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REVIEW





Smoothed Particle Hydrodynamics (SPH) Simulations of Drop Evaporation: A Comprehensive Overview of Methods and Applications

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ABSTRACT: The evaporation of micrometer and millimeter liquid drops, involving a liquid-to-vapor phase transition accompanied by mass and energy transfer through the liquid-vapor interface, is encountered in many natural and industrial processes as well as in numerous engineering applications. Therefore, understanding and predicting the dynamics of evaporating flows have become of primary importance. Recent efforts have been addressed using the method of Smoothed Particle Hydrodynamics (SPH), which has proven to be very efficient in correctly handling the intrinsic complexity introduced by the multiscale nature of the evaporation process. This paper aims to provide an overview of published work on SPH-based simulations related to the evaporation of drops suspended in static and convective environments and impacting on heated solid surfaces. After a brief theoretical account of the main ingredients necessary for the modeling of drop evaporation, the fundamental aspects of SPH are revisited along with the various existing formulations that have been implemented to address the challenges imposed by the physics of evaporating flows. In the following sections, the paper summarizes the results of SPH-based simulations of drop evaporation and ends with a few comments on the limitations of the current state-of-the-art SPH simulations and future lines of research.

KEYWORDS: Drop evaporation; surface tension; heat and mass transfer; phase separation; smoothed particle hydrodynamics (SPH); boiling evaporation; explosive vaporization; droplet/wall interaction

1 Introduction

The evaporation of a liquid is a complex physical process involving the phase transition of the liquid into a vapor state and the motion (and/or deformation) of the liquid-vapor interface. Since mass and energy are transferred simultaneously through the interface, the evaporation is a multiscale and multistep heat transfer problem. The phase transition can take place at different temperatures for which enough thermal energy is stored within the liquid to overcome the forces of surface tension. At the microscopic level, the evaporation occurs when the kinetic energy acquired by the molecules close to the liquid surface is greater than the cohesion exerted by the intermolecular forces within the liquid phase [1,2]. For water drops in warm air, heat is transferred to the drop surface by conduction and convection, while mass (i.e., vapor) is transferred back to the air by diffusion and convection. In particular, the evaporation of small confined liquid systems, such as micrometer- and millimeter-sized drops, have numerous engineering applications and occurs in many natural and industrial processes. For example, raindrops lose some of their mass by evaporation as they fall to the ground. This may happen even when the atmosphere around them is not saturated with the



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vapor of the drops. The basic model of drop evaporation is the diffusion-controlled evaporation of a perfectly spherical drop in a stationary atmosphere, while convective motion that can appear in a moving atmosphere, will add an extra degree of complexity to the problem. Under the effects of convective motions evaporating drops may deform, as indeed occurs in freely falling raindrops where the changing shape geometry affects the evaporation rates. Drops can also evaporate by contact with hot solid surfaces. Good examples are given by the evaporation of sessile and pendant drops (see Erbil [3] for a comprehensive review of this special topic). However, most of our present knowledge of drop evaporation comes from models of homogeneous and single-component drops. If, on the other hand, the drop is composed of a multi-component fluid, as occurs in many industrial applications, the evaporate first, which is then followed by a period where the evaporation rate is limited by the diffusion process in the liquid phase [3–5].

Although drop evaporation is a ubiquitous phenomenon appearing in many processes, it has not yet been modeled and simulated in a physically consistent manner. In general, the study of first-order phase transitions utilizing hydrodynamic plus heat transfer simulations is still today an open topic of research. Other difficulties and challenges are associated with the treatment of sharp discontinuities of fluid properties across the liquid-vapor interface as well as its motion and deformation. Published articles on numerical simulations of drop evaporation by traditional grid-based Eulerian numerical methods have been appearing for more than four decades. Although grid-based methods have succeeded in simulating volumetric effects, they have great difficulties in guaranteeing mass (or volume) preservation at free surfaces, treating inhomogeneities and deformable (or moving) boundaries, and shifting material interfaces [6–9]. In contrast, Smoothed Particle Hydrodynamics (SPH) is a Lagrangian mass-preserving method and has the advantage of being robust at handling free surfaces, extreme boundary deformations, and surface interactions [10,11]. Other attractive features are the Galilean invariance of the discrete hydrodynamic equations which allows for exact modeling of advection and the rather straightforward implementation of additional physical and chemical effects. Since SPH is relatively novel compared to grid-based methods, drop evaporation simulations using SPH date back no more than 25 years. The first SPH simulations of evaporating drops were reported in 2000 by Nugent et al. [12] using classical (local) thermodynamics with the aid of a van der Waals (vdW) equation of state. Since many of the basic features of liquid-vapor phase transitions can be studied in the framework of vdW mean field theory [13,14], the SPH model of Nugent et al. [12] was extended to study phase change flows in an infinite expanse of fluid using non-classical (i.e., non-local) vdW thermodynamics [15,16], where the classical pressure and caloric vdW equations of state are combined with a diffuse-interface model [14]. This model was later used in SPH simulations of spinodal decomposition and homogeneous nucleation [17-20] and explosive boiling [21-23] of liquid droplets. An advantage of these models is that the effects of surface tension are naturally handled by the cohesive term in the vdW pressure equation, while the capillary forces in a diffuse liquid-vapor interface are modeled by the so-called Korteweg tensor [14]. This formulation is quite robust and able to capture the essential physics of phase transition and liquid-vapor coexistence. The coupling between local vdW thermodynamics and the non-classical Korteweg tensor is also referred to in the literature as the vdW square gradient model [15]. In recent work, Harisankar et al. [24] studied the formation of a bare droplet and its evaporation under the addition of a small amount of energy using an SPH formulation similar to the one reported by Nugent et al. [12]. This model was previously applied to simulate the interaction of a fuel droplet with a heated surface [25] and more recently by coupling the SPH hydrodynamics with a Peng-Robinson equation of state to simulate the thermal evolution of an *n*-heptane drop impacting on a hot surface [26].

Other SPH formulations aimed at simulating the evaporation of multiphase flows have also appeared in recent years. In particular, Yang et al. [27] reformulated the SPH hydrodynamic equations to describe the

transport of mass and energy across the liquid-vapor interface with simplified thermodynamics relying on an ideal equation of state where the pressure was assumed to vary linearly with the density. In this approach a continuity equation for the vapor species was added to the system to determine the mass transfer rate across the interface. Since this method was found to be accurate enough to model the evaporation process at the liquid-gas interface and the diffusion of the vapor species into the vapor phase, variants of it were later used to model both the evaporation of bare drops and the evaporation of drops impacting on heated solid surfaces at standard atmospheric and high pressure [28-32]. Most of these variants focus on improvements in the convection-diffusion transport of mass and energy across the liquid-vapor interface. In particular, Xu et al. [31] introduced a time fractional-order convection-diffusion equation to simulate drop evaporation under different environments. They found that their droplet evaporation model conformed to the D^2 law proposed on theoretical grounds by Godsave [33] and Spalding [34], which indicates that the square of the drop diameter decreases linearly with time during the evaporation process. SPH simulations of the evaporation and combustion process of static *n*-hexane single, binary, and multiple droplets were considered by Wang et al. [35], using a Murnaghan-Tait equation of state for the pressure-density relation and a one-step global reaction model for vapor combustion. This framework was also validated against experimental data for methane/air laminar diffusion flames [36]. On the other hand, Li et al. [37] performed SPH simulations to study the effects of drop diameter, impact velocity, liquid evaporation, wall temperature, and inclined wall angle on the impact of a liquid drop on a solid wall using Yang et al.'s [27] SPH formulation with an adaptive spatial resolution (SPH-ASR), and found good agreement between the numerical and experimental results. Using a similar SPH framework, Subedi et al. [38] studied numerically the impact of successive droplets on a heated wall.

A multi-phase, weakly-compressible SPH framework with ideal thermodynamics based on a Murnaghan-Tait equation of state for both the liquid and air phases capable of simulating supercooled large droplets (SLD) impingement at aeronautical speeds while considering the effects of surrounding air was reported by Cui et al. [39]. A similar formulation was extended by Liu et al. [40] to include thermal effects for studying the spreading dynamics and evaporation of sessile and nanofluid droplets. Their model was able to predict the evolution of the droplet from spreading to receding to bouncing on the heated wall. Moreover, the numerically predicted drop diameters were found to agree acceptably well with experimental data from images taken with a high-speed camera. While most of the above-mentioned models are useful in many engineering applications, a deeper insight into the details of evaporating liquid drops will certainly require the use of advanced numerical techniques along with physical and chemical effects. For example, most existing SPH models of drop evaporation are limited to two dimensions with only a few instances involving three-dimensional calculations. On the other hand, several studies start from initial conditions and use empirical parameters that do not strictly correspond to physical reality. However, SPH methods extended to include thermal effects have been demonstrated to be powerful tools for studying the complex dynamics involved in the evaporation of liquid droplets from diffusion-controlled (ordinary) boiling to bubble nucleation to explosive vaporization. This paper aims to provide an overview of the existing SPH formulations and model results of drop evaporation. The paper is organized as follows. A brief on theoretical considerations and formulations necessary for the modeling of drop evaporation is provided in Section 2. Section 3 describes fundamental aspects of the SPH method and introduces the governing equations in discrete form as they are used in the various formulations. An overview of the SPH results obtained for specific topics on drop evaporation is given in Sections 4-6. Section 7 contains a discussion on the limitations of the present state-of-the-art simulations and ends with a brief comment on future work. Finally, Section 8 contains the relevant conclusions.

2 Theoretical Background

The evaporation of liquid drops is a complex physical phenomenon in which the liquid undergoes a transition into a vapor (gas) state. The process is non-stationary and may occur over a wide range of temperatures for which the bulk liquid acquires enough thermal energy to overcome the effects of surface tension. From a molecular point of view, evaporation occurs when the kinetic energy of the surface liquid molecules exceeds the cohesive work exerted by the inner liquid molecules [1,2]. During drop evaporation heat transfer, from the external medium to the drop, and mass transfer, from the drop to the external medium, occur simultaneously, where heat is transferred to the drop by any of three mechanisms, namely conduction, convection, and radiation, while mass transfer to the external medium may occur either by diffusion or convection, or even by both. Under natural conditions, the rate of heat and mass transfer depends on the drop size, the temperature, the relative humidity, and the transport properties of the surrounding medium [3]. In this section, a brief on the basic theoretical aspects behind the numerical modeling of drop evaporation is introduced. However, before continuing, it is important to introduce some basic concepts related to liquidvapor phase transitions. For example, if a homogeneous solution of a given composition is quenched below the region bounded by the binodal (or liquid-vapor coexistence) curve of the phase diagram, the separation of the solution into a liquid and vapor phase may occur either by spinodal decomposition or nucleation. In particular, for quenching into the miscibility gap below the spinodal curve, phase separation occurs spontaneously even for infinitesimally small fluctuations with a high interconnectivity of the two phases. This process is referred to as spinodal decomposition. When quenching takes the solution into the metastable region bounded by the spinodal and binodal curves, the system becomes thermodynamically unstable to the growth of large fluctuations only, leading to the formation of one or more vapor bubbles by nucleation. On the other hand, when a liquid is overheated, it may undergo an extremely rapid evaporation, leading eventually to a thermal or vapor explosion. This process, which is also called explosive vaporization, occurs when the liquid attains its superheat limit, i.e., the maximum temperature below the critical value to which the liquid can be elevated at constant pressure and composition before boiling explosively. At this limit, the liquid enters the metastable region where random density fluctuations of finite size initiate spontaneous nucleation of a vapor bubble, which then expands rapidly accompanied by extremely large evaporation rates and fluid accelerations.

2.1 vdW Thermodynamics

The pressure, p, of a real homogeneous fluid coexisting with its vapor atmosphere can be described in a first approximation by the vdW equation of state

$$p = \frac{Nk_BT}{V - Nb} - \frac{N^2a}{V^2},\tag{1}$$

where *V* is the volume occupied by the fluid, *N* is the number of molecules forming the fluid, k_B is the Boltzmann constant, *T* is the temperature, *a* defines the strength of the attractive force between pairs of molecules, and *b* is the volume of a molecule (or particle). This way *Nb* is the smallest volume to which one can compress all fluid molecules. If $m = \mu m_p$ is the mass of a fluid molecule, where μ is the mean molecular weight and $m_p = 1.6726218 \times 10^{-27}$ kg, then the fluid density is $\rho = mN/V$ from which it follows that $\rho/m = N/V$. Dividing the numerator and denominator in the first and second terms on the right-hand side of Eq. (1) by *N* and N^2 , respectively, and using the above relation for the specific volume ρ/m , Eq. (1) can be written in the alternative form

$$p = \frac{\rho\left(k_B/m\right)T}{1-\rho\left(b/m\right)} - \left(\frac{a}{m^2}\right)\rho^2.$$
(2)

Using the definitions $\bar{k}_B = k_B/m$, $\bar{b} = b/m$, and $\bar{a} = a/m^2$, Eq. (2) takes the final form

$$p = \frac{\rho \bar{k}_B T}{1 - \bar{b}\rho} - \bar{a}\rho^2,\tag{3}$$

which is the form originally introduced by Nugent et al. [12] and later employed by most SPH simulations of evaporating flows based on vdW thermodynamics. In their SPH simulations, Nugent et al. [12] used these parameters in reduced units: $\bar{a} = 2$, $\bar{b} = 1/2$, $\bar{k}_B = 1$, and m = 1 so that the critical density, pressure, and temperature are given by $\rho_{cr} = 2/3$, $p_{cr} = 8/27$, and $T_{cr} = 32/27 \approx 1.19$, respectively. Since then these reduced units have been a standard choice in many simulations of vdW liquid-vapor phase transitions.

The caloric behavior of the vdW fluid is described by the internal energy given by

$$u = \frac{\xi}{2} N k_B T - a \frac{N^2}{V},\tag{4}$$

where the first term on the right-hand side is the kinetic energy of the molecules and the second term is the potential energy of their forces of cohesion [41]. Here, $\xi = 2$ in two dimensions and 3 in three dimensions. Dividing the numerator and denominator of the second term on the right-hand side by *N*, replacing *V*/*N* by m/ρ in the denominator of the second term, and multiplying and dividing the first and second term by m, Eq. (4) becomes

$$u = \frac{\xi}{2} m N\left(\frac{k_B}{m}\right) T - m N\left(\frac{a}{m^2}\right) \rho,\tag{5}$$

where mN is the total mass of the fluid. Using the above vdW parameters in reduced form, the vdW caloric equation takes the final form

$$U = \frac{\xi}{2}\bar{k}_B T - \bar{a}\rho,\tag{6}$$

where U = u/(mN) is the specific internal energy.

The sound speed for this vdW fluid is

$$c_{\rm s} = \sqrt{2\left[\frac{\bar{k}_B T}{(1-\rho\bar{b})^2} - \bar{a}\rho\right]},\tag{7}$$

while the specific heat at constant volume and pressure can be derived to be

$$c_{\rm v} = \bar{k}_B,\tag{8}$$

$$c_{\rm p} = \frac{2\bar{k}_B \left[\bar{k}_B - \bar{a}\rho \left(1 - \rho\bar{b}\right)^2\right]}{\bar{k}_B T - 2\bar{a}\rho \left(1 - \bar{b}\rho\right)^2}.$$
(9)

Since c_v is always positive, the following condition

$$\bar{k}_B T > 2\bar{a}\rho \left(1 - \rho \bar{b}\right)^2,\tag{10}$$

must hold to ensure positivity of c_p . This in turn guarantees that the sound speed is a real number. In addition to inequality (10), complete thermodynamic stability will be guaranteed by the constraint $\rho < 1/\bar{b}$. Although Eqs. (3) and (6) can predict the liquid-vapor phase transition and their coexistence in equilibrium,

the results can only be qualitatively assessed since for nearly all models reported the parameters employed do not correspond to real fluids. Perhaps an exception to this rule is the water evaporation models performed by Xiong et al. [18], who employed vdW parameters \bar{k}_B , \bar{a} , and \bar{b} corresponding to pure water.

