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Investigation of droplet behaviors for spray cooling using level set method

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ABSTRACT

The droplet dynamics and heat removal is one of the popular research streams in spray cooling applications. The increase in the water droplet temperature as a result of its impact on the hot solid surface would determine the efficiency of the heat removal that is crucial in some sensitive applications such as spray cooling in depressurization systems in commercial nuclear power plants. Computer modelling of the underlying mechanism of the liquid droplet interaction with the hot solid surface would be necessary. The accuracy and the reliability of these models are important in simulating the multiphysics phenomena such as droplet dynamics and heat removal. In present work, the level set method coupled with heat transfer was used to simulate the water droplet impact on an isothermal solid surface. The changes in the temperature of water droplet were found to be highly dependent upon its size and the impingement speed. Topological variations in the droplet shape as a result of its impact onto the solid wall would cause abrupt changes in the temperature of the water droplet. In addition, the droplet detachment, coalescence and flattening were found to strongly influence the temperature of the droplet which would evidently affect the heat removal efficiency in the spray cooling systems employed in the commercial nuclear power plants. Furthermore, we demonstrated that the level set method had the ability to produce more accurate estimations of the water droplet dynamics when compared to the Volume-Of-Fluid (VOF) method in simulating the droplet behavior.

1. Introduction

In recent years of advanced improvements in the capability of computers, many physical phenomena can be modelled precisely using computer simulations. In many cases where experimental measurements might be tedious or impossible, there will be a complete reliance on computer simulations. Therefore, the completeness, accuracy and reliability of the models being used in such sensitive areas are vital to the society and the environment. The current powerful computer resources need to be fully exploited, so that precision and accuracy of obtained computational results would be further enhanced. The Computational Fluid Dynamics (CFD) technique is widely used in simulating fluid behavior such as single and multiphase flow in both laminar and turbulent regimes (Norton and Sun, 2006). This technique tends to be computationally expensive and requires relatively large amount of computer resources for large and complex systems. However, considering the powerful computing power available in recent years, simulation of complex fluid behavior has become more convenient.

The investigation of fluid dynamics and heat transfer parameters such as temperature and speed are useful when the heat removal efficiency of spray cooling systems needs to be determined. The importance of the droplet dynamics is mainly due to the many industrial applications, including spray cooling (Jia and Qiu, 2003; Hsieh and Luo, 2016), ink-jet printing (Van Dam and Le Clerc, 2004) and anti-icing (Meuler et al., 2011; Mishchenko et al., 2010). The first method used to simulate the droplet impact on a solid surface was developed by Harlow and Shannon (Harlow and Shannon, 1967) who used the "marker-and-cell" (MAC) finite difference method. The viscosity and the surface tension were neglected in the initial model of MAC to simplify the problem. Tsurutani et al. (1990) introduced the enhanced MAC method that included the surface tension and viscosity, and also heat transfer when considering the spread of a cold liquid droplet on a hot surface.

The Lagrangian formulation was used by Zhao et al. (1996) in order to model the cooling of a liquid microdroplet. The influence

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of liquid properties and interfacial heat transfer during micro-droplet deposition on a glass substrate was studied numerically by Bhardwaj et al. (2007), where the droplet diameter and impact velocity were fixed to be 80 μm and 5 ms^{-1}, respectively. The complexity of the associated transport phenomena was also highlighted (Bhardwaj et al., 2007). On the other hand, the spray cooling system or more fundamentally, the heat removal by the water droplet is an important aspect of nuclear thermal hydraulics which is also necessary to achieve an effective post-LOCA cooling and in many other engineering applications. Li et al. (2011) studied the impact force caused by liquid droplet impingement onto a rigid wall, and showed that the evolution was dominated by the compressibility of the liquid medium. In recent years, the Volume-Of-Fluid (VOF) method has been widely used due to the enhanced computational capacities. Recently, there were excellent and leading studies published in the *Annals of Nuclear Energy* regarding the use of VOF method in numerical simulation of melt interaction with water (Thakre and Ma, 2015; Thakre et al., 2013; Thakre et al., 2015; Gu et al., 2015; Lin et al., 2014), which presented a promising use of the VOF method in simulating complex multiphase systems. In addition to the VOF method, the level set method was devised by Osher and Sethian (Osher and Sethian, 1988), which was developed for interface tracking in two or three dimensions. Moreover, the level set method was used in a variety of applications such as shape recognition (Kimmel et al., 1996), crystal growth, dendrite solidification (Sethain and Strain, 1992), propagation of cold plasma in cell buffer medium (Shahmohammadi Beni and Yu, 2015), cold plasma mixing with blood (Shahmohammadi Beni and Yu, 2017) and two fluid problems (Mulder et al., 1992; Olsson and Kreiss, 2005; Lan et al., 2014; Nagrath et al., 2006; Sussman et al., 1994). Sussman et al. (1999) developed an adaptive level set method for application of incompressible two-phase flow, which was used to simulate the air bubble and water drop in both two-dimensional axisymmetric and fully three-dimensional geometries. A number of methodologies were proposed to improve the initially developed level set method, with the ultimate goal of precisely simulating two-phase flow problems (Peng et al., 1999; Enright et al., 2002; Sussman et al., 1998). The readers are referred to Osher and Fedkiw (2001) and references therein for more details regarding the overview of the level set method. As regards the application of level set method in spray cooling Selvam et al. (2006) used a simplified two-dimensional model to study the effect of gravity on heat transfer of spray cooling with the main focus on the phase change, in which the interface between the liquid and the vapor was tracked by the level set method. In addition, the computer modelling of spray cooling problems and the methods used to solve multiphase flow problems were reviewed (Selvam et al., 2005).

