$

where the source term g denotes the external influences, creation and disappearance during the time evolution. In order to apply the operator splitting method, the equations are transformed into a non-conservation form for the f and the f':

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial z} = g - f \frac{\partial v}{\partial z} \equiv G,$$
 and (C.24)

$$\frac{\partial f'}{\partial t} + v \frac{\partial f'}{\partial z} = G' - f' \frac{\partial v}{\partial z},\tag{C.25}$$

In order to calculate the non-linear hyperbolic equation with a source term, the CIP method employs the two step calculation: advection and non-advection (source term) phases.

1. Advection Phase:

In the advection phase, the left-hand side of Eqs.(C.24) and (C.25) is calculated as linear hyperbolic equation, expressed as follows:

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial z} = 0,$$
 and (C.26)

$$\frac{\partial f'}{\partial t} + v \frac{\partial f'}{\partial z} = 0. \tag{C.27}$$

2. Non-Advection Phase:

In the non-advection phase, the right-hand side of Eqs.(C.24) and (C.25) is calculated to include the influences of the source term, expressed as follows:

$$\frac{\partial f}{\partial t} = G,$$
 and (C.28)

$$\frac{\partial f'}{\partial t} = G' - f' \frac{\partial v}{\partial z},\tag{C.29}$$

The function values from the old time step are employed to calculate the advection phase using the CIP method, thereby generating the intermediate function values f_i^* , and $f_i'^*$. Subsequently, the non-advection phase is calculated using the simple finite difference method in order to obtain the function values in the new time step. The simple finite difference method is described as follows:

$$f_i^{new} = f_i^* + \Delta t \cdot G_i, \qquad \text{and} \qquad (C.30)$$

$$f_i^{\prime new} = f_i^{\prime *} + \Delta t \cdot \left\{ G_i^{\prime} - f_i^{\prime *} \left(\frac{\partial v}{\partial z} \right)_i \right\},\tag{C.31}$$

where G'_i is discretized as follows:

$$G'_{i} = \frac{G'_{i+1} - G'_{i-1}}{z_{i+1} - z_{i-1}} = \frac{1}{z_{i+1} - z_{i-1}} \left(\frac{f^{new}_{i+1} - f^{*}_{i+1}}{\Delta t} - \frac{f^{new}_{i-1} - f^{*}_{i-1}}{\Delta t} \right)$$

$$= \frac{(f^{new}_{i+1} - f^{*}_{i+1}) - (f^{new}_{i-1} - f^{*}_{i-1})}{\Delta t (z_{i+1} - z_{i-1})}.$$
(C.32)

Appendix D A Fast-Running Steam Table Package: WRSTEAMTAB D.1 Outlines of the WRSTEAMTAB

The WRSTEAMTAB is a computer program that calculates the physical properties of liquid water and steam at specific pressures and temperatures. The program generates data points based on the formulas in the 1980 edition of the JSME (The Japan Society of Mechanical Engineers) steam table^(56, 57). The WRSTEAMTAB program interpolates data points from the JSME steam table, and offers rapid calculations than those based on the original formulas.

The JSME steam table, which is included in the WRSTEAMTAB, contains values of density, enthalpy, and their derivatives with respect to pressure and temperature. In the pressure-temperature plane of physical properties, third-order polynomial interpolation is employed, as is the CIP method (see Appendix C). Given that the derivatives are employed at each data point, it is possible to achieve an acceptable degree of accuracy even when utilizing relatively coarse data points. The use of spline interpolation ensures that the values change continuously before and after each data point in the incorporated steam table. The temperature and pressure derivatives of the density and enthalpy, which are necessary for two-phase flow simulations, have no discontinuous derivatives at the data points, thereby, stabilizing the convergence of the simulations.

D.2 Extensions for the Two-Phase Flow Model in Supercritical Regime

Fig. D.1 illustrates the data points of the JSME steam table, which is included in the WRSTEAMTAB. The data points encompass a temperature range of $274 < T_l < 787$ K for liquid water and $281 < T_g < 999$ K for steam, along with a pressure range of $10^3 < P < 10^8$ Pa. The higher temperature range is crucial in order to accurately model the steam explosions, because high-temperature melts are involved. To address a wide range of temperatures ($T_l \sim 800$ K, $T_g \sim 3,000$ K) and pressures ($P \sim 2.0 \times 10^8$ Pa), linear extrapolation or ideal gas approximation is employed for extrapolation at the boundaries of the steam table to the supercritical conditions.

The conventional two-phase flow model has been extended in order to accommodate supercritical conditions, which can arise in steam explosion simulations. In order to facilitate the treatment of supercritical conditions, the saturation curve is extended to the supercritical regime (upper right part of the critical point in Fig. D.1). The saturation curve provides access to the physical properties of both liquid water and steam. The physical properties of liquid water and steam in the supercritical regime, which are not included in the JSME steam table, are determined in a consistent manner or thorough the linear extrapolation. In the supercritical regime, steam exhibits a slightly lower density and a slightly higher enthalpy for than liquid water in order to avoid potential the numerical issues. Consequently, the WRSTEAMTAB is capable of numerical handling of superheated liquid water (with a superheat of approximately 10 K) and supercooled steam (with a supercool of approximately 10 K).



Fig. D.1 The data points of the steam table included in the WRSTEAMTAB that illustrate the various phases of coolant water as a function of pressure and temperature.

D.3 Accuracy of Physical Properties from Steam Table

Figs. D.2–D.6 depict the accuracy of saturation temperature T_{sat} , liquid (coolant water) density ρ_l , liquid (coolant water) enthalpy h_l , steam density ρ_s , and liquid (coolant water) enthalpy h_g . In case of the saturation line extended to the supercritical regime, the physical properties become the same. The extrapolated values are violated because of the steep changes in the physical properties, and simple extrapolation can lead to the discrepancies in the values The WRSTEAMTAB has been designed to mitigate the impact of significant fluctuations in the vicinity of the critical point in the steam table, which could potentially affect the stability of numerical solutions. While this may result in a compromise in accuracy around the critical point, it ensures that sufficient accuracy is maintained in other regions.



Fig. D.2 A comparison between the saturation temperatures (T_{sat}) calculated from the WRSTEAMTAB and those derived from the JSME formula based on the absolute deviation. The absolute deviation is expressed as $T_{sat}^{\text{WRSTEAMTAB}} - T_{sat}^{\text{JSME}}$.



Fig. D.3 A comparison between the coolant water densities (ρ_l) calculated from the WRSTEAMTAB and those derived from the JSME formula based on the relative deviation. The relative deviation is expressed as $(\rho_l^{\text{WRSTEAMTAB}} - \rho_l^{\text{JSME}})/\rho_l^{\text{JSME}}$.



Fig. D.4 A comparison between the coolant water enthalpies (h_l) calculated from the WRSTEAMTAB and those derived from the JSME formula based on the relative deviation. The relative deviation is expressed as $(h_l^{\text{WRSTEAMTAB}} - h_l^{\text{JSME}})/h_l^{\text{JSME}}$.



Fig. D.5 A comparison between the steam densities (ρ_g) calculated from the WRSTEAMTAB and those derived from the JSME formula based on the relative deviation. The relative deviation is expressed as $(\rho_g^{\text{WRSTEAMTAB}} - \rho_g^{\text{JSME}})/\rho_g^{\text{JSME}}$.



Fig. D.6 A comparison between the steam enthalpies (h_g) calculated from the WRSTEAMTAB and those derived from the JSME formula based on the relative deviation. The relative deviation is expressed as $(h_g^{\text{WRSTEAMTAB}} - h_g^{\text{JSME}})/h_g^{\text{JSME}}$.

Appendix E Parameter Adjustments for Steam Explosion Simulations

E.1 Outline of an Adjustment Method

This section presents an enhanced tuning method for a parameter in the steam explosion simulations proposed by Moriyama and Furuya⁽¹³⁾. The models associated with the explosion steps (propagation and expansion stages) in the JASMINE code employ empirical parameters to reproduce the experiments in the following manner:

1. C_{frg}

The fragmentation rate C_{frg} is a parameter defined as the ratio of melt fragments formed from a single premixed melt particle during the fragmentation process in the explosion steps. The C_{frg} is utilized in the formulation of Eq. (2.94).

2. K_{ev}

The heat release partition K_{ev} is a parameter that determines the partition of heat release that contributes to the evaporation of the coolant water during the fragmentation process in the explosion steps.

3. d_{frg}

The diameter of melt fragments d_{frg} during the fragmentation process in the explosion steps is a parameter. The model associated with the explosion steps assumed that the d_{frg} is uniform, and utilized in the formation of Eq. (2.104).

4. $t_{triglife}$

The $t_{triglife}$ is a parameter defined as the time period or duration during which the premixed melt particles are permitted to undergo the fragmentation following triggering in the explosion steps.

The results of the sensitivity analyses indicate that the steam explosion intensity is primarily influenced by the first two empirical parameters, with the last two having a secondary effect. As mentioned in the previous report⁽⁴⁾, it is recommended that the empirical parameters be set to the following values: $C_{frg} =$ 0.35, $K_{ev} = 0.7$, $d_{frg} = 50 \ \mu\text{m}$, and $t_{triglife} = 1 \ \text{ms}$. The recommended values of parameters were determined by comparing simulations with the KROTOS-42 and KROTOS-44 experiments, utilizing alumina melts⁽⁴⁷⁾. The recommended values of parameters were selected with the objective aligning the maximum value of the kinetic energy of the coolant water obtained from the simulations with the single value of the kinetic energy of the coolant water reported in the experiments. The simulation was conducted using the recommended values and replicated the kinetic energy obtained in the FARO-L33 experiment. The FARO-L33 experiments, which utilized a prototypical corium UO₂-ZrO₂ (80:20 wt%) melt, reported that the kinetic energy of the coolant water exhibited a range of values between 100 and 170 kJ⁽⁵²⁾. Moriyama and Furuya⁽¹³⁾ implemented enhancements to the tuning processes of the JASMINE code⁽⁴⁾, with a specific focus on the fragmentation rate C_{frg} . The recommended value of C_{frg} was determined through a comprehensive comparison of the simulations with the experiments, with a particular attention paid to the time series data of the impulses collected at different pressure measurement points. Note that the effects of C_{frg} and K_{ev} on the steam explosion intensity are similar. Given that a solid technical basis for modifying K_{ev} is absence, Moriyama and Furuya⁽¹³⁾ selected to maintain its value and concentrated their efforts on precisely adjusting C_{frg} .

In the experiments, the kinetic energy of the coolant water E_{ki} was estimated based on the assumption of one-dimensional upward movement of the coolant water column situated above each pressure measurement point. It was postulated that the impulses due to the pressure resulting from the steam explosion were converted to the kinetic energy of the coolant in a uniform upward direction.

$$E_{ki} = I^2/(2M),$$
 (E.1)

where I denotes the impulse, and M denotes the mass of the coolant water column. The maximum value of I, derived from the pressure data, is utilized in order to estimate $E_{ki}^{(47)}$. Eq. (E.1) includes I as a quadratic form, and the use of the maximum value can have a significant effect on the uncertainty. Additionally, Eq. (E.1) is dependent on the inverse of M, which is typically smaller and less precise at the upper pressure measurement points due to alterations resulting from void formation and coolant water movement. These factors can result in a considerable degree of uncertainty in E_{ki} at the upper pressure measurement points.

Moriyama and Furuya⁽¹³⁾ proposed that it is more reliable to compare the simulation with the experiments using time series data of I for multiple pressure measurement points. In lieu of a single value of E_{ki} , the following impulse derivatives, ΔI_{sgn} , ΔI_{abs} and ΔI_{max} , were employed for the purpose of comparing the simulation with the experiments:

$$\Delta I_{\rm sgn} = \frac{\int_{t_0}^{t_1} \{ \Delta p_{\rm sim}(t) - \Delta p_{\rm exp}(t) \} \, dt}{\int_{t_0}^{t_0} |\Delta p_{\rm exp}(t)|}, \tag{E.2}$$

$$\Delta I_{\rm abs} = \frac{\int_{t_0}^{t_1} \left| \Delta p_{\rm sim}(t) - \Delta p_{\rm exp}(t) \right| dt}{\int_{t_0}^{t_0} \left| \Delta p_{\rm exp}(t) \right|}, \qquad \text{and} \tag{E.3}$$

$$\Delta I_{\max} = \frac{I_{\max, \ \text{sim}} - I_{\max, \ \text{exp}}}{\left|I_{\max, \ \text{exp}}\right|},\tag{E.4}$$

where the suffixes "sim" and "exp" denote the values derived from the simulations and the experiments, respectively. The symbol $\Delta p(t)$ denotes the pressure relative to the initial pressure value p_{init} [see Eq. (E.5)], and I_{max} denotes the maximum value of I (per area). The time series data of I(t) is defined over the time interval from $t = t_0 - t_1$ at a specific location [see Eq. (E.6)]. Note that a decrease in the I(t) may occur when the p(t) falls below p_{init} ,

$$\Delta p(t) = p(t) - p_{\rm ini}, \qquad \text{and} \qquad (E.5)$$

$$I(t) = \int_{t_0}^{t} p(t)dt$$
. (E.6)

Moriyama and Furuya⁽¹³⁾ conducted the simulations for the KROTOS-42 and FARO-L33 experiments under identical simulation conditions, with the exception that the variation of C_{frg} was from 0.13 to 0.40. Subsequently, the authors evaluated the dependence of ΔI_{sgn} , ΔI_{abs} and ΔI_{max} on changes in C_{frg} .

