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研究課題名（和文） A Multi-physics Compressible-Incompressible Computational Framework for Mechanistic Simulation of Steam Explosion in Fuel-Coolant Interaction

研究課題名（英文） A Multi-physics Compressible-Incompressible Computational Framework for Mechanistic Simulation of Steam Explosion in Fuel-Coolant Interaction

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研究成果の概要（和文）：本研究では、粒子法による非圧縮-圧縮アルゴリズムに基づく新たな沸騰流解析モデルを提案し、また、数値安定性を高めた自由表面粒子判定法と、高精度粒子法表面張力モデルを開発した。さらに、開発したモデルに基づいて、核燃料-冷却材相互作用での蒸気膨張、液相-気相の相変化、溶融表面凝固、クラストレーションなどの重要なマルチフィジックス現象を再現できる新たな粒子法モデルも開発した。
本研究で開発した粒子法モデルを適用して、初期温度や冷却材/融体粘度や臨界破壊応力の感度解析を行い、メルトフラグメンテーションへの影響を検討した。その結果、メルトフラグメンテーションは初期温度に最も大きく影響されることが示された。

研究成果の学術的意義や社会的意義
The proposed models can significantly improve the theory of particle methods and greatly expand the application range of numerical methods.
The proposed method can help to deepen the understanding of the severe accident progression in nuclear power plants.

研究成果の概要（英文）：A novel vaporization model was proposed for particle methods. A new advanced particle method was developed to simulate the key multi-physical phenomena in fuel-coolant interaction.
Sensitivity analysis demonstrated that initial temperature had the most significant influence on melt fragmentation.

研究分野： Nuclear Engineering

キーワード： Particle method　MPS method　SPH method　Vaporization　Solidification　Multiphase flow

１．研究開始当初の背景

(1) The fuel coolant interaction (FCI) plays an important role in the severe-accident management of nuclear power plants. Nevertheless, a direct numerical method was still missing to simulate the key phenomena including vapor expansion, liquid-vapor phase change, melt surface solidification, and crust fracture in FCI. This project mainly aimed to develop a numerical method to simulate these key phenomena in FCI.

(2) Particle methods have great potential for simulating the complicated multiphase flows in FCI, because the Lagrangian nature can automatically track various interfaces. The multiphase models[1], the solidification model[2], and the crust-fracture model[3,4] have been proposed for particle methods. However, the modeling of vapor expansion and liquid-vapor phase change was still challenging. Meanwhile, it was necessary to couple the multiphase models, the solidification model, the crust-fracture model and the vaporization model into one method to simulate the key phenomena in FCI.

(3) The key issue to develop the above particle method was the lack of an effective vaporization model. The high density ratio and high resolution (particle size) ratio were the key difficulties for conventional particle methods. In this situation, a new conception to model vaporization became necessary.

２．研究の目的

(1) To propose a novel vaporization model for the Lagrangian particle methods.

(2) To develop a new advanced multiphase particle method to capture the key phenomena in FCI.

(3) To numerically investigate the influence of different factors on melt fragmentation in FCI.

３．研究の方法

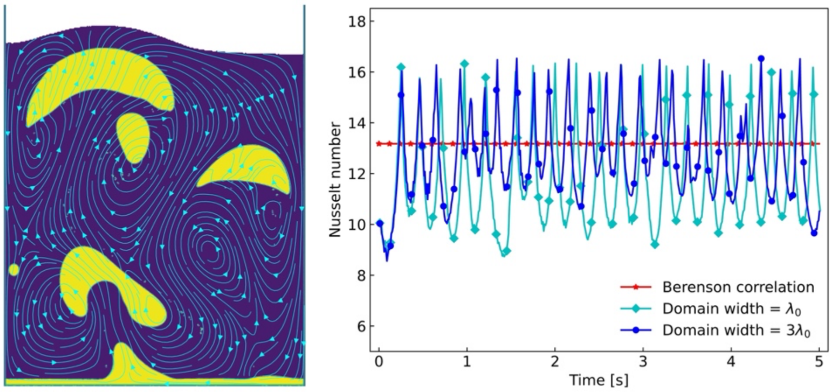
(1) The compressible smoothed particle hydrodynamics (SPH) method and the incompressible moving particle semi-implicit (MPS) method were coupled to propose a novel vaporization model. Various numerical test cases were performed to verify and validate the vaporization model.

(2) The multiphase models, the solidification model, the crust-fracture model, and the new vaporization model were coupled into one particle method to simulate the key phenomena in FCI. All the models were coupled based on a compressible-incompressible algorithm. Each model was verified/validated separately.