In the present work, a complete three-dimensional multiphysics model was built using the Finite Element Method (FEM) to track the droplet movement, impact and rebounce from the solid surface during its impact period, using the level set interface tracking method coupled with heat transfer. The two phases involved in the present work were water and air; this enabled us to perform a sensitivity study on different radii and initial speeds of the water droplet. Due to complexities in the present multiphysics model, the solid surface temperature was assumed to be below the boiling temperature of water. The present work also demonstrated that the level set method provided a better estimation of the experimental results regarding droplet dynamics when compared to the VOF method. The present level set model was found to be promising in the simulation of droplet dynamics and it could be a useful tool for future development and optimization of spray cooling systems in commercial nuclear power plants with special attention to high accuracy and reliability modelling.

2. Materials and methods

The level set method was used to capture the evolution of a water droplet in air as it moved down with the prescribed initial speed under gravity. In this model, the water droplet was initially placed at a specific distance (1.5 cm) from the upper surface of the solid interface, which enabled the interface initialization and further analysis of the ambient air effect on the fluid dynamics and heat transfer of the moving water droplet. The continuous tracking of the water droplet interface with respect to simulation time led to time-dependent scoring of the fluid dynamics and heat transfer parameters which were important for the precise determination of heat removal efficiency.

2.1. Geometry and computation scheme

In order to perform sensitivity studies using the present model, we chose three different radii for water droplets placed in a fixed air column. The summary of the geometries and dimensions of the domains involved in present work are shown in Table 1.

The initial speeds of the water droplets were assumed to be 0.5 and 1.0 ms^{-1} in the downward (-*z*) direction. The overall simulation time of 1 s was employed so that the heat transfer and fluid dynamics parameters could be obtained before, during and after the impact onto the hot solid plate, which had a fixed temperature of 70 °C (i.e., below the boiling temperature of water). The system setup is schematically shown in Fig. 1. The distance between the center of the water droplet and the solid surface was fixed at 1.5 cm for all cases studied in the present paper.

2.2. Level set method coupled with heat transfer

Information on the implementation of the level set method including the major equations in the current multiphysics model will be shown here. The simplified level set variable ϕ defined for a domain denoted by ψ is

$$\phi = \phi(r,t), \ \ r \in \psi \tag{1}$$

where t is the time. Eq. (1) can be converted to an evolution function that describes the moving interface, which in the present case is located between the water droplet and the surrounding ambient air. This evolution function is

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = 0 \tag{2}$$

where u is the velocity. The standard level set function which contains the level set variable ϕ would take different signs at different sides of the interface. Considering a two-phase fluid system consisting of α and β phases, ϕ would be zero at the interface and takes positive or negative values in each domain with different phases, which is controlled by the Heaviside function:

$$\zeta(x) = sign[\phi(x)] = \begin{cases} -1 : \phi < 0 \\ \ \ 0 : \phi = 0 \\ +1 : \phi > 0 \end{cases} \tag{3}$$

The level set function would detect the transition between the two phases using the Heaviside function. However, the abrupt changes between the two phases arising from the sign function

Table 1
Summary of geometries and dimensions for the air column and water droplets.

Domain	Geometry	Dimensions
Air column	Rectangle	$1 \times 1 \times 2$ cm^3
Water droplet	Sphere	radius = 0.1, 0.2, 0.4 cm

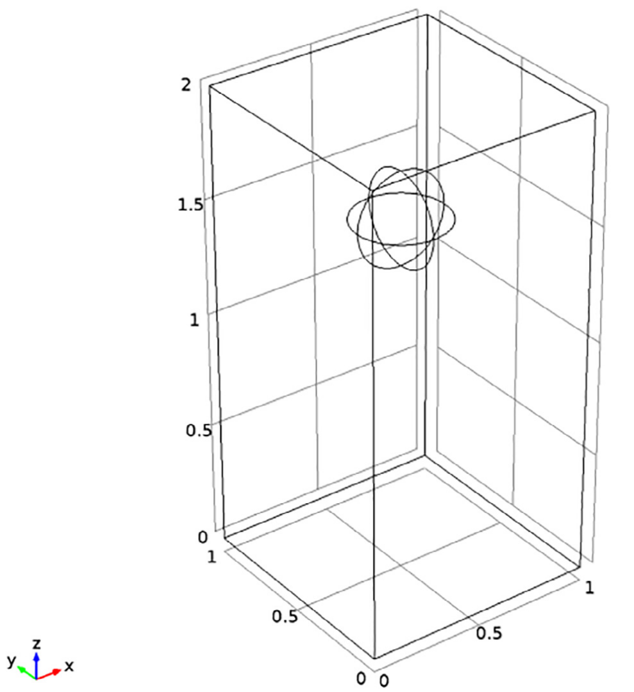

Fig. 1. Schematic diagram showing the initial system setup with dimensions. (Numbers are in the unit of cm.)

will lead to numerical instabilities. To reduce the instabilities in the numerical computations especially when the shape of the water droplet significantly changed as a result of its impact upon the solid surface, the smeared-out Heaviside function was used in the present model:

$$H_s = \begin{cases} 0 & \phi < \epsilon \\ \frac{1}{2} + \frac{\phi}{2} + \frac{1}{2\pi}\sin\left(\frac{\pi\phi}{\epsilon}\right) & -\epsilon \leqslant \phi \leqslant \epsilon \\ 1 & \phi > \epsilon \end{cases} \quad (4)$$

where ϵ was the mesh-dependent half thickness of the interface between the moving fluids. The final level set function used in present work was described as

$$\frac{\partial\phi}{\partial t} + u.\nabla\phi = \gamma\nabla\cdot\left(\varepsilon\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right) \quad (5)$$

