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Transient evaporation of moving water droplets in steam–hydrogen–air environment

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Sarkar Shanthanu, S. Raghuram, Vasudevan Raghavan $*$

Department of Mechanical Engineering, Indian Institute of Technology Madras, Chennai, Tamilnadu 600036, India

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ABSTRACT

During a severe loss of coolant accident in a nuclear reactor, steam and hydrogen are produced by the oxidation of reactor core and get distributed in the containment. A water spray system is employed to cool the mixture as well as to enhance the mixing of the gases to avoid hydrogen accumulation. This paper presents two-phase numerical simulations of transient vaporization of a moving spherical water droplet. The numerical model considers the variation of thermo-physical properties in both liquid- and vapor-phases, as functions of temperature and species concentrations. Multi-component diffusion and surface tension effects are also considered. The model has been validated using experimental results available in literature for hydrocarbon fuel droplet evaporation. Validated model is used to study the evaporation characteristics of moving water droplets under conditions typically observed in nuclear reactor during a loss of coolant accident. The effects of ambient temperature and hydrogen concentration on the vaporization characteristics are studied thoroughly.

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1. Introduction

In a hypothetical severe loss of coolant accident (LOCA) in a nuclear reactor, steam and hydrogen are produced by the oxidation of the reactor core or released from the reactant coolant system and get distributed in the containment. There is a possibility of combustion (or explosion), if the composition of hydrogen–air mixture reaches certain conditions in terms of stoichiometry and temperature. A water spray system is employed to first cool the gas mixture and also to enhance the mixing of the gases to avoid hydrogen accumulation. The effectiveness of the spray system depends on the ambient temperature and the composition of the gas mixture. Since the mixture contains condensable vapor, steam, there is a possibility of steam getting condensed into the spray water droplet. When it happens, the local concentration of hydrogen could increase. It is therefore important to study the vaporization characteristics of moving water droplets under conditions typically found in a nuclear reactor during a loss of coolant accident (LOCA).

Extensive literature reviews are available relating to thorough investigations on droplet vaporization. Haywood et al. [\[1\]](#page--1-0) studied isolated droplet vaporization by using transient two-phase model with variable property evaluation and have predicted the temperature distributions within the droplet. Megaridis and Sirignano [\[2,3\]](#page--1-0) have studied multi-component droplet vaporization by numerically solving the Navier–Stokes equations in axisymmetric coordinates. They have studied the preferential vaporization in a bi-component liquid droplet. Chiang et al. [\[4\]](#page--1-0) have analyzed the evaporation characteristics of a cold fuel drop injected into a hot ambient and studied the effect of varying the transfer number on the vaporization rate and the drag coefficient. Renksizbulut and Bussmann [\[5\]](#page--1-0) investigated the evaporation of decane– hexadecane binary hydrocarbon droplet at intermediate Reynolds numbers. Shih and Megaridis [\[6,7\]](#page--1-0) studied vaporization characteristics of suspended droplets in a laminar convective environment. They also studied the influence of the suspension fiber on the vaporization characteristics. Dwyer et al. [\[8\]](#page--1-0) and Dwyer and Shah [\[9\]](#page--1-0) studied thermal and solutal Marangoni effects for both vaporizing and combusting methanol droplets. They found thermal Marangoni effect to have a profound impact on droplet dynamic behavior. Ha and Lai [\[10,11\]](#page--1-0) used linear stability analysis and energy method respectively, to study Marangoni instability of a vaporizing droplet. They have developed a simplified model to predict the critical thermal and solute Marangoni numbers. They have also studied the effect of varying Lewis number on the critical Marangoni numbers. Savino and Fico [\[12\]](#page--1-0) have studied numerically and experimentally, the role of Marangoni and buoyancy flows in silicone oils with different viscosities and also in hydrocarbons, and have presented correlations between numerical and experimental results.

Daif et al. [\[13\]](#page--1-0) have studied binary fuel (*n*-heptane–*n*-decane) droplet evaporation experimentally, under natural, forced and mixed convective environments. Vaporization characteristics of

[⇑] Corresponding author. Tel.: +91 44 22574712.