(3) The sensitivity analysis of initial temperature, coolant/melt viscosity, and critical fracture stress was performed to investigate their influence on melt fragmentation based on the developed particle method.

４．研究成果

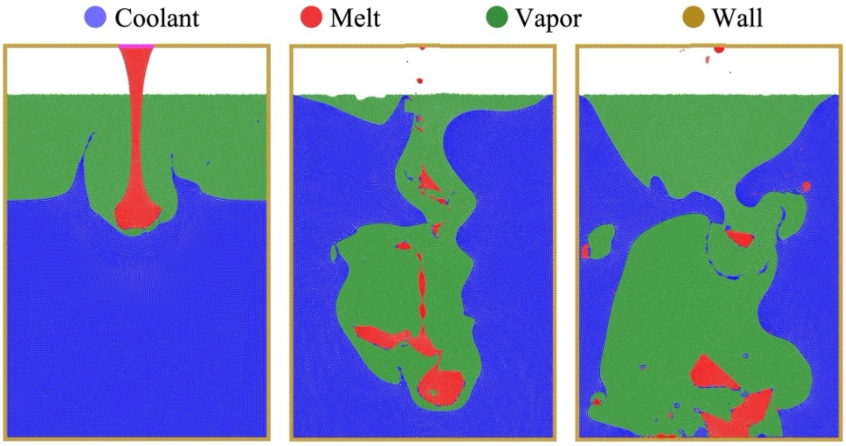
(1) [Committed result] A novel vaporization model for particle methods was proposed. The high density ratio and the high resolution ratio across the interface are the two main challenges for vaporization in particle methods. To overcome these problems in a new perspective, this project proposed a compressible-incompressible approach for the vaporization model. Specifically, the compressible SPH method was adopted to simulate the vapor flow, and the incompressible MPS method was adopted to simulate the melt/coolant flows. In this situation, the liquid particles provided a solid-wall boundary condition for the gas phase, and the gas phase provided a free-surface boundary condition for the liquid phase. Using this technique, a sharp-interface approach for gas-liquid flows was developed. A key problem was the coupling of the surface tension model. When the conventional interface tension model (i.e., CSF) was used, unphysical particle mixing could be easily triggered[5]. To solve this problem, the applicant proposed to employ the free-surface-tension model in the coupling algorithm. Using this technique, the unphysical particle mixing phenomena were avoided. Based on the alternative compressible-incompressible algorithm, the vaporization could be modeled straightforwardly. When an interface particle exhibited a temperature higher than the boiling point, it would insert gas particles at the gas side of the gas-liquid interface. Because (a) the liquid and gas particles were calculated separately and alternatively and (b) the SPH method for the gas phase could automatically regulate particle distributions, the coupling algorithm was stable. The multiphase method for gas-liquid flows were first verified by various bubble-rising simulations. Then, the vaporization model was verified by the classic Stefan and sucking boiling problems. Last, the vaporization model was validated by the horizontal film boiling problem (Fig. 1). The fragmentation and coalescences of interfaces as well as the fast volume increase of the vapor phase were captured reliably by the proposed method. The predicted Nusselt number in the simulations agreed well the experimental Berenson correlation[6], as shown in Fig. 1 (b).



(a) Qualitative result (b) Quantitative result

Fig. 1 The simulated results of film boiling problem by the proposed vaporization model.