In Eq. (5), ε was the thickness of the region where the level set function varied mainly from 0 to 1 using the smeared-out Heaviside function. The term γ was introduced for better numerical stability by reducing the oscillations in the level set function and at the same time keeping the interface thickness constant. The Navier-Stokes momentum and continuity equations were also used in the present work:

$$\rho\frac{\partial u}{\partial t} + \rho(u\cdot\nabla)u = \nabla\cdot[-pI + \mu(\nabla u + (\nabla u)^T] + F \quad (6)$$

$$\frac{\partial p}{\partial t} + \nabla\cdot(\rho u) = 0 \quad (7)$$

where ρ was the density, P was the pressure, u was the velocity and F was the total force acting on the components in the system. Moreover, F could be mathematically represented as $F = \rho g + F_{st} + F_{vf}$ where ρg is the body force, while F_{st} and F_{vf} represented the surface tension and volume force, respectively. Lastly, the heat transfer between the fluids was simulated using the heat equation:

$$\rho C_p\frac{\partial T}{\partial t} + \rho C_p u\cdot\nabla T = -\nabla\cdot(-k\nabla T) + Q \quad (8)$$

where T was the temperature of the system, C_p was the heat capacity at constant pressure and k was the thermal conductivity. The boundary conditions around the simulation box were assumed to be no-slip with thermal insulation and the solid surface located at the bottom of the simulation box was assumed to have a constant temperature of 70 °C throughout the simulation. The present model was implemented in the COMSOL MULTIPHYSICS commercial software and linear discretization was employed to solve the system numerically using the multigrid iterative solver.

3. Results and discussion

3.1. Experimental benchmarking

The experimental results and numerical results (obtained using the VOF method) from Gunjal et al. (2005) were used to compare

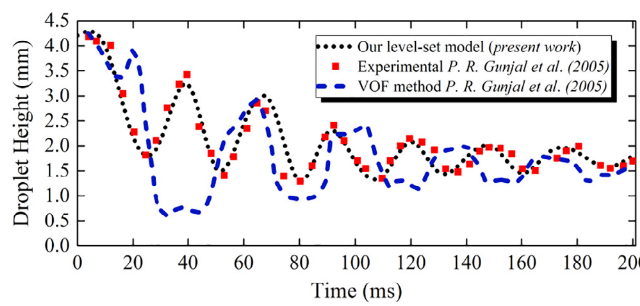

Fig. 2. The water droplet height versus time obtained in experiments and obtained using the VOF method (Gunjal et al., 2005), and obtained using the level set method.

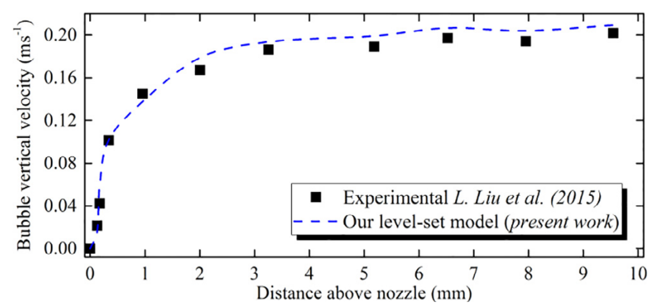

Fig. 3. The vertical velocity component of air bubble obtained experimentally (squares) (Liu et al., 2015) and from the present model (dashed line).

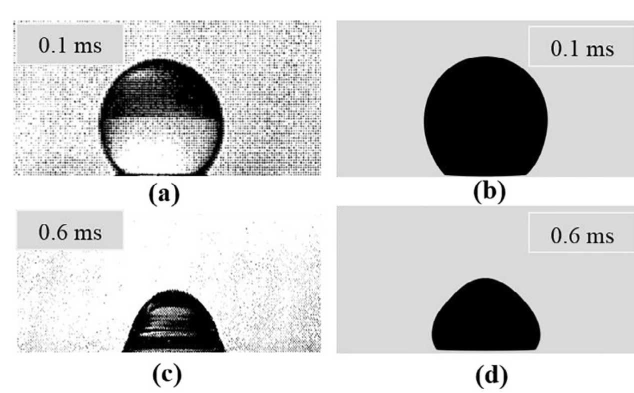

Fig. 4. The shape of the heptane drop upon impact on a stainless steel surface at 24 °C at 0.1 ms from (a) experiment (Chandra and Avedisian, 1991) and (b) the present model; and at 0.6 ms from (c) experiment (Chandra and Avedisian, 1991) and (d) the present model.

with the present results obtained using the level set method. A setup similar to that used by Gunjal et al. was used, with the droplet diameter of 4.20 mm, the initial speed of 0.22 ms^{-1} and the contact angle of 50° (Gunjal et al., 2005). The comparisons of the water-droplet height with respect to the simulation time are shown in Fig. 2.

For the present benchmarking case, the present model showed a better agreement compared to the VOF method with the experimental results. The droplet height was an important variable to be benchmarked since the heat transfer efficiency of the water droplet significantly depended on its shape mainly due to the definition of heat flux (q''). The experimental results from the work of Liu et al. (2015) were used to perform another benchmarking, which involved a 2.77 mm air bubble released under a water column. The vertical velocities of the bubble at different heights above the nozzle were determined, and the comparisons are shown in Fig. 3. Yet another comparison was made between the present model and the experimentally obtained images from the work of Chandra and Avedisian (1991) regarding a 1.5 mm diameter heptane drop impacting on a stainless steel at 24 °C as shown in Fig. 4.

The results from the present level set model were in good agreement with the experimental results (see Fig. 3). For the ease of comparison, Fig. 4(a)–(d) have the same aspect ratio and scale. The shapes of the heptane droplet from the present model were also in good agreement with the experimentally obtained images.