2.2 Other Equations of State

A SPH formulation that has recently been used extensively to simulate many problems involving evaporating multiphase flows relies on ideal thermodynamics by assuming a barotropic equation of state of the form [27].

$$p = c_s^2 \left(\rho - \rho_{\rm ref} \right) + p_{\rm ref},\tag{11}$$

where c_s is a numerical speed of sound (usually set equal to ten times the maximum velocity of the system), ρ_{ref} is a reference density, and p_{ref} is a reference pressure. To prevent negative values of the pressure, the reference pressure is sometimes set arbitrarily to a value higher than atmospheric pressure [30]. When using Eq. (11) the energy equation is written in terms of the temperature so that a caloric equation is not required. The Murnaghan-Tait pressure-density relation [42]

$$p = p_{\rm ref} \left[\left(\frac{\rho}{\rho_{\rm ref}} \right)^{\gamma} - 1 \right], \tag{12}$$

is also frequently used, where $\gamma = 1.4$ for a gas and $\gamma = 7$ for a liquid (or water). The reference pressure is usually set equal to $c_s^2 \rho_{ref} / \gamma$ and, as before, c_s is a numerical sound speed chosen to be ten times the maximum fluid velocity in order to maintain the density fluctuations below 1% of the normal density and ensure weak compressibility [10,43].

On the other hand, Yang et al. [26] reported SPH simulations of the interaction of fuel (*n*-heptane) drops with heated walls using the Peng-Robinson equation of state

$$p = \frac{R_g T}{V_m - b} - \frac{a}{V_m^2 + 2bV_m - b^2},$$
(13)

with realistic fuel properties along with the caloric equation

$$U = cT - a\rho,\tag{14}$$

where R_g is the universal gas constant, V_m is the molar volume, and the parameters *a* and *b* have the same physical meaning as in Eq. (1), with *a* being now calculated as

$$a = \tilde{a} \left[1 + \kappa_{\rm r} \left(1 - \sqrt{\frac{T}{T_{\rm cr}}} \right) \right]^2, \tag{15}$$

where \tilde{a} and κ_r are constants. The value of *c* in Eq. (14) is chosen such that the saturated liquid and vapor enthalpies can be predicted accurately. It is worth mentioning that the specific internal energy is calculated from the energy conservation equation and that the caloric Eq. (6), for a vdW fluid, and (14) are used to obtain the temperature.

2.3 Surface Tension

Surface tension is an interfacial property of any liquid. It arises because liquid molecules at and near the surface are less tightly bound than in the bulk liquid. Therefore, there is an excess of free energy at the

liquid surface and as a result the surface molecules experience inwardly directed attractive forces, which are responsible for the elastic tendency to minimize the surface area. It has units of energy per unit area or, equivalently of force per unit length. In a liquid drop context, the surface tension encodes information of the amount of surface free energy per unit area of the drop [44]. In other words, it is a measure of the cohesive energy in an interface and is the main cause of inducing bubble and drop formation [45,46]. In addition, it is the factor governing the shape of liquid drops, which in turn has a crucial impact on the heat and mass transfer performance of a thermal system [47,48].

The surface tension of a liquid drop can be calculated using the Young-Laplace equation [49,50]

$$\Delta p = \left(p_1 - p_v\right) = \sigma K = \sigma \left(\frac{1}{R_1} + \frac{1}{R_2}\right),\tag{16}$$

where p_1 is the pressure in the interior of the drop, p_v is the pressure of the surrounding vapor atmosphere, σ is the surface tension, K is the mean curvature of the interface, and R_1 and R_2 are the principal radii of curvature. This expression is valid when the interface separating the liquid from the vapor phase is a surface of discontinuity (i.e., a surface of zero thickness). As we shall see later in this section, thermal effects influence the interface thickness, making it more and more diffuse as the heat is increased. For perfect spherical and static drops $R = R_1 = R_2$ and Eq. (16) reduces to the more familiar form

$$\Delta p = \frac{2\sigma}{R}.\tag{17}$$

In model simulations of evaporating drops based either on vdW or Peng-Robinson thermodynamics, surface tension effects are not quantified by adding an artificial input force into the hydrodynamic equations because they arise naturally from the attractive (cohesive) term on the right-hand side of Eqs. (3) and (13). The gradient of the cohesive pressure produces an attractive, long-range surface force perpendicular to the surface itself and pointing towards the liquid phase. Therefore, in these simulations, there is no need to explicitly locate the interface and calculate the local surface curvature. A good example of a three-dimensional, SPH vdW-based calculation of an initially square-shaped drop evolving into a spherical drop by surface tension is displayed in Fig. 1 of Ref. [51].

2.4 Latent Heat

The evaporation of a liquid drop embedded into a hotter medium occurs because heat is transferred from the medium to the drop surface by conduction and/or convection, where it is converted into latent heat (or enthalpy) of vaporization. The amount of vapor that forms above a liquid is proportional to the temperature and therefore it is usually measured as the vapor pressure of the system. At higher heating temperatures, a greater number of surface molecules will acquire enough thermal energy to overcome the intermolecular attraction forces of the liquid and enter the vapor phase, resulting in increasing vapor pressure. A measure of the intermolecular attraction forces between pairs of liquid molecules is the latent heat $\Delta H_{\rm vap}$, which is the necessary energy that a certain amount of liquid must acquire to turn out into vapor without a change of temperature. The relationship between the (saturated) vapor pressure, $p_{\rm v}$, and the latent heat is given by the familiar Clausius-Clapeyron equation

$$p_{\rm v} = A \exp\left(-\frac{\Delta H_{\rm vap}}{R_g T}\right),\tag{18}$$

where A is an experimental constant related to the normal point of boiling. Taking the logarithm on both sides of Eq. (18), yields the expression

$$\ln p_{\rm v} = -\frac{\Delta H_{\rm vap}}{R_g} \frac{1}{T} + C,\tag{19}$$

which is the equation of a straight line of slope $-\Delta H_{\text{vap}}/R_g$. Here *C* is a universal constant which is independent of the particular liquid. In general, the Clausius-Clapeyron equation applies to first-order phase transitions and is frequently used in many SPH drop-evaporation simulations using vdW thermodynamics as a validation benchmark test (see, for example, Refs. [17,18,23,24]), where the gas constant R_g is replaced by \bar{k}_B in reduced units.

2.5 Classical Equations of Hydrodynamics

In the presence of thermal effects the motion of the fluid is described by the physical principles of mass, momentum, energy, and entropy balance. Under a Lagrangian framework, these conservation laws correspond to the set of coupled partial differential equations

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{v},\tag{20}$$

$$\rho \frac{d\mathbf{v}}{dt} = \nabla \cdot \mathbb{T},\tag{21}$$

$$\rho \frac{dU}{dt} = \mathbb{T} : \nabla \mathbf{v} - \nabla \cdot \mathbf{q},\tag{22}$$

$$\rho \frac{dS}{dt} = \Delta_s - \nabla \cdot \left(\frac{\mathbf{q}}{T}\right),\tag{23}$$

where **v** is the fluid velocity vector, S is the specific entropy, \mathbb{T} is the stress tensor given by

$$\mathbb{T} = -p\mathbb{I} + \eta \left(\nabla \mathbf{v} + \nabla \mathbf{v}^t \right) + \left(\zeta - \frac{2}{d} \eta \right) \nabla \cdot \mathbf{v} \mathbb{I},$$
(24)

with I denoting the identity tensor, η the shear viscosity, ζ the bulk viscosity, d the dimension factor, and superscript ^{*t*} meaning transposition, **q** is the heat flux vector

$$\mathbf{q} = -\kappa \nabla T,\tag{25}$$

with κ being the heat conduction coefficient, and

$$\Delta_s = \frac{\kappa (\nabla T)^2}{T^2} + \frac{\eta}{T} \left(\nabla \mathbf{v} : \nabla \mathbf{v} \right), \tag{26}$$

is the entropy production.

SPH simulations of drop evaporation based on Eqs. (20)-(22) were carried out by Nugent et al. [12] and more recently by Harisankar et al. [24] and Yang et al. [26]. On the other hand, Hochstetter et al. [52] performed SPH-based calculations of the evaporation and condensation of liquids using a simplified version of Eqs. (20)-(22) for an incompressible, inviscid fluid under buoyancy effects. In their model, the energy equation was replaced by a heat conduction equation for a homogeneous medium

$$\rho c_{\rm p} \frac{dT}{dt} = \nabla \cdot (\kappa \nabla T), \tag{27}$$

where c_p is the specific heat at constant pressure. Eqs. (20) and (21) coupled with a heat conduction equation written in terms of the enthalpy \mathcal{H} were also employed in recent SPH calculations of the spreading dynamics of nanofluid droplets coupled with thermal evaporation by Liu et al. [40].

In the last five years, most work on drop evaporation has focused on SPH simulations of multiphase flows using the model proposed by Yang et al. [27,28] and variants of it. This model solves Eqs. (20) and (27) coupled to the Navier-Stokes equation for the fluid velocity

$$\rho \frac{d\mathbf{v}}{dt} = -\nabla p + \eta \nabla^2 \mathbf{v} + \mathbf{g},\tag{28}$$

where **g** is the gravitational acceleration. During the process of phase change due to evaporation, the mass and energy transfer across the liquid-vapor interface are modeled by the modified continuity and heat conduction equations

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{v} + \dot{m}^{m},$$
(29)
$$\rho c_{\rm p} \frac{dT}{dt} = \nabla \cdot (\kappa \nabla T) - \Delta H_{\rm vap} \dot{m}^{m},$$
(30)

where \dot{m}^m is the volumetric mass evaporation rate and ΔH_{vap} is the latent heat of vaporization. The mass fraction field of the vapor species in the gaseous phase, *Y*, is calculated using the continuity-like equation for vapor species

$$\rho \frac{dY}{dt} = \nabla \cdot (\rho \mathscr{D} \nabla Y), \tag{31}$$

where \mathscr{D} is the vapor mass diffusivity coefficient. In order to close the system of governing equations, an equation for the mass evaporation rate across the interface is needed, which can be derived from conservation principles to be

$$\rho \dot{m} = \rho \frac{dm}{dt} = \frac{m \nabla \cdot (\rho \mathscr{D} \nabla Y)}{1 - Y},\tag{32}$$

so that $\dot{m}^m = \rho \dot{m}/m$, where *m* is the initial total mass. Under the assumption that there exists equilibrium between the liquid and gas at the interface, the vapor mass fraction there is made equal to the saturated vapor mass fraction given by

$$Y_{\rm s} = \frac{X_{\rm s} M_{\rm v}}{(1 - X_{\rm s}) M_{\rm g} + X_{\rm s} M_{\rm v}},\tag{33}$$

where X_s is the saturated vapor molar fraction, M_v is the vapor molar mass, and M_g is the molar mass of the dry gas, excluding the vapor species. The saturated vapor molar mass is obtained by direct integration of the Clausius-Clapeyron Eq. (18) as

$$X_{\rm s} = \frac{p_{\rm s}}{p_{\rm ag}} = \exp\left[-\frac{\Delta H_{\rm vap}M_{\rm v}}{R_g}\left(\frac{1}{T_{\rm s}} - \frac{1}{T_{\rm boil}}\right)\right],\tag{34}$$

where p_s is the saturated vapor pressure, p_{ag} is the ambient gas pressure, T_s is the interface temperature, and T_{boil} is the boiling temperature at the ambient-gas pressure condition (see Ref. [53] for details on the derivation of Eq. (34)). Using the same model equations, Yang et al. [26] performed further SPH simulations to study the impact of fuel drops on a heated surface.

Variants of their model were also implemented by other authors to simulate drop evaporation [29-32]. Moreover, SPH simulations of the evaporation and combustion of *n*-hexane droplets were carried out by Wang et al. [35] by extending Yang et al.'s [27] model to include a one-step global reaction model of *n*-hexane to calculate the vapor combustion.

2.6 Diffuse Interface

In all classical models of two-phase fluid systems the interface dividing both fluids is assumed to be a surface of discontinuity endowed with surface tension. At the molecular scale, such an interface can be defined as a transition zone of typical width a few tens of Angströms. In contrast, the interfacial zone in a diffuse-interface model is defined by a continuous variation of an order parameter, such as the density, according to the molecular theory of capillarity [13]. In this case, the interface has an inner structure and a finite width through which the densities of both fluids are connected smoothly. Across the volume of the diffuse interface, all physical quantities are defined in terms of density variation. The diffuse-interface model has been successfully used to study diffusion mechanisms during processes of solidification and phase transitions [54–56]. In particular, Antanovskii [57] performed model simulations of binary fluids with heat and mass transfer using the fluid composition as an order parameter. Similar models were also used to study spinodal decomposition as well as drop migration and coalescence processes by thermocapillary effects [58,59]. More recent simulations based on the diffuse-interface model coupled with vdW thermodynamics were reported by many authors to study liquid-vapor phase transitions by spinodal decomposition and homogeneous nucleation [17-20] and explosive vaporization in drops [21-23] as well as by heterogeneous nucleation in infinitely extended fluids [16,60]. Diffuse interfaces arise naturally in the description of fluids near their critical point. It is well-known that at subcritical temperatures two fluid phases separated by an interface may coexist in equilibrium. However, as the critical point is approached from below the binodal curve, the diffuse interface becomes thicker and thicker, and the effects of surface tension decrease. Eventually, at the critical point, the interface becomes infinitely diffuse and the surface tension vanishes. In the context of critical phenomena, there are in the literature a few works dealing with the dynamics of diffuse interfaces. For example, Felderhof [61] derived the equations governing the dynamics of diffuse interfaces near the critical point using a Lagrangian formalism, while Langer et al. [62] studied the condensation of a vapor near its critical point using a coarse-grained approximation.

2.6.1 Mean-Field Approximation

In the mean-field approximation, the thermodynamics of the liquid-vapor transition phase and the diffuse interface are described by the vdW capillarity model [14]. In this model the free energy per unit volume of the fluid is given by

$$F(\rho, T, \nabla \rho) = F^{0}(\rho, T) + \frac{\lambda}{2} \nabla \rho \cdot \nabla \rho, \qquad (35)$$

where *F* is the volumetric free energy of the fluid, F^0 is its classical part, and λ is the capillarity coefficient, which depends only on the intermolecular potential. The non-local term, $\nabla \rho$, is necessary to ensure physical consistency and therefore a correct description of the diffuse interface. Noting that the differential of *F* can be written as

$$dF = -sdT + Gd\rho + \phi \cdot d(\nabla \rho), \tag{36}$$

where *s* is the entropy, *G* is the Gibbs free enthalpy, and ϕ is a vector to be defined later. The Second Law of Thermodynamics states that the entropy attains a maximum in a closed and isolated system in equilibrium.

Noting that the internal energy u = F + sT and using Eq. (36), the above statement is equivalent to

$$\delta \int_{V} \left[s + \mathcal{L}_{1}u(s,\rho,\nabla\rho) + \mathcal{L}_{2}\rho \right] dV = 0, \tag{37}$$

where δ is the variation, *V* is the fluid volume, and \mathcal{L}_1 and \mathcal{L}_2 are two constant Lagrange multipliers. Working out Eq. (37), the equilibrium conditions for the liquid and vapor phases are given by

$$T = \text{constant}, \quad \widehat{G} = G - \nabla \cdot \vec{\phi} = \text{constant}.$$
 (38)

These two conditions imply, respectively, that the temperature and generalized Gibbs free enthalpy must be uniform at equilibrium. By differentiation of Eq. (36) with respect to ρ , the equilibrium condition on both sides of the interface becomes

$$\frac{\partial F}{\partial \rho} = \widehat{G} = G - (\nabla \cdot \vec{\phi}) = \text{constant}, \tag{39}$$

where it has been made use of the identity

$$\vec{\phi} \cdot d(\nabla \rho) = \nabla \cdot (\vec{\phi} d\rho) - (\nabla \cdot \vec{\phi}) d\rho.$$
(40)

Since at equilibrium $G \to G^0 = \partial F^0 / \partial \rho$, it follows from Eq. (39) and differentiation of Eq. (35) that

$$\vec{\phi} = \lambda \nabla \rho, \tag{41}$$

and the equilibrium condition becomes

$$\frac{\partial F^0}{\partial \rho} - \lambda \nabla^2 \rho = \text{constant},\tag{42}$$

where $F^0 = F^0(\rho, T_0)$ and T_0 is the equilibrium temperature of the system. The explicit dependence of F on $\nabla \rho$ in Eq. (35) describes the internal structure of the diffuse interface and interprets the excess energy there as the surface tension. The equilibrium condition (42) is also valid for a bubble or droplet at equilibrium. In particular, by assuming a spherical coordinate system whose origin coincides with the center of the inclusion and constraining the system to spherical symmetry it is possible to derive the Laplace Eq. (17) from Eq. (42).

