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Modeling of droplet impact on a heated solid surface with a diffuse interface model

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ABSTRACT

A Diffuse Interface Model (DIM) is employed to model droplet impact on a heated solid surface. The DIM uses an especially constructed solid wall boundary condition which enables simulations with different wetting conditions of the solid surface. The model is also extended to include the effects of surface roughness on the behavior of the contact line dynamics. Multiple simulations are carried out to demonstrate the capabilities of the presented model. The simulation results demonstrate the influence of the wetting properties of the solid, with a higher cooling rate for hydrophilic than for hydrophobic wetting conditions. Surface roughness of the solid surface increases the cooling rate of the solid by enhancing the heat transfer between solid and fluid.

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1. Introduction

Insight into the dynamics of droplet impact on solid surfaces is relevant for various industrial processes such as spray cooling, spray painting and coating. Spray cooling, for example, is a good way of achieving high heat fluxes in systems where cooling of components is vital for efficiency and performance (Liang and Mudawar, 2017b). Droplet impact and spreading on solid surfaces are also relevant for understanding natural phenomena such as the water repellent properties of the lotus leaf. In the present study, an attempt is made to account for a number of process conditions which, to the best of the authors knowledge, are rarely included in previous studies of droplet impact (see for example Khatavakar et al. (2007)). These factors are: the occurrence of phase transition, solid surface roughness and a non-uniform temperature of the solid surface.

When a spray of fine droplets impacts a heated surface, the droplets spread on the surface to form a thin liquid film. They subsequently evaporate, removing heat from the solid due to the latent heat of evaporation in addition to heat removal via convection and diffusion. The high surface to volume ratio of the spray leads to a fairly uniform spatial distribution of heat removal. The momentum of individual droplets allows liquid to penetrate more easily through a possibly existing vapor layer and to actually reach the heated surface. The critical heat flux for spray cooling is therefore typically higher than for pool boiling at similar superheat (Liang and Mudawar, 2017b).

The impingement of a droplet on a heated wall is a process difficult to model due to the large number of parameters which influencing the process and due to the complex nature of phase-transitional flows (Breitenbach et al., 2018). The parameters which influence the process include droplet parameters (diameter, impact velocity), fluid properties (saturation temperature, mass density, dynamic viscosity, surface tension) and wall characteristics (surface roughness, wetting contact angle) (Liang and Mudawar, 2017a). In the present study, a Diffuse Interface Model (DIM) based on the Navier-Stokes-Korteweg equations in combination with the Van der Waals equation of state. The temperature distribution of the solid is modeled with the heat diffusion equation.

In DMs the liquid-vapor interface is postulated to be a region with strong but smooth transition of physical properties between the bulk values. Multiple DMs have been developed for numerical simulations of moving interfaces on a fixed grid, which include the Volume of Fluid (VOF) method (Hirt and Nichols, 1981) and the level-set method (Adalsteinsson and Sethian, 1995). These methods account for the effects of surface tension by using a body force that acts in a narrow region which represents the interface. The VOF and level-set method could be classified as numerical diffuse
interface methods. In these methods the width of the interface is a numerical artifact and not based on any physical process. A different approach is used in the physical Diffuse Interface Methods. In these methods the width of the interface is determined by relating the Helmholtz free energy of the fluid to the mass density gradient distribution at the liquid-vapor interface (Anderson et al., 1998). Besides being more thermodynamically consistent, the advantage of this approach is that the phase-change process as well as the displacement and topology change of the interface are all naturally embedded in the governing equations and do not require any additional models or special treatment of the interface region. DIMs have been used to model a wide range of different phenomena such as the dynamics of rising bubbles (Ding et al., 2007), cavitation phenomena (Magaletti et al., 2016), boiling processes (Shen et al., 2017) and droplet collisions (Gelissen et al., 2018).

One can distinguish two types of physical Diffuse Interface Methods, which are both based on an extended version of the Navier-Stokes equations. These are the Navier-Stokes-Cahn-Hilliard (NSCH) equations (Feng (2006), Liu et al. (2016), Shokpour Roudbari et al. (2018)) and the Navier-Stokes-Korteweg (NSK) equations (Pencenko et al. (2010), Tian et al. (2015), Liu et al. (2015)). Both equation sets reduce to the Navier-Stokes equations in the absence of an interface. In the present study the NSK equations are used, since fluid compressibility and phase-change, which play an important role in spray cooling, are naturally included in these equations.

Droplet impacts are governed by the dynamics of the contact line. Many computational methods methods have been extended to allow for the presence of moving contact lines in simulated two-phase flows (Sui et al., 2014). In the present study a solid wall boundary condition for DIM is presented which accounts for partial wetting behavior in the contact line dynamics. This solid wall boundary condition uses an especially constructed wall-fluid interaction energy function, following the approach of Sibley et al. (2013) The tendency of the system to minimize the Helmholtz free energy is exploited to achieve partial wetting of the solid wall boundary. Special attention is given to the effect of surface roughness on the behavior of the contact line. Even the smoothest surfaces are not perfectly homogeneous and exhibit geometrical heterogeneities. The effect of these heterogeneities on the behavior of the contact line needs to be accounted for in order to mimic the actually observed motion of the contact line in experimental investigations (see for example Tang et al. (2017)). This can be achieved by introducing a non-uniform contact angle, where the non-uniformity is derived from artificially constructed surface roughness profiles. In the present study a method for characterization of surface roughness via spectral analysis is also presented. The surface roughness profiles are constructed with the help of fractal theory, an approach inspired by the work of Russ (2013).

An extensive theoretical investigation of the influence of surface roughness on contact line behavior can be found in the work of Savva et al. (2011a,b), where the authors investigated two-dimensional droplet spreading on a substrate with surface roughness. The authors demonstrate that the droplet wets the substrate less as the substrate roughness increases.

The structure of the paper is the following. In Section 2 the governing equations are introduced accompanied by a brief description of the numerical method. In Section 3 boundary conditions are presented for both a solid wall boundary and an open boundary. Also, a method for the characterization of surface roughness based on fractal theory is presented. In Section 4 droplet impacts on a heated solid surface are systematically studied, and the influence of the wetting condition of the solid surface as well as the influence of surface roughness is investigated. In Section 5 the conclusions are summarized.

2. Governing equations

The structure of this section is the following. In Section 2.1 the governing equations for the fluid domain are presented. In Section 2.2 the governing equations for the solid domain. In Section 2.3 the Van der Waals equation of state is introduced, together with the Van der Waals theory of capillarity. Section 2.5 a brief overview of the numerical method used for the discretization of the governing equations.