3.2. Grid sensitivity analysis

For all simulated cases in this paper, numerical convergence was verified through simulations with different grid resolutions,

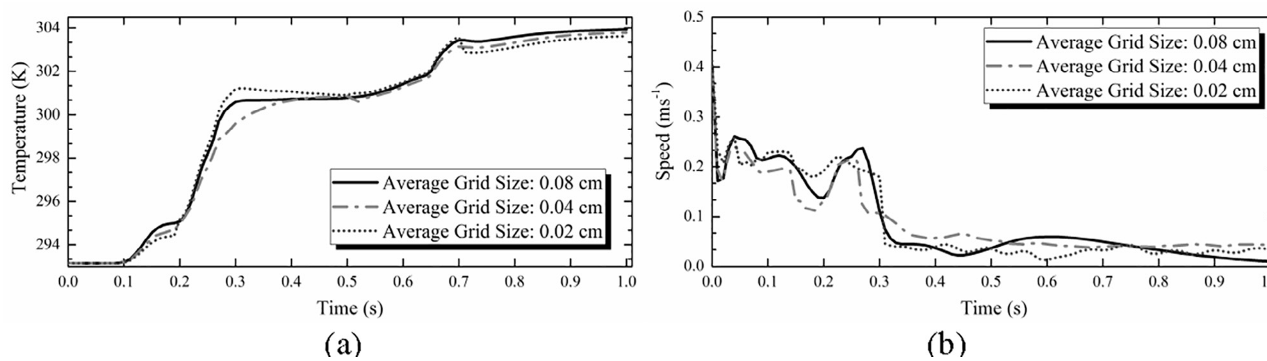

Fig. 5. Grid sensitivity analysis for (a) temperature and (b) speed for a droplet with a 0.2 cm radius and an initial speed of 0.5 ms^{-1}.

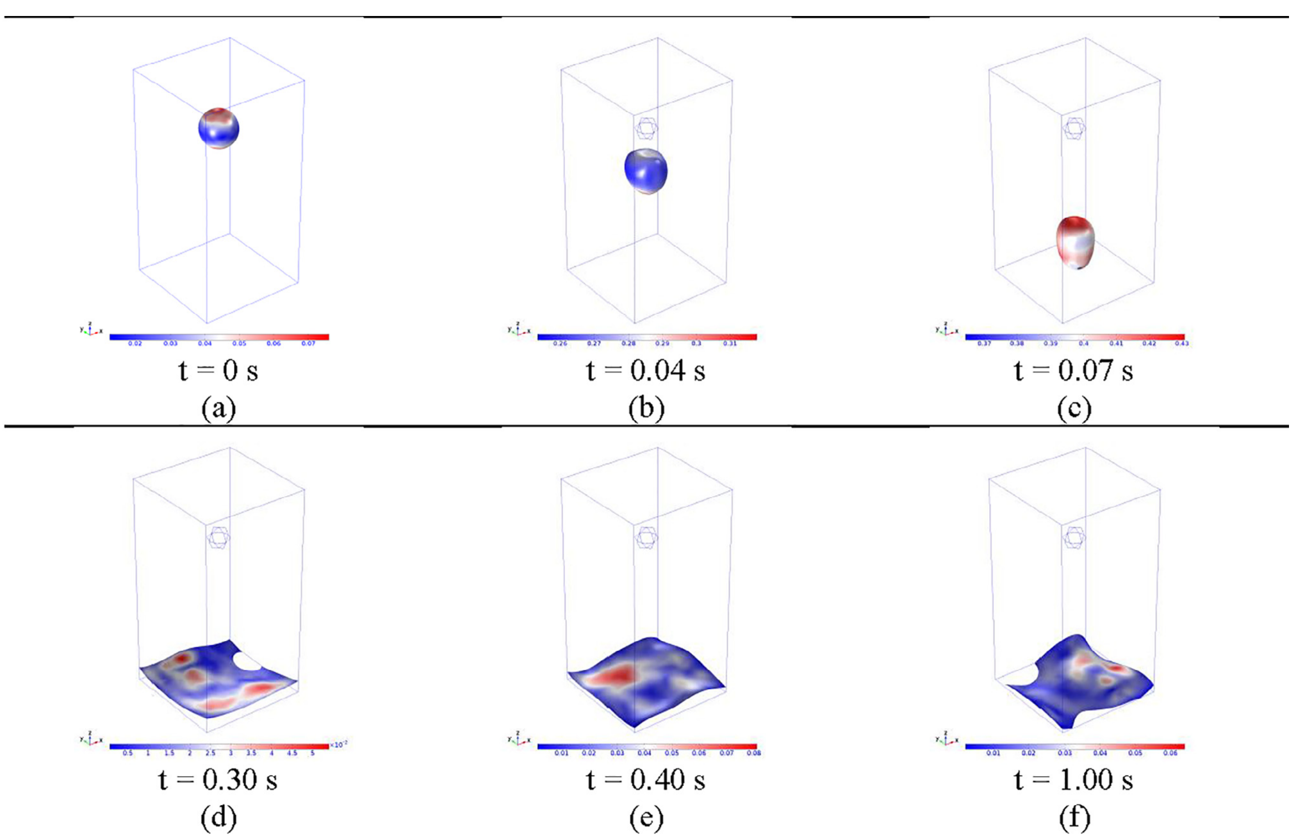

Fig. 6. Shape of the water droplet with 0.1 cm radius and initial speed of 0.5 ms^{-1} at (a) 0 s, (b) 0.04 s, (c) 0.07 s, (d) 0.30 s, (e) 0.40 s and (f) 1.00 s. Different colors correspond to different speeds (in ms^{-1}) as shown in the color bar. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

and no significant discrepancies were observed for the convergence and the final results. To perform a feasible grid sensitivity analysis for the temperature and speed of the droplet, a droplet with a 0.2 cm radius and an initial speed of 0.5 ms^{-1} was chosen. Three different average grid sizes of 0.08, 0.04 and 0.02 cm were analyzed. Variations in the obtained results as shown in Fig. 5 were not significant, so the grid or mesh convergence of the present model was ensured.

The results on grid sensitivities in Fig. 5(a) and (b) showed some variations, which were likely due to the iterative method (i.e., multigrid iterative solver) used to solve the present numerical problem, and which were unavoidable.