2.6.2 Modified Hydrodynamic Equations

The dependence of the fluid energy on the non-local term $\nabla \rho$ needs modification to the classical hydrodynamics Eqs. (20)–(23) to allow the description of the internal structure of the liquid-vapor interface and the interpretation of the surface tension as an energy concentrated there. Since the thermodynamic behavior of the fluid is not classical, the form of the classical mass, momentum, and energy balance equations must be expanded, and the following closure relations can be derived [14,15,23]

$$\mathbf{q} + \vec{\phi} \frac{d\rho}{dt} = -\kappa \nabla T \Rightarrow \mathbf{q} = -\kappa \nabla T - \vec{\phi} \frac{d\rho}{dt},\tag{43}$$

$$\mathbb{T} + \left(p - \rho \nabla \cdot \vec{\phi}\right) \mathbb{I} + \vec{\phi} \nabla \rho = \mathbb{S} \Rightarrow \mathbb{T} = \left(-p + \rho \nabla \cdot \vec{\phi}\right) \mathbb{I} - \vec{\phi} \nabla \rho + \mathbb{S},\tag{44}$$

where now the heat flux vector **q** not only involves the classical Fourier heat conduction but also a nonclassical contribution referred to as the interstitial working [63], while $\mathbb{S} = \mathbb{T} + p\mathbb{I}$ is the viscous stress tensor. The tensor \mathbb{S} must satisfy the condition $\mathbb{S} : \nabla \mathbf{v} \ge 0$ to comply with the Second Law of Thermodynamics. Using the above closure relations, the modified system of balance equations becomes

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{v},\tag{45}$$

$$\rho \frac{d\mathbf{v}}{dt} = \nabla \cdot (\mathbb{T} + \mathbb{K}), \tag{46}$$

$$\rho \frac{dU}{dt} = (\mathbb{T} + \mathbb{K}) : \nabla \mathbf{v} + \nabla \cdot (\kappa \nabla T) + \nabla \cdot \left(\lambda \nabla \rho \frac{d\rho}{dt}\right), \tag{47}$$

$$\rho \frac{dS}{dt} = \frac{1}{T} \mathbb{S} : \nabla \mathbf{v} + \frac{1}{T} \nabla \cdot (\kappa \nabla T), \tag{48}$$

where \mathbb{K} is the Korteweg stress tensor defined as

$$\mathbb{K} = \frac{\lambda}{2} \left(\rho \nabla^2 \rho + \frac{1}{2} \nabla^2 \rho^2 \right) \mathbb{I} - \lambda \nabla \rho \nabla \rho.$$
⁽⁴⁹⁾

This tensor vanishes as the system approaches the critical point as does the surface tension. The third term on the right-hand side of Eq. (47) is a non-classical energy flux associated with the capillarity coefficient λ and admits a different interpretation compared to all other terms. For instance, in the bulk of the liquid and vapor phases, this term vanishes because $d\rho/dt \rightarrow 0$, while in the interface it is different from zero and represents the vaporization rate. As a liquid particle crosses the interface it becomes a vapor particle and therefore $d\rho/dt < 0$ since its density decreases. This implies that the term is related to the propagation of latent heat through the interface. Although Eq. (48) is not necessary, it is solved to guarantee that the Second Law of Thermodynamics is always satisfied. The two terms on the right-hand side represents the entropy generation due to the irreversible processes of viscous dissipation and heat conduction, whose combined contribution must always be greater than zero so that the entropy maximizes (i.e., $dS \rightarrow 0$) as the system reaches equilibrium.

3 Fundamentals of the SPH Method

The SPH method was independently introduced in the literature in 1977 by Lucy [64] and Gingold et al. [65] for the numerical simulation of astrophysical flows of arbitrary geometry and at different spatial scales in three-space dimensions (3D). Since its invention, the method has found its way into an everincreasing number of research areas, including applications to different fields of physics, biology, engineering, health sciences, and computer graphics. SPH is grid-free and relies on a Lagrangian description of the fluid, where the fluid is represented by a finite number of discrete particles (or interpolation points). Unlike traditional mesh-dependent schemes, SPH is easy to handle under complicated physics and deformable boundaries. In this section, we shall first introduce some fundamental aspects of SPH followed by details on the discretization of the continuum equations of thermohydrodynamics.

3.1 General Remarks on SPH

SPH is based on interpolation theory and uses as a starting point the well-known Dirac sifting property

$$f(\mathbf{x}) = \int_{\Omega} f(\mathbf{x}') \delta(\mathbf{x} - \mathbf{x}') d^{n} \mathbf{x}',$$
(50)

where $f(\mathbf{x})$ is a continuous and differentiable function defined in the domain $\Omega \in \mathbb{R}^n$, \mathbf{x} is a generic point in Ω , $\delta(\mathbf{x} - \mathbf{x}')$ is the Dirac- δ distribution, and n (= 1, 2, or 3) denotes the spatial dimension. In contrast to conventional grid-based schemes, SPH consists of two approximations, namely the *kernel* and the *particle* approximation. The kernel approximation of $f(\mathbf{x})$ is obtained by replacing the Dirac- δ distribution in the integrand of Eq. (50) by a bell-shaped interpolation function, $W(||\mathbf{x} - \mathbf{x}'||, h)$, such that

$$\langle f(\mathbf{x}) \rangle = \int_{\Omega} f(\mathbf{x}') W(\| \mathbf{x} - \mathbf{x}' \|, h) d^{n} \mathbf{x}',$$
(51)

where $\langle f(\mathbf{x}) \rangle$ is the so-called kernel (or smoothed) estimate of $f(\mathbf{x})$ and h is the smoothing length specifying the radius of influence of the kernel. In most modern applications of SPH, a compactly supported kernel is employed so that W = 0 for $|| \mathbf{x} - \mathbf{x}' || \ge kh$, where k is some dilation factor usually ≤ 2 . In general, the kernel must satisfy the normalization condition

$$\int_{\Omega} W(\|\mathbf{x} - \mathbf{x}'\|, h) d^{n} \mathbf{x}' = 1,$$
(52)

and in order to be a suitable interpolation function it must approach the Dirac- δ distribution in the limit when $h \rightarrow 0$. The kernel must also satisfy some other properties, for example, to be a positive-definite, a monotonically decreasing, and an even function. For a fluid of density $\rho(\mathbf{x})$, Eq. (51) is more conveniently written as

$$\langle f(\mathbf{x}) \rangle = \int_{\Omega} \left[\frac{f(\mathbf{x}')}{\rho(\mathbf{x}')} \right] W(\| \mathbf{x} - \mathbf{x}' \|, h) \rho(\mathbf{x}') d^n \mathbf{x}'.$$
(53)

Direct differentiation of Eq. (53) with respect to coordinate **x** yields the expression for the kernel estimate of the gradient $\nabla f(\mathbf{x})$

$$\langle \nabla f(\mathbf{x}) \rangle = \int_{\Omega} \left[\frac{f(\mathbf{x}')}{\rho(\mathbf{x}')} \right] \nabla W(\| \mathbf{x} - \mathbf{x}' \|, h) \rho(\mathbf{x}') d^n \mathbf{x}',$$
(54)

where ∇ is the nabla operator. Noting that $\partial W/\partial x = \partial W/\partial x'$ and the same for the partial derivatives of W with respect to y and z, it is a simple matter to show that

$$\nabla' W(\parallel \mathbf{x} - \mathbf{x}' \parallel, h) = -\nabla W(\parallel \mathbf{x} - \mathbf{x}' \parallel, h),$$

where ∇' is the nabla operator with respect to the primed coordinates \mathbf{x}' . On the other hand, it is also easy to show that the gradient of the kernel estimate of $f(\mathbf{x})$ is exactly equal to the estimate of the $\nabla f(\mathbf{x})$, leading to the well-known identity $\nabla \langle f(\mathbf{x}) \rangle = \langle \nabla f(\mathbf{x}) \rangle$. Similarly, the kernel estimate of the divergence of a vector function, say $\mathbf{f}(\mathbf{x})$, admits the following representation

$$\langle \nabla \cdot \mathbf{f}(\mathbf{x}) \rangle = \int_{\Omega} \left[\frac{\mathbf{f}(\mathbf{x}')}{\rho(\mathbf{x}')} \right] \cdot \nabla W(\| \mathbf{x} - \mathbf{x}' \|, h) \rho(\mathbf{x}') d^{n} \mathbf{x}'.$$
(55)

In a similar form the kernel estimate of the gradient of a vector function, f(x), can be obtained from Eq. (54) by simply replacing the scalar function, f(x), with the vector function, f(x).

The particle (or SPH) approximation is obtained by dividing the computational domain, Ω , into *N* small Lagrangian cells of volume Ω_a (with a = 1, 2, ..., N) and boundaries $\partial \Omega_a$ so that an interpolation point (or particle) is defined within each cell at position $\mathbf{x}_a \in \Omega_a$. A mass, m_a , and density, ρ_a , are assigned to each particle *a* such that the sum of all particle masses equals the total mass of the system. Fig. 1 shows schematically the discretization procedure in a portion of the computational domain. The circle centered at the location of the observation particle *a* represents the spherical volume of the kernel support, Ω_s . The particles that fall within the kernel support are the neighbors of particle *a*. Using the mean value theorem so that $\mathbf{x}_b \in \Omega_b$ for each neighbor *b* of the observation particle *a* and identifying the term $\rho(\mathbf{x}')d^n\mathbf{x}'$ in the integrand of Eq. (53) with the differential mass m_b of a neighbor particle, the SPH approximation of Eq. (53) can be written as the summation interpolant

$$f_a = \sum_{b=1}^{n_{\text{neigh}}} m_b \frac{f_b}{\rho_b} W_{ab},\tag{56}$$

where $f_a = \langle f(\mathbf{x}_a) \rangle$, $\rho_b = \rho(\mathbf{x}_b)$, and $W_{ab} = W(||\mathbf{x}_a - \mathbf{x}_b||, h)$. As it is common practice in SPH notation, the subscript *a* is used to denote a generic observation particle and the subscript *b* to denote its neighboring companions. Following similar steps, the SPH approximation of Eq. (54) becomes

$$(\nabla f)_a = \sum_{b=1}^{n_{\text{neigh}}} m_b \frac{f_b}{\rho_b} \nabla_a W_{ab}.$$
(57)

Higher accuracy for the estimation of the gradient can be obtained using the alternative representation

$$(\nabla f)_a = \frac{1}{\rho_a} \sum_{b=1}^{n_{\text{neigh}}} m_b (f_b - f_a) \nabla_a W_{ab}, \tag{58}$$

which guarantees that the gradient vanishes exactly when $f(\mathbf{x})$ is a constant. Other representations are guided by momentum conservation requirements [11,67,68]. For example, consistent approximations to the pressure forces and compressional work in the momentum and energy equations, which lead to improved angular momentum conservation, are achieved using the symmetrized form

$$(\nabla f)_a = \rho_a \sum_{b=1}^{n_{\text{neigh}}} m_b \left(\frac{f_a}{\rho_a^2} + \frac{f_b}{\rho_b^2} \right) \nabla_a W_{ab}.$$
(59)

In addition, a convenient SPH replacement of Eq. (55) for the divergence of a vector function, which is frequently encountered in the literature, is given by the expression

$$(\nabla \cdot \mathbf{f})_a = \frac{1}{\rho_a} \sum_{b=1}^{n_{\text{neigh}}} m_b (\mathbf{f}_b - \mathbf{f}_a) \cdot \nabla_a W_{ab}.$$
(60)

Other variants of Eqs. (58) and (60) can be found in the literature where the factor $1/\rho_a$ is replaced either by $1/\rho_b$ or $1/\bar{\rho}_{ab} = 2/(\rho_a + \rho_b)$, which are all of comparable accuracy. A peculiar feature of SPH is that the discrete particle equations are assembled by replacing the field functions and gradients with their basic SPH interpolation formulae.



Figure 1: Schematic drawing showing the SPH discretization and the kernel support. Figure taken from Sigalotti et al. [66]

3.2 The SPH Heat Conduction Equation

In almost all SPH studies of evaporation and condensation processes, the heat conduction Eq. (27) is written in particle form using the formulation introduced by Cleary et al. [69], namely

$$\frac{dT_a}{dt} = \frac{1}{c_p} \sum_{b=1}^{n_{\text{neigh}}} \frac{m_b}{\rho_a \rho_b} \frac{4\kappa_a \kappa_b}{(\kappa_a + \kappa_b)} \frac{T_{ab} \mathbf{x}_{ab} \cdot \nabla_a W_{ab}}{(\| \mathbf{x}_{ab} \|^2 + \varepsilon)},\tag{61}$$

where $T_{ab} = T_a - T_b$, $\mathbf{x}_{ab} = (x_a - x_b)\mathbf{i} + (y_a - y_b)\mathbf{j} + (z_a - z_b)\mathbf{k}$ in rectangular coordinates, $\|\mathbf{x}_{ab}\|^2$ is the squared distance between particle *a* and its neighbor *b*, and $\varepsilon = 0.01h^2$ to prevent singularities when two particles become too close to each other. This standard SPH formulation is numerically stable and ensures continuity of heat fluxes across discontinuities in material properties [31,40,61,70].

3.3 Smoothed Particle Equations of Evaporating Multiphase Flows

A model based on Eqs. (28)–(32) was proposed by Yang et al. [27] to simulate heat and mass transfer across liquid-vapor interfaces, which was then employed in many recent SPH simulations of evaporating multiphase flows [28–30,32,71]. In SPH particle form these equations read as follows:

$$\frac{d\rho_a}{dt} = \sum_{b=1}^{n_{\text{neigh}}} m_b (\mathbf{v}_a - \mathbf{v}_b) \cdot \nabla_a W_{ab} + \dot{m}^m, \tag{62}$$

$$\frac{d\mathbf{v}_{a}}{dt} = -\sum_{b=1}^{n_{\text{neigh}}} m_{b} \left(\frac{p_{a} + p_{b}}{\rho_{a}\rho_{b}} + \Pi_{ab} \right) \nabla_{a} W_{ab} + \sum_{b=1}^{n_{\text{neigh}}} \frac{m_{b}}{\rho_{a}\rho_{b}} \frac{4\eta_{a}\eta_{b}}{(\eta_{a} + \eta_{b})} \frac{(\mathbf{v}_{a} - \mathbf{v}_{b})\mathbf{x}_{ab} \cdot \nabla_{a} W_{ab}}{(\|\mathbf{x}_{ab}\|^{2} + \varepsilon)} + \mathbf{g}, \tag{63}$$

$$\frac{dT_a}{dt} = \frac{1}{c_p} \sum_{b=1}^{n_{\text{neigh}}} \frac{m_b}{\rho_a \rho_b} \frac{4\kappa_a \kappa_b}{(\kappa_a + \kappa_b)} \frac{T_{ab} \mathbf{x}_{ab} \cdot \nabla_a W_{ab}}{(\||\mathbf{x}_{ab}\|^2 + \varepsilon)} - \frac{\Delta H_{\text{vap}}}{\rho c_p} \dot{m}^m, \tag{64}$$

$$\frac{dY_a}{dt} = \sum_{b=1}^{n_{\text{neigh}}} \frac{m_b}{\rho_a \rho_b} \frac{(\rho_a D_a + \rho_b D_b)(Y_a - Y_b) \mathbf{x}_{ab} \cdot \nabla_a W_{ab}}{(\| \mathbf{x}_{ab} \|^2 + \varepsilon)}.$$
(65)

Note that the viscous acceleration in the Navier-Stokes Eq. (28) and the right-hand side of the continuity-like equation for vapor species (31) are set in particle form using the same SPH replacement for

the conduction Eq. (61). The term Π_{ab} is an artificial viscosity proposed by Monaghan [43], defined as

$$\Pi_{ab} = \frac{-\alpha \bar{c}_{ab} \mu_{ab} + 2\beta \mu_{ab}^2}{\bar{\rho}_{ab}},\tag{66}$$

if $(\mathbf{v}_a - \mathbf{v}_b) \cdot \mathbf{x}_{ab} < 0$ and 0 otherwise, where $\mu_{ab} = [h(\mathbf{v}_a - \mathbf{v}_b) \cdot \mathbf{x}_{ab}]/(||\mathbf{x}_{ab}||^2 + \varepsilon)$, $\bar{c}_{ab} = (c_a + c_b)/2$ is the average sound speed associated with particles *a* and *b*, and $\bar{\rho}_{ab} = (\rho_a + \rho_b)/2$. The parameters α and β control the strength of the artificial viscosity.