2.1. Navier-Stokes-Korteweg equations

The Navier-Stokes-Korteweg (NSK) equations are a system of non-linear partial differential equations, expressing the conservation of mass, momentum, and energy. The non-dimensional form of the NSK equations are obtained by introducing scaling quantities, as is demonstrated in Desmarais (2016); Gelissen et al. (2018). The scales for the mass density, temperature and pressure are chosen to be the corresponding quantities at the critical point of the fluid: \( \rho_c \), \( T_c \) and \( P_c \). The velocity and characteristic time scale are derived as follows:

\[
    u_0 = \sqrt{ \frac{P_c}{\rho_c} } \quad t_0 = \frac{L}{u_0},
\]

with \( L \) the domain length. Non-dimensionalizing the NSK equations yields the following dimensionless quantities:

\[
    Re = \frac{\rho u_0 L}{\mu}, \quad We = \frac{u_0^2 L^2}{\rho c}, \quad Pr = \frac{\mu \xi}{\lambda}, \quad c_v = \frac{1}{R} \xi
\]

with \( Re \) the Reynolds number, \( \mu \) the dynamic viscosity of the fluid, \( We \) the Weber number, \( K \) the capillary coefficient, \( Pr \) the Prandtl number, \( \lambda \) the thermal conductivity of the fluid. The specific heat at constant volume of the fluid is non-dimensionalized with the universal gas constant \( R \) as the characteristic scale. The non-dimensional form of the NSK equations reads:

\[
\begin{align*}
    \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) &= 0 \\
    \frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u \otimes u + pI - \tau - \xi) &= 0 \\
    \frac{\partial \rho E}{\partial t} + \nabla \cdot \left( (\rho E + P)u - (\tau + \xi) \cdot u + q + j_f \right) &= 0
\end{align*}
\]

with \( u \) the velocity vector, \( P \) the pressure, \( \tau \) the viscous stress tensor, \( \xi \) the capillary stress tensor, \( \rho E \) the total energy density, \( q \) the heat flux and \( j_f \) the interstitial working flux. The influence of gravity is neglected in the present study. To close this system of equations, an equation of state is required which relates the pressure with the temperature, mass density and internal energy of the fluid. An equation of state is introduced in Section 2.3.

It is assumed that the fluid is Newtonian and that the so-called Stokes hypothesis holds. The viscous stress tensor is then equal to:

\[
    \tau = \frac{1}{Re} \left( \nabla u + \nabla u^T - \frac{2}{3} \nabla \cdot u I \right)
\]

Surface viscosity effects are neglected, which is a common assumption for an interface in a single component fluid without surfactants (Slattery et al., 2007). The capillary stress tensor is expressed in terms of the local mass density and its spatial gradients:

\[
    \xi = \frac{1}{We} \left( \rho \nabla^2 \rho + \frac{1}{2} | \nabla \rho |^2 I - \nabla \rho \otimes \nabla \rho \right)
\]

This expression for the capillary stress tensor is a simplified version of the original formulation proposed by Korteweg. It was derived by using Noether’s theorem and assuming a constant capillary coefficient (Anderson et al., 1998; Papatzacos, 2000). The
capillary stress tensor represents a force that pushes the system towards thermodynamic equilibrium and is zero at local thermodynamic equilibrium.

The heat flux is expressed as a function of the temperature gradient (Fourier’s law):

$$ q = -\frac{8c}{3RePr} \nabla T $$

(6)

with $T$ the temperature. The dimensionless numbers in this expression follow from non-dimensionalizing of the governing equations but the factor in front of the gradient can be reduced to just the thermal conductivity $\lambda$ of the fluid.

Dunn and Serrin (1985) demonstrated that the original formulation of the capillary stress tensor is incompatible with the Clausius-Duhem inequality if the energy equation is not extended with an additional “non-classical” term. This term ensures that the volumetric rate of entropy production is strictly positive and has contributions from thermal and viscous dissipation only. The term is commonly called the “interstitial work flux” and is expressed as:

$$ j_k = \frac{1}{We} (\rho \nabla \cdot \mathbf{u}) \nabla \rho $$

(7)

The total energy density is defined as:

$$ \rho E = \rho e + \frac{1}{2} \rho |\mathbf{u}|^2 + \frac{1}{2} We \left| \nabla \rho \right|^2 $$

(8)

which represents the sum of the internal energy, kinetic energy, and interfacial energy. The expression for the internal energy depends on the equation of state of the fluid, as is explained in Section 2.3.

It should be noted that the capillary stress tensor is non-dissipative, i.e. does not lead to additional dissipation in the system. This can be proven by substituting the expressions for the capillary stress tensor, viscous stress tensor, interstitial work flux and total energy density into the energy balance equation, which can then be reduced to the heat equation (see Lamorgese et al. (2017), equation 157, 158 and 159). The source term in this heat equation indicates that for a single component system the conversion of mechanical energy into heat is only due to dissipation of momentum.

Because fluid properties can vary significantly between the phases of the fluid while they should be differentiable, a smooth transition between the values of these properties should exist at the liquid-vapor interface. The Diffuse Interface Model in the present study uses the mass density as the parameter to distinguish between the different phases, so it makes sense to use the local mass density as the input parameter for any interpolating function to determine fluid properties. A number of requirements have to be fulfilled by such an interpolating function:

- The interpolating function and its first derivative need to be continuous.
- The first derivative of the interpolating function needs to be zero at the points between which it interpolates ($\rho_v \leq \rho \leq \rho_i$).
- The interpolating function has to remain at a constant value outside the interpolated domain ($\rho < \rho_v$ and $\rho > \rho_i$).

These requirements eliminate any polynomial or exponential interpolating function. A hyperbolic tangent function appears to be a good choice. Taking for example the dynamic viscosity as the fluid property that needs to be interpolated between the liquid and vapor mass density, the following expression can be used:

$$ \mu(\rho) = \frac{1}{2} \left( \mu_1 + \mu_v \right) + \frac{1}{2} \left( \mu_1 - \mu_v \right) \tanh \left( \frac{8(\rho - \frac{1}{2} (\rho_1 + \rho_v))}{\rho_i - \rho_v} \right) $$

(9)

with $\mu_1$, $\mu_v$ the liquid/vapor dynamic viscosity and $\rho_i$, $\rho_v$ the liquid/vapor mass density at the vapor-liquid equilibrium. Not only the dynamic viscosity but also the thermal conductivity of the fluid is interpolated with a hyperbolic tangent function. Within the non-dimensional equations the dynamic viscosity and the thermal conductivity of the fluid are included in the definition of the Reynolds and Prandtl number, which causes these numbers to be a function of the local mass density ($Re = Re(\rho)$ and $Pr = Pr(\rho)$). In the present study the dynamic viscosity of the vapor is 5 times smaller than the dynamic viscosity of the liquid. Similarly the thermal conductivity is a 100 times smaller in the vapor than in the liquid.

2.2. Heat diffusion equation

Heat diffusion in a solid without heat source is governed by the following (dimensional) equation:

$$ \frac{\partial \tilde{T}}{\partial \tilde{t}} - \frac{\lambda_s}{\rho_s c_p} \nabla^2 \tilde{T} = 0 $$

(10)

with $\lambda_s$ the thermal conductivity, $c_p$ the specific heat capacity and $\rho_s$ the mass density. The product of specific heat capacity and mass density is the volumetric heat capacity and represents the ability of a material to store thermal energy. The ratio of thermal conductivity to the volumetric heat capacity is called the thermal diffusivity and it determines the rate of heat diffusion in a solid.