E.2 Sensitivity Analyses for Parameter Values

0.454

0.647

0.820

0.977

CF5

CF6

CF7

CF8

0.25

0.30

0.35

0.40

Table E.1 illustrates the impact of variation of the fragmentation rate C_{frg} on the impulse derivatives between the simulations and the experiments. The impulse derivatives ΔI_{sgn} , ΔI_{abs} , and ΔI_{max} were estimated using the average pressure over the locations from K0 to K3 for the KROTOS-44 experiment, and from 490 mm to 1,165 mm for the FARO-L33 experiment.

the simulation	ne simulations (JASMINE) and the experiments (KRO10S-44 and FARO-L33).							
		ŀ	KROTOS-44			FARO-L33		
Case	C_{frg}	${\it \Delta}I_{ m sgn}$	$\varDelta I_{\rm abs}$	$\varDelta I_{\rm max}$	$\varDelta I_{\rm sgn}$	$\varDelta I_{\rm abs}$	ΔI_{max}	
CF1	0.13	-0.0969	0.192	0.0356	-0.517	0.517	-0.401	
CF2	0.15	0.00702	0.176	0.143	-0.427	0.427	-0.309	
CF3	0.17	0.1037	0.195	0.242	-0.340	0.340	-0.224	
CF4	0.20	0.241	0.262	0.383	-0.212	0.216	-0.105	

0.699

0.797

0.972

1.13

-0.013

0.179

0.351

0.508

0.172

0.247

0.377

0.523

0.0731

0.240

0.388

0.521

0.454

0.647

0.820

0.977

Table E.1 A discrepancy in the impulse derivatives can be attributed to the variations in C_{frg} between the simulations (JASMINE) and the experiments (KROTOS-44 and FARO-L33).

Note that the average pressure was estimated by excluding the pressures measured at the upper locations in the vicinity of the coolant water surface. This was done to account for the potential for inaccuracy in pressure measurements resulting from the significant elevation in the surface of the coolant water at the premixing steps. The absolute values of $\Delta I_{\rm sgn}$, $\Delta I_{\rm abs}$, and $\Delta I_{\rm max}$ were minimized by varying C_{frg} , which are highlighted in bold. In the KROTOS-44 experiment, the values of $\Delta I_{\rm sgn}$ and $\Delta I_{\rm max}$ exhibited a minimum at $C_{frg} = 0.13$, and 0.15, respectively. In the FARO-L33 experiment, the minimum values of all impulse derivatives occur at $C_{frg} = 0.25$.



Fig. E.1 A correlation between the impulse derivatives ΔI_{sgn} and ΔI_{abs} , depending on C_{frg} , estimated from the simulations (JASMINNE) and the experiments (KROTOS-44 and FARO-L33).



Fig. E.2 A correlation between the impulse derivatives ΔI_{max} , depending on C_{frg} estimated from the simulations (JASMINE) and the experiments (KROTOS-44 and FARO-L33).

Figs. E.1 and E.2 illustrate the correlation between the ΔI_{sgn} , ΔI_{abs} and ΔI_{max} , and C_{frg} . As C_{frg} increases, both ΔI_{abs} and ΔI_{max} demonstrate a corresponding increase (see Fig. E.1 and Fig. E.2). Notwithstanding the minimum ΔI_{max} at $C_{frg} = 0.13$ for the KROTOS-44 experiment and $C_{frg} = 0.25$ for the FARO-L33 experiment (see Fig. E.2), the ΔI_{abs} exhibits derivatives of approximately 20% at $C_{frg} = 0.13$ for the KROTOS-44 experiment and $C_{frg} = 0.25$ for the FARO-L33 experiment (see Fig. E.2), the ΔI_{abs} exhibits derivatives of approximately 20% at $C_{frg} = 0.13$ for the KROTOS-44 experiment and $C_{frg} = 0.25$ for the FARO-L33 experiment (see Fig. E.1). The simulations appear to be most similar to the experiments at $C_{frg} = 0.15$ for the KROTOS-44 experiment and $C_{frg} = 0.25$ for the FARO-L33 experiment (see Fig. E.1). The simulations appear to be most similar to the experiments at $C_{frg} = 0.15$ for the KROTOS-44 experiment and $C_{frg} = 0.25$ for the FARO-L33 experiment, as indicated by the ΔI_{sgn} and ΔI_{abs} . In the previous report⁽⁴⁾, the optimal value is $C_{frg} = 0.35$. The value results in larger ΔI_{sgn} and ΔI_{abs} , with approximately 80% for the KROTOS-44 experiment and 40% for the FARO-L33 experiment.

E.3 Determination of a Parameter Value

Figs. E.3 and E.4 present a comparison of the time series data of the impulses obtained from the simulations at the pressure measurement points for the KROTOS-44 experiment ($C_{frg} = 0.15$) and the FARO-L33 experiment ($C_{frg} = 0.25$). The simulations indicate that the impulses at the lower locations are larger than those at the upper locations, which is consistent with the difference in the coolant water mass inertia depending on location, as expressed in Eq. (E.1). The experiments, however, indicate that the larger impulses are observed at the upper locations. In particular, the data from "EXP.K3" exhibit a larger value than those from "EXP.K0", "EXP.K1", and "EXP.K2", as illustrated in Fig. E.3. The observed behavior suggests that the shock wave may have intensified in an uneven manner, which could be attributed to the non-uniform distribution of the premixed melts. The previous method proposed by Huhtiniemi et al.⁽⁴⁷⁾, which employed the largest impulse estimated among the pressure measurement points, may result in a considerable overestimation (see Fig. E.5). The present method, proposed by Moriyama and Furuya⁽¹³⁾, which utilizes a greater number of available impulses, appears to be a more reasonable approach for determining the parameter.

Figs. E.5 and E.6 present a comparison of the kinetic energy estimated from the impulses between the simulations and experiments. The figures include the estimated values from the experiments (labeled as "EXP."), the reported value (labeled as "EXP. reported"), and the estimated values from the simulations (labeled as "CF1" to "CF8."). With regard to the KROTOS-44 experiments (see Fig. E.5), the kinetic energy derived from the impulses designated as K0-K2 in the experiments ranges from 60 to 80 kJ, while K3 exceeds 170 kJ. The kinetic energy designated as K3 is in close agreement with the reported value by Huhtiniemi et al.⁽⁴⁷⁾. The kinetic energy designated as CF7 ($C_{frg} = 0.35$), which was recommended in the previous report⁽⁴⁾, is in close agreement with the reported value by Huhtiniemi et al.⁽⁴⁷⁾. The kinetic energy designated of CF2-CF4 ($C_{frg} = 0.15 - 0.20$) are comparable to those of K0-K2. With regard to the FARO-L33 experiment (see Fig. E.6), the kinetic energy from the impulses in the simulations of 93-261 kJ by Annunziato et al.⁽⁴⁹⁾ or 100-170 kJ by Magallon⁽⁵²⁾ (indicated in the figure). The kinetic energy from the impulses in the simulation of CF5 and CF6 ($C_{frg} = 0.25$ and 0.30) agrees with the reported value by Magallon⁽⁵²⁾.



Fig. E.3 A comparison of the impulses between the experiments ("EXP.") and simulations ($C_{frg} = 0.15$) ("SIM.") estimated from the pressures at each sensor location for the KROTOS-44 experiments.



Fig. E.4 A comparison of the impulses between the experiments ("EXP.") and the simulation ($C_{frg} = 0.25$) ("SIM.") estimated from the pressures at each sensor location for the FARO-L33 and experiments.

In consideration of the preceding discussions, Moriyama and Furuya⁽¹³⁾ proposed that the newly recommended value for the fragmentation rate should be $C_{frg} = 0.25$. The simulations conducted in both the KROTOS-44 (alumina) and the FARO-L33 experiments demonstrated that the impulses estimated from the experiments were not significantly underestimated. It is important to note, however, that the KROTOS-44 simulations result in an overestimation of approximately 40% in the impulse (see Fig. E.1). The recommended value for C_{frg} is satisfactory, particularly in view of the importance of accurately evaluating the FARO experiments, which are conducted under the conditions that are relatively close to the prototypical conditions, compared to the KROTOS experiments.



Fig. E.5 A comparison of the kinetic energy of the coolant water for the KROTOS-44 experiment: the estimated from impulses in the experiments ("EXP. "), the reported value ("EXP. reported"), and the estimated from impulses in the simulations ('CF1 to CF8').



Fig. E.6 A comparison of the kinetic energy of the coolant water for the FARO-L33 experiment: the estimated values from impulses in the experiments ("EXP."), the reported value ("EXP. reported"), and the estimated values from impulses in the simulations ("CF1 to CF8").

Appendix F Input File and Contents

The input file, which has been prepared in a plain text format, is read line by line and interpreted according to the order of the data (input valuables). The interpreter offers a range of preprocessing functions, including the ability to add comments, include additional files, and echo data. The following sections provide an overview of the preprocessing functions, the order of data and the contents included in the input file.

F.1 Preprocessing Functions

Limitation of Line Length

The input file is constrained to a maximum line length of 140 characters. The initial 132 characters are interpreted as data to be read by the interpreter, while the remainder part of the line is disregarded as an index field, can be utilized to put line numbers, for example.

Functions: Comments

The input file can include comment lines. Any characters following the string "//" are considered to be comments and ignored, as demonstrated in the following example.

// this is a comment line.
3 5 12.6 // anything after "//" is ignored.

C-style commenting is available through the use of the "/*" and "*/" characters to enclose the comment, as demonstrated in the following example.

/* node */ 15 /* element */ 6
23.8 /*
this is a comment.
*/ 56.7

The nested usage of the "/**/" pair, as demonstrated in the example below, is not permitted in order to ensure the successful completion of the process.

/* /* this is an example of nesting. */ */

Functions: Directives

The input file can be processed in accordance with the specified directives. The directives are identified by one of the following keywords at the beginning of a line.

#include <file name>:

The directive is employed to incorporate a distinct file at the designated position within the input file. It should be noted that the use of the directive in a nested fashion is not permitted.

#listoff:

The directive is employed to prevent the replication of input data. By default, the input data is replicated in the "list output file", which is the output file for the two-phase flow simulations.

#liston:

The directive is employed to restart the replication of the input data. When the directive is specified, the echoing process commences with the next input data.

F.2 Input Variables and Ordering

The input file is comprised of the following sections. The input data is identified based on its position (order) within the input file. The values in () indicate the default or recommended values.

Flag for Namelist Options

This section specifies a flag that controls a namelist option utilization for the input file.

Variable	Туре	Description
iopt	integer	flag to control the namelist options
		0 = NO use
		1 = use

Input File Title

This section specifies the input file title as a string of 132 characters.

Variable	Туре	Description
title	character	input file title in A132 Format

If "iopt" = 1, the program will proceed to read the namelist options from the subsequent sections. The format of the namelist options is based on the syntax of Fortran namelist input.

Namelist Options: Common Flags and Parameters (Two-Phase Flow)

This section specifies the common flags and parameters for the two-phase flow simulations. In the absence of any specified flags or parameters, the default values ate automatically employed.