In this model, the effects of surface tension are calculated by adding a term of the form [72]

$$\mathbf{F}_{s} = \frac{\sigma}{\rho} K \mathbf{n} \delta^{s}, \tag{67}$$

to the right-hand side of Eq. (28), where σ is the coefficient of surface tension, K is the surface curvature, **n** is the unit vector normal to the surface, and δ^s is a delta function. The unit normal vector is defined in terms of the gradient of a color function C, where $\mathbf{n} = \nabla C / |\nabla C|$ and the surface curvature is given by $K = -\nabla \cdot \mathbf{n}$ [29]. In smoothed particle form the expressions for the gradient of the color function and the surface curvature is given by [73]

$$\nabla C_a = \frac{\rho_a}{V_a} \sum_{b=1}^{n_{\text{neigh}}} \frac{V_a^2 + V_b^2}{\rho_a + \rho_b} \nabla_a W_{ab},\tag{68}$$

$$K = -\nabla \cdot \mathbf{n}_{a} = d \frac{\sum_{b=1}^{n_{\text{neigh}}} V_{a}(\mathbf{n}_{a} - \mathbf{n}_{b}) \cdot \nabla_{a} W_{ab}}{\sum_{b=1}^{n_{\text{neigh}}} |V_{a} \mathbf{x}_{ab} \cdot \nabla_{a} W_{ab}},$$
(69)

where $V_a = m_a/\rho_a$ is the volume associated with particle *a* and *d* is a dimension factor. Note that when particles *a* and *b* are of different phases then the color function $C_{ab} = 1$ and zero otherwise. The surface tension force (67) admits the following SPH representation [28,29]

$$\mathbf{F}_{s,a} = -\frac{\sigma d}{\rho_a V_a} (\nabla \cdot \mathbf{n})_a (\nabla C)_a.$$
⁽⁷⁰⁾

Most recent SPH simulations using the above formulation have focused mainly on studying drop evaporation as a result of contact with a heated solid surface. To model the vapor generated by the liquid drop after contact with a heated wall an additional force, \mathbf{F}_{w} , must be added to the right-hand side of Eq. (28), which simulates the effects of wall temperature, T_{w} , and ambient pressure, p_{amb} , on either drop rebound from the wall or film splashing when $T_{w} > T_{boil}$. This force is calculated according to the following prescription

$$\mathbf{F}_{w} = \frac{1}{2} C_{w} \left[\left(\frac{T_{w}}{T_{\text{boil}}} \right)^{2} - 1 \right] \left(\frac{p_{\text{amb}}}{p_{\text{atm}}} + 1 \right) \frac{p_{\text{ref}}}{\rho_{l} \rho_{w}} \nabla_{l} W_{\text{lw}}, \tag{71}$$

where p_{atm} is the atmospheric pressure, p_{ref} is the reference pressure in Eq. (11), and the subscripts l and w denote the liquid and wall particles, respectively. The coefficient C_w is usually set equal to 0.9. The boiling temperature, T_{boil} in Eqs. (34) and (71) is calculated using the Clausius-Clapeyron equation (see Ref. [28] for more details). As a final step, the volumetric mass flux at the liquid-vapor interface, \dot{m}^m , is calculated using the smoothed particle representation

$$\dot{m}^{m} = \sum_{l} \frac{2\rho_{v}m_{l}\mathscr{D}_{v}(\mathbf{x}_{v} - \mathbf{x}_{l}) \cdot \nabla_{v}W_{vl}}{\rho_{l}(\|\mathbf{x}_{vl}\|^{2} + \varepsilon)(1 - Y_{v})}(Y_{v} - Y_{l}),$$
(72)

where the subscript v denotes vapor particles. Note that the term \dot{m}^m on the right-hand side of Eq. (62) works only for vapor particles interacting with liquid particles near the liquid-vapor interface. This is so because during evaporation only the vapor density changes. Moreover, since the energy of the liquid phase is reduced as the latent heat is consumed by evaporation, the second term on the right-hand side of Eq. (64) has to be calculated only for liquid particles within the interface [28]. The rate of mass transfer when a liquid particle evaporates into a vapor particle is given by the relation

$$\dot{m}_{vl} = -\dot{m}_{lv} = \frac{2m_v m_l \mathscr{D}_v (\mathbf{x}_v - \mathbf{x}_l) \cdot \nabla_v W_{vl}}{\rho_l (\|\|\mathbf{x}_{vl}\|^2 + \varepsilon)(1 - Y_v)} (Y_v - Y_l),$$
(73)

so that the total mass change rates of vapor and liquid particles are

$$\dot{m}_{\rm v} = \sum_{\rm l} \dot{m}_{\rm vl},\tag{74}$$

$$\dot{m}_1 = \sum_{v} \dot{m}_{1v}.$$
(75)

The saturated vapor mass fraction and vapor molar mass are calculated using Eqs. (33) and (34), respectively. During evaporation, the mass of vapor particles will increase at the interface, while that of liquid particles will consequently decrease. This implies that the mass of SPH particles changes during the numerical simulation. Therefore, to prevent large differences in the mass among particles about the same phase, Yang et al. [28] have implemented the criterion that when a mass particle exceeds a large critical value, the particle splits into two small particles, while on the contrary, if the mass particle is smaller than a small critical value, the particle merges with its nearest neighboring particle. For more details on the particle splitting and merging procedures, the interested reader is referred to Refs. [28,74].

3.4 Smoothed Particle Non-Classical Equations Describing a Diffuse Interface

An alternative SPH scheme to the one developed more recently by Yang et al. [27,28], known as the van der Waals square gradient model, was introduced in the literature by Charles et al. [15] in late 2011 to study the nanoscale condensation of water. This model is based on an extension of Nugent et al.'s [12] formulation to include non-classical thermodynamics through a diffuse-interface description, where the inhomogeneous interfacial region is described as smoothly varying in density. This model has been extensively applied by many authors to study first-order phase transitions and equilibrium properties of vdW multiphase systems, resulting from ordinary evaporation [17–20] and explosive vaporization [21–23] of liquid drops, and is based on the modified balance Eqs. (45)–(48), which admit the following smoothed particle representations

$$\frac{d\rho_a}{dt} = \rho_a \sum_{b=1}^{n_{\text{neigh}}} \frac{m_b}{\rho_b} \mathbf{v}_{ab} \cdot \nabla_a W_{ab}, \tag{76}$$

$$\frac{d\mathbf{v}_a}{dt} = \sum_{b=1}^{n_{\text{neigh}}} m_b \left(\frac{\mathbb{T}'_a}{\rho_a^2} + \frac{\mathbb{T}'_b}{\rho_b^2} \right) \cdot \nabla_a W_{ab} + 2\bar{a} \sum_{b=1}^{n_{\text{neigh}}} m_b \nabla_a W_{ab}^H + \sum_{b=1}^{n_{\text{neigh}}} m_b \left(\frac{\mathbb{K}_a^H}{\rho_a^2} + \frac{\mathbb{K}_b^H}{\rho_b^2} \right) \cdot \nabla_a W_{ab}^H, \tag{77}$$

$$\frac{dU_{a}}{dt} = \frac{1}{2} \sum_{b=1}^{n_{\text{neigh}}} m_{b} \left(\frac{\mathbb{T}'_{a}}{\rho_{a}^{2}} + \frac{\mathbb{T}'_{b}}{\rho_{b}^{2}} \right) : \mathbf{v}_{ba} \nabla_{a} W_{ab} + \tilde{a} \sum_{b=1}^{n_{\text{neigh}}} m_{b} \mathbf{v}_{ba} \cdot \nabla_{a} W_{ab}^{H}
+ \frac{1}{2} \sum_{b=1}^{n_{\text{neigh}}} m_{b} \left(\frac{\mathbb{K}_{a}^{H}}{\rho_{a}^{2}} + \frac{\mathbb{K}_{b}^{H}}{\rho_{b}^{2}} \right) : \mathbf{v}_{ba} \nabla_{a} W_{ab}^{H} + \sum_{b=1}^{n_{\text{neigh}}} \frac{m_{b}}{\rho_{a}\rho_{b}} \frac{4\kappa_{a}\kappa_{b}}{(\kappa_{a} + \kappa_{b})} \frac{T_{ab}\mathbf{x}_{ab} \cdot \nabla_{a} W_{ab}}{(\|\mathbf{x}_{ab}\|^{2} + \varepsilon)}
+ \lambda \sum_{b=1}^{n_{\text{neigh}}} \frac{m_{b}}{\rho_{a}\rho_{b}} \left(\frac{d\rho_{a}}{dt} + \frac{d\rho_{b}}{dt} \right) \frac{\rho_{ab}\mathbf{x}_{ab} \cdot \nabla_{a} W_{ab}}{(\|\mathbf{x}_{ab}\|^{2} + \varepsilon)},$$
(78)

$$\frac{dS_a}{dt} = \frac{1}{2T_a} \sum_{b=1}^{n_{\text{neigh}}} m_b \left(\frac{\mathbb{S}_a}{\rho_a^2} + \frac{\mathbb{S}_b}{\rho_b^2} \right) : \mathbf{v}_{ba} \nabla_a W_{ab} + \frac{1}{T_a} \sum_{b=1}^{n_{\text{neigh}}} \frac{m_b}{\rho_a \rho_b} \frac{4\kappa_a \kappa_b}{(\kappa_a + \kappa_b)} \frac{T_{ab} \mathbf{x}_{ab} \cdot \nabla_a W_{ab}}{(\|\mathbf{x}_{ab}\|^2 + \varepsilon)}, \tag{79}$$

where $\mathbf{v}_{ab} = \mathbf{v}_a - \mathbf{v}_b$, $\mathbb{T}' = \mathbb{T} - \bar{a}\rho^2 \mathbb{I}$, \mathbb{K} is the Korteweg tensor given by Eq. (49), and $W_{ab}^H = W(||\mathbf{x}_{ab}||, H)$ is the kernel function evaluated at a longer smoothing length $(H \ge 2h)$. This is a necessary condition to improve interfacial stability in the evaluation of the attractive, long-range central forces implied by the vdW cohesive term $-\bar{a}\rho^2$ in Eq. (3) and the Korteweg forces. Stable SPH representations are used to evaluate the components of the Korteweg tensor in Eqs. (77) and (78) (see Ref. [17] for more details). The second term on the right-hand side of Eqs. (77) and (78) accounts for the effects of surface tension so that there is no need for additional force terms. Eq. (79) for the the time rate of change of the entropy has been introduced by Díaz-Damacillo et al. [23] in recent work to measure the consistency of the simulations with the Second Law of Thermodynamics. Instead of the value of the particle entropy, S_a , the main interest lie in the change of entropy for each particle over time: $\Delta S_a^{l \rightarrow l+1} = S_a^{l+1} - S_a^l$, where *l* denotes the time level. The total entropy change in a timestep is then given by

$$\Delta S^{l \to l+1} = \sum_{a=1}^{N} \Delta S_a^{l \to l+1},\tag{80}$$

so that $\Delta S^{l \to l+1} \ge 0$ for all timesteps to satisfy the Second Law of Thermodynamics.

4 SPH Models of Drop Evaporation with Standard Classical Thermodynamics

The first SPH simulations of drop circularization by surface tension and evaporation at subcritical temperatures were reported by Nugent et al. [12]. In their two-dimensional models, the liquid-to-vapor phase transition in evaporating drops was calculated using a vdW equation of state. Unlike most SPH simulation models of free-surface flows at that time, surface tension was not handled as an input parameter since it arises naturally from the cohesive part of the vdW equation of state. At the vapor-liquid interface, the vdW cohesive action translates into an attractive, long-range force normal to the interface that points toward the bulk of the liquid phase, so that there is no need to explicitly track the surface since the details of the local surface curvature are reproduced automatically. The SPH governing equations employed by Nugent et al. [12] include the summation interpolant for the particle density

$$\rho_a = \sum_{a=1}^{\text{neigh}} m_a W_{ab},\tag{81}$$

which conserves mass exactly and replaces the smoothed particle continuity Eq. (76) to second-order accuracy. The momentum balance equation is the same as Eq. (77) without the last term on the right-hand

side, while the specific internal energy is as Eq. (78) but without the third and fifth terms on the right-hand side and with the smoothed heat conduction term given instead by the symmetrized representation

$$-\sum_{a=1}^{\text{neigh}} m_a \left(\frac{\mathbf{q}_a}{\rho_a^2} + \frac{\mathbf{q}_b}{\rho_b^2} \right) \cdot \nabla_a W_{ab}, \tag{82}$$

where $\mathbf{q} = -\kappa \nabla T$ is the heat flux vector. On the other hand, Nugent et al. [12] first noticed that to obtain stable spherical (circular) drops and handle the effects of surface tension properly, the short- and longrange components of the vdW equation of state must be evaluated separately. In particular, they noticed that improved interfacial stability can be obtained by increasing the interaction range of the cohesive term in the momentum and energy equations to a smoothing length $H(\geq 2h)$ compared to *h* for all other forces. This distinction between short- and long-range forces (second term on the the right-hand side of Eqs. (77) and (78)) leads to the cohesive contributions for the acceleration and heating

$$\frac{d\mathbf{v}_a}{dt} = 2\bar{a} \sum_{b=1}^{n_{\text{neigh}}} m_b \nabla_a W_{ab}^H,\tag{83}$$

$$\frac{dU_a}{dt} = \bar{a} \sum_{b=1}^{n_{\text{neigh}}} m_b \mathbf{v}_{ba} \cdot \nabla_a W_{ab}^H, \tag{84}$$

respectively. The right-hand side of Eq. (83) strongly resembles the form used by Morris et al. [75] to estimate the surface normals for the calculation of surface curvatures with SPH in the framework of the continuum-surface-force (CSF) method. The choice of H was determined by the same considerations that led to interfacial stability with the CSF method. Thus, the forces represented by Eq. (83) largely cancel in the bulk of the liquid, except for a small strip of width H around the drop surface, where liquid particles are constrained to move inward in the opposite direction to the outward surface normal, leading to a net surface tension due to the local surface curvature. As the interpolating function, Nugent et al. [12] used the quartic spline kernel introduced by Lucy [64]

$$W(r,h) = \begin{cases} \frac{5}{\pi h^2} \left(1 + \frac{3r}{h}\right) \left(1 - \frac{r}{h}\right)^3 & \text{if } r < h, \\ 0 & \text{if } r \ge h, \end{cases}$$

$$\tag{85}$$

which is appropriate in two-space dimensions. In all simulations, they used 2500 SPH particles of equal mass $(m_a = m)$ and started the simulations from a square-shaped drop by imposing periodic boundary conditions on a much larger square box. As was already mentioned in Section 2.1, Eqs. (3) and (6) were employed with vdW parameters m = 1, $\bar{a} = 2$, $\bar{b} = 0.5$, and $\bar{k}_B = 1$ in reduced units. In these units the shear and bulk viscosity coefficients were set to $\eta = 1$ and $\zeta = 0.1$, while a heat conductivity $\kappa = 5$ this large was used to reduce the density fluctuations and allow a rapid adjustment of the temperature. The smoothing lengths were set to h = 5 and H = 2h = 10.

Square drops of length L = 50, starting with subcritical temperatures ($T < T_{cr}$), were evolved until circular drops in thermo-mechanical equilibrium were obtained as shown in Fig. 2. In particular, Fig. 2a shows a circular equilibrium drop formed from a subcritical temperature T = 0.2. In this case the drop rounds off by surface tension effects without evaporating. As the initial temperature is increased to T = 0.6 (Fig. 2b), 0.87 (Fig. 2c), and 1.05 (Fig. 2d), circular drops surrounded by a vapor atmosphere are formed in equilibrium. Evidently, the evaporation rate at the surface of the liquid drop increases with increasing initial temperature as shown in Fig. 2d, which started with a temperature close to the critical value ($T_{cr} = 32/27 \approx 1.185$).