The introduction of appropriate scales to non-dimensionalize the heat diffusion equation yields:

$$ \frac{T_c \partial T}{t_0 \partial t} - \frac{\lambda_s}{u_0 p_i c_p L} \frac{T_c}{L^2} \nabla^2 T = 0 $$

(11)

after defining $t_0 = \frac{L^2}{u_0}$, using the same characteristic velocity and length scale as for the NSK equations, this expression can be rewritten as:

$$ \frac{\partial T}{\partial \tilde{t}} - \frac{\lambda_s}{u_0 p_i c_p L} \nabla^2 T = 0 $$

(12)

which is equal to:

$$ \frac{\partial T}{\partial \tilde{t}} - \frac{1}{Pe} \tilde{t} \nabla^2 T = 0 $$

with $Pe = \frac{u_0 p_i c_p L}{\lambda_s}$

(13)

for the Peclet number. The heat diffusion equation is thus non-dimensionalized with the same velocity and length scales as used for the NSK equations.

2.3. Van der Waals equation

To close the system of equations introduced in Section 2.1, an equation of state is required which relates the pressure with the temperature, mass density and internal energy of the fluid. The equation of state needs to be valid for both phases in which the fluid can exist, and be able to handle the phase transition between these phases. The Van der Waals equation (Van der Waals, 1873) is the simplest example of this:

$$ \tilde{P} = \frac{R \tilde{T}}{1 - b \tilde{P}} - a \tilde{P}^2 $$

(14)

with $\tilde{P}$ the pressure, $\tilde{T}$ the temperature and $R$ the specific gas constant. The coefficients $a$ and $b$ represent the average attraction between the molecules and the volume excluded by the molecules, respectively. Although $a$, $b$ and $R$ differ for every fluid considered, the Van der Waals equation can be recast into a fluid independent form according to the law of corresponding states, which gives:

$$ P = \frac{8RT \rho}{3 - 3\rho^2} $$

(15)
with the reduced temperature $T = \frac{T}{T_e}$, reduced pressure $P = \frac{P}{P_e}$ and reduced mass density $\rho = \frac{\rho}{\rho_e}$.

The internal energy of a fluid is a function of the local temperature and local mass density. The general equation for specific internal energy in terms of $dT$ and $d\rho$ reads:

$$de = c_v dT + \left( P - T \frac{\partial P}{\partial T} \right) \frac{d\rho}{\rho^2}$$

(16)

for a Van der Waals fluid this expression reduces to:

$$e = \frac{8}{3} c_v T - 3 \rho$$

(17)

2.4. Van der Waals theory of capillarity

In his theory of capillarity, Van der Waals proved that the Helmholtz free energy of a fluid cannot depend only on local variables, such as the local mass density and temperature, since this would cause the thickness of a liquid-vapor interface and the surface tension coefficient to be zero. A non-local term needs to be included in the expression for the Helmholtz free energy:

$$\mathcal{F} = \mathcal{F}_b + \frac{1}{2 We} |\nabla \rho|^2$$

(18)

where $\mathcal{F}_b$ refers to the bulk of the two phases and $|\nabla \rho|^2$ represents the non-local contribution (Rohde, 2005). The expression for the Weber number contains the capillary coefficient $K$. Its value can be derived from accurate measurements of the surface tension coefficient of a liquid-vapor interface. For a Van der Waals fluid, the expression for the bulk Helmholtz free energy per unit volume takes the form:

$$\mathcal{F}_b(\rho, T) = \frac{8}{3} c_v T \rho (1 - \ln(T)) + \frac{8}{3} T \rho \ln \left( \frac{\rho}{\rho_e} \right) - 3 \rho^2$$

(19)

Note that this expression has only local variables. The properties of a planar liquid-vapor interface can be derived from the excess of Helmholtz free energy $\Delta \mathcal{F}$ in the multiphase region (represented by the gray area in Fig. 1). If thermodynamic equilibrium is assumed then it is possible to derive the following expression (Cahn and Hilliard, 1958):

$$\Delta \mathcal{F} = \mathcal{F}_b - \mathcal{F}_l = \frac{1}{2 We} \left( \frac{d\rho}{dx} \right)^2$$

(20)

where $\mathcal{F}_l$ is called the bi-tangent (Fig. 1) and $x$ the spatial coordinate. It is possible to derive the following relation from the definition of the surface tension coefficient of a planar interface:

$$\sigma_{lv} = \frac{1}{We} \int_{-\infty}^{\infty} \left( \frac{d\rho}{dx} \right)^2 dx$$

(21)

With Eq. 20 it is possible to rewrite this expression as:

$$\sigma_{lv} = \frac{1}{We} \int_{\rho_l}^{\rho_u} \frac{d\rho}{\rho} \frac{d\rho}{\rho^2} = \frac{1}{We} \int_{\rho_l}^{\rho_u} \sqrt{2 We \Delta \mathcal{F}} d\rho$$

(22)

with $\rho_l, \rho_u$ the mass density of the vapor and liquid at saturation conditions. The vapor-liquid equilibrium can be found by applying Maxwell’s equal area rule, as was demonstrated previously, see for example Gelissen et al., 2018.

By using Eq. 22 it is possible to find an interpolation function for the surface tension coefficient as a function of temperature. As long as the Van der Waals equation is used the following function is sufficiently accurate for $T \in [0.4, 1.0]$:

$$\sigma_{lv}(T) = \sqrt{\frac{71.8056}{We}} (1 - T)^{1.5}$$

(23)

It is also possible to find an expression for the enthalpy of evaporation $l_h$ required or generated during phase change. The Clausius-Clapeyron equation gives the following expression:

$$l_h(T) = T \left( \frac{1}{\rho_l} - \frac{1}{\rho_u} \right) \frac{d\rho}{dT}$$

(24)

with $T$ the temperature and $\hat{\rho}$ the saturation pressure, which is the pressure at vapor-liquid equilibrium. Also for the enthalpy of evaporation an interpolation function can be found:

$$l_h(T) \approx 15.08 \sqrt{1 - T}$$

(25)

This expression demonstrates how the magnitude of the enthalpy of evaporation depends on the temperature. However, it is not used in the numerical simulations, since its effect is naturally included in the peak.

The normalized surface tension coefficient and enthalpy of evaporation of a Van der Waals fluid for $T \in [0.4, 1.0]$ is visualized in Fig. 2. Both surface tension coefficient and enthalpy of evaporation are zero at the critical point ($T = 1.0$) and increase with fluid temperature decreasing.

2.5. Numerical method

Numerical methods for discretization of the NSK equations have to cope with additional difficulties when compared to single-phase compressible flow simulations. One such difficulty is that the capillary stress tensor causes dispersive behavior of the solution, since it contains a second-order spatial derivative of the mass density. Also, the Van der Waals equation of state has a non-convex part which causes a mixed hyperbolic-elliptic nature of the governing
equations. This prevents the use of upwind based discretization methods, which are commonly used for compressible flow simulations. The discretization method used in the present study is the same as the one used by Gelissen et al. (2018), which is based on a discretization technique developed by Cockburn and Gau (1996). It uses a second-order accurate finite-volume method for spatial discretization and the third-order accurate TVD Runge-Kutta time integration method developed by Shu and Osher (1988). Second-order central difference schemes are employed to calculate the derivatives in the flux expressions. The finite volume method is preferred over other discretization methods since it is strictly conservative.