Variable	Туре	Description
cvm	real	coefficient of the virtual mass term for two-phase flow $(-)$ (0.0)
sdtim	real	interval for message output in time step (sec) (0.1)
sdstp	integer	interval for message output in calc. step (sec) (1000)
editop	integer	flag to control the output variables (0)
		0 = primary variables only
		1 = additional variables
		2 = additional variables (all)
idebug	integer	flag to control the debug information output (0)
		0 = NO output
		1 = output
idbeos	integer	flag to control the EOS data output in case of convergence failure (0)
		0 = NO output
		1 = output ("out.db" is output)
istdiff	integer	flag to control the auxiliary diffusion model replicate the diffusion of
		steam in the gas phase not to create gaps in steam concentration by
		enhancing the intermixing of gas components (1)
		0 = NO use
		1 = use
ddst	real	diffusion coefficient of steam for the auxiliary diffusion model $(-)$ (0.1)
fhtint	real	fraction of the heat transfer from the melts directly deposited at the
		liquid-gas interfaces for evaporation (-) (0.02)
tlsupqcut	real	cut-off superheating of water that limits the heat transfer from the melts
		to bulk water (K) (0.5)
fhigkill	real	attenuation factor for the heat transfer coefficient ("hig") between
		superheated steam and the liquid-gas interfaces in the cells with heat
		transfer from the melts if "ihighil0=0" (-) (0.1)
fhilkill	real	attenuation factor for the heat transfer coefficient ("hil") between
		subcooled water and the liquid-gas interfaces in the cells with heat
fcondres	raal	(-) (0.001)
TCONUTES	1001	interfaces when NC gases exist in the gas phase, attenuation effects by
		NC gases accumulation near the interfaces (-) (0.02)

Variable	Туре	Description
fevapres	Real	attenuation factor for the evaporation heat transfer at the liquid-gas
		interfaces when NC gases in the gas phase; attenuation effects by NC
		gases dilution near the interfaces (-) (0.5)
dtminqvbd	real	lower limit for the denominator of "qvbd/delt" in the evaporation
		term: the "qvbd" means the heat input from melt in a single cell for a
		single time step. If the time step is decreased due to convergence failure,
		the "qvbd/delt" increases and worsen the convergence. "dtminqvbd"
		limits the increase of the source term and continue the calculation. Note
		that the energy conservation is consistently maintained.
ihighil0	integer	flag to control the heat transfer coefficient ("hig" and "hil") between
		water and the liquid-gas interfaces (0)
		$0 = \text{ default (for premixing step)}^{*1}$
		1 = NO heat transfer or "hig=hil=0"
		2 = limited the heat transfer (for explosion step) *2
		relaxation time to suppress rapid changes in the heat transfer coefficient
taueqxplg	real	("hig") between superheated steam and the liquid-gas interfaces due to
		high superheated steam when "ihighil0=2" $(1.0 \times 10^{-3} \text{ sec})$
irsarla0	integer	flag to control the heat transfer between NC gases and water or steam
		(0)
		0 = default
		1 = NO heat transfer or "rsa=rla"
ici0	integer	flag to control the interface friction between the liquid-gas interfaces
		for two-phase flow (0)
		0 = default
		1 = NO interface friction or "cix=ciy=ciz=0"
fcfmist	real	attenuation factor of the interface friction for droplet flow $(-)$ (1.0)
fcfbubb	real	attenuation factor of the interface friction for bubbly flow $(-)$ (1.0)
ieqdia	integer	flag to control the model to determine bubble or droplet sizes for two-
		phase flow (1)
		0 = Weber number using local relative velocity
		1 = equilibrium between gravity, drag, and buoyancy
nftran	real	exponent of interpolation function for two-phase friction in the
		transition regime $\alpha = 0.3 - 0.75$. The bubbles escapes of coolant water
		in larger values (1.0-4.0) (-) (1.0)

Variable	Туре	Description
icimj	integer	number of columns applied for the annular flow model ranging from the
		center $(1 - nx")$ of the simulation domain (-) (0)
islvr	integer	flag to control the matrix solver of pressure equations (0)
		0 = Band-Gauss
		1 = Incomplete LU BCG

^{*1}The "hig" and "hil" for the bubbly flow regime are employed when $\alpha < 0.30$, the "hig" and "hil" for the annular flow regime are employed when $\alpha > 0.75$, and the "hig" and "hil" in the bubbly and annular flow regimes are taken as the sum of each multiplied by the steam and liquid volume fraction.

^{*2}The "hig" is determined when supercooled steam: $T_g < T_{sat}$ and $\alpha < 1.0 \times 10^{-6}$ (steam is present), or high superheated steam $T_g > (T_m + T_{sat}) / 2$. Otherwise, the "hig=0". The "hil" is determined when superheated water: $T_l > T_{sat}$ and $\alpha > 1.0 \times 10^{-6}$ (water is present). Otherwise, the "hil=0".

Namelist Options: Time Step and Output Interval (Commons)

This section specifies the variables utilized in the simulation, delineating the time step and output interval. The number of iterations controls the time step in order to ensure the pressure convergence. The pressure convergence is controlled based on the convergence criteria. The Courant limit is employed to ensure that the time step remains sufficiently small.

Variable	Туре	Description
sttime	real	start time for the simulation (sec)
endtim	real	end time for the simulation (sec)
deltmx	real	maximum time step (sec)
deltmn	real	minimum time step (sec)
edtim	real	output time interval for the "list output" (sec)
pltim	real	output time interval for the "plot output" (sec)
httim	real	output time interval for the "history output" (sec)
itrinc	integer	iteration limit to increase the time step as early convergence (-) (5)
itrred	integer	iteration limit to decrease the time step as late convergence (-) (10)
fdtinc	real	factor to increase the time step (-) (1.20)
fdtred	real	factor to decrease the time step $(-)$ (0.95)

Namelist Options: Convergence Criteria (Two-Phase Flow)

This section specifies the variables utilized in the convergence criteria. When maximum number of iterations for the pressure convergence ("maxitr") are exceeded, the iteration is terminated, the time step is reduced by 80%, and the pressure convergence is attempted once more. The pressure convergence is achieved when the relative residual is smaller than the convergence criterion ("epscnv").

Variable	Туре	Description
maxitr	integer	maximum number of iterations for the pressure convergence (-) (20)
epscnv	real	conversion criterion based on the relative residual (-) (1.0×10^{-4})

Namelist Options: Output Cells Position (Two-Phase Flow)

This section specifies the cells for output to the "history output." The number of cells ("nhstcell") needs to be specified first. Then, the i-th cell index in the x/r-direction ["ihst(i)"] and z-direction ["khst(i)"] needs to be specified ($1 \le i \le$ "nhstcell"), which are read in the following format:

read(iwkunt, *) (ihst(i), khst(i), i=1, nhstcell)

Variable	Туре	Description
nhstcell	integer	number of cells output to the "history output" (-) (maximum 50)
ihst(i)	integer	<i>i</i> -th cell index in the x/r -direction (-)
khst(i)	integer	<i>i</i> -th cell index in the <i>z</i> -direction (-)

Namelist Options: Water Levels Output (Two-Phase Flow)

This section specifies the x/r-positions of the water levels output to the "history output." The number of the x/r positions ("nwlevel") is specified first. Then, the i-th cell index in the x/r-direction ["iwlev(i)"] needs to be specified ($1 \le i \le$ "nwlevel"), which are read in the following format:

read(iwkunt, *) (iwlev(i), i=1, nwlevel)

Variable	Туре	Description
nwlevel	integer	number of the x/r -positions of the water levels output to the "history output" (-) (maximum 20)
iwlev(i)	integer	<i>i</i> -th cell index in the x/r -direction (-)

In order to detect the water levels, the void fraction α is scanned from the top of a cell column at the specified position until the first cell is identified where $\alpha < \alpha_{lev}$. The cell index where $\alpha < \alpha_{lev}$ in the z-direction is designated as k_{lev} . The criterion is $\alpha_{lev} = 0.8$. The water levels are determined using the methods designated as "leva" and "levb".

leva:

Assuming that the water surface is situated between the k_{lev} -th and k_{lev} + 1-th cells, the water level at the z-position where $\alpha = \alpha_{lev}$ is determined using a linear interpolation between the zpositions of the k_{lev} -th and k_{lev} + 1-th cells centers.

levb:

Assuming that the water surface is situated inside the k_{lev} -th cell, the water level at the z-positions where $\alpha = \alpha_{lev}$ is determined using a liner interpolation between the top and bottom of the k_{lev} -th cell boundaries.

Namelist Options: Meshes of Simulation Domain (Two-Phase Flow)

This section specifies the number of the meshes in each direction. As the JASMINE code is only available only in the 2D cylindrical (r-z) coordinate system, the value of "ny=1" for a single cell in the y/θ -direction (i.e., a single grid) can be specified.

Variable	Туре	Description
nx	integer	number of the meshes in the x/r -direction (-)
ny	integer	number of the meshes in the y/θ -direction (-) (1)
nz	integer	number of the meshes in the z -direction (-)

Namelist Options: Non-Condensable Gas Components (Two-Phase Flow)

This section specifies the non-condensable gases included within the simulation domain. The number of the non-condensable gas components ("ngas") needs to be specified first. Then, the gas components ["kindgs(i)"] needs to be specified for the i-th component ($1 \le i \le$ "ngas"). If "ngas=0", the simulation domain is devoid of non-condensable gases, and the gas phase is constituted only by steam.

Variable	Туре	Description
ngas	integer	number of the non-condensable gas components (-) (maximum 20)
kindgs(i)	integer	index of the i-th non-condensable gas component
		1 = air
		2 = hydrogen

Variable	Туре	Description
		3 = helium
		4 = nitrogen
		5 = argon

Namelist Options: Coordinate, Boundary and Gravity (Two-Phase Flow/Melts)

This section specifies the coordinate systems, the boundary conditions, and the gravity direction. It should be noted that for the inlet boundaries ["igbcz=1"], velocities must be specified at the boundary cells, and for the outlet boundaries ["igbcz=2"], pressures must be specified at the boundary cells.

Variable	Туре	Description
igeom	integer	flag to control the coordinate system (0)
		0 = Cylindrical
		1 = Cartesian
cyclic	integer	flag to control the boundary condition in the y/θ -direction (0)
		0 = wall (slip)
		1 = cyclic
ngrav	integer	flag to control the gravity direction (0)
		$0 =$ the z-direction at $g_z = -9.807$ m/s ²
		1 = specified arbitral values and directions
igbcz(1)	integer	flag to control the boundary at bottom $(k = 0)$ in the z-direction
		0 = wall (slip)
		1 = inlet
		2 = outlet
igbcz(2)	integer	flag to control the boundary at top $(k = "nz"+1)$ in the z-direction
		0 = wall (slip)
		1 = inlet
		2 = outlet

Namelist Options: Inner Walls in Simulation Domain (Two-Phase Flow)

This section specifies the inner walls that represent the vessel or structural walls. The number of the inner walls needs to be specified first. Then, the position of the inner walls needs to be specified for the i-th inner wall ($1 \le i \le \text{"nxwall"/"nzwall"}$). It should be noted that the inner walls in the x/r-direction need to be specified first, followed by the those in the z-direction.

Variable	Туре	Description
nxwall	integer	number of the inner walls in the x/r -direction (-) (maximum 20)
ixwall(i)	integer	cell boundary index in the x/r -direction of the <i>i</i> -th inner wall (-)
ixwall(1,i)	integer	cell center index at bot. in the z-direction of the i -th inner wall (-)
ixwall(2,i)	integer	cell center index at top in the z -direction of the i -th inner wall (-)
nzwall	integer	number of the inner walls in the z -direction (-) (maximum 20)
kxwall(i)	integer	cell boundary index in the z -direction of the i -th inner wall (-)
kxwall(1,i)	integer	cell center index at cent. in the x/r -direction of the <i>i</i> -th inner wall (-)
kxwall(2,i)	integer	cell center index at edge in the x/r -direction of the <i>i</i> -th inner wall (-)

Namelist Options: Mesh Position of Simulation Domain (Two-Phase Flow)

This section specifies the mesh positions in the simulation domain, as defined by the "nx," ny," and "nz" values. As the JASMINE code is only available only in the 2D cylindrical (r-z) coordinate system, the mesh positions for a single cell (or a single grid) in the y/θ -direction can be specified.

Variable	Туре	Description
z	real	cell boundary positions in z-direction (required "nz"+1 data) (m)
rad	real	cell boundary positions in x/r -direction (required "nx"+1 data) (m)
th	real	cell boundary positions in y/θ -direction (required "ny"+1 data) (m)

Namelist Options: Gravity Components and Directions (Two-Phase Flow/Melts)

This section specifies the gravity components and directions. If "ngrav=1", the following data must be specified. It should be noted that the following data is automatically applied to the melt simulations.

Variable	Туре	Description
gc	real	absolute value of the gravitational acceleration (m/s ²)
gravx	real	cosine in the x/r -directional (-)
gravy	real	cosine in the y/θ -directional (-)
gravz	real	cosine in the z-directional (-)

Namelist Options: Initial Variables within Simulation Domain (Two-Phase Flow)

This section specifies at the initial conditions or variables for the two-phase flow simulations. The volume and surface area of the two-phase flow simulations are automatically adjusted to correspond with the geometrical volume and surface area. The volume fractions and temperatures of the water and steam are uniformly set for the entire simulation domain, according to the following data set.