In a very recent work Harisankar et al. [24] used Nugent et al.'s [12] model to study the formation of bare liquid drops by surface tension and their evaporation when a small amount of energy, corresponding to 10% of the maximum particulate specific internal energy is added to the evolving drop every time step till 10,000 time steps after which the heat supply was stopped. In essence, their model differed from Nugent et al.'s [12] approach only in the choice of the kernel function. In this case, Lucy's [64] kernel was replaced by the hyperbolic-shaped kernel function introduced by Yang et al. [76], namely

$$W(q,h) = \alpha_d \begin{cases} q^3 - 6q + 6 & \text{if } 0 \le q < 1, \\ (2-q)^3 & \text{if } 1 < q < 2, \\ 0 & \text{if } q \ge 2, \end{cases}$$
(86)

where $q = r/h = ||\mathbf{x} - \mathbf{x}'|| /h$, while $\alpha_d = 1/(7h)$, $1/(3\pi h^2)$, and $15/(62\pi h^3)$ in one-, two-, and three-space dimensions, respectively. Unlike other kernels used in the literature, this kernel is claimed to possess positive second-order derivatives over its compact support. This is a desirable property because it guarantees that repulsive forces between pairs of SPH particles do not vanish as they become close enough during a compression. In addition, under a negative stress (i.e., positive pressure) the calculation remains stable against the tensile instability. This instability may result in unphysical clustering of SPH particles or a complete blow-up of the particle positions to infinity [77–80]. As an example, the structure of the bare drop displayed in Fig. 2a is plagued by a tensile instability which is evident by the clustering of SPH particles in concentric circular rings separated by void spaces. In the absence of such instability we would expect the liquid phase to be characterized by a uniform distribution of particles.



Figure 2: Stable circular drops in equilibrium with their vapor atmosphere formed from a square-shaped vdW liquid of initial subcritical temperature (a) $T_0 = 0.2$, (b) 0.6, (c) 0.87, and (d) 1.05 in reduced units. In all cases N = 2500 SPH particles were used in a square box of side L = 50. Figure taken from Nugent et al. [12]

Harisankar et al. [24] simulated the complete vaporization of a model circular drop of initial temperature T = 0.43 and density $\rho = 1.76$ in reduced units. As more heating is supplied to the drop, the drop temperature

increases and its size decreases with time as more liquid particles are converted into vapor particles. Since the simulation was confined to a square box of side L = 120 with impenetrable walls, the average vapor density was seen to increase as a result of continued evaporation. Fig. 3 shows snapshots of the evaporation process at different times during the evolution along with the corresponding radial density and pressure profiles of the drop-vapor coexisting system. The core density of the drop shrinks and the pressure goes up and down within the liquid-vapor interface. This dip is the result of an unphysical loop displayed by the vdW equation of state at a subcritical temperature due to the hard-core repulsion, indicating an unstable state across the interface. The depth of the pressure dip decreases with time and eventually disappears at t = 2200 when the drop has completely vaporized. They also studied the effects of varying the box size, finding that the boiling temperature decreases as the box size increases, while the drop size remains unaltered. A similar formulation was previously employed by Ray et al. [25] to study the phenomenon of liquid oscillation, the binary collision of vdW drops at high velocity, and the vapor-liquid equilibrium of a vdW drop. They stressed the importance of using a variable smoothing length to accurately capture the physics of a sparse vapor medium. They also found that as the critical temperature is approached, the liquid-vapor interface becomes blurred in agreement with expectations at supercritical environments.

The drop evaporation by impingement on heated surfaces is a related topic of research that has attracted great interest in science and engineering due to its occurrence in many industrial processes, such as, for example, spray cooling, fuel injection, fire suppression systems, inkjet printing, and fuel spray in internal combustion engines, among many other applications. Numerous recent SPH simulations relying on variants of the Nugent et al.'s [12] approach have been performed to study the spreading and evaporation of drops impacting upon heated solid surfaces. In particular, Yang et al. [26] performed three-dimensional simulations of the interaction of fuel (n-heptane) drops with heated surfaces. They used 125,000 SPH particles to represent the drop and 3000 particles to model the solid wall. To predict the liquid-vapor equilibrium, the Peng-Robinson Eq. (13) was employed along with the caloric Eq. (14) and the cohesive parameter as defined by Eq. (15). In order to remove the tensile instability, the hyperbolic-shaped kernel (86) was used. This model was validated against experimental observations of the spreading of ethanol drops after their impact on a heated surface [81,82]. Fig. 4 shows the time evolution of the experimentally measured spread size of 2.4 mm diameter ethanol drop after impacting on a surface at 24° C with a velocity of 3.1 m s⁻¹ [81] as compared with the numerical results (left) and the experimental spread factor of *n*-heptane drops impacting a stainlesssteel surface at different temperatures between 24° C and 200° C with a velocity equal to 0.93 m s⁻¹ [82] as compared with the numerical predictions (right). In both cases the numerical simulations were found to reproduce fairly well the trends of the experimental data.

The evolution of a 1.5 mm diameter *n*-heptane drop impinging on a heated surface at different temperatures is depicted in Fig. 5 at discrete times. In order to better illustrate the liquid surface deformation the vapor atmosphere around the drop has been removed. In all cases, during the first ms after contact with the surface, the drop spreads into a thin film. Thereafter the retarding effects of surface tension, liquid viscosity, and friction forces between the liquid and the wall slow down the spreading, while the liquid at the center has enough inertia to form a visible cusp. As the wall temperature is increased, the spreading rate decreases. For instance, as shown in the right frame of Fig. 4, at wall temperatures just above 100°C, the spread diameter reaches a maximum and then shrinks as the drop recoils due to surface tension. The Leidenfrost temperature is reached at 200°C when a thin layer of vapor is formed between the liquid and the wall. At this temperature and above, the drop completely recoils and rebounds from the surface. Further simulations with varying impact velocities (i.e., varying Weber numbers, We = $\rho v^2 D/\sigma$, where *v* is the drop velocity at impact and *D* is its diameter) show that at all temperatures there is a critical We beyond which the drop disintegrates into secondary droplets. As the wall temperature increases the critical We decreases, reaching

a minimum value at the Leidenfrost temperature above which the We number remains the same. Fig. 6 shows three different regimes of drop breakup for a wall temperature of 350°C well above the Leidenfrost point for increasing We. From left to right these three regimes can be identified as "receding breakup", "drop disintegration", and "splashing". The impingement of an oil drop on walls with different conditions was further studied by Ma et al. [70] in order to better understand the splashing mechanism in engine conditions. They proposed a new splashing sub-model to determine the ratio of splashed mass during the impact process which is thought to be the main factor influencing the mixture.



Figure 3: Sequence of snapshots showing the evolution to complete vaporization of a bare drop consisting of 1740 SPH particles with an initial temperature T = 0.43 in reduced units (left column). The middle and right columns display the corresponding radial density and pressure profiles. Figure taken from Harisankar et al. [24]



Figure 4: (Left) Time evolution of the spread diameter of a 2.4 mm diameter ethanol drop impacting on a solid wall at $T_w = 24^{\circ}$ C with a velocity of 3.1 m s⁻¹. (Right) Time evolution of the spread factor, defined as the ratio of the liquid diameter on the wall after impact with the original liquid diameter, of *n*-heptane drops impacting on a stainless-steel surface at different temperatures with a velocity of 0.93 m s⁻¹ (symbols: experimental measurements; lines: numerical results). Figure taken from Yang et al. [26]



Figure 5: Deformation of a 1.5 mm diameter *n*-heptane drop at three different times after impact on a surface at different temperatures. The vapor atmosphere around the spreading drop due to evaporation has been removed for clarity. Figure taken from Yang et al. [26]

A modified SPH model to simulate the spreading dynamics of nanofluid droplets on heated walls was recently proposed by Liu et al. [40], where the fluid surface tension and wetting absorption during droplet wetting on a solid surface is modeled by adding a source force, \mathbf{F}_s , in the momentum equation, defined as the sum within the kernel support domain of the attractive force among particles, \mathbf{F}_{ab} , given by the expression [83]

$$\mathbf{F}_{ab} = s_{ab} \cos\left(\frac{1.5\pi}{3h} \parallel \mathbf{x}_a - \mathbf{x}_b \parallel\right) \frac{\mathbf{x}_a - \mathbf{x}_b}{\parallel \mathbf{x}_a - \mathbf{x}_b \parallel},\tag{87}$$

if $\| \mathbf{x}_a - \mathbf{x}_b \| \le h$ and 0 otherwise, where s_{ab} is the strength of the surface tension. In addition, natural convection inside the drop is accounted for by adding a buoyancy force, \mathbf{F}_b , due to temperature differences given by

$$\mathbf{F}_{\rm b} = \mathbf{g}\beta(T - T_{\rm ref}),\tag{88}$$

where **g** is the gravitational acceleration vector, β is the coefficient of thermal expansion, and T_{ref} is a reference temperature. In this case, a water droplet is modeled using the Murnaghan-Tait pressure-density

relation given by Eq. (12) with added nanoparticles whose effective properties are formulated according to Liu et al.'s [40], Eqs. (8)–(12). The drop evaporation model is described by solving a SPH heat conduction equation of the form given by Eq. (61) but with the particle temperature replaced by the particle enthalpy, \mathcal{H} , in the temporal derivative with

$$\mathscr{H} = \begin{cases} c_{\rm p} T & \text{if } T < T_{\rm boil}, \\ c_{\rm p} T_{\rm boil} + \mathscr{U} & \text{if } T \ge T_{\rm boil} & \text{and } 0 \le U \le \Delta H_{\rm vap}, \end{cases}$$

where \mathscr{U} is the heat absorbed during the phase change. As a further remark, when the temperature reaches the boiling point, T_{boil} , the particle density is adjusted in linear relation with the internal energy from liquid density to zero according to [84]

$$\rho_a = \left(1 - \frac{\mathscr{U}}{\Delta H_{\rm vap}}\right) \rho_0,\tag{89}$$

where ρ_0 is the initial drop density.



Figure 6: Drop deflagration after impact on a surface at $T_w = 350^{\circ}$ C well above the Leidenfrost point. Three different regimes of drop breakup are shown from left to right for increasing We numbers. Figure taken from Yang et al. [26]

Based on the above SPH model, Liu et al. [40] simulated the wetting and de-wetting dynamics of sessile nanofluid droplets on a solid surface from non-heating to sub-boiling to super-boiling temperatures. In particular, when a nanofluid droplet impacts a sub-boiling heating plate the buoyancy force causes a slight change in the local velocity direction near the drop bottom where the temperature is characterized by a layered gradient. At a sub-boiling surface temperature of 80°C the drop evolves dynamically changing its shape due to the impact on the surface without experiencing boiling evaporation (see Liu et al.'s [40], Fig. 11). During drop spreading, thermal transfer from the heated plate induces a temperature field near the drop bottom, while during the receding phase a temperature gradient is present in the cap droplet. The temperature gradient causes the appearance of buoyancy forces within the drop near the heated surface.

In particular, looking at Fig. 11 of Liu et al. [40], the experimentally observed drop morphology during its spreading and receding phase is very well reproduced by the SPH simulation. However, as these authors mention two different patterns may arise depending on the drop impact inertia. For instance, at more violent impacts (higher inertia) the high impact velocity at the drop bottom brings the heat to the edge of the drop, leading to high temperatures near the contact line. Conversely, as discussed above, at lower inertia little heat flow occurs along the spreading direction, and more heat is transferred to the drop center so that the temperature decreases from the drop center to its edge.

At super-boiling temperatures of the heated plate, boiling evaporation is seen to play a dominant effect on the de-wetting stage. In this case, the experiments and the simulations also reveal two different patterns, this time depending on the heating temperature and thermal transfer. At moderate super-boiling the drop experiences intense boiling at its maximum spreading (i.e., wetting) on the surface, undergoing liquid film bursts and bubble explosion. However, during the spreading, receding, and evaporation the drop always remains in contact with the heated surface. This occurs at plate temperatures $\leq 130^{\circ}$ C. At temperatures higher than this the drop boils as it spreads over the surface. At its maximum spreading sustained boiling destroys the pinning of the contact line and the drop recedes quickly, leading to a drop rebound from the heated surface. Fig. 7 shows details of the dynamics after the impact of a 20°C nanofluids droplet on a super-boiling heated plate at 150°C and We = 24.4. The upper two rows display experimental images of the impact of a deionized water drop with nanosilver particles and the bottom rows display the results of the SPH simulation for the same sequence of discrete times.



Figure 7: Impact of a nanofluids droplet on a sub-boiling heated surface at $T_w = 150^{\circ}$ C. The drop has a temperature of 20°C and impacts on the surface with We = 24.4. The shape evolution as obtained experimentally (upper two rows of images) is compared with the numerical simulation (bottom two rows). Figure taken from Liu et al. [40]

5 SPH Models of Multispecies Flow Drop Evaporation

In general, the dynamics of drop evaporation involve phase change and energy transfer at the liquidvapor interface along with the diffusion of vapor species in the vapor phase. As was described in Section 3.3, Yang et al. [27] proposed a reformulation of the classical model based on Eqs. (28)–(32), where a continuity equation for the vapor species was added to simulate the vapor mass fraction in the vapor phase. To account for the vapor mass increase and the liquid mass decrease during the process of liquid-vapor phase transition and avoid large mass differences at the liquid-vapor interface they introduced a particle splitting and merging technique, which was formulated in such a way as to conserve mass, momentum, and energy. Yang et al.'s [27] model and variants of it have been successfully applied to study the evaporation of static drops embedded in a heated gas. However, most studies were addressed to investigate the evaporation of liquid drops impacting on a heated surface.

Although most existing model simulations of drop impact on heated surfaces are validated for conditions at atmospheric pressure, Yang et al. [28] solved Eqs. (28)–(32) complemented by the pressure-density relation (11) to simulate the impact of a 50 μ m diameter *n*-heptane drop on a hot surface, using the SPH discretization scheme given by Eqs. (62)–(65) along with the provisions described by relations (66)–(75). They conducted a large number of simulations for impact velocities in the range between 4 and 20 m s⁻¹ (corresponding to We numbers between 27 and 680), surface temperatures in the range 27°C–300°C, and ambient pressures ranging from atmospheric to 20 bars. Based on the outcomes of their simulations they identified six different regimes, namely spreading, breakup, contact splash, partial rebound, rebound, and film splash. In particular, drop spreading is observed at low We numbers and relatively low wall temperatures. In this case, after impact, the drop spreads on the surface forming a film. The film stops spreading and reaches a maximum diameter by the time the kinetic energy of the drop vanishes. Thereafter, it recedes by surface tension effects until an equilibrium state is achieved. At higher We numbers and wall temperatures, the drop spreading produces a larger and thinner film with subsequent breaking on the surface. Yang et al.'s [28] Fig. 2 displays a picture of these two regimes at *p* = 1 bar. For instance, spreading is observed when We = 100 and $T_w = 27^{\circ}$ C, while breakup occurs when We = 430 and $T_w = 100^{\circ}$ C.

At We = 430 and raising the surface temperature to 150° C, the rim of the liquid film moves upward during spreading forming a crown structure, which soon thereafter breaks up into tiny secondary droplets, while the remainder of the film remains attached to the wall surface and fragments as shown in Fig. 8a. This outcome was referred to by Yang et al. [28] as contact splash. As the temperature is raised to 300°C, the splashing becomes more violent even when We = 240 as shown in the column sequence of Fig. 8b. In this case, a crown of secondary droplets forms which are lifted from the wall. During the next 30 μ s, the liquid which is still attached to the wall surface forms a ring like structure before fragmenting into new droplets which then levitate over the solid surface. In order to distinguish this outcome from the previous one, Yang et al. [28] called this regime film splashing. Since the Leidenfrost temperature of *n*-heptane is about 200° C at a pressure of 1 bar, it was reasonable to expect film splashing to occur at wall temperatures above 200°C. At We number as low as 50 and p = 1 bar partial rebound was seen to occur at wall temperatures around 180°C, while total rebound started to appear at slightly higher wall temperatures ($T_w = 200^{\circ}$ C). In these cases, the drop flattens over the surface which is then pulled back by surface tension regaining its spherical shape and detaching from the hot surface. If during rebound from the surface part of the drop remains attached to it (when $T_w < 200^{\circ}$ C), the regime is called partial rebound, while when no liquid remains attached to the hot surface, the regime is called rebound, which is seen to occur at $T_w \ge 200^{\circ}$ C and We < 200. On the other hand, the outcome of drop evolution changes when increasing the ambient pressure. For example, at 20 bars the Leidenfrost temperature is higher than the boiling temperature. The Leidenfrost temperature is sensitive to the ambient pressure and increases with increasing ambient pressure.