For the discretization of the Heat Diffusion equation the finite-difference method is used where the second-order central schemes leads to a five-point stencil for the spatial discretization. Time integration is done with the same Runge-Kutta method as used for the NSK equations. Both discretizations use the same grid-size and time-step.

3. Boundary conditions

This section contains the implementation of the boundary conditions. In Section 3.1 the solid wall boundary condition for DIM is introduced, which includes a contact angle that represents the wetting properties of the solid wall boundary. In Section 3.2 a method for characterization of surface roughness profiles is presented, which is subsequently used for constructing artificial surface roughness profiles. In Section 3.3 a mechanism is introduced that enables inclusion of the effects of surface roughness of the solid wall boundary on the contact angle. In Section 3.4 the coupling between the solid domain and the fluid domain is discussed. Finally, Section 3.5 introduces an open boundary condition which is used for the top boundary of the domain.

3.1. Solid wall boundary condition

When a liquid drop is brought into contact with a solid surface that is mechanically rigid and both smooth and homogeneous down to molecular scale, the drop may spread over the surface until it becomes a uniform film or it lies on a limited area of the surface. These two modes of liquid-solid contact are called complete wetting and partial wetting. The degree of partial wetting can be expressed in terms of the contact angle $\theta$, the angle measured through the liquid phase from the solid surface at the point where the liquid-vapor interface meets the solid surface. At equilibrium the value of $\theta$ is related to the solid-vapor, solid-liquid and liquid-vapor surface tension coefficients according to the Young equation:

$$\sigma_{lv} \cos(\theta) = \sigma_{sv} - \sigma_{sl}$$  \hspace{1cm} (26)

The Young equation can, within the context of the present study, best be interpreted as the solution of the minimization problem of the Helmholtz free energy (Roura and Fort (2004)) instead of a force balance at the three-phase contact line, which is how it is commonly presented in literature.

The formulation of a solid wall boundary condition begins with the definition of the wall-fluid interaction energy function, which determines the affinity of the wall with the saturated phases. A third-order polynomial function with a minimum at both the liquid and vapor mass density was proposed by Sibley et al. (2013), as an extension/improvement to the work of Seppecher (1996) and Jacqmin (2000). This will ensure convergence towards either the liquid or vapor mass density in case of density fluctuations at the wall. Additionally, the wall-fluid interaction energy function should match the surface tensions $\sigma_{sv}$ and $\sigma_{sl}$ used in Young's law. These requirements result in the following conditions (Sibley et al., 2013):

$$\frac{d\phi_v}{d\rho} (\rho_v) = 0 \quad \frac{d\phi_v}{d\rho} (\rho_l) = 0 \quad \phi_v(\rho_v) = \sigma_{sv} \quad \phi_v(\rho_l) = \sigma_{sl}$$  \hspace{1cm} (27)

These four conditions require at least a third-order polynomial if all conditions are to be satisfied. The chosen wall-fluid interaction energy function and its first derivative with respect to $\rho$ read:

$$\phi_v(\rho) = \frac{(\rho - \rho_l)^2(2\rho + \rho_l - 3\rho_v)\sigma_{sv} - (\rho - \rho_v)^2(2\rho + \rho_v - 3\rho_l)\sigma_{sl}}{(\rho_l - \rho_v)^3}$$  \hspace{1cm} (28)

$$\frac{d\phi_v}{d\rho} (\rho) = \frac{6(\rho - \rho_l)(\rho - \rho_v)(\sigma_{sv} - \sigma_{sl})}{(\rho_l - \rho_v)^3}$$  \hspace{1cm} (29)

which is a third-order polynomial with the same shape as proposed by Sibley et al. (2013). Young’s law can be substituted into the last expression which results in:

$$\frac{d\phi_v}{d\rho} (\rho) = \frac{6(\rho - \rho_l)(\rho - \rho_v)\sigma_{lv} \cos(\theta)}{(\rho_l - \rho_v)^3}$$  \hspace{1cm} (30)

with $\sigma_{lv}$ the liquid-vapor surface tension and $\theta$ the contact angle. The convention is that the contact angle is the angle between the interface and the solid surface as measured through the liquid phase in a plane perpendicular to the tangent of the contact line on the surface (Fig. 7).

According to Sibley et al. (2013) and Desmarais (2016) the partial wetting condition at the wall can be formulated as:

$$\frac{d\phi_v}{d\rho} (\rho) + \frac{1}{\text{We}} \nabla \rho \cdot \mathbf{n} = \gamma \left( \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho \right)$$  \hspace{1cm} (31)

with $\mathbf{n}$ the unit vector normal to the wall and $\gamma$ a relaxation parameter. For simplicity the assumption is made of instantaneous wall-fluid energy equilibrium ($\gamma = 0$).

A solid (non-permeable) wall combined with the no-slip boundary condition results in the following expressions for the velocity vector:

$$\mathbf{n} \cdot \mathbf{u} = 0 \quad \mathbf{t} \cdot \mathbf{u} = 0$$  \hspace{1cm} (32)

with $\mathbf{n}$ the vector normal to the wall and $\mathbf{t}$ any vector tangential to the wall. Even if a no-slip boundary condition is applied at the wall, the contact line can still move as a result of the diffusive fluxes stemming from the capillary stress tensor. The problems surrounding the stress singularity at the moving contact line (the so-called Huh-Scriven paradox (Huh and Scriven, 1971)) do not exist when the interface is diffuse, because the interface can move due to diffusion and phase-transition.

The combination of Eqs. 31 and 32 represents a solid wall boundary condition under isothermal conditions. However, in the present study droplet impact on a heated solid surface is investigated, which means that also an expression for the temperature at the solid wall boundary is required. The derivation of such an expression is presented in Section 3.4.

3.2. Characterization of surface roughness

Roughness determines many functional properties of surfaces, such as adhesion, friction and thermal conductance across contact interfaces. It is the main reason why macroscopic bodies usually do not adhere to each other with any measurable strength. Surface roughness is generally described as the short-wavelength fluctuations of a solid surface topography. Both the amplitude and wavelength of these fluctuations determine the characteristics of the surface roughness. Real solid surfaces are never perfectly smooth, additionally they may also have surface impurities and the composition may vary with location. The analysis of the characteristics of surface roughness reveals fractal-like behavior, i.e. within
a limited range of length scales the statistical properties of the surface roughness are invariant to the length scale (Russ, 2013; Majumdar and Bhushan, 1990). Euclidean geometry is the traditional basis for understanding and describing geometry. However, as pointed out by Mandelbrot in his book The Fractal Geometry of Nature (Mandelbrot, 1982), fractal geometry is often superior to Euclidean geometry in representing the characteristics of many natural processes and objects. The key property of a fractal is self-similarity or self-affinity between different length scales.