Variable	Туре	Description
alpn0	real	volume fraction for steam (-)
pn0	real	pressure (Pa)
tvn0	real	steam temperature (K)
tln0	real	water temperature (K)

The velocities of the gas and liquid phases must be specified in accordance with the following data. It should be noted that the gas phase includes the non-condensable (NC) gas components if "ngas \geq 1".

Variable	Туре	Description
vvxr0	real	gas (including NC gases) velocity in the x/r -direction (m/s)
vvyt0	real	gas (including NC gases) velocity in the y/θ -direction (m/s)
vvz0	real	gas (including NC gases) velocity in the z-direction (m/s)
vlxr0	real	water velocity in the x/r -direction (m/s)
vlyt0	real	water velocity in the y/θ -direction (m/s)
vlz0	real	water velocity in the z -direction (m/s)

If "ngas≥1", the volume fractions, and temperatures of the non-condensable gases must be specified. It should be noted that the following data must be specified for each gas component.

Variable	Туре	Description
alp0a	real	volume fraction of a non-condensable gas (-)
ta0	real	non-condensable gas temperature (K)

Namelist Options: Specified Rectangular Sections (Two-Phase Flow)

This section specifies the variables of the two-phase flow simulations at specified rectangular sections. The number and position of the rectangular sections must be specified. The rectangular sections are employed to modify the initial variables in only specific areas.

Variable	Туре	Description
nmararea	integer	number of the rectangular sections to modify the initial variables (-)
is	integer	cell center index in the x/r -direction that specifies start point
		(diagonal) of a rectangular section (-)
ks	integer	cell center index in the z -direction that specifies start point (diagonal)
		of a rectangular section (-)
ie	integer	cell center index in the x/r -direction that specifies end point
		(diagonal) of a rectangular section (-)
ke	integer	cell center index in the z -direction that specifies end point (diagonal)
		of a rectangular section (-)

Subsequently, the volume fractions, and temperatures of the two-phase flow simulations are uniformly set for the specified rectangular sections based on the following data. If "ngas≥1", the volume fractions, and temperatures for the non-condensable gases must be specified in the order of components, as indicated in the following data set.

Variable	Туре	Description
alpst	real	volume fraction of steam in a rectangular zone (-)
tv	real	steam temperature in a rectangular zone (K)
tl	real	water temperature in a rectangular zone (K)
alpgs	real	volume fraction of a non-condensable gas in a rectangular zone (-)
tvgs	real	non-condensable gas temperature in a rectangular zone (-)

In order to specify the volume fractions of steam and non-condensable gases, it is necessary to consider the two-phase equilibrium for cells at the initial conditions. When the initial system pressure is 0.2 MPa, and the initial water temperature is 342 K (subcooling 50 K), the volume fractions* of steam and non-condensable gases in the two-phase equilibrium at the specified pressure (0.2 MPa) and temperature (342 K) must be provided. It can be assumed that the temperatures of the gas components are equivalent to the water temperature.

For example, the initial void fractions are set at 0.999 for the cover gas cells, 0.001 for the water cells, and 0.500 for the water surface cells. The supporting tool "initparp" program calculates the volume fractions of steam "alpst" and non-condensable gases "alpgs" for a given pressure and temperature

^{*}The modeling of multi-component gases is achieved through the volume fractions rather than partial pressures in the JASMINE code. For further details, please refer to the User's Guide.

based on the specified void fractions for the cover gas, water, and water surface as follows. The command prompt, represented by the symbol, "\$," serves as a header for the command lines.

```
$ initparp 0.2e6 342 0.999 0.001 0.5
p= 2.0000e+05 T= 342.00 (Tsub= 50.91)
=> pst= 2.9629e+04 alpst/alp=pst/p= 1.4814e-01
alp alpst alpgs
0.99900 1.4800e-01 8.5100e-01
0.00100 1.4814e-04 8.5185e-04
0.50000 7.4072e-02 4.2593e-01
```

Namelist Options: Inlet and Outlet Boundaries (Two-Phase Flow)

This section specifies the two-phase flow variables at the boundary conditions for the inlet ("igbcz=1") or outlet ("igbcz=2") boundaries at the bottom or top of the simulation domain. It should be noted that the variables of the bottom boundary must be specified first, followed by those of the top boundary. If "igbcz=2", the dz needs to be specified. The size and volume of the boundary cells outside of the simulation domain are determined based on the value of the "dz". If "igbcz=1", the dz is not utilized, and the size and volume of the boundary cells are set to be identical to those of the adjacent cell within the simulation domain.

Variable	Туре	Description
dz	real	boundary cell size for the <i>z</i> -direction (m)

Subsequently, the volume fractions, temperatures, and velocities of the two-phase flow at the boundary cells must be specified. If the positive values are specified at the following data set, the uniform values are applied to all boundary cells.

Variable	Туре	Description
alpha	real	volume fraction of steam at boundary cells (-)
press	real	pressure at boundary cells (Pa)
tempv	real	steam temperature at boundary cells (K)
templ	real	water temperature at boundary cells (K)

If any of the variables are assigned as negative values, the cell-dependent values are retrieved from the following data set. It is necessary to specify the number of values corresponding to those of boundary cells. It should be noted that the velocities are always regarded cell-dependent values.

Variable	Туре	Description
alpha	real	volume fraction of steam at a boundary cell (-)
press	real	pressure at a boundary cell (Pa)
tempv	real	steam temperature at a boundary cell (K)
templ	real	water temperature at a boundary cell (K)
vvz	real	gas (including NC gases) velocity at a boundary cell (m/s)
vlz	real	water velocity at a boundary cell (m/s)

The cell-dependent values are read in the following format. Here, k = 0 denotes the bottom boundary, while k = "nz"+1 denotes the top boundary, respectively.

```
do 100 j = 1, ny
```

read(iwkunt, *) (vel(i, j, k) , i = 1, nx)

100 continue

The velocities specified here replace the initial values specified in the section, "Initial Variables within Simulation Domain (Two-Phase Flow)." When dealing with the inlet boundaries, the velocities specified here become the inlet velocities.

Variable	Туре	Description
vvz	real	gas velocity at a boundary cell (m/s)
vlz	real	water velocity at a boundary cell (m/s)

If "ngas≥1", the volume fractions and temperatures of the non-condensable gases at the boundary cells must be specified. If the positive values are specified at the following data set, the uniform values are applied to all boundary cells.

Variable	Туре	Description
alp0a	real	volume fraction of a non-condensable gas at boundary cells (-)
ta0	real	non-condensable gas temperature at boundary cells (K)

If any of the variables are assigned as negative values, the cell-dependent values are retrieved from the following data set. It is necessary to specify the number of variables corresponding to those of boundary cells. It should be noted that the following data set must be specified for each gas component.

Variable	Туре	Description
alp0a	real	volume fraction of a non-condensable gas at a boundary cell (-)
ta0	real	non-condensable gas temperature at a boundary cell (K)

Namelist Options: Common Flag and Variables (Melt)

This section specifies the flag that controls the utilization of the melt simulation. If "imelt=0", the following section are NOT read, and the program will proceed solely with the two-phase flow simulation.

Variable	Туре	Description
imelt	integer	flag to use the melt simulation (1)
		0 = NO use
		1 = use
prmpp_iedg	integer	cell boundary index in x/r -direction specifies the range of movement
		for the melt components (melt pool and particles)
prmj_ktop	integer	cell boundary index in z -direction specifies the location of melt jet
		inlet, and the range of movement for the melt components
prmj_nsub	integer	number of cell sub-divisions in z -direction of the simulation domain
		to simulate melt jet in finer grids (4)

Namelist Options: Initial Variables (Melt Jet)

This section specifies the initial variables for the melt jet inlet. The number of the data points must be specified. Subsequently, the time, velocity and diameter of the melt jet inlet corresponding to the data point must be specified at the following data set $(1 \le i \le "prmj_nini")$.

Variable	Туре	Description
prmj_tempini	real	melt jet temperature (K)
prmj_nini	integer	number of the data points to specify the inlet velocity and diameter
		of the melt jet inlet (-) (maximum 500)
prmj_tini(i)	real	<i>i</i> -th time of the melt jet inlet at <i>i</i> -th data point (s)
prmj_vini(i)	real	<i>i</i> -th velocity of the melt jet inlet at <i>i</i> -th time (m/s)
prmj_dini(i)	real	<i>i</i> -th diameter of the melt jet inlet at <i>i</i> -th time (m)

The velocity and diameter are interpolated or extrapolated over time. A liner interpolation is applied between the values just before and after the time in ranges of "prmj_tini(1)" and "prmj_tini (prmj_nini)." The values at "prmj_tini(1)" are extrapolated before "prmj_tini(1)," and the values at "prmj_tini(prmj_nini)" are extrapolated after "prmj_tini(prmj_nini)."

Namelist Options: Initial Variables (Melt Particle)

This section specifies the initial variables associated with the melt particles. The JASMINE code allows arbitrary placement of the melt particles at any desired time and position. The number of the particle groups must be specified, followed by the particle group information.

Variable	Туре	Description
nparin	integer	number of the particle groups put within the simulation domain (-)

For the physical consistency, the particle groups exhibit with inconsistent sizes, diameters, and densities. The user must ensure that the number of melt particles in a single group does not exceeds the filling or packing limit that is feasible in reality. If particle groups are added to the simulation domain, the corresponding volume is deduced from the two-phase flow volume.

Variable	Туре	Description
x	real	center position of a particle group in the x/r -direction (m)
z	real	center position of a particle group in the z-direction (m)
vx	real	velocity in the x/r -direction (m/s)
vz	real	velocity in the z -direction (m/s)
rgx	real	1/2 size of a particle group in the x/r -direction (m)
rgz	real	1/2 size of a particle group in the <i>z</i> -direction (m)
dp	real	uniform diameter of melt particles (m)
tav	real	average temperature of melt particles, initially same value is applied
		for the surface temperature (m)
np	real	number of melt particles in a particle group (-)
tstart	real	start time to put the particle groups in the simulation domain (s)
frequency	integer	total frequency to put the particles groups (-)
tint	real	time interval to put the particle groups (s)

Namelist Options: Common Flags and Parameters (Melt Jet)

This section specifies the common flags and parameters for the melt jet model. The constitutive models and parameters are must be specified in accordance with the following data set.

Variable	Туре	Description
prmj_brkmdl	integer	flag to select the model to determine the jet-breakup length (3)
		0 = Saito/type 1 model
		1 = Saito/type 2 model
		2 = Saito/type 3 model
		3 = Moriyama model
prmi sacvx	real	coefficient to determine the velocity in the x/r -direction of the melt
		particles based on the volume flux of the melt jet C_{vx} (-) (5.0)
		weight coefficient to determine the velocity in the z-direction of the
prmj_sacvzwt	real	melt particles based on the velocity in the z -direction of the melt jet
		or two-phase flow C_{vzwt} (-) (5.0)
nrmi sacent	real	coefficient to determine the mass flux from the volume flux of the
pimj_sacene		melt jet due to the melt particle formation C_{ent} (-) (1.0)
numi condio	real	equivalent or uniform diameter D_e of the melt particles detached
pimj_saedia		from a melt jet (m)
prmj_saedia	real	friction factor for the melt jet C_{frc} (-) (1.0)

The Saito/type 1 model employs the ambient fluid density as the local water density, which is a function of the water level. The Saito type 2 model employs the ambient fluid density in accordance with the cross-section averaged two-phase density, with a cutoff if less than 1/1000 of the melt density. The Saito type 3 model employs the ambient fluid density in accordance with the cross-sectional averaged void fraction α_{av} . If $\alpha_{av} < 0.5$, the density is almost identical to that of water. If $\alpha_{av} < 0.75$, the density is that of the cross-sectional averaged density. If α_{av} is less than 1/1000 of the melt density, the density is considered to be cutoff. The Moriyama model selects either the Taylor type or Saito type models according to Bo_J with the same concept of the ambient fluid density as the Saito type 3 model. The user must examine the D_e parametrically in order to ascertain whether the simulations align with the experiments, including those pertaining to the steam explosion loads: $D_e \sim 2-6$ mm for corium melts, and $D_e \sim 10$ mm for alumina melts.

Namelist options: Common Flags and Parameters (Melt Particle)

This section specifies the common flags and parameters for the melt particle model. The constitutive models and parameters need to be specified in accordance with the following data set.