E-mail addresses: [raghavan@iitm.ac.in,](mailto:raghavan@iitm.ac.in) vrag108@gmail.com (V. Raghavan).

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heptane–decane binary droplets having several initial blend compositions, at temperatures in the range of 350 K–360 K and at atmospheric pressures were reported. The experimental results in terms of surface regression data have been compared against those obtained using Sirignano model and the results were in good agreement. Wilms [\[14\]](#page--1-0) performed laser based levitation of pure and blended hydrocarbon fuel droplets and their vaporization characteristics at low pressure and low temperature conditions were studied. Though much work has progressed in this field, the application of droplet evaporation in the containments in nuclear reactors has been neglected in the literature.

Many works are available in the literature related to sprays used in nuclear reactor during an LOC accident. Royl et al. [\[15\]](#page--1-0) have developed a 3-D-field code for the simulation of steam/hydrogen distribution and combustion in complex nuclear reactor containment geometries. Jongtae et al. [\[16\]](#page--1-0) have developed a 3-D CFD code to analyze the effect of sprays on the behavior of steam and hydrogen produced in the reactor vessel and released into the containment during hypothetical severe LOC accidents. Babic and Kljenak [\[17\]](#page--1-0) have performed CFD spray simulations for nuclear reactor safety applications using a Lagrangian approach for spray modeling. Porcheron et al. [\[18\]](#page--1-0) investigated experimentally, the heat and mass transfer in sprays, used for containment applications in the TASQAN facility. Rabe et al. [\[19\]](#page--1-0) has studied droplet coalescence in spray systems used in nuclear reactors for containment safety. Fossaic et al. [\[20\]](#page--1-0) have investigated experimentally the droplet size and velocity distributions at the outlet of a swirling spray nozzle used in pressurized water reactor containment. Mimouni et al. [\[21\]](#page--1-0) studied the CFD modeling of wall steam condensation by using a two-phase flow approach. They have focused their study on condensation heat transfer that plays a major role in many accidents in the containment of nuclear reactors.

Even though several studies have been conducted relating to sprays used in a nuclear reactor during a severe LOCA, a fundamental study of vaporization of water droplets from the spray has been very scarce. Therefore in this work, a comprehensive two-phase numerical model has been employed to study the fundamental transient behavior involved in both liquid- and gas-phases during the evaporation of moving water droplets under conditions typically found in a nuclear reactor during LOCA. The numerical model has been modified from its initial version reported in Raghuram and Raghavan [\[22\],](#page--1-0) to adapt to the present problem. The numerical model has been validated using the experimental data available in Daif et al. [\[13\]](#page--1-0) for suspended hydrocarbon droplets evaporating under a forced convective air environment. The validated numerical model is used to study the effects of ambient temperature and hydrogen concentration in the gas-phase on the evaporation characteristics of moving water droplets.

2. Numerical model

The numerical model simulates the evaporation of a liquid droplet with initial radius R_0 in a low pressure convective gas/vapor environment. To simplify the complex problem, the following assumptions have been invoked in the numerical model: (1) laminar and axisymmetric flow, (2) droplet remains spherical throughout its lifetime (due to low Weber number), (3) Dufour and Soret effects are negligible in both phases, (4) negligible gravity, (5) negligible thermal radiation (only low temperatures are considered), (6) pressure diffusion is negligible in both phases and (7) viscous dissipation and pressure work are negligible. All the thermophysical properties of all the species in gas- and liquid-phases are evaluated as functions of temperature using correlations from Reid et al. [\[23\]](#page--1-0) and appropriate mixing rules are used to calculate the mixture properties.