A conventional measurement of surface roughness is the root-mean-square (RMS) roughness value: the square root of the sum of squares of the deviations of individual values from the mean value divided by the number of data points. However, the RMS roughness value is incapable of containing the complete characterization of the roughness profile and is dependent on the length of the sample and the resolution of the measurement device. Spectral analysis in combination with fractal theory can be used to achieve more complete characterization of surface roughness profiles.

In the present study the assumption is made that the surface roughness is isotropic and that the roughness profiles can be expressed as a continuous function. The roughness profiles are composed of sinusoidal components with different amplitudes and phase-angles. If \( N \) is the number of grid points available, then it is assumed that there are \( N \) different components in the roughness profile. It is possible to decrease the wavelength down to the Nyquist limit (\( \lambda = \frac{8}{N} \)), but this is not recommended since it will not be possible to accurately capture these components on the grid. Additionally, in DIM the width of the liquid-vapor interface corresponds to approximately 10 grid points. It is assumed that any components in the roughness profile much smaller than the width of the liquid-vapor interface will not have a significant influence on the contact line behavior. The formula for the Fourier series of the roughness profile reads:

\[
X_n = n \Delta x \quad \text{for} \quad n = 0, 1, \ldots, N - 1
\]

\[
Z(x_n) = \sum_{k=1}^{N/4} r_k \cos \left( \frac{2\pi}{\lambda_k} x_n + \phi_k \right)
\]

The wavelength of each of these components is:

\[
\lambda_k = \frac{L}{k} \quad \text{for} \quad k = 1, 2, \ldots, \frac{N}{4}
\]

The zeroth wave (\( k = 0 \)) represents the average of the signal, henceforth assumed to be zero by choice of the \( \tilde{Z} \)-plane (\( \tilde{Z} = r_0 = 0 \)). To facilitate the writing, the combination of amplitude and phase-angle of each wave is expressed as a complex number, with the modulus \( r \) representing the amplitude and the argument \( \phi \) the phase-angle of each wave. The signal can then be expressed as a set of complex numbers, according to the following expression:

\[
\tilde{Z}(\lambda_k) = \begin{cases} 
\alpha_k \lambda_k^{H+1} e^{-\phi_k} & \text{if} \quad \lambda_k \geq \lambda_r \\
\alpha_k \lambda_k^{H+1} e^{-\phi_k} & \text{if} \quad \lambda_k < \lambda_r
\end{cases}
\]

with \( \alpha, \lambda, \) and \( H \) constants, \( j^2 = -1 \) and \( |Z(\lambda_k)| = r_k \). The phase-angle \( \phi_k \) is obtained from a random number generator which ensures a uniform distribution between \([0, 2\pi]\) for the generated numbers. The constant \( \lambda_r \) represents the roll-off wavelength. If there is no roll-off wavelength (for example in fracture-produced surfaces) then the behavior is fractal-like up to the longest length scale. However, most surfaces of engineering interest have a roll-off wavelength. Waves with wavelengths equal or larger than the roll-off wavelength no longer increase in amplitude (Fig. 3). The constant \( H \) represents the Hurst exponent and it determines how the roughness profile changes as the lateral length scale changes. The constant \( \alpha \) is a scaling factor which can be determined from the RMS roughness value. The area under the spectrum represents the variance of the roughness profile, or the square of the RMS roughness value. By using Parseval’s theorem it is possible to relate the scaling factor \( \alpha \) to \( R_{\text{RMS}}^2 \):

\[
R_{\text{RMS}}^2 = \frac{1}{N} \sum_{n=0}^{N-1} |\tilde{Z} - Z(x_n)|^2 = \alpha \sum_{k=0}^{N/4} |\tilde{Z}(\lambda_k)|^2
\]

Roughness profiles follow from computing an inverse Fourier transformation on constructed Fourier spectra. Both 1D (Fig. 4) and 2D (Fig. 5) roughness profiles are easily obtained with the method presented in this section. In the present study simulations
of droplet impacts on surfaces with different roughness profiles are presented. For each simulation the values of $R_{\text{rms}}$, $H$, $\lambda_t$ are specified.

3.3. Surface roughness and contact angle

The influence of roughness on wetting phenomena has already been explored in earlier work. On a hydrophobic rough substrate Wenzel (1936) predicted enhanced wettability due to surface roughness. The Wenzel model introduces a roughness factor in the Young equation, which is the ratio of the actual area of a rough surface to the geometric projected area of the surface. However, the definition of this roughness factor is incompatible with the approach outlined in the previous section, since the actual area of a fractal surface is by definition infinite, leading to an infinite roughness factor. An extension to the Wenzel model was proposed by Cassie and Baxter (1944). In the Wenzel wetting model the liquid is assumed to fill all the surface asperities. In the Cassie-Baxter wetting model the liquid does not penetrate into all the surface asperities, rather the liquid sits upon asperities which still contain pockets of vapor or gas. The Cassie-Baxter model is often used to explain the wetting phenomena of super-hydrophobic surfaces, best example of which is probably the Lotus effect (see Marmur (2004)). The transition between the Wenzel and Cassie-Baxter wetting regime is still a topic of ongoing research, see for example Yang et al. (2018). In the present study all the simulations with surface roughness are assumed to be in the Wenzel regime. The mechanism that enables inclusion of the effects of surface roughness on the contact angle is introduced below.

First it is necessary to make the distinction between the intrinsic contact angle $\theta_i$ and the apparent contact angle $\theta_A$, as illustrated in Fig. 6. The intrinsic contact angle depends only on the liquid and solid material properties. The apparent contact angle is a function of the spatial coordinates and is determined by the intrinsic contact angle and the surface roughness profile. The following expression can be used for the apparent contact angle profile:

$$\gamma(x, y) = \arctan\left(\frac{\nabla \rho}{||\nabla \rho||} \cdot \nabla Z\right)$$

(33)

$$\theta_A(x, y) = \theta_i - \gamma(x, y)$$

with $Z(x, y)$ the function describing the roughness profile and $\frac{\nabla \rho}{||\nabla \rho||}$ the contact line normal vector, as illustrated in Fig. 7. The apparent contact angle is subsequently used in the solid wall boundary condition introduced in Section 3.1.

It is not possible to model the transition from the Wenzel regime to the Cassie-Baxter regime with the approach outlined in this section. Modeling this transition would require fully capturing the surface roughness topology with the computational grid, preferably by adaptive grid refinement at the contact line (see for example Yang et al. (2018)).