Variable	Туре	Description
prmpa_mergecrt	real	criteria for relative overlap when merging particle groups (-) (0.2)
prmpa_cdamppar	real	attenuation factor for the velocity when two particle groups collide
		with each other $(-)$ (0.5)
prmpa_cdampwal	real	attenuation factor for the velocity when a particle groups collide with
		a wall (-) (0.1)
prmpa_crnump	integer	criteria for number of the particle groups released into the simulation
		domain; pre-groups to real-groups (-) (10-5000)
prmpa_crhist	integer	criteria for number of the steps released into the simulation domain;
		pre-groups transferred to real-groups (-) (1000)
prmpa_ccfrc	real	factor for the melt particles-fluid friction based on the solid sphere
		correlation (-) (1.0)
prmpa_chtc	real	factor for the melt particles-fluid heat transfer coefficient (also used
		for melt pool-fluid heat transfer coefficient) (-) (1.0)
prmpa_nattrad	real	exponent of function for radiation heat transfer attenuation from melt
		particles due to void formation; small values (< 1) allow radiation to
		persist into higher void fractions (-) (1.0)
prmpa_coxd	real	factor for the oxidation of melt particles; currently NOT implemented
		(-) (1.0)
prmpa_mh2max	real	mass of hydrogen produced per unit mass of melts; currently NOT
		implemented (kg/kg) (2.4×10^{-3})
prmpa_fhtstl	real	attenuation factor for the heat transfer from the particle groups settled
		on the floor (-) (0.1)
prmpa_dminpar	real	minimum particle size that can participate in the secondary breakup
		in the premixing step (m) (1.0×10^{-3})
prmpa_ivxran	integer	flag to control the applications of random factor for velocity in x/r -
		direction at particle group releases (1)
		0 = NO use
		1 = use
prmpa_ibrkcri	integer	flag to control the temperature criteria for the secondary breakup of
		the melt particles (-1)
		$0 = T_{av} > T_{melt}$
		$1 = T_{sf} > T_{sol}$
		$2 = T_{sf} > T_{sol}$ or $T_{av} > T_{liq}$
		-1 = NO secondary breakup

Variable	Туре	Description
prmpa_inotdrp	integer	flag to control the model to lower the surface temperature of the melt
		particles (0)
		0 = NO use
		1 = use
prmpa_imrgtsf	integer	flag to control the temperature criteria for the melt particles-pool
		merging (1)
		$0=T_{av}>T_{melt}$
		$1=T_{sf}>T_{sol}$
prmpa_ihtpack	integer	flag to control the attenuation for the heat transfer from the particle
		groups settled on the floor (1)
		0 = NO use
		1 = use
prmpa_inomerge	integer	flag to disable the merging the particle groups to track particle groups
		profiles (0)
		0 = NO disable
		1 = disable

The symbols T_{av} denotes the average temperature of a single melt particle; T_{sf} denotes the surface temperature of a single melt particle; and T_{melt} denotes the melting point, which is defined as the midpoint between the liquidus T_{liq} and solidus T_{sol} temperatures of the melt.

Namelist options: Common Flags and Parameters (Melt Pool)

This section specifies the common flags and parameters for the melt pool model. The constitutive models (heat transfer, surface temperature and ambient pressure) for the melt pool are selected in accordance with the following data set.

Variable	Туре	Description
prmp_inoht	integer	flag to control the heat transfer from melt pool to two-phase flow (0)
		0 = enable
		1 = disable
prmp_inotdrp	integer	flag to control the surface temperature drop of the melt pool (0)
		0 = enable
		1 = disable
Variable	Туре	Description
--------------	---------	---
prmp_inopamb	integer	flag to control the ambient pressure term induced by two-phase flow
		in the momentum equation for the melt pool for stability (1)
		0 = enable
		1 = disable

Namelist Options: Common Flags and Parameters (Melt Fragment)

This section specifies the common flags and parameters for the melt fragment model. In the explosion step, the melt jet is automatically transformed into the melt particles, while the melt pool is disregarded in terms of the heat transfer due to its smaller surface area compared to the melt jet and melt particles.

Variable	Туре	Description
prmf_ixpl	integer	flag to control the restart mode
		0 = premixing step
		1 = explosion step/type1
		2 = explosion step/type2

If "prmf_ixpl=2", the melt jet is NOT transformed into the melt particles. The simulations restarted after the explosion step starts has commenced, as the melt jet is no longer present within the simulation domain.

Variable	Туре	Description
prmf_ifrgmdl	integer	flag to control the model for the fine fragmentation (0)
		0 = Carachalios (1983) model
		1 = Yuen (1994) model
prmf_cfrg	real	ratio of fine fragments formed from a single premixed melt particle
		during the fine fragmentation process C_{frg} (-) (0.25)
prmf_ifrgcri	integer	flag to control the temperature criteria for the fine fragmentation (0)
		$0=T_{av}>T_{melt}$
		$1=T_{sf}>T_{sol}$
		$2=T_{sf}>T_{sol} \ {\rm or} \ T_{av}>T_{liq}$
nnmf ifnacni	integer	flag control the attenuation factor for the rate of fine fragment mass
brmt_tti.Act.T		due to the void formation $(2)^{*3}$
		0 = interaction with two-phase fluid

Variable	Туре	Description
		$1 =$ interaction with only water, attenuation by $1 - \alpha$
		$2 =$ interaction with only water, cutoff in range $\alpha = 0.30 - 0.75$
prmf_ikevmdl	integer	flag control the model to distribute the heat from fine fragments to evaporation or bulk water heating (0)
		$0 = \text{ constant value or "prmf_ckevfrg"}$
		1 = original model, NOT tested
prmf_ckevfrg	real	heat release partition K_{ev} for the evaporation of coolant water during the fine fragmentation process when "prmf_ikevmdl=0" (-) (0.7)
prmf_cvicfrg	real	constant for the original model, NOT tested (-)
prmf_cqfrg	real	factor of the heat transfer from fine fragments $(-)$ (1.0)
prmf_ttriglife	real	time period or duration during which the premixed melt particles are allowed to undergo the fine fragmentation $t_{triglife}$ (s) (1.0×10 ⁻³)
prmf_ptrig	real	criteria for local triggering in a cell pressure; needs to be higher than the initial pressure and lower than pressure pulse caused by steam explosions (Pa) $(5.0 \times 10^5 - 1.0 \times 10^7)$
prmf_nmtrig	integer	number of times allowed for a particle group can be made into fine fragments by triggering during $t_{triglife}$ (< 5) (1)
prmf_dfrg	real	uniform or equivalent diameter of fine fragments d_{frg} during the fine fragmentation process (m) (5.0×10 ⁻⁵)
prmf_dmminfrg	real	minimum particle diameter that can participate in fine fragmentation; "prmf_dfrg" is used when "prmf_dmminfrg=0" (0)

^{*3}If "prmf_ifrgcri=0", the mean density and velocity of two-phase flow are utilized to ascertain the rate of fine fragment mass \dot{m}_f . If "prmf_ifrgcri=1", the density and velocity of the liquid phase are utilized for the \dot{m}_f , and the attenuation factor $1 - \alpha$ is applied to the \dot{m}_f . If "prmf_ifrgcri=2", the \dot{m}_f is determined in the same manner when "prmf_ifrgcri=1", but no attenuation factor is applied where $\alpha < 0.30$. The \dot{m}_f is determined in the same manner when "prmf_ifrgcri=1", and the attenuation factor $(0.75 - \alpha)/0.45$ is applied to the \dot{m}_f where $0.30 < \alpha < 0.75$. The \dot{m}_f is not determined or out of fine fragmentation where $\alpha > 0.75$.

The default parameters have already been determined based on the simulations. Nevertheless, practical guidance on how to adjust the parameters for the explosion step has been provided for users who require assistance in the parameter adjustments. To modify the peak and width of the pressure pulse (or kinetic energy output), users must adjust "prmf_cfrg" and "prmf_ttriglife." If satisfactory agreement is achieved with respect to the pressure pulse, yet unsatisfactory with respect to the fine fragment mass, it is advisable to modify "prmf_ckevfrg" value. To maintain the pressure pulse size while increasing the fine fragment mass, it is recommended to utilize a larger "prmf_cfrg" and a smaller "prmf_ckevfrg."

F.3 Input Preparation Tips

F.3.1 Input Troubles

If the JASMINE code proves problematic when utilizing the prepared input file, it is recommended that the following points be considered in order to identify and address the issue:

Case1: incorrect order of the input data

The input data is read in the order specified in the input file and subsequently provided to the designated target variables. If the order of the input data is incorrect, the input data will not be provided to the designated target variables, which results in a runtime error.

Case2: Over line limit of the input data

The input data is read to the 132nd character, after which it is ignored or not read. Should the input data be written beyond the specified length, it will not be read and may result in a runtime error or anomalous simulation outcome.

If the user is unable to identify any errors in the input file, it is recommended that the JASMINE code be compiled with the appropriate options to enable debug information. The debug-enabled load module may indicate the location of the error, thereby enabling the user to identify the underlying causes. If the load module is unable to provide meaningful information, it is recommended that a symbolic debugger, such as "gdb," be employed in order to ascertain the actual data read during the input process.

F.3.2 Melt Jet Velocity and Diameter

The inlet condition of the melt jet is specified by the input variables: "prmj_tini", "prmj_vini", and "prmj_dini". The user must specify time-dependent velocity and diameter at the inlet position. It is of the utmost importance to ensure that the velocity and diameter of the subsequent parts of the melt jet do not exceed those of the preceding ones.

A faster-moving component of the melt jet will overtake the preceding component, resulting in an increase in the diameter of the preceding component due to the one-dimensional nature of the melt jet model. The numerical issues can be attributed to the melt jet with an excessively wide diameter. In reality, the preceding component of the melt jet can be penetrated by the subsequent component, resulting in the formation of a heading vortex due to sideways motions. The one-dimensional model is unable to accommodate phenomena of this nature.

To circumvent the numerical issues, the sample input files establish a constant velocity over time or with a declining trend. Alternatively, if a slower initial velocity is deemed necessary for any reason, it is possible to circumvent the numerical issues by employing a small diameter at the corresponding components of the melt jet. The supporting tool "mdischarge" program calculates the time-dependent velocity for gravity-driven poring, which originates from a vessel or funnel. The tool considers the transient liquid melt discharge, whereby the velocity continues to increase until it reaches the steady state velocity due to static heat- or gravity-driven acceleration. Consequently, the initial velocity can be relatively low. It is of utmost importance to exercise caution when utilizing the velocity trends obtained by the "mdischarge" program.

Appendix G Output Files and Contents

The output file contains both for the two-phase flow (ACE3D) and melt simulations. The filename of the output files for the two-phase flow simulations can be specified using the command line options. The filename of the output files for the melt simulations is fixed by default. In addition to the output files, a series of brief messages indicating the progress or status of the simulations or warnings are displayed as standard output (stdout) in the absence of any redirections to a file.

G.1 Two-Phase Flow Simulations (ACE3D)

G.1.1 List Output (output_file)

The "list output" in a plain text format contains the cell variables, error messages, and other pertinent information for the two-phase flow simulations (ACE3D). The format is an $x/r \times z$ table for each cell variable at a specified time step. The contents can be employed for the purpose of quick checking of the simulations. In the header section, the contents of the input file and the cell variables for the simulation geometry (listed in the following table) are displayed in the format of an $x/r \times z$ table for each cell.

Variable	Description
vol	total fluid volume (total cell volume – total melt volume) (m ³)
fa-xr	cross-sectional area of the cell in the x/r -direction (m ²)
fa-yt	cross-sectional area of the cell in the y/θ -direction (m ²)
fa-z	cross-sectional area of the cell in the z-direction (m^2)

In the main section, the contents of the list output can be controlled using the "editop", which is configured using the input file. If "editop=0" is specified, only the primary variables (as listed in the subsequent table) are output in the list output.

Variable	Description
alpstn	steam volume fraction (-)
alpn	void fraction or total volume faction (-)
pn	total pressure (Pa)
tvn	steam temperature (K)
tln	water temperature (K)
rovmix	gas density (kg/m ³)
vvxrn	gas velocity in the x/r -direction (m/s)
vvzn	gas velocity in the z-direction (m/s)
vlxrn	water velocity in the x/r -direction (m/s)
vlzn	water velocity in the z -direction (m/s)
alpgsn#	#-th non-condensable gas volume fraction (-)
tvgsn#	#-th non-condensable gas temperature (K)

If "editop=1" is specified, the additional variables (as listed in the subsequent table) are output in addition to the primary variables.