3.3. Graphical representation

In order to facilitate visualization of the results, snapshots from selected cases are shown in the Figs. 6(a)–(f) up to 9(a) and (b). Different colors correspond to different speeds (in ms^{-1}) as shown in the color bar in the figures.

3.4. Fluid dynamics and heat transfer results

The fluid dynamics and heat transfer results for the droplet were obtained for the impact time period of 1 s, and the results were averages over the water droplet domain or the air domain. The time-dependent analysis was required for the water droplet impacting on the hot solid surface. The variations in the droplet temperature averaged over its domain are shown in Fig. 10 (a) and (b) for 0.5 and 1.0 ms^{-1}, respectively. Three different droplet radii were studied to investigate the effect of droplet size on the amount of heat extracted from the isothermal solid surface.

The temperature of the water droplet was highly dependent upon its shape and the speed, so their variations would cause abrupt changes in the temperature of the water droplet when it approaches, impacts on and rebounces from the solid surface.

The water droplet with a radius of 0.1 cm reached a higher temperature compared to the larger droplets (with radii of 0.2 and 0.4 cm). For the water droplet with a radius of 0.1 cm, the temperature was higher for the water droplet with a larger initial speed of 1.0 ms^{-1}. For the droplets with radii larger than 0.1 cm, their initial speeds did not affect the maximum temperature, but changed the pattern of temperature increase. For example, an abrupt increase in the droplet temperature was observed at ~0.2 s only for the initial speed of 0.5 ms^{-1}. The differences among droplets with different sizes were mainly due to their different spreading on the solid surface, which significantly affects the droplet temperature due to the different heat transfer efficiencies. In the present work, the system was confined in the x and y directions by no-

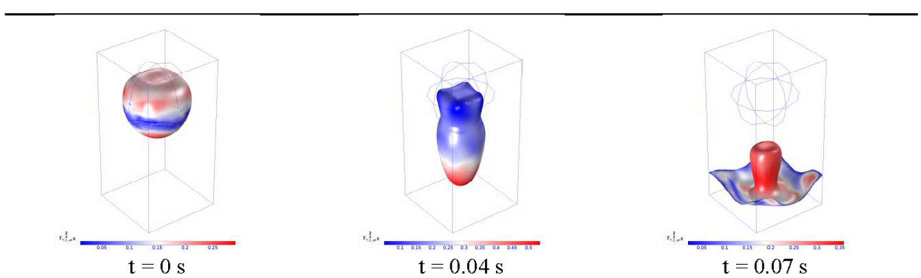

Fig. 7. Shape of the water droplet with 0.4 cm radius and initial speed of 0.5 ms^{-1} at (a) 0 s, (b) 0.04 s, (c) 0.07 s, (d) 0.30 s, (e) 0.40 s and (f) 1.00 s. Different colors correspond to different speeds (in ms^{-1}) as shown in the color bar. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

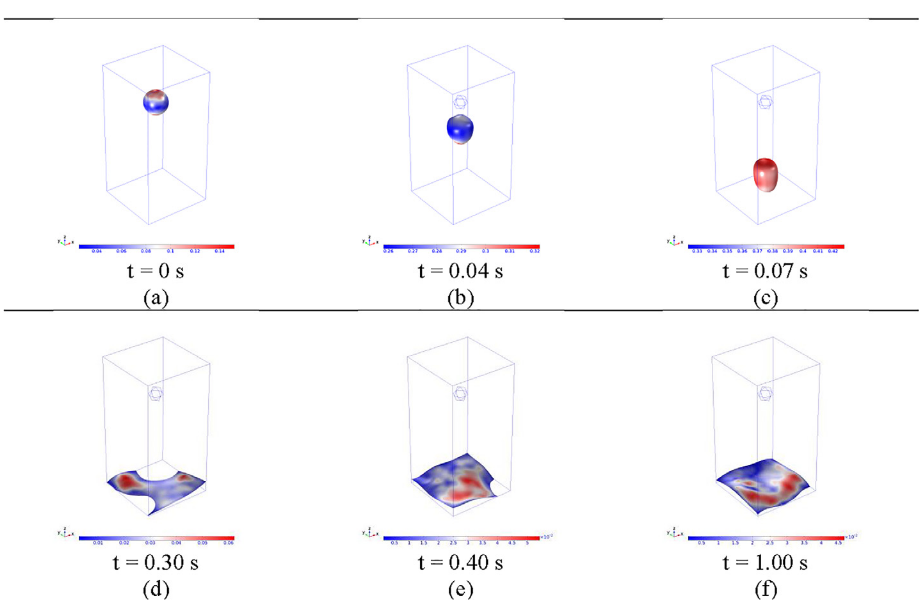

Fig. 8. Shape of the water droplet with 0.1 cm radius and initial speed of 1.0 ms^{-1} at (a) 0 s, (b) 0.04 s, (c) 0.07 s, (d) 0.30 s, (e) 0.40 s and (f) 1.00 s. Different colors correspond to different speeds (in ms^{-1}) as shown in the color bar. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