3.4. Interfacial contact between solid and fluid

When a warm solid surface comes into contact with a colder fluid, the strive towards thermal equilibrium dictates that the solid and fluid instantly assume the same temperature at the contact interface. The value of the temperature at the contact interface can be determined from the heat-flux balance equation: the heat-flux out of the solid equals the heat-flux into the liquid and vice versa. The following expression holds for the heat-flux at the contact interface:

$$\lambda_s \nabla \cdot \vec{f}_l|_s = \lambda_s \nabla \cdot \vec{f}_l|_f$$

(34)

with $\lambda_s$, $\lambda_f$ the thermal conductivity of the solid and fluid, respectively. Note that $\lambda_f = \lambda_f(\rho)$; the thermal conductivity of the fluid depends on the phase of the fluid, with the liquid having a higher thermal conductivity than the vapor. After introducing the same scaling quantities as for the governing equations, Eq. 34 is equal to:

$$\frac{1}{\kappa} \nabla \cdot \vec{T}|_s = \frac{1}{RePr} \nabla \cdot \vec{T}|_f$$

with $\kappa = \frac{\rho c_v}{\rho c_p}$

(35)

The value of $\kappa$ represents the ratio between the volumetric heat capacity of the fluid with respect to the volumetric heat capacity of the solid. The unit vector $n$ normal to the contact interface and outward from the solid follows from:

$$\vec{n} = \left(\frac{\partial Z}{\partial x}, \frac{\partial Z}{\partial y}, 1\right)^T, \quad \vec{n} = \frac{\vec{n}}{||\vec{n}||}$$

(36)

with $Z(x, y)$ the function describing the surface roughness profile. In a three-dimensional Cartesian coordinate system the balance equation can be expanded to:

$$\frac{1}{\kappa Pe} \left(\begin{array}{l} n_x \frac{\partial T}{\partial x} + n_y \frac{\partial T}{\partial y} + n_z \frac{\partial T}{\partial z} \end{array}\right)|_s = \frac{1}{RePr} \left(\begin{array}{l} n_x \frac{\partial T}{\partial x} + n_y \frac{\partial T}{\partial y} + n_z \frac{\partial T}{\partial z} \end{array}\right)|_f$$

(37)

A first-order finite difference stencil is used for the derivative in the z-direction:

$$\frac{\partial T}{\partial z}|_s = \frac{T_s - T}{\frac{1}{2} \Delta z}, \quad \frac{\partial T}{\partial z}|_f = \frac{T - T_f}{\frac{1}{2} \Delta z}$$

(38)

with $T_s$ and $T_f$ the temperature in the adjacent cells at the contact interface and $\frac{1}{2} \Delta z$ the distance between the contact interface and the first cell center. The solution for $T$ of the following equation yields the temperature field at the contact interface:

$$(RePr + \kappa Pe) T_s + \frac{1}{2} (\kappa Pe - RePr) \Delta z \left(\begin{array}{l} n_x \frac{\partial T}{\partial x} + n_y \frac{\partial T}{\partial y} \end{array}\right) = RePr T_s + \kappa Pe T_f$$

(39)

Full discretization leads to a system of linear equations which needs to be solved, preferably with the use of an optimized sparse matrix solver.
An additional effect of the surface roughness at the solid wall boundary needs to be included in the numerical simulations: the surface area of the cell boundaries at the contact interface is enlarged due to the roughness profile, as is illustrated in Fig. 8. To include this effect it is necessary to introduce the conservation integral equation upon which the Finite Volume Method is based:

$$\frac{\partial U_i}{\partial t} + \frac{1}{V_i} \oint_{S_i} F(U) \cdot n dS = 0$$

(40)

with $U_i$ the cell average of an arbitrary variable, $V_i$, $S_i$ the cell volume and cell outer surface and $n$ the unit vector pointing outward from the solid. When a uniform Cartesian grid is used this expression reduces to:

$$\frac{\partial U_i}{\partial t} + \frac{1}{h} \sum F(U) \cdot n = 0$$

(41)

with $h = \Delta x = \Delta y = \Delta z$ the grid spacing. As a consequence of the surface roughness, the surface area between the solid and fluid domain exceeds the projected surface area. It is assumed that the volume of the cells is not influenced by the surface roughness. To adjust for the increased surface area, the following additional factor for the fluxes at the solid-fluid interface is required:

$$\alpha = \sqrt{1 + \left(\frac{\partial Z}{\partial x}\right)^2 + \left(\frac{\partial Z}{\partial y}\right)^2}$$

(42)

This factor needs to be applied to the fluxes at the contact interface.

3.5. Open boundary condition

In most studies of multiphase flow simulations with a Diffuse Interface Model either periodic or symmetry boundary conditions (BCs) are used at the boundaries of the domain. These type of BCs are convenient because they are relatively easy to implement in a simulation code. However, it is not always possible or desirable to use these BCs. This means that either Dirichlet or Neumann BCs need to be imposed at some of the boundaries of the computational domain. The use of Dirichlet or Neumann BCs effectively closes the computational domain for waves intending to propagate through the boundaries, since these BCs cause these waves to be reflected back into the domain. These reflected waves disturb the solution computed inside the domain, leading to different results as a consequence of the finite size of the domain (Desmarais and Kuerten, 2014). To overcome this problem open BCs have been developed, which have been especially constructed such that they will not reflect waves intending to propagate through the boundaries of the domain.

The open BCs used in the present study are based on the technique presented by Hedstrom (1979) and were originally developed for the Euler equations. The technique was extended by Dutt (1988) for use with the Navier-Stokes equations by employing perturbation theory with the viscous stress tensor treated as the perturbation term. Desmarais and Kuerten (2014) developed an adaptive domain extension technique in order to use open BCs for the Navier-Stokes-Korteweg equations. In the present study the latter extensions are not included, the open BC presented in this section can therefore only be used as long as the liquid-vapor interface does not come into contact with the open boundary and velocity gradients near the open boundary are not too high.

The first step in the derivation of open BCs is the simplification of the NSK equations by neglecting the viscous and capillary stress tensor, which simplifies the NSK equations to the Euler equations. The next step is to obtain the hyperbolic structure of the equations by means of a linearization procedure: each variable is split into an average and a fluctuating part (for example: $\rho = \bar{\rho} + \rho'$). The linearized form of the governing equations then becomes:

$$\frac{\partial U}{\partial t} + A_k \frac{\partial U}{\partial x} + A_y \frac{\partial U}{\partial y} + A_z \frac{\partial U}{\partial z} = \mathbf{0}$$

(43)

with vector $U$ and Jacobian matrices $A$ expressed as:

$$U = \begin{pmatrix} \rho' \\ u' \\ v' \\ w' \\ \rho E' \end{pmatrix}$$

$$A_k = \begin{pmatrix} \bar{u} & \bar{\rho} & 0 & 0 & 0 \\ 0 & \bar{u} & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{u} & 0 \\ 0 & \frac{\bar{u} \rho}{\rho E} & \frac{\bar{u} \rho}{\rho E} & (\bar{\rho E} + \bar{\rho}) & 0 \\ 0 & 0 & 0 & 0 & \bar{w} \end{pmatrix}$$

$$A_y = \begin{pmatrix} \bar{v} & 0 & 0 & 0 & 0 \\ 0 & \bar{v} & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{v} & 0 \\ 0 & \frac{\bar{v} \rho}{\rho E} & \frac{\bar{v} \rho}{\rho E} & (\bar{\rho E} + \bar{\rho}) & 0 \\ 0 & 0 & 0 & 0 & \bar{w} \end{pmatrix}$$

$$A_z = \begin{pmatrix} \bar{w} & 0 & 0 & 0 & 0 \\ 0 & \bar{w} & 0 & 0 & 0 \\ 0 & 0 & \bar{w} & 0 & 0 \\ 0 & \frac{\bar{w} \rho}{\rho E} & \frac{\bar{w} \rho}{\rho E} & (\bar{\rho E} + \bar{\rho}) & 0 \\ 0 & 0 & 0 & 0 & \bar{w} \end{pmatrix}$$