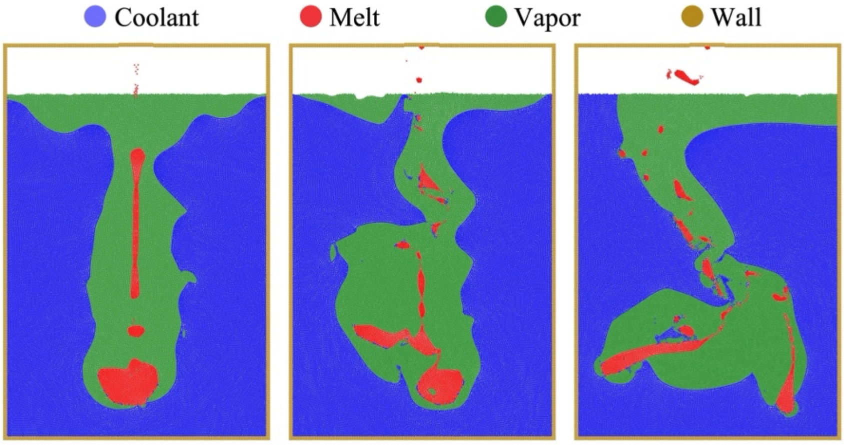
(2) [Committed result] An advanced particle method to simulate the key phenomena in FCI was developed. The multiphase models, the solidification model, the vaporization model, and the crust-fracture model were combined into one particle method to simulate the key phenomena in FCI. Before the coupling, each model had been verified and validated separately. In the developed particle method, three phases, the gas/vapor, coolant, and melt phases, were considered. The coupling processes in one time step were as follows. ① The gas phase was simulated by the compressible SPH method. Due to the alternative algorithm, the gas simulation was independent from other phases. ② The heat transfer among all the phases were calculated. ③ The viscosity of the liquid phase was updated based on temperature. The solid-liquid phase change was modeled by abruptly changing the viscosity. Due to the advanced time-integral algorithm for highly viscous fluids[2], the numerical creeping problem could be effectively avoided, and the crust fracture could be considered by the strain rate. ④ The pressure Poisson equation and the pressure gradient force of the melt and coolant phases were calculated semi-implicitly using the MPS multiphase models. ⑤ The viscosity diffusion of the melt and coolant phases were computed using an implicit algorithm for viscosity. Because the viscosity terms were calculated after the pressure terms, the numerical creeping of the solidified crust were effectively prevented[2]. ⑥ The particle shifting method was employed for the melt and coolant phases to regulate the particle distributions and maintain simulation stability. ⑦ The crust-fracture model was implemented. Specifically, when the historical mean stress of viscosity was higher than the critical fracture stress, the local crust inside the interaction radius would be remelted to simulate the fracture[3,4]. ⑧ The vaporization model was considered. Specifically, when the temperature of an interface liquid particle was higher than the boiling point, this particle would generate gas particles based on the difference between its temperature and its boiling point. In this manner, the multiphase models (Step ④ and ⑤), the solidification model (Step ③ and ⑤), the crust-fracture model (Step ⑦), and the vaporization model (Step ⑧), were all considered in one advanced particle method. The simulated results of pouring melt into coolant at three typical moments were presented in Fig. 2. The main phenomena in FCI, vapor expansion, liquid-vapor phase change, melt solidification (by increasing viscosity), and melt fragmentation, were captured. Due to the violent vaporization, the gas-liquid interfaces were rather unstable. The top free surface was regarded as an outlet boundary condition for the gas and coolant phases considering the gas expansion.



(a) Time = 0.1 s (b) Time = 0.2 s (c) Time = 0.3 s

Fig. 2 Simulated snapshots of pouring melt into coolant using the developed particle method.

(3) [Committed result] The sensitivity analysis of various factors on melt fragmentation was performed. Based on the developed advanced particle method, the influence of the initial temperature, the melt/coolant viscosity, and the crust fracture model on melt fragmentation was investigated. The typical results of sensitivity analysis under different conditions were shown in Fig. 3. First, the effect of initial temperature of melt was discussed. The boiling point of coolant was 373.15 K, and the solidification temperature of melt was assumed as 800 K. The melt and coolant exhibited a conductivity of 300 W/m/K and a specific heat capacity of 400 J/kg/K. When the melt had an initial temperature of 820 K, the melt fragmentation was minor, as shown in Fig. 3 (a). When the initial temperature was increased to 1000 K, the melt fragmentation was obvious, as shown in Fig. 3 (b). Therefore, the melt fragmentation became more violent with the increase of the initial temperature of melt. Second, the influence of melt/coolant viscosity was investigated. When the melt or coolant viscosity was increased by 10, 100, and 1000 times, it was observed that the melt fragmentation behaviors did not change essentially, considering the random fragmentation caused by the violent vaporization. Particularly, as shown in Fig. 3 (c), even when the melt and coolant viscosities were simultaneously increased by 1000 times, the fragmentation pattern was not changed essentially. Thus, the melt/coolant viscosity did not significantly affect the melt fragmentation under the current conditions. Third, the influence of the crust fracture model was discussed. The performed simulations demonstrated that the melt fragmentation patterns did not vary essentially no matter the crust fracture model was enabled or disabled. The reason was as follows. Because the employed resolution was not fine enough, the solidified melt surface was discontinuous in the performed simulations. Therefore, the melt mainly broke up just from the discontinuous unsolidified surface of melt. That is to say, the sufficiently fine resolution must be employed to capture the thin and continuous solidification at the melt surface, and then the influence of critical fracture stress on melt fragmentation could be discussed reliably. Considering that the parallelization of the present asynchronous algorithm is out of the scope of this project, the specific quantitative discussion on the effect of crust fracture will be further investigated in future after an efficient parallel framework can be developed for the present particle method.