Variable	Description
rov	steam density (kg/m ³)
rol	water density (kg/m ³)
ev	steam internal energy (J)
el	water internal energy (J)
tsat	saturation temperature (K)
rovgs#	#-th non-condensable density (kg/m ³)
evgs#	#-th non-condensable internal energy (J)

If "editop=2" is specified, the all variables (as listed in the subsequent table) are output in addition to the primary and additional variables.

Variable	Description
cinxr	interface friction coefficient in the x/r -direction [(N/m ³)/(m/s) ²]
cinz	interface friction coefficient in the z-direction $[(N/m^3)/(m/s)^2]$
hig	interface heat transfer coefficient in the gas phase (W/K)
hil	interface heat transfer coefficient in the liquid phase (W/K)
gamm	evaporation rate for the two-phase flow $[kg/(m^3 \cdot sec)]$
tlsub	water subcooling (K)
tvsup	steam superheat (K)
qvbdl	hear input from melt to water (J)
qvbd2	hear input from melt to steam (J)
qvbd3	hear input from melt to evaporation (J)
qvbdg#	heat input from melt to #-th non-condensable gas (J)

It should be noted that a hash symbol (#) denotes the non-condensable gas component $(1 \le \# \le "ngas")$. If "ngas>1" is specified, the variables for the non-condensable gases are output in the list output.

G.1.2 Plot Output (plot_file)

The "plot output" in a binary (unformatted) format contains the primary variables for the two-phase flow simulations (ACE3D). The supporting tools, "readplot" and "mkrsdat" programs, read the data of the plot output in a specified time or step. The contents can be employed for the purposes of plotting figures and restarting simulations. The format of the "plot output" is found in "plotf.f."

G.1.3 History Output (hist_file)

The "history output" in a columnar text format contains the history of the total mass and energy of each component for the two-phase flow (ACE3D), the water level, and the cell variables for cells specified in the input file. One line of the "history output" comprises the variables outputted at each time step. Lines that do not contain the output variables are preceded by a hash symbol (#).

No.	Variable	Description
01	time	time (sec)
02	wat-mass	water mass (kg)
03	vap-mass	steam mass (kg)

No.	Variable	Description
04	nc1-mass	non-condensable gas 1 mass (kg)
05	nc2-mass	non-condensable gas 2 mass (kg)
06	mlt-mass	melt mass (kg)
07	wat-iene	water internal energy (J)
08	vap-iene	steam internal energy (J)
09	nc1-iene	non-condensable gas 1 internal energy (J)
10	nc2-iene	non-condensable gas 2 internal energy (J)
11	wat-enth	water enthalpy (J)
12	vap-enth	steam enthalpy (J)
13	nc1-enth	non-condensable gas 1 enthalpy (J)
14	nc2-enth	non-condensable gas 2 enthalpy (J)
15	mlt-iene	melt internal energy (basis: 300 K)*1 (J)
16	heat-ex	total heat transferred from melt to fluid (J)
17	gamma	total phase change rate (kg/s)
18	fld-kene	fluid kinetic energy (J)
19	fld-ken2	fluid kinetic energy (employed another scheme for v)* ² (J)
20	fld-upmo	fluid upper momentum (N·s)
21	fld-dnmo	fluid downward momentum (N·s)
22	wat-lev	water level averaged in the x/r -direction under the assumption that the water surface exists when the void fraction $\alpha_{lev} = 0.8$ (m)
23	leva0001	water level using "leva" method at specified location or ring (m)
24	levb0001	water level using "levb" method at specified location or ring (m)
25	leva0003	
26	levb0003	(this example outputs water levels at 3 rings $i = 1, 3, and 5$)
27	leva0005	
28	levb0005	
29	pres0101	pressure at a specified location, e.g. $(i,k) = (1,1)$ (Pa)
30	tsps0101	saturation temperature a specified location (K)
31	alst0101	steam volume fraction at specified location (-)

No.	Variable	Description
32	alg10101	non-condensable gas 1 volume fraction at specified location (-)
33	alg20101	non-condensable gas 2 volume fraction at specified location (-)
34	vm/v0101	melt volume fraction at specified location (-)
35	tv0101	steam temperature at specified location (K)
36	tl0101	water temperature at specified location (K)
37	tg10101	non-condensable gas 1 temperature at specified location (K)
38	tg20101	non-condensable gas 2 temperature at specified location (K)
39	vv 0101	steam abs. velocity at specified location (m/s)
40	vl 0101	water abs. velocity at specified location (m/s)
		the data at specified locations is to be continued

It should be noted that the contents of the column following the 25th depend on the number of locations for the output of water levels or cell variables specified in the input file. The values of the output variables, namely, mass and energy, among others, pertaining to the two-phase flow and melt simulations are for a sector of a cylinder with the azimuthal angle given as the size of the first and sole y/θ -direction $\Delta\theta$ specified in the input file. The total quantity for the entire system is calculated by multiplying $2\pi/\Delta\theta$.

G.2 Melt Simulations

G.2.1 Melt Jet List Output (out.j)

The "out.j" in a plain text format contains the cell variables for the melt jet simulations. This information is output at the same time as the "list output" of the two-phase flow simulations. The format is an array of z columns, one for each cell variable, at a specified time step. The contents can be employed for the purposed of plotting figures and quick checking of the simulations.

No.	Variable	Description
01	k	cell index of melt jets in the z-direction (-)
02	zjc	cell center position (m)
03	zjb	cell boundary position (m)
04	flj	mass flux or $A_J \rho_J$ (kg/s)
05	f2j	internal energy flux (J/s)
06	velj	velocity (m/s)

No.	Variable	Description
07	Rj	radius (m)
08	tempj	temperature (k)
09	Rj+bound	boundary layer thickness + radius (m)

G.2.2 Melt Pool List Output (out.p)

The "out.p" in a plain text format contains the cell variables for the melt pool simulations. This information is output at the same time as the "list output" of the two-phase flow simulations. The format is an array of x/r columns, one for each cell variable, at a specified time step. The contents can be employed for the purpose of plotting figures and quick checking of the simulations.

No.	Variable	Description
01	i	cell index of melt pools in the x/r -direction (-)
02	хрс	cell center position (m)
03	xpb	cell boundary position (m)
04	wp	cell width at cell center position (m)
05	wpb	cell width at cell boundary position (m)
06	flp	mass flux or $A_P \rho_P$ (kg/s)
07	f2p	internal energy flux (J/s)
08	velp	velocity (m/s)
09	hp	height (m)
10	tempp	temperature (k)
11	tempsfp	surface temperature (k)

G.2.3 Melt Particle List Output (out.par)

The "out.par" in a plain text format contains the cell variables for the melt particle simulations. This information is output at the same time as the "list output" of the two-phase flow simulations. The format is a particle-group number column for each cell variable at a specified time step. The contents can be employed for the purpose of plotting figures and quick checking of the simulations.

No.	Variable	Description			
01	grpno.	particle group index (-)			
02	хр	center position of the particle group in the x/r -direction (-)			
03	zp	center position of particle group in the z -direction (-)			
04	vx	velocity in the x/r -direction (-)			
05	vz	velocity in the z -direction (-)			
06	rx	half of the particle group size in the x/r -direction (-)			
07	rz	half of the particle group size in the z -direction (-)			
08	massp	mass of a single melt particle in the particle group (kg)			
09	tav	average temperature of the particle group (K)			
10	tsf	surface temperature of a melt particle (K)			
11	enerp	internal energy (J/kg)			
12	nump	number of melt particles in the particle group (-)			
13	diap	particle diameter (m)			
14	foxp	oxidation fraction (NOT implemented at present)			
15	dbnd	thermal boundary layer thickness of a melt particle (m)			
16	qflux	heat flux at a melt particle surface (W/m ²)			
17	iht	index of heat transfer mode of the particle group (-)			
		0 = convection in a liquid phase			
		1 = nucleate boiling			
		2 = transition boiling			
		3 = film boiling			
		4 = convection in a gas phase			

G.2.4 Melt Fragment List Output (out.frg)

The "out.frg" in a plain text format contains the cell variables for the melt fragment simulations. This information is output at the same time as the "list output" of the two-phase flow simulation. The format is a particle-group number for each cell variable at a specified time step. The contents can be employed for the purpose of plotting figures and quick checking of the simulations.

No.	Variable	Description			
01	іра	particle group index (-)			
02	ifrg	fragment group index (-)			
03	istate	index for fragmentation status (-)			
		0 = OUT of fragmentation			
		1 = under fragmentation			
04	ttrig	triggering time for the fragment group (sec)			
05	mass	fragment mass (kg)			
06	dia	fragment diameter (m)			
07	temp	fragment temperature (K)			
08	rho	fragment density (kg/m ³)			
09	ene	fragment internal energy (J)			
10	htrate	heat release rate (W/kg)			
11	htpart	heat released partition contributes to the evaporation (-)			

G.2.5 Melt Dump Output (out.mdp)

The "melt dump output" in a binary (unformatted) format contains the primary variables utilized in the melt simulations. This information is output at the same time as the "plot output" of the two-phase flow simulations. The supporting tool, "mkrsdat," program reads data from the "melt dump output" for a specified time or step. The contents can be employed for the purpose of restarting simulations. The format of the "melt dump output" is found in "meltdump.f."

G.2.6 Melt History Output (out.mlt)

The "melt history output" in a columnar text format contains the total mass, internal energy, and mass fraction of each component for the melt. This information is output at the same time as the "history output" of the two-phase flow simulations. One line of the melt history output comprises the variables outputted at each time step. One line of the " melt history output" comprises the variables outputted at each time step. Lines that do not contain the output variables are preceded by a hash symbol (#).

No.	Variable	Description				
01	step	step (-)				
02	time	time (sec)				
03	massmelt	total melt mass (kg)				
04	enermelt	total melt internal energy (basis: 300 K)*1 (J)				
05	surfmelt	total melt surface area (m ²)				
06	npamax	total number of particle groups (-)				
07	jet	total mass fraction of melt jet (-)				
08	pool	total mass fraction of melt pool (-)				
09	par	total mass fraction of melt particles (-)				
10	volumemtot	total melt volume (m ³)				
11	heatmtot	total heat transfer rate from melt to two-phase flow (W)				
12	focemxtot	total force from melt to fluid in the x/r -direction (N)				
13	focemztot	total force from melt to fluid in the z -direction (N)				
14	zjlead	leading edge position of melt jet (m)				
15	zparlead	leading edge position of particle group in the z -direction (N)				
16	xparlead	leading edge position of particle group in the x/r -direction (N)				
17	hydrgmtot	total hydrogen generation rate (NOT implemented at present)				
18	dmmpar	mass median diameter of melt particles (m)				
19	dmapar	surface equivalent diameter of melt particles (m)				
20	massmms	total mass of melt jet & particles with temperatures				
		$T_{sf} > T_{sol}$ (kg)				
21	tmms	average temperature of melt jet & particles with temperatures T > T (K)				
22	massmma	total mass of melt jet & particles with temperatures				
		$T_{av} > T_{melt}$ (kg)				
23	tmma	average temperature of melt jet & particles with temperatures				
		$T_{av} > T_{melt}$ (K)				
24	masspms	total mass of melt jet & particles with temperatures $T \rightarrow T$ in the premiud variance $(a < 0.75)$ (1)				
25		$I_{sf} > I_{sol}$ in the premixed regions ($\alpha \le 0.75$) (kg)				
25	masspilla	$T_{av} > T_{melt}$ in the premixed regions ($\alpha \le 0.75$) (kg)				

No.	Variable	Description			
26	masspmaj	total mass of melt jet with temperatures			
		$T_{av}>T_{melt}~$ in the premixed regions ($\alpha \leq 0.75$) (kg)			
27	masspmapa	total mass of melt particles with temperatures			
		$T_{av}>T_{melt}~$ in the premixed regions ($\alpha \leq 0.75)$ (kg)			
28	surfpma	total surface area of melt jet & particles with temperatures			
		$T_{av}>T_{melt}~$ in the premixed regions ($\alpha \leq 0.75$) (m²)			
29	surfpmaj	total surface area of melt jet with temperatures			
		$T_{av}>T_{melt}~$ in the premixed regions ($\alpha \leq 0.75)~({\rm m^2})$			
30	surfpmapa	total surface area of melt particles with temperatures			
		$T_{av}>T_{melt}~$ in the premixed regions ($\alpha \leq 0.75)~({\rm m^2})$			
31	enermma	total internal energy of the melt with temperatures (basis: 300 K)* ¹			
		$T_{av} > T_{melt}$ (J)			
32	enerpma	total internal energy of the melt with temperatures (basis: 300 K)* ¹			
		$T_{av}>T_{melt}~~{ m the~premixed~regions}~(lpha\leq 0.75)~~{ m (J)}$			
33	massfrg	total mass of melt fragment (kg)			
34	enerfrg	total internal energy of melt fragment (basis: 300 K)*1 (J)			

The values of the output variables, namely, mass and energy, among others, pertaining to the two-phase flow and melt simulations are for a sector of a cylinder with the azimuthal angle given as the size of the first and sole y/θ -direction $\Delta\theta$ specified in the input file. The total quantity for the entire system is calculated by multiplying $2\pi/\Delta\theta$.