For each variable the average that is used in the linearization procedure equals the value at the boundary where the BC is applied. In the present study the open BC is applied at the top boundary of the domain ($z = L$), where the contributions by $A_y$ and $A_z$ can be neglected. The following expression for the open BC is found with the method of characteristics:

$$\left( \frac{\partial W}{\partial t} + \mathcal{L} \right)_{z=L} = 0$$

where

$$\mathcal{L} = \begin{pmatrix} R \cdot (U_{ff} - U) & \text{if } \lambda_i < 0 & \text{incoming wave} \\ \Lambda \cdot \frac{\partial W}{\partial x} & \text{if } \lambda_i > 0 & \text{outgoing wave} \end{pmatrix}$$

$$L \cdot A_y \cdot R = \Lambda$$

and

$$W = R \cdot U$$

(44)

with $\Lambda$ the eigenvalue matrix (with eigenvalues $\lambda_i$) and $L$, $R$ the left and right eigenvectors of Jacobian matrix $A_y$. The sign of the eigenvalue distinguishes outgoing from incoming waves. The vector $U_{ff}$ contains the far-field conditions, which correspond to a stagnant vapor at a constant temperature. The gradient $\frac{\partial W}{\partial x}$ must be calculated using a one-sided difference scheme that is pointing outwards.

Successful application of the open BCs is only possible if the eigenvalues of the Jacobian matrices are real. This is the reason why the open BCs can only be used as long as the liquid-vapor interface does not come in the close vicinity of the open boundary, since this would cause the eigenvalues to become complex.
4. Simulation results

4.1. Simulation setup

The dimensions of the computational domain are displayed in Fig. 9. The computational grid is Cartesian and uniform with 200 grid points in each direction for the fluid domain, and 20 grid points in z-direction for the solid domain. Simulations on finer grids showed no significant differences in the simulations results. The initial mass density field is constructed with a hyperbolic tangent function in the shape of a single droplet positioned in the middle of the domain and with a velocity towards the solid wall. The thickness of the liquid-vapor interface is approximately $L_i \approx 0.0676L$ which corresponds to the width of approximately 13.5 grid points. This implies that the interface is well resolved. The initial temperature field of the fluid is uniform with $T_{f,i=0} = 0.85$. The initial temperature of the solid is also uniform with $T_{s,i=0} = 0.95$. An overview of all the simulation parameters for the simulation results in this section can be found in Tables 1 and 2.

The Navier-Stokes-Korteweg equations are used for the fluid domain and the heat diffusion equation is used for the solid domain. The fluid and solid domains are coupled by implementing the special boundary condition described in Section 3.1 that takes into account the wetting properties of the solid and ensures continuity of the temperature field and conservation of heat-flux at the contact interface between solid and fluid. In some of the simulations the effect of surface roughness of the solid wall is included by constructing the artificial surface roughness profile described in Section 3.2, which yields an expression for the apparent contact angle as a function of the spatial coordinates. Periodic boundary conditions are used at the left/right and front/back boundaries. The open boundary condition described in Section 3.5 is used at the top boundary. The solid domain is indicated in black, also with periodic boundary conditions at the left/right front/back boundaries and an adiabatic boundary condition at the bottom boundary.

A timestep of $\Delta t = 2 \times 10^{-6} t_0$ was used in all the simulations, with $t_0$ the characteristic timescale derived from the domain length and characteristic velocity (Eq. 1). This implies that discretization errors due to the time stepping are negligibly small. In the visualizations of the simulation results the liquid-vapor interface is represented by a two dimensional surface mesh that was constructed using the Lewiner marching cubes algorithm (Lewiner et al., 2003), where the mass density field was used as the volume data. Only 2 of the 6 simulation cases are visualized in this section (Figs. 10 and 14). However, all simulation cases have been visualized as videos with the video-files added as supplementary material to this article.

4.2. Simulation results of droplet impact

4.2.1. Droplet impacts on a smooth surface with different wetting conditions

Figs. 10 shows a simulation of a liquid droplet impacting on a smooth uniformly heated solid surface with contact angle $\theta_i = 90^\circ$ (Case 1). The temperature field in the solid is visualized by contour plots of two cross-sections. In all simulations the droplet spreads in radial direction from the center of impact, eventually reaching a disk shape at its maximum spreading diameter. Next the liquid starts to recede back towards the center of impact, as a consequence of the capillary forces which aim to minimize the surface area of the liquid-vapor interface. A full droplet rebound is observed in the simulation with hydrophobic wetting conditions ($\theta_i = 120^\circ$, Case 2) where the droplet detaches from the solid surface after the receding movement. The detached droplet does not fall back onto the solid surface because the effect of gravity is not included. In the other two simulations a sessile droplet remains on the solid surface after the receding, the shape of which is determined by the wetting condition and the surface tension coefficient between liquid and vapor.

Because the heat conduction coefficient of the vapor is 100 times smaller than the heat conduction coefficient of the liquid and the solid, a non-uniform temperature field in the solid can be observed from the moment the liquid droplet touches the wall (Fig. 10). The contour plots visualized in this figure shows the topview and a cross-section of the solid during the simulations. The effect of the wetting condition becomes more visible in Fig. 11 which shows the average temperature of the whole solid domain during the droplet impacts. The highest cooling rate is observed for the hydrophilic wetting conditions ($\theta_i = 60^\circ$, Case 3), and the lowest cooling rate for the hydrophobic wetting conditions ($\theta_i = 120^\circ$, Case 2). This can be explained by the difference in wetted surface area of the solid, which is higher for hydrophilic wetting conditions. A larger wetted surface area will lead to more heat transfer between solid and fluid. Fig. 12 shows the total volume of the droplet, the surface area of the liquid-vapor interface and the total kinetic energy of the liquid during the droplet impacts and the solid-liquid interfacial area. The total volume of the droplet decreases during the impact process due to evaporation of some of the liquid. After the moment of impact at $t \approx 0.8$ the surface area of the liquid-vapor interface decreases rapidly for a short moment, which corresponds to the rapid wetting of the solid surface in the first few moments of the impact. The decrease is shortly counteracted by the spreading of the droplet, which is at its maximum at $t = 5.3$, as can also be observed from the kinetic energy plot. The hydrophilic wetting

![Fig. 9. Sketch of a 2D cross-section at $y = 0.5$ of the computational domain with the initial configuration of a single droplet positioned in the middle of the domain and with a velocity towards the solid wall. The solid domain is indicated in black.](image-url)

<table>
<thead>
<tr>
<th>Simulation</th>
<th>$\theta_i$</th>
<th>$R_{\text{rms}}$</th>
<th>$H$</th>
<th>$\alpha$</th>
<th>$P_e$</th>
<th>$\kappa$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>90°</td>
<td>0</td>
<td>n/a</td>
<td>n/a</td>
<td>50</td>
<td>1</td>
</tr>
<tr>
<td>Case 2</td>
<td>120°</td>
<td>0</td>
<td>n/a</td>
<td>n/a</td>
<td>50</td>
<td>1</td>
</tr>
<tr>
<td>Case 3</td>
<td>60°</td>
<td>0</td>
<td>n/a</td>
<td>n/a</td>
<td>50</td>
<td>1</td>
</tr>
<tr>
<td>Case 4</td>
<td>90°</td>
<td>0.01L, 0.8</td>
<td>0.5L</td>
<td>100</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>Case 5</td>
<td>90°</td>
<td>0.01L, 0.7</td>
<td>0.75L</td>
<td>50</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Case 6</td>
<td>90°</td>
<td>0.01L, 0.7</td>
<td>0.75L</td>
<td>50</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

Table 1: Overview of the dimensionless simulation parameters for the simulation results in this section.