Figure 8: Impact of a 50 μ m diameter drop on a heated wall at atmospheric pressure (p = 1 bar): (a) contact splash at We = 430 and wall temperature of 150°C and (b) film splash at We = 240 and wall temperature of 300°C. Figure taken from Yang et al. [28]

In a recent paper, Sohag et al. [29] reported three-dimensional SPH simulations of the impact of 50 μ m diameter drops of *n*-heptane and *n*-decane on heated solid surfaces in high-pressure environments, using Yang et al.'s [27,28] formulation. They considered surface temperatures between 27°C and 400°C and pressures up to 20 bars for impacts with We = 50. They validated their scheme against experimental results of the impact of *n*-heptane drops on a drywall heated at temperatures of 35°C, 150°C, and 300°C and at 1 bar pressure for We ~ 50 [85] (see their Fig. 2). For all three wall temperatures, the morphological changes of the drop after the impact as predicted by the SPH simulations were found to be in good qualitative agreement with the experimental results. Fig. 9 shows the morphology of an *n*-heptane drop impacting on a wall at 300°C and different ambient pressures as compared with the experimental observations of Chausalkar et al. [85]. The comparison between simulation and experiment was not conducted on a timescale basis. At higher pressure the fluid saturation temperature of *n*-heptane increases from 98.5°C at 1 bar to 232°C at 15 bars, which delays the onset of drop evaporation and therefore the formation of the vapor layer that causes the floatation of the drop on the heated surface. This explains the delay at the onset of drop rebound when increasing the ambient pressure from 1 to 15 bars.



Figure 9: Impact of a 50 μ m diameter *n*-heptane drop on a heated wall of temperature $T_w = 300^\circ$ at We = 50 and different ambient pressures of 1, 5, and 15 bars. The numerical simulations are compared with experimentally taken images [85]. Figure taken from Sohag et al. [29]

The simulations reported by Sohag et al. [29] focused on two different drop-impact regimes: spread and rebound. They found that the ambient pressure has little effect in changing the maximum liquid film spread. For example, Fig. 10 shows the temporal dependence of the spread factor for the *n*-heptane drop at wall temperature of 300°C and We = 50 for different ambient pressures. However, under film boiling the occurrence of the maximum spread is delayed when the ambient pressure is increased from 1 to 20 bars. Their simulations also predict the experimental variation of the difference between the Leidenfrost and liquid saturation temperature ($T_1 - T_s$) for the *n*-decane and *n*-heptane drops with the ambient pressure. Yang et al.'s [27,28] formulation was also used by Xiao et al. [30] to study in two-space dimensions the evaporation of static single and binary drops. In particular, they found that the evaporation time of a single droplet conformed to the D^2 law proposed by Godsave [33] and Spalding [34]. For interacting binary droplets in the process of evaporation, they found that only when the ratio of droplet separation over drop diameter is greater than 8 the evaporation process is not influenced by the binary drop interaction.



Figure 10: (a) Numerically predicted variation of the spreading factor as compared with experimental observations [86] after impact at We \approx 57 of a water drop on a heated surface of temperature $T_w = 125^\circ$ and (b) comparison of the variation of the spreading factor with experimental data [86] and results from simulations with the rational-cubic interpolation program (RCIP) [87] after impact of a water drop at We = 100 on a heated wall at 125°C. Figure taken from Sohag et al. [29]

An extension of Yang et al.'s [27,28] SPH formulation has been employed by Wang et al. [35] to provide a framework for direct numerical simulations (DNS) of drop evaporation and combustion processes. In particular, the movement of drops in an infinite flow field is allowed by implementing non-reflective boundary conditions in a limited area along with heat and mass transfer and chemical reaction processes. Their formulation includes a solution of the continuity Eq. (20), the momentum Eq. (28), augmented by a surface tension term of the form given by Eq. (67) using Qiang et al.'s [88] formulation for the color function and its gradient, the energy equation

$$\rho c_{\rm p} \frac{dT}{dt} = -p \nabla \cdot \mathbf{v} + \nabla \cdot (\kappa \nabla T) + \Phi + Q, \tag{90}$$

where Φ is the viscous dissipation, defined in terms of the strain rate tensor, and *Q* is the heat released from the chemical reactions, and the species conservation equation

$$\rho \frac{dY_{\rm s}}{dt} = -\nabla \cdot \left(\rho Y_{\rm s} V_{\rm s}\right) + R_{\rm s},\tag{91}$$

where Y_s is the mass fraction of species *S*, V_s is the diffusion velocity of species *S*, and R_s is the mass generation rate of *S* in the chemical reactions. A weakly compressible SPH scheme is enforced by adopting the Murnaghan-Tait equation of state (12) for the pressure. During drop evaporation heat is absorbed by the liquid from the outside and part of this heat is used by the outer drop liquid molecules to undergo a continuous phase transition to a vapor state. In the process of phase transition the liquid mass fraction, $\bar{\alpha}$, of an SPH particle is varied from 0 to 1, where $\bar{\alpha} = 1$ means that the SPH particle is fully liquid, while $\bar{\alpha} = 0$ means that it has become completely gaseous. In general, $\bar{\alpha}$ is calculated according to

$$\nabla \bar{\alpha} = \frac{\nabla Q}{mh_{fg}},\tag{92}$$

where ∇Q represents the heat absorbed by the SPH particle and *m* is its mass. As $\bar{\alpha}$ changes from 1 to 0, the particle density, heat transfer coefficient, and diffusion coefficient change according to the prescriptions $\bar{\alpha}\rho$,

 $\bar{\alpha}\kappa$, and $\bar{\alpha}\mathscr{D}$, respectively. This ensures the conservation of mass, momentum, and energy. The combustion process was modeled by the one-step irreversible reaction mechanism of *n*-hexane:

$$v_F \text{Fuel} + v_O \text{Oxidizer} \rightarrow v_P \text{Product} + Q,$$
(93)

where *Q* is the heat released and the stoichiometric coefficients v_F , v_O , and v_P are obtained from the global reaction

$$C_6H_{14} + \frac{19}{2}O_2 \to 6CO_2 + 7H_2O.$$
 (94)

The combustion heat of *n*-hexane is 45,104.82 kJ kg⁻¹ and the oxidizer is air whose nitrogen component does not participate in the reaction. Therefore, the stoichiometric coefficient v_0 is set equal to 15.14. The SPH discretization of the hydrodynamic equations was made following similar replacements to those shown in Eqs. (62)–(65), except for the pressure gradient in the momentum equation which was replaced using the symmetrized form (59) (see Wang et al.'s [35] Eqs. (24)–(30)).

Wang et al. [35] applied their scheme to the simulation of drop evaporation in a forced convection environment and the combustion of static single and multiple drops. In the first case, the evaporation of a 200 μ m diameter *n*-hexane drop at an initial temperature of 342 K is calculated under the effects of an external hot nitrogen stream (at 850 K) flowing at different velocities. Fig. 11a shows the mass fraction distribution of vapor from the *n*-hexane fuel drop at 0.3 ms when the external inflow velocity is 5 m s⁻¹, while Fig. 11b displays the corresponding temperature distribution. At such high velocity, most of the vapor phase is blown downstream of the drop forming a long tail in the direction of the main external nitrogen stream. They further considered the combustion of single and multiple drops in a static environment. However, their results for drop combustion in a forced convective environment look more interesting. Fig. 12 displays the results of droplet combustion under increasing inflow velocities: (a) 1.0 m s^{-1} , (b) 2.0 m s^{-1} , and (c) 5.0 m s⁻¹. At an inflow of 1.0 m s⁻¹, the combustion mode is similar to that of a static drop where the flame is completely wrapped around the drop. When the inflow velocity increases to 2.0 m s⁻¹, the flame is behind the drop, while at 5.0 m s⁻¹ the flame is farther away from the drop forming a longer tail, which resembles a parachute. In all three cases, the effects of convection are to produce a more severe chemical reaction in the downstream region where the flame temperature is higher. The structure and combustion modes displayed in Fig. 12 were successfully compared with the experimental results of the combustion of acetone oil drops [89].

The drop evaporation after impact on the liquid film in a horizontal falling film evaporator was recently studied by Fan et al. [32] using Yang et al.'s [27,28] SPH formulation. The horizontal tube falling film evaporation is a promising technology that is widely applied in refrigeration and water treatment systems with great advantages in the heat and mass transfer efficiency and low cost [90–92]. The evaporation process of a drop impacting on a liquid film in falling-film heat exchangers not only relates to the flow and spreading dynamics after impact but also to the thermodynamic process of phase transition. Apart from related work by Xu et al. [31], Cui et al. [39], and Wang et al. [91], among other scholars, there are only a few instances in the literature dealing with SPH applications to liquid film evaporation. As a validation test case, Fan et al. [32] simulated the evaporation evolution of an ethanol droplet after impact on a heated surface, finding a fairly good agreement with ad hoc experimental observations for an ethanol drop of equivalent diameter $D_{equiv} = (D_h^2 D_v)^{1/3} = 1.89$ mm impacting on a heated wall with an initial velocity of 0.89 m s⁻¹, where D_h and D_v are, respectively, the horizontal and vertical drop diameters. After 0.3 s in the evolution, they found that the drop spreading rate matched the experimental data within 6%.



Figure 11: Numerical results for the evaporation of a 200 μ m *n*-hexane drop at an initial temperature of 342 K in a hot nitrogen stream initially at 850 K and flowing from bottom to top with a velocity of 5 m s⁻¹. (a) Distribution of the *n*-hexane gas components and (b) temperature distribution at 0.3 ms. Figure taken from Wang et al. [35]



Figure 12: Predicted temperature field during the combustion of a 100 μ m diameter *n*-hexane drop in a stream of hot air moving from bottom to top with a velocity of (a) 1 m s⁻¹, (b) 2 m s⁻¹, and (c) 5 m s⁻¹. A full-envelope flame is seen in (a), while a tail and parachute flame are seen in (b) and (c), respectively. Figure taken from Wang et al. [35]

A schematic drawing of the evaporation model of drop impact on the liquid film employed by Fan et al. [32] is displayed in Fig. 13. The falling drop of radius 0.1 mm and temperature 313 K is placed at the center of a rectangular domain filled with gas at 333 K. The same initial temperature was used for the liquid film, while the wall temperature was set to 341 K. As the drop impacts the liquid film, a small crown first forms, which then spreads out as the drop merges gradually with the liquid film. When the initial drop velocity grows from 1 to 3 m s⁻¹, the contact area with the liquid film and the drop temperature both increase, implying that at higher falling velocities temperature equilibrium between the drop and liquid film takes longer. Fig. 14 shows details of the drop morphology and system temperature during and after the drop-liquid film impact for varying initial drop velocity from 1 to 3 m s⁻¹. Only the central top part of the semi-circular liquid film displayed in Fig. 13a is shown. When the drop temperature is increased at a given falling velocity, the liquid film around the merging drop is significantly affected by the drop temperature as its rate of evaporation becomes more pronounced, while the overall liquid film away from the drop impact region is little affected. These scholars also studied the impact of multiple droplets on the liquid film, finding that the time required

for them to reach thermal equilibrium with the liquid film is longer compared to that for a single drop at the same initial velocity.



Figure 13: (a) Schematic drawing of a water drop in air impacting on a hot liquid film resting on a heated arched surface and (b) computational model domain. Figure taken from Fan et al. [32]

In a recent paper, Xu et al. [31] argued that SPH simulations of phase transitions based on ideal thermodynamics through the use of Eqs. (11) and (12) may not be accurate enough due to the decrease of liquid particles during evaporation. In order to improve the accuracy of SPH drop evaporation calculations, they proposed a formulation based on Eqs. (20), (27), and (28) coupled with Eq. (11) for the pressure-density relation, Eq. (31) for the mass fraction of the vapor species, and a time-fractional order convection-diffusion equation for the temperature of the form [93–95]

$${}_{0}^{C}\mathscr{D}_{t}^{\alpha}T_{ab}^{n} = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left[c_{0}^{(\alpha)}T_{ab}^{\alpha} - \sum_{k=1}^{n-1} \left(c_{n-k-1}^{(\alpha)} - c_{n-k}^{(\alpha)} \right) T_{ab}^{k} - T_{n-1}^{(\alpha)} - T_{n-1}^{(\alpha)}u_{ab}^{0} \right],$$
(95)

where $T_{ab} = \mathscr{D}(T_a - T_b)$ is the so-called response function, τ is the timestep, Γ is the gamma function, and α is the fractional order. The coefficients $c_k^{(\alpha)}$ are defined as follows:

$$c_{k}^{(\alpha)} = \begin{cases} a_{0}^{(\alpha)} + b_{0}^{(\alpha)} & \text{if } k = 1, \\ a_{k}^{(\alpha)} + b_{k}^{(\alpha)} - b_{k-1}^{(\alpha)} & \text{if } 1 \le k \le n-2, \\ a_{k}^{(\alpha)} - b_{k-1}^{(\alpha)} & \text{if } k = n-1, \end{cases}$$

for n > 1 and $c_0^{(\alpha)} = a_0^{(\alpha)} = 1$ for n = 1. Here a_k and b_k are, respectively, the diffusion and convective coefficients defined as

$$\begin{aligned} a_k^{(\alpha)} &= (k+1)^{1-\alpha} - k^{1-\alpha}, \\ b_k^{(\alpha)} &= \frac{1}{2-\alpha} \left[(k+1)^{2-\alpha} - k^{2-\alpha} \right] - \frac{1}{2} \left[(k+1)^{1-\alpha} - k^{1-\alpha} \right], \end{aligned}$$

for $0 \le k \le n - 1$. Eq. (95), known as the Caputo time fractional derivative, is added to the right-hand side of the smoothed particle representation of Eq. (27) given by Eq. (61). With this provision the classical thermal conduction equation becomes a fractional order differential equation that better simulates the liquid-vapor phase transition when ideal thermodynamics is employed. Values of the fractional order between $\alpha = 0.1$ and 0.7 were tried for the evaporation of an equilibrated drop. As shown in Fig. 15, the value that

better reproduced the theoretical variation of the drop diameter with time (i.e., the D^2 law) was $\alpha = 0.1$, corresponding to a drop survival time of 0.54 s.



Figure 14: Temperature distribution at different times after the impact of a water drop initially at a temperature of 313 K on a hotter liquid film at a temperature of 333 K. The snapshots show the drop evaporation at different times in the top part of the arched liquid film for drop impact velocities of (a) 1 m s⁻¹, (b) 2 m s⁻¹, and (c) 3 m s⁻¹. In all cases, the solid arched surface was at an initial temperature of 341 K. Figure taken from Fan et al. [32]

With the above-modified scheme, Xu et al. [31] simulated the phase transition process of drops impacting on hot flat, and curved solid surfaces. Fig. 16 shows the evolution of a 0.3 mm diameter drop with an initial temperature of 573 K in a gaseous medium of the same temperature during impact on a hot arched surface. As the drop hits the surface it evaporates rapidly and a vapor film forms between the drop and the surface, which makes it float and reduces its evaporation rate. Fig. 17 shows how the spreading length and the evaporation rate of the drop vary with time. During drop evaporation, the ambient gas temperature decreases as most energy is absorbed by the evaporation process. Since the temperature of the hot surface is kept constant, the gas temperature rises again when the drop has completely evaporated.



Figure 15: Temporal variation of the squared diameter of a static droplet undergoing evaporation. The colored symbols correspond to varying values of the fractional order selection (α) using the SPH method corrected by the convection-diffusion Eq. (95). The straight solid line is the theoretically calculated D^2 law, which predicts a time survival for this drop of 0.54 s. Figure taken from Xu et al. [31]



Figure 16: Snapshots showing a 0.3 mm diameter drop falling in a hot gas environment (at 573 K) and impacting on a semi-circular surface at 373 K with a velocity of 0.5 m s⁻¹. Figure taken from Xu et al. [31]



Figure 17: Variation of the spreading length and evaporation rate with time for the drop impact model of Fig. 16. Figure taken from Xu et al. [31]

In a further study, Subedi et al. [38] simulated the impact of a drop train on a hot surface at different impingement frequencies using a variant of Yang et al.'s [27,28] SPH formulation, where a Shepard filtering [96]

$$\rho_a \to \left(\sum_{b=1}^{n_{\text{neigh}}} \frac{m_b}{\rho_b} W_{ab}\right)^{-1} \sum_{b=1}^{n_{\text{neigh}}} m_b W_{ab},\tag{96}$$

is applied after a certain number of timesteps to redefine the particle density so that large numerical fluctuations that may occur in the course of the simulation are effectively minimized. In addition, the XSPH technique introduced by Monaghan [43]

$$\widehat{\mathbf{v}}_{a} = \mathbf{v}_{a} + \varepsilon \sum_{b=1}^{n_{\text{neigh}}} \frac{m_{b}}{\widetilde{\rho}_{ab}} \left(\mathbf{v}_{a} - \mathbf{v}_{b} \right) W_{ab}, \tag{97}$$

is used to smooth out the velocities and maintain an orderly movement of particles. Their method was first validated against experimental observations of a drop train impacting on a drywall for the radial position of the crown's rim normalized to the drop diameter [97], finding a good level of agreement (see Subedi et al.'s [38], Fig. 2). The crown rim propagation and crater formation dynamics were also tested against the experimental measurements provided by Zhang et al. [98] for the impingement of a stream of hydrofluoroether (HFE)-7100 droplets on a pre-wetted surface for varying We numbers and impact frequencies. The numerical results were also found to be in reasonable agreement with the experimentally measured crown's rim propagation for a falling 240 μ m diameter drop train with We = 280.