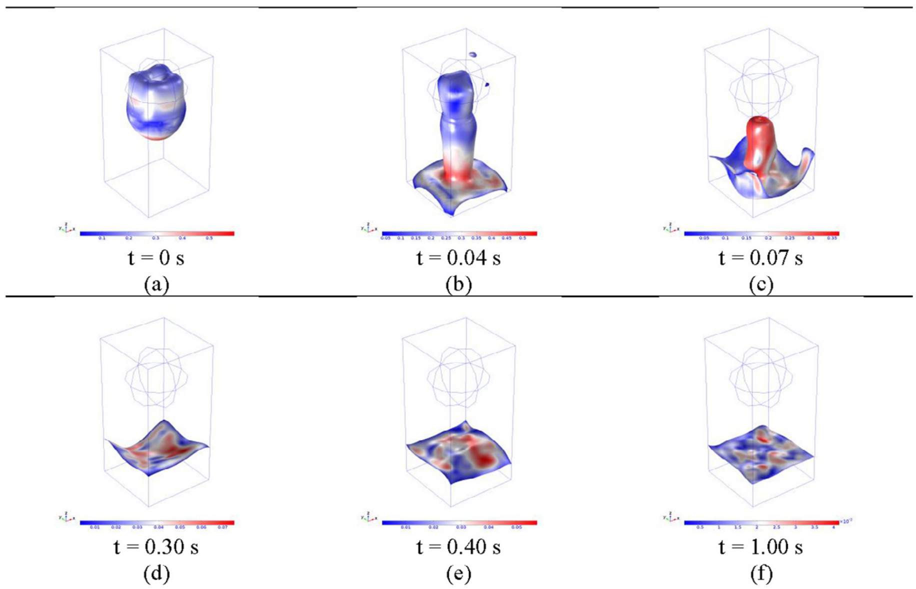

Fig. 9. Shape of the water droplet with 0.4 cm radius and initial speed of 1.0 ms^{-1} at (a) 0 s, (b) 0.04 s, (c) 0.07 s, (d) 0.30 s, (e) 0.40 s and (f) 1.00 s. Different colors correspond to different speeds (in ms^{-1}) as shown in the color bar. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

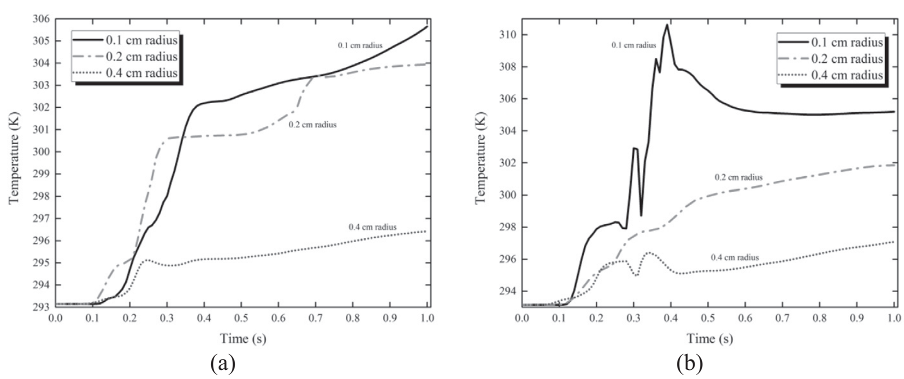

Fig. 10. Droplet temperature during its impact onto the solid surface with initial downward speeds of (a) 0.5 ms^{-1} and (b) 1.0 ms^{-1}.

slip walls with an area of 1 × 1 cm^2 so the large droplets produced thicker water films on the solid surface, which slowed down the temperature rise of these droplets during the impact. On the other hand, for the droplet with a radius of 0.1 cm, a higher initial speed enhanced the heat transfer efficiency due to its flattening on the hot solid surface as a result of faster and more powerful impact.

The temperature increase of the water droplets followed a stabilized pattern beyond ~0.4 s for all configurations and initial speeds, except for the droplet with a radius of 0.1 cm and an initial speed of 1.0 ms^{-1}. In the latter case, the drop in the temperature was due to the formation of detached water droplet fractions as a result of the high-speed impact, some of which did not have contact with the hot solid surface before coalescence with the fraction which had already contacted the hot solid surface. The complex variations of the water droplet temperature were mainly due to the involvement of phenomena such as spreading, detachment and coalescence, which could all be precisely tracked using the present three-dimensional computer program. The results for the initial speed of 0.5 ms^{-1} shown in Fig. 10(a) were smoother than those for the initial speed of 1 ms^{-1} shown in Fig. 10(b) mainly because the water droplets with larger initial speeds underwent larger topological changes when they hit the solid surface, which significantly affected the heat transfer between the droplets and the solid surface.

The ambient air temperatures during the impact of water droplets with initial speeds of 0.5 and 1.0 ms^{-1} are shown in Fig. 11 (a) and (b), respectively. The heat transfer mechanism that leads to temperature rise in the air domain consists of two parts, namely, (1) heat transfer between air and the hot solid surface and (2) heat transfer from the water droplet to air during its spreading and rebounce period beyond ~0.4 s, the air temperature increased at higher rates for droplets with smaller radii or higher initial speeds. During the period of approach and impact, the air temperature increased at a slightly higher rate for larger droplet size mainly due to better heat transfer to the ambient air as a result of the velocity field formed in air by the movement of these droplets. In summary, the liquid droplet had a minimal role in transferring heat to air. Instead, droplets might decrease the heat transfer to air, and consequently, the heat transfer to air was higher for smaller droplets (see the final air temperature rise in Fig. 11). During the approaching period, the droplet caused air to flow upwards by occupying its volume and hence enhanced the heat transfer.