Table 2: Overview of the wetting conditions and roughness profile parameters for the simulation results in this section.
condition gives the largest spreading. An even more significant influence of the wetting condition is observed during and after the receding of the droplet. Hydrophilic wetting conditions can be observed to enhance the evaporation rate. More significant oscillation of the droplet after impact can be observed for $\theta_i = 90^\circ$ (Case 1), as indicated by the minima and maxima in the kinetic energy plot. The full droplet rebound in the simulations with the hydrophobic wetting condition ($\theta_i = 120^\circ$, Case 2) can clearly be observed by the horizontal line after $t \approx 3.5$ in the volume and surface area plots.

The influence of the periodic boundary conditions can clearly be observed in the contour plots of the temperature of the solid, with the corners of the domain maintaining a higher temperature on average.
Fig. 11. Average temperature of the solid domain during droplet impacts on a smooth surface with different wetting conditions (Case 1, 2 and 3).

Fig. 12. Total volume of the droplet, surface area of the liquid-vapor interface, surface area of the liquid-solid interface and total kinetic energy of the liquid during simulations of droplet impacts on a smooth surface with different wetting conditions (Case 1, 2 and 3).

Fig. 13. Average temperature of the solid domain during droplet impacts with different thermal properties of the solid (Case 1 and 4).
4.2.2. Droplet impact on a smooth surface with different solids

Fig. 13 shows the average temperature of the whole solid domain during droplet impacts with different thermal properties of the solid. In Case 4 the heat capacity of the solid ($\rho_s c_p$) is 2 times larger than it is in Case 1, while the thermal conductivity ($\lambda_s$) is the same. It can clearly be observed in Fig. 13 that the cooling of the solid is slower and smaller in Case 4 than it is in Case 1, which is consistent with a larger heat capacity.

4.2.3. Droplet impact on a rough surface

Fig. 14 shows a simulation of a liquid droplet impacting on a uniformly heated solid surface with surface roughness and with
intrinsic contact angle $\theta_i = 90^\circ$ (Case 5). The intrinsic contact angle represents the average of the contact angle values imposed at the solid surface. The variation in contact angle values is determined by the surface roughness profile, as is explained in Section 3.3.

In the simulations with a smooth surface, the spreading/receding of the droplet has perfect axial-symmetry, with the center axis located at the point of impact and parallel to the z-axis. The influence of the surface roughness can be observed in a small asymmetry in the spreading/receding of the liquid droplet and also in the asymmetry in the temperature profiles of the cross-sections of the solid. Fig. 15 shows the average temperature of the whole solid domain during the droplet impacts for Case 1, 5 and 6. It is clearly visible that surface roughness increases the cooling rate of the solid, an increase of approximately 1.5% in cooling rate is observed in this comparison. The increased cooling rate can be explained by the increased surface area of the contact interface between the solid and the fluid due to the surface roughness.

Fig. 16 shows the total volume of the droplet, the surface area of the liquid-vapor interface, surface area of the liquid-solid interface and the total kinetic energy of the liquid during the droplet impacts. In the first two plots there is a negligible difference between case 5 and 6, hence only case 1 and 5 are plotted in the first two plots.
between Case 5 and 6, hence only Case 1 and 5 are plotted in the first two plots. A small increase in evaporation rate of the liquid is observed for the simulations with surface roughness (Case 5 and 6) caused by the increased heat transfer between the solid and the fluid. The total kinetic energy in the liquid remains on average at a higher level for the rough surface than for the smooth surface. This can be explained by taking into account the manner in which the roughness profile influences the moving contact line, as was illustrated in Fig. 6. A moving contact line will experience more disturbances on a rough surface and these disturbances will increase the total kinetic energy of the fluid.

In general there are only minor differences between Case 5 and 6, which is to be expected since the surface roughness profiles used in these simulations have the same RMS value. The purpose of this comparison is to study the sensitivity of cooling rate of the solid with respect to the Hurst exponent $H$ and roll-off wavelength $\lambda_r$ of the roughness profile. The simulation results indicate that this sensitivity is small. Additional simulations with different RMS values for the roughness profile indicate that the cooling rate is significantly more sensitive to changes in this parameter.

5. Conclusions

In the present study a Diffuse Interface Model derived from thermodynamics is employed to investigate droplet impacts on a heated solid surface in a vapor environment. The effects of phase transition, surface roughness and non-uniform temperature of the solid surface are included in the simulation method. Phase transition is naturally included in the governing equations of the DIM used in the present study. Surface roughness is included by making the distinction between the intrinsic contact angle $\theta_i$ and the apparent contact angle $\theta_a$, with the apparent contact angle a function of the surface roughness profile. Surface roughness profiles are constructed (and subsequently also characterized) with fractal theory. The heat equation is used to model heat diffusion in the solid. The solid and fluid domain are coupled by a boundary condition that ensures conservation of the heat flux and continuity of the temperature field and also takes into account the surface roughness.

Simulation results demonstrated that the wetting properties of the solid surface influence the cooling of the solid during the droplet impact process. Hydrophobic wetting conditions lead to a higher cooling rate of the solid. Hydrophobic wetting conditions not only lead to a lower cooling rate, also a full droplet rebound is observed after the droplet has receded from its maximum spreading.

Surface roughness of the solid surface increases the cooling rate of the solid by enhancing the heat transfer between solid and liquid. This effect has also been observed in experimental investigations on the effect of surface roughness on heat transfer between solid and liquid (Pais et al., 1992; Silk et al., 2006), as long as the liquid is still able to properly wet the solid (the Wenzel regime). If the surface roughness becomes too large such that it will impede the wetting (the Cassie-Baxter regime), then it is expected that heat transfer will be significantly reduced as a result of surface roughness.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

E.J. Gelissen: Conceptualization, Methodology, Software, Investigation, Visualization, Writing - original draft.
C.W.M. van der Geld: Conceptualization, Supervision, Project administration, Writing - review & editing, Funding acquisition.
M.W. Baltussen: Conceptualization, Supervision, Writing - review & editing, J.G.M. Kuerten: Conceptualization, Supervision, Project administration, Writing - review & editing, Funding acquisition.

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Supplementary material

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