In particular, Subedi et al. [38] simulated the vertical impingement of consecutive 50 μ m diameter drops on a heated surface ($T_w = 323$ K) at a velocity of 10 m s⁻¹ (We = 170) at frequencies of 10, 20, 30, 40, and 50 kHz, Reynolds number Re = 850, and We^{0.5}Re^{0.25} = 70.4. The parameter We^{0.5}Re^{0.25} was found to provide a better representation of the splashing threshold than We (see Ref. [99] for more details). They found that the splashing characteristics are dependent on the frequency, with more splashing resulting from higher impact frequencies. However, the liquid film thickness after the impact of consecutive drops is a function of several parameters, including the kinematic viscosity, impingement frequency, surface conditions, drop size, and ambient pressure. On the other hand, the propagation of the crown rim can be inhibited by increasing the ambient pressure.

6 SPH Models of Drop Evaporation with Non-Local Thermodynamics

An alternative formulation for the numerical description of liquid-vapor phase transitions combines the pressure and caloric vdW equations with a diffuse-interface model, as was already reviewed in Section 2.6. In this formulation, the thermodynamics is based on the vdW mean-field theory and therefore the dynamics of evaporation require modification of the classical equations of hydrodynamics as given by the set of Eqs. (45)–(48), whose smoothed particle representations are given by Eqs. (76)–(79).

A simplified version of Eqs. (45)-(47), where the third term on the right-hand side of the internal energy Eq. (47) is dropped, was implemented by Sigalotti et al. [17] to investigate the evaporation of liquid drops starting from a square shape for a range of initial densities and temperatures. They found that drops with initial subcritical temperatures $T_0 < 0.6$ and densities $0.661 \le \rho_0 \le 1.322$ in reduced units undergo spinodal decomposition (i.e., spontaneous separation of the liquid and vapor phases as a consequence of drop evaporation) and achieve thermo-mechanical equilibrium with mean drop temperatures higher than the initial ones, while drops with $T_0 > 0.6$ achieve thermo-mechanical equilibrium with mean temperatures lower than the initial values. On the other hand, drops starting with temperatures $T_0 \le 0.3$ and a density close to the liquid zone of the phase diagram ($\rho_0 \approx 1.652$) (see their Fig. 1a) formed stable liquid drops with almost no vapor phase, while for $T_0 > 0.3$ equilibrated drops formed with a very sparse external vapor atmosphere. Fig. 18 shows the final stable liquid drops coexisting with their vapor atmosphere at temperatures from top to bottom of about 0.46, 0.64, 0.66, and 0.75 and decreasing liquid densities. The first row of pictures display an equilibrium drop with $\rho \approx 1.75$ surrounded by a sparse vapor atmosphere. Drops with lower initial densities experience higher evaporation rates and therefore the evolution ends up with stable drops of smaller size and much denser vapor atmospheres as shown in the remaining rows of frames in Fig. 18. As shown in Fig. 19, the densities and temperatures of the coexisting liquid and vapor were found to closely match the binodal curve as predicted by the vdW equation of state in accordance with the Maxwell construction tie-line.

The same model formulation was further used by Sigalotti et al. [21] to simulate the evaporation and explosive vaporization of initially square-shaped drops with densities in the range between 0.31 and 1.64 in reduced units. For a fixed density, a sequence of models was produced by raising the initial drop temperature in order to predict the point separating normal boiling at subcritical heating from explosive boiling at the superheat limit. Values of $\rho \gtrsim 1$ are more representative of a liquid, while drops with a lower density are closer to the vapor zone of the phase diagram and are likely to exhibit higher evaporation rates at a fixed heating temperature. The response of a drop to instantaneous, uniform heating is therefore sensitive to the initial density, ρ_0 , and heating temperature, T_0 . As the heating is increased, the simulations revealed four different regimes: (a) a subcritical heating regime in which the drop undergoes spinodal decomposition (i.e., spontaneous evaporation at the drop surface boundary), the process ends up with a stable circular dropembedded in its vapor; (b) a near-critical heating regime in which the drop nucleates a transient central bubble. In this case, the bubble grows for a short time and then contracts upon itself and disappears, leaving in many cases a stable drop of noncircular shape surrounded by a vapor atmosphere; (c) a superheating regime in which the drop nucleates an unstable central bubble, leading to fragmentation of the liquid layer into stable secondary drops floating in their vapor atmosphere. Fig. 19 shows the equilibrium densities and temperatures of the coexisting liquid and vapor as obtained from these simulations; and (d) a superheating regime in which the nucleated bubble grows violently, leading to an explosive vaporization. In this case, the liquid layer breaks up into tiny droplets, which with their accompanying vapor, expand rapidly from the site of the explosion. Fig. 20 shows snapshots of the density and temperature at discrete times during the evaporation and fragmentation of a drop model with $\rho_0 \approx 1.64$ and $T_0 = 2.09$ in reduced units. The calculations predicted a superheat limit for this vdW fluid of $\approx 0.81T_{crit} = 0.96$, which is close to the theoretical value of $T_s = 1$,

predicted at ambient pressure p = 0 (see Ref. [100]). This theoretical value was found to agree reasonably well with experimental measurements [101].



Figure 18: Stable vdW liquid drops in their vapor atmosphere after evaporation by spinodal decomposition. The equilibrium temperatures from top to bottom are 0.46, 0.64, 0.66, and 0.75 in reduced units. The normalized distribution of SPH particle densities overlayed on the phase diagram is shown in the left column of plots, while the particle positions showing the liquid and vapor phases and the spatially rendered mass density field are shown in the middle and right columns, respectively. The color-scale bar and numbers on the right indicate the density contrast in reduced units. Figure taken from Sigalotti et al. [17]



Figure 19: Equilibrium densities and temperatures for the vdW evaporation drops that produced stable liquid drops of finite size floating in their own vapor. The symbols discriminate among the model's initial conditions (see Fig. 1 of Ref. [21]). Figure taken from Sigalotti et al. [21]

Water boiling on hydrophilic and hydrophobic surfaces was further simulated by Xiong et al. [18] by solving the SPH Eqs. (76)–(78), where the fifth term on the right-hand side of Eq. (78) was replaced by a volume-based external energy source (see their Eqs. (12) to (15)). In contrast with previous SPH simulations of liquid-vapor coexistence with non-local thermodynamics, they used dimensionless vdW parameters corresponding to water in terms of reference values of length (2.81 nm), temperature (562 K), time (1 ns), and mass (1.274×10^{-23} kg), which are the same scaling parameters for SPH simulations of water condensation tabulated by Charles et al. [15]. This way the results in dimensionless form can all be transformed to physical units. In particular, Xiong et al. [18] performed simulations of water evaporation and drop formation on hydrophilic, neutral, and hydrophobic surfaces. The Clausius-Clapeyron Eq. (19) was used to estimate the latent heat. Fig. 21 shows the fitting of ln *p* vs. 1/T after thermodynamic equilibrium between water and its vapor atmosphere is achieved. The slope corresponds to $-\Delta H_{vap}/R_g = -9.265$ in dimensionless units, which in physical units gives a value of 2403.3 kJ kg⁻¹ for the latent heat of evaporation. This value agrees with the experimental result within an error of 6%.

The same SPH model was employed by Xiong et al. [22] to simulate the vaporization of superheated drops in a vacuum and in a vapor chamber, this time using reference length, temperature, mass, and time scales of 5.326 nm, 546 K, 7.295 × 10⁻²³ kg, and 1.356×10^{-11} s, respectively. The amount of thermal energy supplied to the drop was quantified in terms of the parameter SD = $T_0 - T_{eq}$, which they called superheated degree (SD), where T_0 is the initial drop temperature and T_{eq} is the equilibrium temperature. Fig. 22 displays the different evaporation patterns encountered by a drop of initial density $\rho_0 = 1.05$ when SD is raised from 0.05 to 1.9 in dimensionless units. At low heating (SD = 0.05), the drop undergoes only surface evaporation. When SD = 0.2, the drop nucleates a central bubble and undergoes simultaneous surface evaporation forming a liquid ring. A similar process occurs for SD = 0.6 and 1.0 except that now the liquid ring fragments into a number of secondary droplets. For SD = 1.0 the fragmentation is the result of an explosive evaporation. At an extremely high SD(= 1.9) explosive vaporization takes place. In this case, phase separation occurs so rapidly that this pattern was called flash boiling. They simulated the evaporation of drops with initial densities in the range $0.7 \le \rho_0 \le 1.75$ by introducing an equivalent superheated degree SD = SD/ σ_{eq} , where σ_{eq} is the drop surface tension at equilibrium, finding that the surface evaporation occurs when SD < 1/3, while bubble

nucleation may occur when $1/3 \le S\overline{D} < 1$. Fragmentation and explosive fragmentation of the liquid ring was observed in the interval $1 \le S\overline{D} < 3$ and flash boiling only at $S\overline{D} \ge 3$.



Figure 20: Snapshots of the density (upper plots) and temperatures (lower plots) showing the evaporation process of a vdW drop initially with $\rho_0 \approx 1.64$ and $T_0 = 2.09$ in reduced units. This model nucleated an unstable growing central bubble which induced fragmentation of the outer liquid layer into three stable droplets. The color-scale bar and numbers indicate the density and temperature contrasts. Figure taken from Sigalotti et al. [21]



Figure 21: Linear fitting of $\ln p$ as a function of 1/T to obtain the latent heat of evaporation for water coexisting with its vapor atmosphere. Figure taken from Xiong et al. [18]

In a more recent work, Díaz-Damacillo et al. [23] solved the SPH Eqs. (76)-(79) with the aid of the hyperbolic kernel introduced by Yang et al. [76] to study the evaporation of suspended equilibrium vdW drops. In this case, the fifth term on the right-hand side of Eq. (78) was added for the first time in order to provide a correct description of the thermal evolution and structure of the liquid-vapor interface. Starting from equilibrated circular drops with mean densities $1.20 \le \rho \le 1.78$ and temperatures in the range $0.297 \le$ $T \leq 0.732$, they simulated the evaporation process for overheating at supercritical temperatures. Depending on the mean density and overheating temperatures, they found five different patterns, namely (a) surface evaporation, leading to smaller drops in equilibrium with their vapor atmosphere; (b) bubble nucleation at the drop center accompanied by surface evaporation, where the central bubble first expands and then collapses upon itself; (c) slow fragmentation, where the liquid ring breaks into two or more motionless secondary droplets; (d) fast fragmentation, where the liquid ring fragments into a number of small droplets, which expand radially outward; and (e) explosive vaporization, leading to deflagration of the drop. This last pattern resembles the flash-boiling pattern encountered by Xiong et al. [22]. Fig. 23 shows snapshots at different times during the slow fragmentation of a drop initially with $\rho = 1.50$ and $T \approx 0.732$ after overheating with a supercritical temperature of 2.4 in reduced units. The last frame on the bottom right shows the path of the liquid and vapor on the phase diagram. This model experienced a bubble nucleation accompanied by slow surface evaporation and underwent deep quenching into the miscibility gap during the fragmentation process into 11 slowly expanding droplets in equilibrium with their surrounding vapor. In general, when the drops are uniformly overheated, the out-of-equilibrium liquid undergoes rapid quenching into either the miscibility gap (below the spinodal curve given by the dashed line) or between the spinodal and binodal curves. In the former case, the drop is likely to undergo spinodal decomposition by surface evaporation, while in the latter case the drop nucleates a central bubble.



Figure 22: Rendered density field showing different evaporation patterns for a vdW drop initially with $\rho_0 = 1.05$ submitted to increasing uniform heating. Figure taken from Xiong et al. [22]



Figure 23: Rendered density field at different times during the evaporation of an equilibrium circular vdW drop initially with a mean density $\bar{\rho} \approx 1.50$ and mean temperature $\bar{T} \approx 0.732$ in reduced units after overheating with a supercritical temperature T = 2.4. The path of the liquid (red) and vapor (blue) on the phase diagram is shown in the bottom right frame. Figure taken from Díaz-Damacillo et al. [23]

In general, when liquid drops with microparticles evaporate completely on a surface, they leave a stain on it. This is typical of the so-called coffee ring effect by which the evaporated coffee drops leave a distribution pattern of particles that are more concentrated around the contact line. If the coffee drops contain

nanometer particles, as they evaporate they leave instead a uniform stain of particles where they appear to be distributed evenly within the contact line. In contrast to coffee rings, this pattern deposition particle is called a coffee splat. These phenomena have been recently studied both experimentally and numerically by Xiong et al. [20], using the same vdW-based SPH formalism used previously by the same authors [18,22] coupled with a rigid particle model of finite-size microparticles, and a point-particle model for the nanoparticles. They considered the case of a drop placed on a wall of initial density $\rho_0 = 1.3875$ and temperature $T_0 = 0.6$, containing randomly distributed rigid and point particles and coexisting in equilibrium with a vapor phase of density $\rho_v = 0.008\rho_0$. Their scheme was validated against the evaporation of a sessile drop of 10 μ L on a heated surface at 75°C. Experimentally this drop took about 120 s to completely evaporate. The simulation was performed using 10,000 initially uniformly spaced SPH particles and a smoothing length equal to twice the initial inter-particle spacing. Fig. 24 shows the temporal evolution of the drop volume as it evaporates compared with the experimental data.



Figure 24: Temporal variation of the volume of an evaporating sessile drop of 10 μ L on a hot surface of 75°C. The drop completely evaporates after 120 s. The result of the SPH simulation is compared with experimental observations for a deionized water drop. Figure taken from Xiong et al. [20]

Although the results shown in Fig. 24 are sufficiently convincing of the reliability of SPH to deal with problems of drop evaporation, the validity of the formulation proposed by Xiong et al. [20] was further tested against experimental observations of the flow field during evaporation of a 10 μ L drop seeded with polystyrene spherical particles of diameter 10 μ m as tracers. The flow structure inside the drop during evaporation was photographed using particle image velocimetry (PIV) techniques and a high-resolution camera, while the SPH simulation was performed using 40,000 SPH particles. Fig. 25 shows the experimentally observed flow field (left image) as compared with the SPH results (right plot). For greater clarity, the steam particles were removed from the numerical flow field plot. The numerically obtained flow field reproduces very well the experimental data, with the flow structure characterized in both cases by two dominant counter-rotating vortices.

The morphology of an evaporating drop with rigid particles of diameter 0.25 (in dimensionless units; see Xiong et al.'s [20] Table 1 where the dimensionless and physical parameters are listed) is shown in Fig. 26. In this case, as the drop evaporates the rigid particles expand outwards following the steam out of the drop. However, when the diameter of the rigid particles is increased they always stay inside the drop. By comparison, the effect of point particles is depicted in Fig. 27 for the same superheat operated in Fig. 26 (i.e., $\Delta T = 0.1$ in dimensionless units). As the drop evaporates, the particles gradually expand so that the precipitation range gradually increases over time. In general, the simulations revealed that for rigid particles their precipitation and the forms emerging on the wall are mainly affected by the wall wettability [102]. At high wall temperatures, the coffee ring effect is weakened, while hydrophilic surfaces produce larger coffee

rings compared to hydrophobic ones. On the other hand, droplets with a high concentration of point particles deposited on a high-temperature hydrophobic wall are likely to form uniform coffee splats, rather than coffee rings. As Xiong et al. [20] concluded this feature may be important to produce uniformly distributed and easily controlled nanostructure coatings through droplet evaporation.