(a) Case 1:
$T_{init} = 820$ K
$\mu_{coolant} = 0.001$ Pa·s
$\mu_{melt} = 0.005$ Pa·s

(b) Case 2:
$T_{init} = 1000$ K
$\mu_{coolant} = 0.001$ Pa·s
$\mu_{melt} = 0.005$ Pa·s

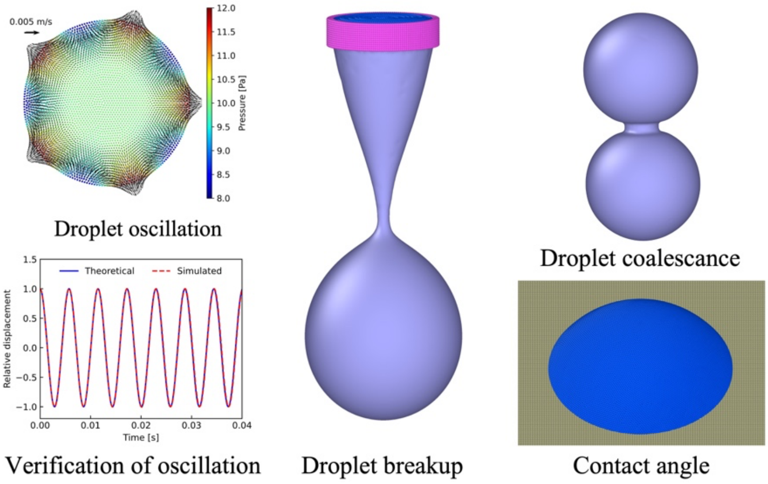
(c) Case 3:
$T_{init} = 1000$ K
$\mu_{coolant} = 1.0$ Pa·s
$\mu_{melt} = 5.0$ Pa·s

Fig. 3 The snapshots of melt fragmentation at time = 0.2 s simulated under different conditions.

(4) [Related result] Stable novel free-surface detection conditions for the high-order particle methods were proposed. In the present asynchronous compressible-incompressible algorithm, a free-surface particle method must be employed to simulate the liquid phases. Therefore, a high-order free-surface particle method can greatly improve the accuracy of the developed particle method above. However, when the high-order schemes were adopted, the instability at free surfaces was the key bottle-neck problem. Based on a theoretical error accumulation analysis, the instability at free surface was attributed to a positive feedback loop of biased errors. The accumulation rate of the biased errors could be estimated from the employed high-order schemes. Based on this error analysis, novel free-surface detection conditions were proposed. It is demonstrated that the proposed conditions could effectively enhance the stability of the high-order schemes. In this manner, a general, stable, and accurate free-surface particle method based on the consistent high-order schemes was proposed for the first time.

(5) [Related result] A new high-order free-surface-tension model was proposed for particle method. In the present alternative compressible-incompressible algorithm, the free-surface-tension model must be employed, because the conventional interface-tension model (CSF model) can trigger unphysical particle

mixing[5]. The following three improvements were made. First, the free-surface-tension force was converted to a pressure boundary condition. In this situation, the high-order schemes must be adopted to ensure that the pressure boundary condition was precisely imposed. Second, a new surface-normal particle shifting method was proposed for the free-surface particles based on the reconstructed free surfaces using curve fitting. Third, a new contact angle model was developed by inserting an imaginary particle at the intersection point of free-surface and wall boundaries. With the three improvements, a new high-order free-surface-tension model was proposed. The simulated results of different test cases using the developed models were presented in Fig. 4, where the droplet simulations using the free-surface particle method were greatly enhanced.



Droplet oscillation

Droplet coalescance

Verification of oscillation Droplet breakup Contact angle

Fig. 4 Different droplet simulations using the high-order free-surface-tension model.

(6) [Future work] A high-efficient parallelization framework for the developed particle method is the future work. Due to the asynchronous calculation of the compressible gas phase and the incompressible liquid phases, the parallelization of the present method is challenging. Parallelization is necessary to capture the multi-scale fragmentation phenomena in FCI, which can enable quantitative sensitivity analysis of more factors on the melt fragmentation.

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５．主な発表論文等

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掲載論文のDOI（デジタルオブジェクト識別子） 10.1002/fld.4878	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 －

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３．雑誌名 Computer Methods in Applied Mechanics and Engineering	６．最初と最後の頁 113425～113464
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2022年

〔図書〕　計0件

〔産業財産権〕

〔その他〕

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６．研究組織

	氏名 （ローマ字氏名） （研究者番号）	所属研究機関・部局・職 （機関番号）	備考

７．科研費を使用して開催した国際研究集会

〔国際研究集会〕　計0件

８．本研究に関連して実施した国際共同研究の実施状況

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