The speeds of droplets with initial speeds of 0.5 and 1.0 ms^{-1} during approach, impact and rebounce periods are shown in

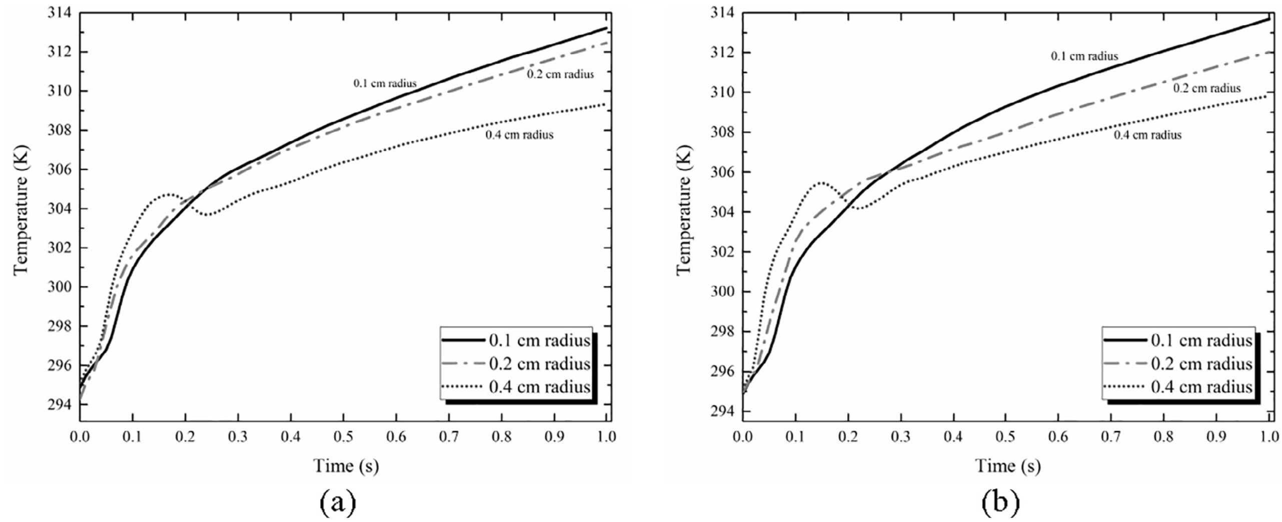

Fig. 11. Ambient air temperatures during the impact of water droplets with initial speeds of (a) 0.5 ms^{-1} and (b) 1.0 ms^{-1}.

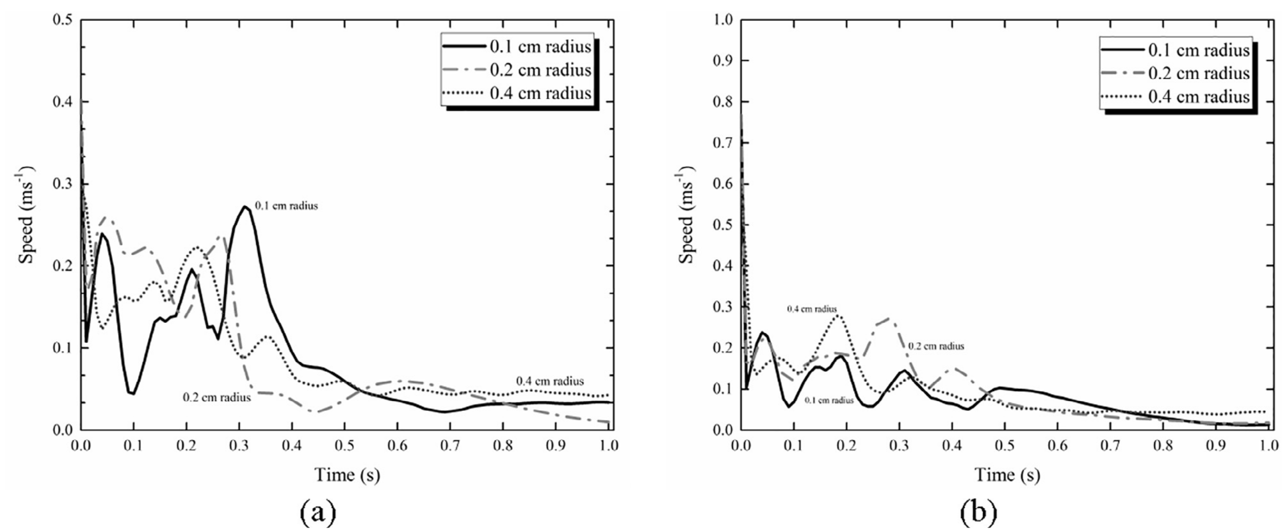

Fig. 12. Speed of droplets with initial speeds of (a) 0.5 ms^{-1} and (b) 1.0 ms^{-1} during approach, impact and rebounce periods.

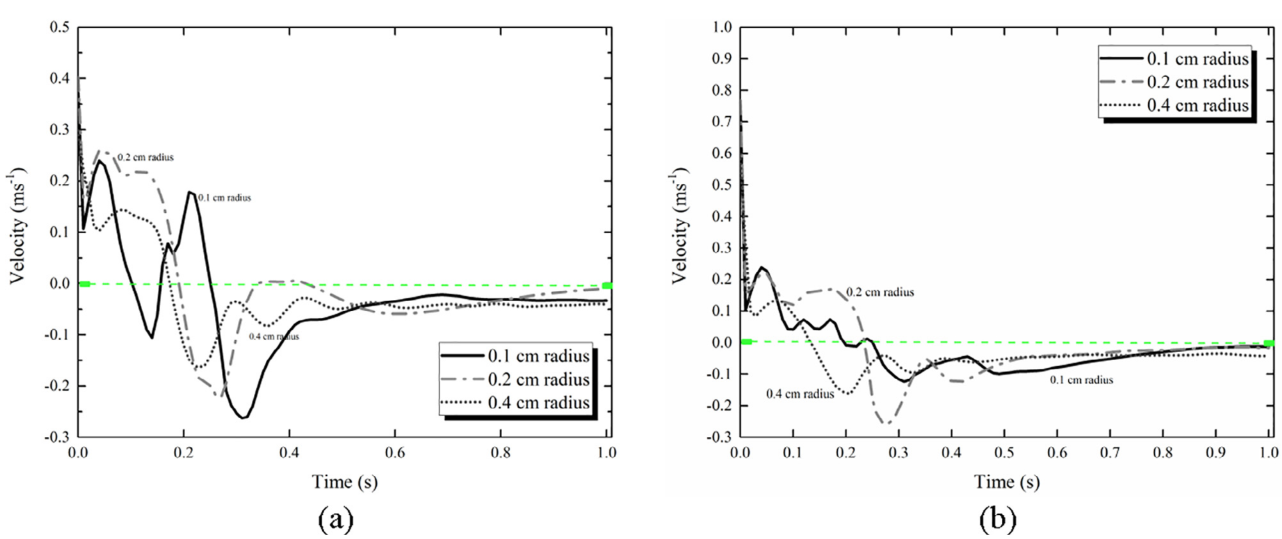

Fig. 13. Velocities of the water droplet during their approach to, impact on and rebounce from the solid surface with initial droplet speeds of (a) 0.5 ms^{-1} and (b) 1.0 ms^{-1}. Positive velocities corresponded to downward motion of the water droplet while negative velocities corresponded to upward motion of the water droplet. (Dashed green line: zero velocity.) (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