G.2.7 Melt-Two Phase Flow Output (out.m2f)

The "melt-two phase flow output" in a plain text format contains the cell variables for the exchanges between the melt and two-phase flow simulations, including volume, force, and heat. The format is an $x/r \times z$ table for each cell variable at a specified time step. The contents can be employed for the purpose of quick checking of the simulations.

Variable	Description		
volumem/volume_cell	ratio of melt volume to cell volume (-)		
forcem(x)	force from melt to fluid in the x/r -direction (N)		
forcez(z)	force from melt to fluid in the z -direction (N)		
heatm	heat transfer from melt to fluid (W)		

Variable	Description
heatmew	heat transfer contributes to evaporation (W)
temperm	average temperature of melt (K)
hydrgm	hydrogen production mass (NOT implemented at present)
massmf/(massm+massmf)	mass fraction of melt fragment (-)

*¹The base melt temperature is 300 K, which means that the internal energy of the melt at 300 K is equal to zero. The thermal energy at room temperature (300 K) is employed in order to evaluate the ratio of thermal energy to kinetic energy, which is the energy conversion rate of a steam explosion.

*²The "fld-kene" employs the velocity values at the cell center, as estimated by the average of velocity values at adjacent cell boundaries, while the "fld-kene2" employs the velocity values at the cell center, as estimated by the linear interpolated velocity values at adjacent cell boundaries.

Appendix H Practical Program Usages

H.1 Environmental Requirements

The common programming style utilized in the JASMINE code is FORTRAN 77. The supporting tools included in the distribution package is written in either FROTRAN77 or Perl scripts. The graphical presentation is achieved through the utilization of the Gnuplot software. The JASMINE 3.3c and supporting tools have been tested on the Ubuntu 20.04 (native and on WSL2) operating system. The software version is GNU Fortran 9.4.0, Perl 5.30.0, and Gnuplot 5.2.8. It is necessary to ascertain that the hardware is capable of supporting the CPU, RAM, and storage requirements. A system with an Intel Core is CPU, 8GB of RAM, and a 500GB SSD would be a suitable or necessary option.

H.2 Building Program Packages

The distribution package contains the archive files, "jasmine33c.tgz" and "33c-verif.tgz." The archive files are generated on the Linux ex4 file system. It should be noted that the symbolic link may not be preserved if the archive files are extracted in other operating systems, such as Windows. The extraction of the archive files will result in the generation of corresponding directories: "jasmine33c/" and "33c-verif/."

The "jasmine33c.tgz" file contains the source code files and directories. The directory structure for the source code in the "jasmine33c/" directory is as follows:

3d/-+source/	ACE3D sources			
+include/	include files			
+object/	object files			
t/+src/	MELT sources			
sttab/	steam table source			
st/	post processing programs (FORTRAN)			
01/	pre/post processing scripts (Perl)			
1/	binary (executable) files			
s/	manual			
ples/	sample inputs			
	<pre>3d/-+source/ +include/ +object/ .t/+src/ sttab/ st/ ol/ st/ ol/ ss/ ples/</pre>			

The "jasmine33c/" directory contains files and directories as follows: for illustrative purposes, a list of these items is shown below, with the "/" symbol denoting directories and the "\$" symbol denoting the command prompt. The plain text files, designated with the extension ".txt," utilize the Unix line break, represented by the character code LF. The character code for Japanese documents is UTF-8.

\$ ls
ace3d/ CHANGES.txt Makefile mktar README.txt tool/ vimfs
bin/ docs/ melt/ post/ samples/ VERSION wrsttab/

In the "jasmine33c/" directory, the "make" command is employed to compile the load modules. The variable "PROP," which is utilized in the "Makefile" file, specifies the melt material package that is linked to the load modules. The "Makefile" file, located in the "jasmine33c/" directory is responsible for controlling the melt material specification through the value of "PROP." The user can modify the configuration by editing the "Makefile" file to select the value of "PROP" or by providing it on the command line in the following manner:

```
$ make PROP=alumina2
```

The corresponding load modules are created in the "bin" directory: "jasmine.alumina2," "celldatex.alumina2," "pmmass.alumina2," and "triginfo.alumina2." It should be noted that the load module "jasmine.alumina2" executes the JASMINE code utilized in the "alumina2" melt, and the load modules "celldatex.alumina2," "pmmass.alumina2," and "triginfo.alumina2" serve as supporting tools, facilitating extraction and calculation based on the simulations obtained from the JASMINE code or "jasmine.alumina2."

The "Makefile" files for each component (e.g., melt and two-phase flow) are located in the corresponding subdirectories. The following "Makefile" files are employed in the compilation process for each component of the source code.

ace3d/Makefile melt/src/Makefile wrsttab/Makefile post/Makefile post/triginfo/Makefile The header section of the "Makefile" file in the "jasmine33c/" directory enumerates the available melt material package names. The source code for each component of the melt can be found in the "melt/src/" directory, where the file name is "mprop_<name>.F." When the user requires the alteration of the compiler software or compiler options, it is necessary to edit the "Makefile" in order to incorporate the requisite compiler commands and options.

```
# choose melt material by giving PROP macro from the command line like
# make PROP=xxxxx
# available candidates are as follows.
#PROP=corium
                  # corium of FARO/KROTOS (UO2 80:ZrO2 20wt%) (default)
#PROP=corium2
                  # corium with lower melting point (for BWR)
                  # tsol/tmelt/tlig = 2420/2545/2670
#PROP=corium3
                  # corium of TROI-13 (UO2 70:ZrO2 30wt%, near eutectic)
#PROP=alumina
                  # alumina
#PROP=alumina2
                  # alumina properties for SERENA-T3 KROTOS
#PROP=zirconia
                  # zirconia
#PROP=ss304
                  # stainless steel 304L
#PROP=fe
                  # iron tmelt=1810K
#PROP=fe3c
                  # iron with 3% carbon tsol/tmelt/tlig=1427/1498/1568K
                  # ZrO2 49:Al2O3 51wt% tsol/tmelt/tliq=2163/2182/2200K
#PROP=zao
#PROP=zwo
                  # ZrO2 15.7:WO3 84.3wt% eutectic tmelt=1504K
                  # Bi2O3 42.6:WO3 57.4wt% eutectic tmelt=1143K
#PROP=biwo
```

To illustrate, if a load module with debug information and no optimization is desired for source-level debugging, the following command should be entered in the "Makefile" files under the "ace3d", "melt", and "wrsttab" subdirectories for the GNU Fortran compiler.

The "bin" directory contains the load modules, which have been generated from FORTRAN source code or have been created as symbolic links to the Perl scripts in the "tool" directory. In order to for the JASMINE code and supporting tools to be invoked on the user's command line, it is necessary to include the "bin" directory in the user's PATH environment variable. If the user employs the Bash shell, the following addition to the user's home directory's ".bashrc" file will set the PATH variable.

```
export PATH=$PATH:$HOME/jasmine33c/bin
```

It is assumed that the source archive has been extracted in the user's home directory. To delete the object files and load modules, the user can utilize the "make" targets "clean" and "binclean," respectively.

\$ make clean # to erase object files
\$ make binclean # to erase load modules

The "33c-verif.tgz" file contains the verification and validation data, including inputs, outputs, and plots presented in the user's guide (report), with the exception of the steam table. The data set is voluminous, comprising approximately 1.9 GB. The data set for the steam table can be found in the corresponding source directory within the "jasmine33c/" directory.

H.3 Summary of Supporting Tools

The distribution package includes a site of supporting tools for both the pre- and post-processing. The supporting tools are provided in the form of FORTRAN programs and Perl scripts as follows:

Fortran programs

mkrsdat:

The "mkrsdat" program is designed to generate the restart data file, designated as "rs.dat," which is created from one time step of data from the plot output "plot_file" and the melt dump "out.mdp."

readplot:

The "readplot" program is designed to extract the specified data from the "plot_file" in order to plot figures. The "readplot" program is principally invoked via the "mkmcprof" program.

celldatex.PROP:

The "celldatex.PROP" program is designed to extract the specified data from the "plot_file" and "out.mdp" files. The output data is either cell data tables or grid data format for use with Gnuplot.

pmmass.PROP:

The "pmmass.PROP" program is designed to calculate the premixed mass of the melt particles. The calculation can be altered based on the specific melt condition and void fraction criteria.

triginfo.PROP:

The "triginfo.PROP" program is designed to extract the specified data, regarding to the melt particle. from the "plot_file" and "out.mdp" files, which allows to judge the appropriateness for the trigger for steam explosions.

propwr:

The "**propwr**" program invokes the steam table, the WRSTEAMTAB, to calculate the physical properties of the water. The load module is located in the "wrsttab/" directory.

Perl scrips:

initparp:

The "initparp" program calculates the volume fractions of steam "alpgs" and non-condensable gas "alpgs", which are utilized in an input file, based on the two-phase flow equilibrium.

mkjasminp:

The "mkjasminp" program generates the input files for both the premixing and explosion steps from a single prototype input file, which contains all of the requisite information for both steps.

mkmcprof:

The "mkmcprof" program consolidates the specified data extracted from the "plot_file" and "out.mdp" into a single file, and then generates a Gnuplot script to plot figures of the two-dimensional distribution of the melts and water (void fraction).

mktptile:

The "mktptile" program extracts the specified data from the "plot_file" and then generates a Gnuplot script to plot figures of the tile chart of the water (pressure/void fraction).

mktpvect:

The "mktpvect" program extracts the specified data from the "plot_file" and then generates a Gnuplot script to plot figures of the vector chart of the water (velocity).

meshplot:

The "meshplot" program extracts the specified data from the "plot_file" and then generates a Gnuplot script to plot figures of the meshing in the simulation domain.

Following the compilation of the JASMINE code, the load modules are located in the "bin/" directory. The supporting tools are designed to provide their functions when called without any command line options. The "README" files in the "bin/" or "post/" directory provide a concise overview of the functions. The source code files for the supporting tools in Fortran programs or Perl scripts can be found in the "post/" or "tool/" directories.

H.4 Execution Procedures

Prior to the execution of the program, the user is required to prepare a designated work directory, for example, "./work," and then locate the load module (executable) with the work directory.

H.4.1 Normal Mode: Premixing Simulations

For the premixing simulations in the normal mode, the following command and arguments should be specified. The filename of the output files for the two-phase flow simulations can be specified using the command line options. The filename of the output files for the melt simulations is fixed.

\$ jasmine.{PROP} -i input_file -o output_file -p plot_file -h hist_file

The load module is designated as "jasmine. {PROP}," where {PROP} represents the name of the physical property package for melts compiled to address the inflexible handling of physical property packages for melts. Ideally, separate load modules should be prepared for each property package for melts. The specifications of the command line options are delineated as follows:

-i input_file:

In order to read the input file located in the current directory, namely "./work," the argument "-i" and the file name must be specified via the command line options. The input file is essential component of the command and arguments, and therefore cannot be omitted.

-o output_file:

For the "list output" in a text format for the two-phase flow simulations, the argument "-o" and the file name can be specified via the command line options. In the absence of the information, the default path and file name, namely "./work/outlist," will be employed.

-p plot_file:

For the "plot output" in a binary format for the two-phase flow simulations, the argument "-p" and the filename can be specified via the command line options. In the absence of the information, the default path and file name, namely "./work/plotfile," will be employed.

-h hist_file:

For "history output" in a text format for the two-phase flow simulations, the argument "-h" and the file name can be specified via the command line options. In the absence of the information, the default path and file name, namely "./work/histfile," will be employed.

H.4.2 Restart Mode: Premixing Simulations

For the premixing simulations in the restart mode, the following procedures, Step 1. to 5., must be carried out. The restart mode is a valuable and helpful function for effective debugging when a simulation failure occurs. The user can attempt to execute the simulations in the restart mode from a few steps prior to the simulation failure, and with a minimum output data time, in order to identify the reasons for the simulation failure.

Step 1. The preparation of a separated directory for the restart mode simulation

A restart mode simulation generates a new set of output files. If the restart mode simulation is executed within the same directory as the original simulation, the overwrite of specific output files (melt outputs) may result in the loss of data.