Figure 25: Experimentally observed velocity field within a sessile drop evaporating on a heated surface at 75°C (left image) as compared with the velocity distribution obtained from the SPH simulation (right plot). Figure taken from Xiong et al. [20]



Figure 26: Snapshots showing the morphology of an evaporating sessile drop of 10 μ L seeded with rigid microparticles on a heated wall at a temperature of 50°C. Figure taken from Xiong et al. [20]



Figure 27: Snapshots showing the morphology of an evaporating sessile drop of 10 μ L seeded with rigid nanoparticles on a heated wall at a temperature of 50°C. Figure taken from Xiong et al. [20]

7 Limitations of the Present State-of-the-Art SPH Simulations and Future Lines of Research

Drop evaporation is a complex phenomenon involving a liquid-to-vapor phase transition. The complexity of the subject has been highlighted by Erbil [3] in his comprehensive review of the basic theory of evaporation of sessile and suspended liquid drops. The understanding of the physical processes involved during droplet evaporation under natural and industrial conditions is an important topic of research in many disciplines and has gained a wide audience over the last ten years due to the greater amount of documented experimental observations available and the emergence of increasingly sophisticated numerical methods and models. The subject has also important technological applications in an ever-increasing number of areas in science and engineering.

Among the different existing numerical methods that have been applied to study the problem of drop evaporation in its various forms, SPH has emerged as a relatively young and promising numerical method capable of modeling small to medium-sized systems from nanometric to millimetric length scales. Although significant progress has been achieved in consolidating its mathematical foundations, the method still suffers from some drawbacks, such as the lack of complete proofs of convergence and the standardization of techniques [103]. These problems leave behind a number of features that require intensive investigation. However, despite these caveats, SPH has been successfully employed in the simulation of finite-sized systems requiring the solution of the equations of fluid dynamics with heat transfer. In particular, state-of-the-art SPH simulations of droplet evaporation are based on two different formulations, which are extensions of the one implemented by Nugent et al. [12]. One formulation was introduced by Yang et al. [27] for the simulation of evaporating multiphase fluid flows, where the usual conservation laws were complemented with a continuity equation for the vapor species to simulate the vapor mass fraction in the gas phase. The second formulation, known as the vdW square gradient model, was introduced by Charles et al. [15], which uses non-classical thermodynamics based on the vdW mean-field approximation of capillarity. A number of limitations are common to both types of SPH simulations. Comments on the more relevant limitations will be provided in what follows.

7.1 Need for More Three-Dimensional Simulations

Most SPH simulations in the literature are limited to two-space dimensions, while a more realistic approach will require to model drop evaporation in three-space dimensions. Three-dimensional SPH simulations of evaporating drops have been reported in a few cases by Xiong et al. [18] for water drop boiling in contact with hydrophilic and hydrophobic surfaces and in Refs. [20,26,28,29,38,40] for fuel and nanofluids droplets impacting on a heated surface. However, there is almost a complete lack of three-dimensional SPH simulations of evaporating droplets suspended in static and convective atmospheres. On the other hand, three-dimensional simulations of non-evaporating drops have been presented by Acevedo-Malavé [51] for studying the dynamics of drop spheroidization under the effects of surface tension, and more recently, by Yang et al. [104] for studying drop impact on dry surfaces and Chaussonnet et al. [105] for studying the tree fragmentation of a mother drop in the context of biofuel production.

7.2 Need for Consistent Thermodynamics

Almost all SPH simulations of drop impact on heated surfaces using Yang et al.'s [27] SPH formulation rely on the use of ideal pressure-density relations so that surface tension effects are modeled by just adding an artificial force term to the momentum equation and a heating term to the energy equation based on a prescribed algorithm to mimic the cohesive action. In contrast, the SPH simulations of drop evaporation based on vdW thermodynamics display a liquid-to-vapor phase transition similar to that of a real fluid, while the long-range, attractive, inter-particle interaction force implicit in the cohesive term of the vdW equation of state results in surface tension. A drawback of some of these models is that the results can only be qualitatively assessed because the liquid-vapor equilibrium is predicted using vdW parameters in reduced (dimensionless) units and therefore they do not deal with realistic fluids [19,21–23]. However, Xiong et al. [18] studied drop evaporation in contact with hot surfaces using vdW thermodynamics with vdW parameters appropriate for water and Yang et al. [26] simulated the interaction of *n*-heptane drops with a heated surface using a Peng-Robinson equation of state. Future SPH simulations of evaporating drops must use real equations of state along with characterization of the fluid in order to provide true comparisons with experiments.

7.3 Need for Temperature- and Density-Varying Transport Coefficients

A further important limitation that is common to all SPH simulations of evaporating drops lies in the assumption that the coefficients of viscosity and thermal conduction are constant, while in general for real liquids these coefficients are functions of density and temperature. For example, it is well-known that the shear and bulk viscosity coefficients of most liquids decrease with increasing temperature. It is common in numerical work to use the empirical relation [106,107]

$$\eta(T) = A \exp\left(-BT\right),\tag{98}$$

to model the dependence of the shear viscosity coefficient on temperature, where A and B are empirically determined parameters [106]. Similarly, the thermal conductivity also decreases with temperature for most real liquids [107]. This can have important effects on the vapor conductivity especially in cases where the drop undergoes homogeneous nucleation followed by explosive vaporization. The dynamics of the bubble growth and the intensity of the explosion depend on the heat exchange between the vapor and the liquid layer around it [108]. In addition, for poorly conducting liquids, the rate of heat transfer from the liquid to the vapor decreases and, as a consequence, the dynamics of the bubble growth will be affected. Therefore, the assumption of constant transport coefficients limits the possibility of quantitative comparisons with experimental observations of the ordinary and explosive boiling of liquid drops. However, despite this, the landscape of SPH simulations of evaporating drops remains largely focused on constant viscosity and heat conductivity conditions. For instance, recent work on the characterization of fuel drop impact on wall films using Yang et al.'s [27] SPH formulation with constant transport coefficients was reported by Pan et al. [109,110]. A weakly compressible SPH formulation for thermo-capillary phase change problems involving solid, liquid, and gas phases using constant transport coefficients for application to selective laser melting was implemented by Meier et al. [111], which is an emerging metal additive manufacturing technique. More recently, Patwary et al. [112] reported three-dimensional SPH simulations of fuel droplets interacting with a heated wall at different ambient pressures and Weber numbers based on constant viscosity. In particular, they studied secondary atomization and proposed an empirical correlation relating the mean secondary droplet size to the ambient pressure in the film-boiling regime. Moreover, Subedi et al. [113] simulated the Leidenfrost behavior of a droplet stream impinging on a hot wall using Yang et al.'s [27] SPH formalism, finding that when the ambient pressure is increased splashing is impeded and the film concentrates inwards near the impingement point. The use of constant viscosity and thermal conduction coefficients has not only been a shortcoming of most SPH simulations, but also of simulations with other numerical methods [114–117].

Recently, the effects of variable viscosity have been studied in droplet collision dynamics for complex fluid systems, where interactions between liquid/liquid and liquid/air interfaces are involved [118]. In this case, however, the temperature dependence of viscosity on droplet collisions for both Newtonian and non-Newtonian fluids has been simulated using Direct Numerical Simulations with the aid of a Volume-of-Fluid method. For the liquid the temperature-dependent viscosity was modeled using the Arrhenius-type equation

$$\ln \eta(T) = \ln \eta(T_{\rm ref}) = \frac{E_{\rm a}}{R} \left(\frac{1}{T} - \frac{1}{T_{\rm ref}} \right), \tag{99}$$

where T_{ref} is a reference temperature taken to be 293.15 K, $\eta(T_{ref}) = 5.7 \times 10^{-2}$ Pa s, E_a is the activation energy varied between 22.06 and 59.55 kJ mol⁻¹, and *R* is the universal gas constant. The air viscosity was taken to be 1.836×10^{-5} Pa s. The study was also extended to investigate experimentally the dynamics of drop impact on a sapphire surface heated between 40°C and 90°C. In particular, local temperature gradients in the viscosity

were seen to influence the spreading and heating of drops compared to numerical predictions of drop impact on hot surfaces by excluding the local effects of temperature on viscosity.

A new SPH scheme developed for simulations of multi-component fluid mixing with thermally-driven buoyancy and temperature-dependent viscosity was presented by Reece et al. [119,120]. In this case, the SPH scheme was applied to study vitrification processes in the nuclear industry for waste immobilization before long-term storage. A list of ten different equations for viscosity as a function of temperature is provided by Reece [120]. However, of these equations the preferred ones for modeling melt viscosities of glasses in the vitrification of nuclear waste are those given by [121]

$$\ln \eta = A + \frac{B}{T} + \frac{C}{T} \exp\left(\frac{D}{T}\right),\tag{100}$$

$$\ln \eta = A + \ln \left(\eta_{T_g} - A \right) \left(\frac{T_g}{T} \right), \tag{101}$$
$$\ln \eta = \eta_{\infty} + \frac{K}{T} + \exp \left(\frac{C}{T} \right), \tag{102}$$

where *A*, *B*, *C*, *D*, and *K* are empirical parameters. In Eq. (101), T_g is the glass transition temperature and $\eta_{T_g} = 10^{12}$ Pa s. Application of this scheme to a vitrification melter for single-phase and two-phase flows with temperature-dependent viscosities reveals a three-dimensional flow instability taking place due to mixing and suggesting a different flow regime in the melter that has to be investigated further.

A notable analytical model for the heating and evaporation of a single component liquid drop was developed by Cossali et al. [122], which includes a temperature-dependent density, diffusivity, thermal conductivity, and specific heat of the gas species. They performed a comparison of the effects of variable properties on heat and evaporation rates with predictions of a constant property model for six different species, including water, acetone, ethanol, *n*-hexane, *n*-octane, and *n*-dodecane. In particular, the thermal conductivity of a pure gaseous substance was approximated by the power-law correlation

$$\kappa(T) = rT^q,\tag{103}$$

which is consistent with monoatomic gases at low density [123], where q = 1/2. For polyatomic gases the above temperature dependence can still be used but with different values of q (see Table 1 of Cossali et al. [122] for the values of r and q about the different species). The analytical model can be extended to non-spherical drops. Whereas experimental measurements of the evaporation rate of spheroidal drops show consistency with the D^2 -law [124], this provides a good scenario for comparing the results with analytical models of non-spherical drops with constant properties of the gaseous phase [125–128].

7.4 Non-Newtonian Fluid Drops

Rheologically complex fluids and materials are of great importance in numerous processing operations in the industry. In general, good examples of these materials are polymer solutions and biological fluids. Other examples are given by coated sheets, optical fibers, and plastics, which are important in many manufacturing processes. Therefore, more efficient production methods and manufacturing procedures can be designed by improving our understanding of their physical behavior. In response to this, a great amount of research dealing with the characterization, modeling, and simulation of non-Newtonian fluid flows using grid-based traditional numerical methods has been performed during the last three decades. In comparison only a few SPH simulations have been reported to date.

The first simulations of non-Newtonian fluid flows using SPH were reported in 2002 by Ellero et al. [129], where a corotational Jaumann-Maxwell model was employed to describe the viscoelastic behavior of the fluid. Shortly after, Shao et al. [130] studied the dynamics of viscoelastic fluid flows with free surfaces using a modified form of the Cross model. The ability of SPH to simulate transient viscoelastic fluid flows was assessed by Ellero et al. [131]. They simulated the start-up flow between parallel plates for a viscoelastic (Oldroyd-B) and an upper-convected Maxwell (UCM) fluid at a low Reynolds number, finding very good agreement with available analytical solutions. Later on, in 2007, Hosseini et al. [132] simulated non-Newtonian fluid flows using standard SPH techniques, including power-law, Herschel-Bulkley, and Bingham-plastic models. They considered three different test cases, namely a non-Newtonian dam-break problem, flow through a viscometer for different non-Newtonian fluids, and a laminar mudflow on a mild slope. The impact of Oldroyd-B and UCM fluid drops on a rigid plate was further investigated by Fang et al. [133]. Their results for the Newtonian and Oldroyd-B fluids were found to reproduce quantitatively well those obtained by Tomé et al. [134] using finite-difference methods. Xu et al. [135] reported three-dimensional SPH simulations of non-evaporating, Newtonian, and non-Newtonian drops impacting on a solid wall, in which the viscosity was modeled using the Cross model. Their results indicate that the Newtonian droplet spreads out by keeping a convex shape during the impact, while the non-Newtonian drop behaved differently due to the shear-thinning effect, achieving a larger spreading radius than its Newtonian counterpart. Their SPH scheme was also applied to two-dimensional simulations of transient viscoelastic fluid flows, where the polymer dynamics was described by the evolution of continuous Brownian configuration fields [136]. More recently, Tembely et al. [137] performed simulations of drop impact on different substrates for Newtonian and polymer solutions using a Volume-of-Fluid method. Moreover, Shi et al. [138] extended the δ -plus-SPH, proposed by Molteni et al. [139], for modeling non-Newtonian multiphase flows. On the other hand, the visualization of impacting non-Newtonian drops has enormous applications in animated computer games as well as in many applied areas ranging from engineering to medical simulations. In response to this, SPH has also gained ground in the computer graphics community to create realistic drop simulations and animations [140]. From this survey of non-Newtonian SPH models it is clear that the method has become sufficiently mature to be able to simulate the evaporation of non-Newtonian drops in its various contexts.

7.5 The Issue of Spatial Resolution

A further important factor is the issue of spatial resolution. For example, as resolution is increased quantitative differences can appear in the morphology of the system and the number of secondary droplets produced in overheated drops undergoing rapid or even explosive fragmentation. In addition, resolution can also influence the breakup times of the liquid layer due to bubble growth and the structure of the diffuse liquid-vapor interface. There are almost no publications showing convergence studies in SPH droplet simulation. However, Xu et al. [135] demonstrated that increasing the resolution from 55,552 to 749,078 particles in Newtonian and non-Newtonian drop impact simulations has little effect on the results when measured in terms of the evolution of the drop width. This situation will certainly change in drop simulations of fragmentation and explosive vaporization where a plethora of tiny droplets accompanied by vapor are produced. Therefore, in order to clarify how spatial resolution affects the drop evaporation process, it is necessary to carry out three-dimensional convergence studies in these cases and assess the validity of the numerical predictions by direct comparison with experimental data.

Since there is great interest in engineering applications where the liquid-vapor equilibrium is crucial to the development of predictive models of evaporating fuel droplets in engines for spray combustion, future simulations must include chemical reactions in order to simulate the evaporative combustion in multi-component fuel drops. On the other hand, considering the influence of the various conditions that

may intervene during the drop/wall interaction process, more experimental results are needed to refine the model simulations. The level of prediction of SPH drop evaporation models will depend on several factors, including improved physics, chemistry, and spatial resolution. Of course, the computational tool can be extended to include realistic thermodynamic properties to simulate other fuels and predict the outcome of drop/wall interaction at practical operating conditions. In addition to the evaporation of drop impact on heated surfaces, more simulations are needed to study the evaporation and combustion of fuel drops in convective environments. These models are of particular importance because most liquid fuels are atomized before entering the combustion chamber and undergo combustion in the form of droplet groups. The reliability of the predictions must necessarily be tested by comparing the SPH results with molecular dynamics simulations and experimental measurements.

8 Conclusions

In this paper, we provide an overview of the published work on SPH-based simulations of liquid drop evaporation. The review covers articles published since 2000 when the first SPH simulations of evaporating drops were conducted. To assist non-expert readers, the paper includes an introductory section on the theoretical background necessary for the numerical modeling of drop evaporation. A separate section introduces some fundamental aspects of the SPH method, along with the governing equations and current state-of-the-art formulations employed in these simulations. Subsequent sections provide a brief description of relevant results obtained using different formulations for drop evaporation in static and convective hot environments, as well as during impact on a heated surface or liquid film. The evaporation of sessile drops due to contact with a hot wall is also reviewed as a specific case of drop impingement on a solid surface. The overview concludes with a section discussing the limitations of current SPH model simulations and suggesting potential directions for future research. Upon reviewing the various published studies, it is evident that the SPH method has become a powerful tool for simulating both ordinary and explosive boiling of small liquid drops in a hot atmosphere, as well as drop evaporation upon contact with a hot surface. These simulations have demonstrated a high level of predictive accuracy, particularly in cases where direct comparisons with experimental data were available.

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