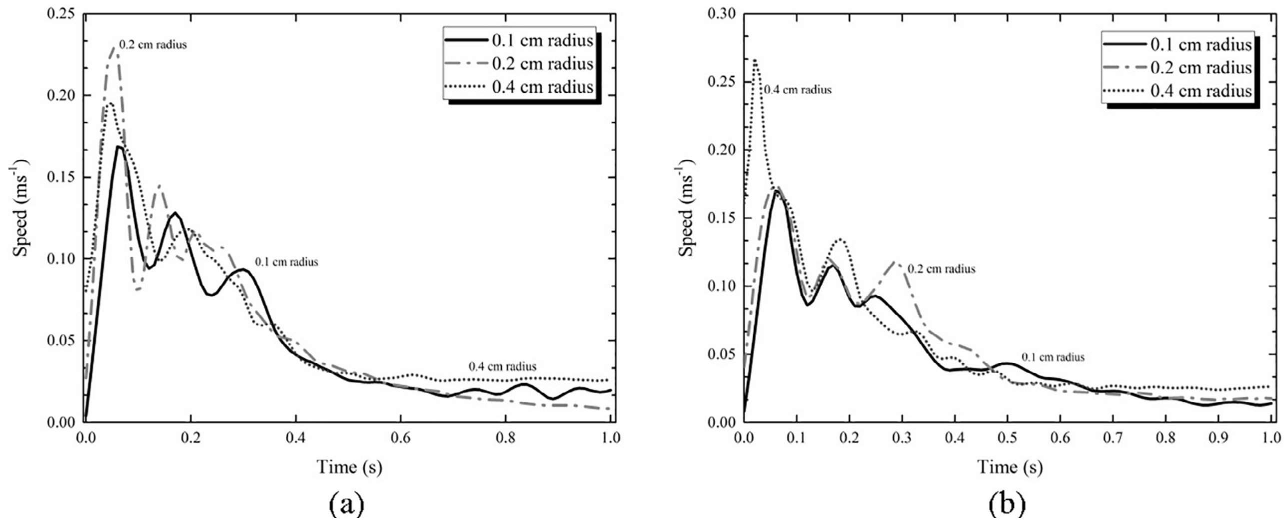

Fig. 14. Variations in air speed during the movement period of water droplets with initial droplet speeds of (a) 0.5 ms^{-1} and (b) 1.0 ms^{-1}.

Fig. 12(a) and (b), respectively. The oscillations were due to the rebounce of the droplets from the solid surface, where a fraction of their energies had been lost due to the impact, which determined the heights reached by the droplets. The oscillations became negligible after ~0.5 s measured from the instant of release. To follow the water droplets more closely, the velocities of the droplets are shown in Fig. 13(a) and (b) from their release until they come to rest.

The velocities scored for the droplet domain are shown in Fig. 13(a) and (b) for different initial droplet speeds. Positive velocities corresponded to downward motion of the water droplet while negative velocities corresponded to upward motion of the water droplet. The results showed that droplets with higher initial speeds had smaller rebounce speeds, which was explained by their more severe flattening leading to their contacts with the sides of the simulation box under the no-slip boundary condition. Therefore, the dynamics of the droplet would be influenced by the confinement of the system, in addition to the surface properties and morphologies.

The velocities scored for the ambient air are shown in Fig. 14 (a) and (b) for different initial droplet speeds. The ambient air in the system was initially stationary, and the movement of the water droplet and its impact on the solid surface would affect the air velocity. Interestingly, oscillations in the water-droplet velocity field were translated to the air due to the confinement of the system that accounted for the drag between the two fluids. However, the effects of the droplet on the surrounding air was only significant in the beginning (0 to ~0.3 s) when changes in the droplet velocity were large enough to exert influence on the air domain which had a much larger volume than the droplet.

4. Conclusions

The present numerical model could simulate the impact of water droplets with different sizes and initial speeds onto a hot solid surface. Here, more details including the radii and initial speed of the water droplet impacting on a solid surface were analyzed. The present work addressed the very important issue of cooling, the success of which would be essential for many industrial purposes and for nuclear power plant safety. This 3D model constructed using the level set method provided reliable results which could compare satisfactorily with experiments. The present model showed better agreement with previously published experimental data when compared to the VOF method. From the results obtained in the present work, the variations in the temperature of the water droplets were mainly due to differences between their spreading pattern on the solid surface which determined the heat transfer efficiency between the solid surface and the water droplet. Moreover, the temporal changes in the temperature of the water droplets with an initial droplet speed of 0.5 ms^{-1} were smoother than those with an initial droplet speed of 1.0 ms^{-1}, which was explained by the significant topological changes of the water droplets with larger initial speeds when they impinged the solid surface. Despite the desirable aspects of the present level set method described above, the method required substantial computational resources when compared to the VOF method. Furthermore, the current version of the model was built for solid surface temperatures below the phase transition temperature of water. In future, we aim at using this model to study the interaction of melts with the coolant and to further compare the results from the level set method with those from the widely used VOF method.

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