Step 2. The same input file copied from the directory of the original simulation

The input file utilized for the original simulation serves also as the input file for the restart mode simulation. Provided that the physical consistency remains unaltered, the input file can be modified. The filename of the input file is designated to be "in" in the following explanations.

Step 3. The preparation of a restart data file (rs.dat)

The post-processing tool "mkrsdat," extracts the data from the "plot_file," and the "out.mdp," both of which are based on the original simulation.

The extracted data is utilized to create the "rs.dat" in a binary (unformatted) format. In order for the data from the original simulation, the filename of the plot output file and the melt dump file are the "pl" and "out.mdp," located in the work directory "../work," to be extracted, the following command, which invoke the "mkrsdat" program, should be specified. In order to extract the data in the specific step, namely "1234," it is necessary to specify the argument "-s."

\$ mkrsdat ../work/pl ../work/out.mdp [-s 1234]

Step 4. The preparation of a restart instruction file (rsi)

A restart instruction file, designated "rsi," is in a text file format and contains the instructions for modifying cell variables to perform a restart mode simulation. It should be noted that the pressure or volume fraction change must be implemented prior to the specification of the saturation temperature in the "rsi," as such information is indispensable for determining the saturation temperature. The format of the "rsi" is described as follows:

```
// restart instruction file: example
11
                                   Description
11
11
                                    // makes comments that is ignored
// restart data file name and path
../work/rs.dat
// modifications (these override the data read from restart datafile)
// named: number of data modification items
g
// time and step (having no cell index)
time 0.
                                 // time given at the start of restart
delt 1d-9
                                 // time step at the start of restart
                                 // flag to reset delt and dvol()
step 1
// if step=0 is specified, delt is automatically reset to min. limit
// before the first two-phase flow evolution calc.
// (after the first melt evolution calc.), and
// also, fluid volume change in cells dvol() is reset to 0.
// delt specification is necessary at the start of explosion calc.
// because premixing calc delt is usually too large.
// time, delt, step (not set to 0) can be left as it is (as in restart data)
// for plain or normal continuation of the calc.
// cell data modification
// available items:
// pn alpstn alpgsn1 alpgsn2 ... tvn tln tvgsn1 tvgsn2 ...
// vvx vvy vvz vlx vly vlz
// name i k value
pn 3 3 2.4e5
                            // variable name, cell index(i, k), value
alpstn 3 3 0.100
// alpgsn# tvgsn#: # is one digit int for gas no.
alpgsn1 3 3 0.100
                           // volume fraction of a non-condensable gas
tvn 3 3 1000.
tln 3 3 s
                            // "s" means the saturation temperature
tvgsn1 3 3 1000.
                            // non-condensable gas 1 temperature
```

Step 5. The execution of the restart mode in the premixing step

Finally, the following command and arguments must be specified. In the restart mode, the restart instruction file, designated "rsi," should be to be specified using the command line options "-r."

f jasmine.{PROP} −i in −o output_file −p pl −h hist_file −r rsi

H.4.3 Restart Mode: Explosion Simulations

The explosion simulations only be executed in the restart mode. In the case of pressure propagation simulations alone, a brief premixing simulation must be executed. If "prmf_ixpl=1" is specified in the input file, the restart mode for the explosion simulation will be initiated. The explosion simulations are different from those of the premixing simulations in the following respects:

Melt jet conversion into melt particles:

For the first time, the melt jet is transformed into the melt particles. In a subsequent restart mode following the first explosion simulation, the transformation is deemed invalid due to absence of a melt jet within the simulation domain. In order to explicitly suppress the transformation, it is necessary to specify "prmf_ixpl=2" in the input file.

No interaction of melt particles:

The processes of heat transfer, breakup, or merging of melt particles are neglected in the explosion simulation. The formation of fine fragments is postulated to be a consequence of the hydrodynamic interaction. The rapid release of heat from the fine fragments exerts a dominant effect on the evaporation and heating up of the surrounding water.

In order to conduct the explosion simulations in the restart mode, it is necessary to implement the following modifications to the input file and the restart instruction file.

Optimal time steps: input file

"ihighil0=2" should be specified in order to suppress the heat transfer between the gases and water at the liquid-gas interface. For the explosion simulations, the heat transfer should be limited only for evaporation of the bulk water. A sufficiently small for "dtminqvbd" value $(1.0 \times 10^{-8} \ll \text{time step})$ should be applied to suppress the convergence failure.

Optimal time steps: input file

The optimal time step and output time step should be specified. It is recommended that 2 μ s be utilized for the maximum time step for the simulations, with 0.1 ms being for the optimal output time step.

External trigger: restart instruction file

A high-pressure bubble is placed in a specific trigger cell as an external trigger in the simulation domain. It is essential to provide the pressure and volume fraction of the non-condensable gas in the trigger cell.

The pV value of the non-condensable (NC) gas utilized for the external trigger should be aligned with the experimental conditions or within an acceptable range. A temperature of approximately 1,000 K is optimal for the NC gas in order to avoid the potential issues due to the temperature decrease by the adiabatic expansion of the NC gas. If the triggering mechanism utilizing the pressurized NC gas is employed in the experiments, the non-condensable gas should be included from the premixing simulation.

H.5 Simulation Procedure Example

This section presents examples of the simulation procedure using the sample input for a PWR ex-vessel steam explosion, which is contained in the "samples/pwrev" directory. The following files are located within the directory.

\$ ls			
in.ev.proto	README.txt	rsi	runjas.sh

in.ev.proto:

The prototype or common input file. The lines for the premixing step are marked with "//!PM" and those for the explosion step are marked with "//!EX."

rsi:

The restart instruction file that contains the instructions to modify the cell variables in order to perform the restart mode simulation for the explosion step.

runjas.sh:

The Bash script file contains the command to initiate the premixing and explosion simulations. The "runjas.sh" file eliminates the need for manual input of commands.

README.txt:

The "README.txt" file also presents the code execution practices or simulation procedure examples using the sample input for a PWR ex-vessel steam explosion described in this section.

In order to initiate the simulations, the user must execute the following command in the "pwrev" directory. This will then cause the "runjas.sh" to execute the following processes:

\$ sh runjas.sh

1. The directories are created for the premixing and explosion simulations, which are labelled "PM" and "EX," respectively. The input files are created within each directory.

- 2. The premixing simulation is initiated in the "PM" directory. The output files resulting from the two-phase flow simulations: "ou," "hi," and "pl," and from the melt simulations: "out.j," "out.p," "out.par," "out.mlt," "out.mdp," and "out.m2f" are created in the "PM" directory.
- 3. The restart data file, designated "rsdat," is created in the "PM" directory ("PM/rsdat").
- 4. The explosion simulation is initiated in the "EX" directory. The output files are analogous to those created in the premixing simulation, though no "out.j" is, and an additional "out.frg" file is created in the "EX" directory.

The command prompt, represented by the symbol "\$," serves as a header for the command lines. The sample commands and outputs displayed on the terminal are as follows: The runtime messages are partially omitted by "...," and descriptive comments are added by "...<

```
_____
$ mkdir PM EX
$ mkjasminp -p in.ev.proto > PM/in.pm
$ mkjasminp -e in.ev.proto > EX/in.ex
$ cd PM
$ jasmine.corium -i in.pm -o ou -p pl -h hi
problem title = Ex-Vessel
present time
               = 0.000000
step number
             = 0
delt
             = 1.0000E - 09
iteration no
               = 0
courant limit = 0.00000E+00
melt dtlim(j) = 1.75316E-03
melt dtlim(p) = 1.00000E-02
melt dtlim(pa) = 1.00000E-02
melt npamax
             = 0
present time
               = 0.1000095
step number
             = 561
. . . .
melt dtlim(p) = 1.00000E-02
melt dtlim(pa) = 1.41171E-03
melt npamax
               = 408
0 *jasmine* job terminated normally.
```

```
... check the plot file output times ...
$ readplot pl
getting geometry data
getting time=
               0.0000000 nstep=
                                    0
getting time= 0.0500095 nstep=
                                   311
getting time= 0.1000095 nstep=
                                   561
. . . .
getting time= 2.9000095 nstep=
                                   14561
getting time= 2.9500095 nstep=
                                   14811
getting time=
               3.0000095 nstep=
                                   15061
... choose time 0.7s and make restart data ...
$ mkrsdat pl out.mdp -t 0.7 -o rsdat
plot file: pl
melt-dump file: out.mdp
output time : 0.700000
output file : rsdat
output file opened... : rsdat
plot file opened...
 getting geometry data
 getting time=
                  0.0000000 step=
                                         0
 getting time=
                  0.0500095 step=
                                       311
 getting time=
                  0.1000095 step=
                                       561
 getting time=
                  0.1500095 step=
                                       811
 getting time=
                  0.2000095 step=
                                      1061
. . . .
 getting time=
                  0.6500095 step=
                                      3311
 getting time=
                  0.7000095 step=
                                      3561
** Output for step
                     3561
melt-dump file closed.
output file closed.
$ cd ../EX
$ jasmine.corium -i in.ex -o ou -p pl -h hi -r ../rsi
** RESTART-MODE ** restart-inst-file= ../rsi
problem title = Ex-Vessel
** data read from restart-inst-file **
```

```
restart-data-file= ../PM/rsdat
*setrestart* particle data geom.
*setrestart* nparprop : 16
*setrestart* niparprop: 3
*setrestart* nfrgprop : 8
** RESTARTING **
 step= 1
 time= 0.00000000
 data modification points: 8
 1:time 0
 2:delt 1e-9
 3:step 1
 4:pn 1 1 10e6
 5:alpgsn1 1 1 0.662
 6:tvgsn1 1 1 1000
 7:alpstn 1 1 1e-4
 8:tvn 1 1 1000
 explosion mode. jet recasted to particles.
 npamax= 632
present time = 0.0000000
step number = 1
    = 1.0000E-09
delt
iteration no = 2
courant limit = 0.00000E+00
melt dtlim(j) = 8.13490E-04
. . .
courant limit = 1.95983E-03
melt dtlim(j) = 8.13490E-04
melt dtlim(p) = 1.00000E-02
melt dtlim(pa)= 1.70654E-05
melt npamax = 632
0 *jasmine* job terminated normally.
$ cd ..
 _____
```

Following the premixing and explosion simulations, the supporting tool "mkmcprof" is available for the rendering of snapshots of the simulations. In order to execute the rendering process for the premixing simulation on the command prompt, the following steps should be taken in the "PM" directory.

```
_____
$ cd PM
$ ls
hi
      log
                  ou
                         out.m2f out.mlt out.par rsdat
in.pm log.mkrsdat out.j out.mdp out.p
                                           pl
$ mkmcprof -i pl -r 2.75 -h 7.00 -a -m -w in.pm -png -np -f 2840
  -t 0.02 0.2 0.5 1.0 2.0 3.0
Making output directory if not exist ...
Doing readplot processes ...
tile format output for scalar data.
cut-off vol. frac.: 1.000E-03
out-dir: mcpf
var-name: alpn
epstime: 0.0200000
getting geometry data
getting time= 0.0000000 nstep=
                                0
getting time= 0.0500095 nstep=
                                311
getting time=
              0.1000095 nstep=
                                561
getting time= 0.1500095 nstep=
                                811
getting time=
               0.2000095 nstep=
                                1061
outfile=mcpf/001
getting time=
               0.2500095 nstep=
                                1311
getting time=
              0.3000095 nstep=
                                1561
. . . .
> time= 2.700010
> time= 2.750009
> time= 2.800009
> time= 2.850010
> time= 2.900009
> time= 2.950010
> time= 3.000009 -> write mcpf/par/005
```

Making a gnuplot script								
Done.	Done.							
Gnuplot :	script is	mcpf/gp						
(execute	it from c	urrent di	r.)					
\$ mcpf/g	\$ mcpf/gp							
gnup	lot window	displays	the graph	nics				
mous	mouse click on the graphic proceeds							
to t	to the next							
\$ ls mcpf								
001	002	003	004	005	gp*	p/	wall	
001.png	002.png	003.png	004.png	005.png	j/	par/		

In the aforementioned example, the snapshots or graphics for times 0.2, 0.5, 1.0, 2.0, and 3.0 sec are drawn on the screen and subsequently saved in PNG files with the following names: The files are "001.png," "002.png," and so on. The snapshots are located in the default output directory, designated as "mcpf." The simulation data for the two-phase flow and melt for the selected time steps are saved in the "mcpf" directory as files bearing the sequence of numbers ("001," "002," and so on).

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