2.1. Governing equations

The governing equations are described in axisymmetric spherical polar $(r - \theta)$ coordinates. Continuity equation in both gas- and liquid-phases is given by,

$$
\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho v_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \rho v_\theta) = 0, \tag{1}
$$

where ρ is the density, t is time and v_r and v_θ , are the radial and tangential components of the velocity vector, v , respectively. The momentum balance in the radial direction in both phases is governed by,

$$
\frac{\partial}{\partial t}(\rho v_r) + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho v_r^2) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \rho v_\theta v_r) \n= \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \mu \frac{\partial v_r}{\partial r} \right] + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \mu \left(\frac{1}{r} \frac{\partial v_r}{\partial r} \right) \right] + S_r,
$$
\n(2)

where S_r is the *r*-momentum source term given as:

$$
S_r = -\frac{\partial p}{\partial r} - \frac{2}{3} \frac{\partial}{\partial r} [\mu \nabla \cdot \mathbf{v}] + \frac{1}{r^2} \frac{\partial}{\partial r} \left[\mu r^2 \frac{\partial v_r}{\partial r} \right] + \frac{1}{r \sin \theta}
$$

$$
\times \frac{\partial}{\partial \theta} \left[\mu \sin \theta \left(\frac{\partial v_\theta}{\partial r} - \frac{v_\theta}{r} \right) \right] - \frac{2\mu}{r} \left[\frac{2v_r}{r} + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_\theta}{r} \cot \theta \right]
$$

$$
+ \frac{\rho v_\theta^2}{r} - \rho \cos \theta \frac{dU_\infty}{dt}.
$$
 (3)

The momentum balance in the tangential direction in both phases is governed by,

$$
\frac{\partial}{\partial t}(\rho v_{\theta}) + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho v_r v_{\theta}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \rho v_{\theta}^2) \n= \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \mu \frac{\partial v_{\theta}}{\partial r} \right] + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \mu \left(\frac{1}{r} \frac{\partial v_{\theta}}{\partial \theta} \right) \right] + S_{\theta},
$$
\n(4)

where S_θ is the θ -momentum source term given as:

$$
S_{\theta} = -\frac{1}{r} \frac{\partial p}{\partial \theta} - \frac{2}{3} \frac{1}{r} \frac{\partial}{\partial \theta} [\mu \nabla \cdot \mathbf{v}] + \frac{1}{r^2} \frac{\partial}{\partial r} \left[\mu r \frac{\partial v_r}{\partial \theta} \right] - \frac{1}{r^2} \frac{\partial}{\partial r} (\mu r v_{\theta}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left[\mu \sin \theta \left(\frac{1}{r} \frac{\partial v_{\theta}}{\partial \theta} \right) \right] + \frac{2}{r \sin \theta} \frac{\partial}{\partial \theta} \left[\mu \sin \theta \frac{v_r}{r} \right] + \frac{\mu}{r} \left[\frac{\partial v_{\theta}}{\partial r} + \frac{1}{r} \frac{\partial v_r}{\partial \theta} - \frac{v_{\theta}}{r} \right] - \frac{2\mu}{r} \cot \theta \left[\frac{v_r}{r} + \frac{v_{\theta}}{r} \cot \theta \right] - \rho \frac{v_{\theta} v_r}{r} + \rho \sin \theta \frac{dU_{\infty}}{dt}
$$
(5)

In Eqs. (3) and (5), p is the pressure, μ is the dynamic viscosity and U_{∞} is the relative velocity between the droplet and surrounding medium. The conservation of species, in terms of mass fractions of the components in the gas-phase, is governed by,

$$
\frac{\partial(\rho Y_i)}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho v_{r,i} Y_i) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \rho v_{\theta,i} Y_i) \n= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \rho D_{im} \frac{\partial Y_i}{\partial r} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \rho D_{im} \left(\frac{1}{r} \frac{\partial Y_i}{\partial \theta} \right) \right], \ni = 1 \text{ to } N - 1,
$$
\n(6)

where Y_i is mass fraction of species *i*, *N* is the total number of species in the gaseous phase and is equal to 4, D_{im} is the diffusion coefficient of species i diffusing into the gas-phase mixture. The conservation of energy in both phases (denoted by g and l) includes enthalpy transport due to species diffusion and is governed by,

$$
\frac{\partial}{\partial t}(\rho T) + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho v_r T) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \rho v_{\theta} T) \n= \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \frac{k}{c_p} \frac{\partial T}{\partial r} \right] + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{k}{c_p} \left(\frac{1}{r} \frac{\partial T}{\partial \theta} \right) \right] + S_{Ej}, \nj = g, l
$$
\n(7)

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