Simulation of Surface Wetting by Droplets Using a Phase Field Model

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In the proposed phase field model a continuous order parameter indicates the phase distribution (liquid/gas). An energy density functional which is defined by three contributions yields the total energy of the system. An equilibrium state is then computed by minimizing this energy of the system using an evolution equation. Details of the algorithmic implementation are discussed by illustrative examples.

1 Introduction and Phase Field Model

For the production as well as for many applications of machine components a reliable prediction of wetting phenomena is very important. In this context the wettability and the so called contact angle are of interest and can be investigated using molecular simulations with force fields. Since those molecular simulations are very costly with regard to the numerical effort they are limited to certain length and time scales. The presented phase field model is intended to transfer the knowledge from molecular simulations to larger scales which are relevant in engineering applications. The continuous order parameter φ of this model indicates if the gas or the liquid phase is preset at a certain location

$$\varphi = \begin{cases} 0 & \text{, for gas} \\ 1 & \text{, for liquid} \end{cases}. \tag{1}$$

Based upon this order parameter an energy functional F that represents the total energy of the domain Ω is formulated

$$F = \int_\Omega \left[12\frac{\gamma_{GL}}{\varepsilon} f(\varphi) + \frac{3}{4}\gamma_{GL}\varepsilon|\nabla\varphi|^2 \right] \mathrm{d}V + \frac{c}{2}\left(\int_\Omega h(\varphi)\mathrm{d}V - V_0 \right)^2 + \int_{\partial\Omega} [h(\varphi)\gamma_{SL} + (1-h(\varphi))\gamma_{SG}]\,\mathrm{d}S. \tag{2}$$

The first component includes the separation and gradient terms which are commonly found in phase field models. Here, γ_{GL} is the surface tension/energy between the gas and the liquid phase. The weights for the separation and gradient terms are chosen such that the width of the transition zone can by adjusted by the parameter ε. The function $f(\varphi)$ is the double well potential

$$f(\varphi) = \varphi^2(1-\varphi)^2. \tag{3}$$

The second component of (2) adds a penalty term that controls the droplet volume with V_0 being the target volume and c being a penalty parameter. Without this penalty term the minimization of the energy contributed from the first part would cause the drop to vanish. In order to be able to adjust the contact angle between droplets and structured surfaces the third component models the energy contribution of the component surface, [1]. Therefore, γ_{SL} is the surface tension between the solid surface and the liquid and γ_{SG} the surface tension between the solid surface and the gas phase. A regularized interpolation function from [2]

$$h(\varphi) = \varphi^3(6\varphi^2 - 15\varphi + 10) \tag{4}$$

ensures the numerical applicability of the volume constraint as well as the surface contribution. Instead of directly computing saddle points (and thereby feasibly minima) of (2) an Allen-Cahn type evolution equation is used

$$\dot{\varphi} = -M\frac{\delta F}{\delta \varphi} \tag{5}$$

where δF is the first variational derivative of F and M is the mobility. Once the vicinity of the solution is reached

$$\int_\Omega 0.5\left(\frac{\dot{\varphi}}{M}\right)^2 \mathrm{d}V \leq \text{tolerance} \tag{6}$$

the evolution equation is no longer used and $\delta F = 0$ is solved directly.

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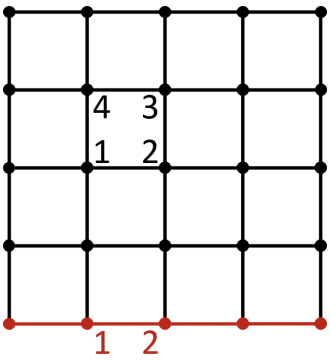

Fig. 1: Discretization with 4-node and 2-node elements.

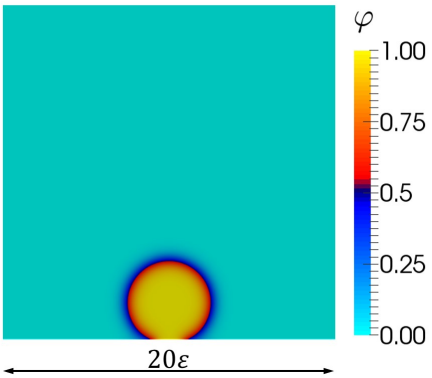

Fig. 2: Drop on hydrophobic surface, input parameters are reported in Table 1.

Table 1: Input parameters (and contact angle) for drop on surface and drop on spikes.

Parameter	Value
γ_{GL}	1.000
γ_{SG}	0.134
γ_{SL}	1.000
ε	0.5
M	0.5
c	10
Θ	150°

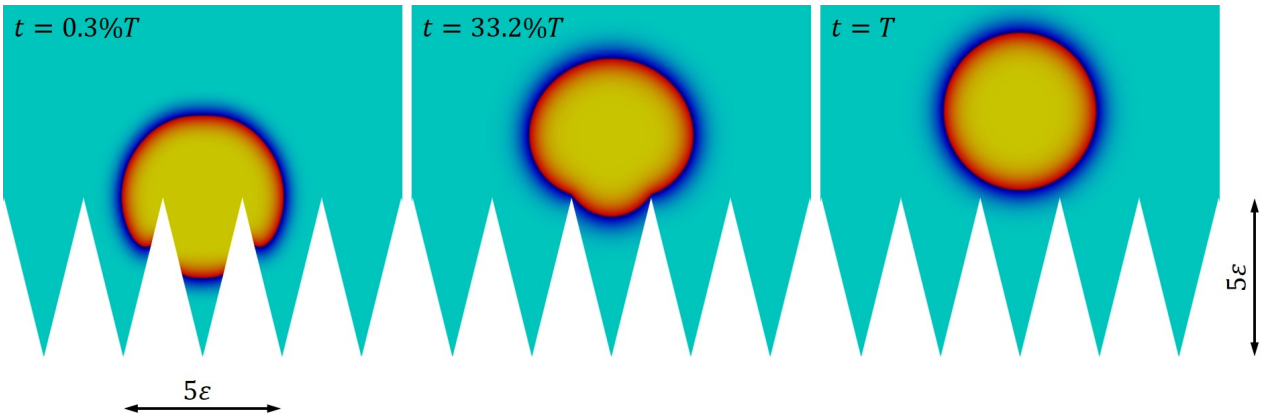

Fig. 3: Drop on hydrophobic spikes at different solution states, input parameters are reported in Table 1.

2 Numerical Validation

The finite element method is used to discretize the proposed model. Regarding the two dimensional case the energy contribution of the first and second component of (2) are discretized by 4-node elements (black elements in Fig. 1) and the third component of (2) (the energy contribution of the surface) is discretized by 2-node elements (red elements in Fig. 1). In the following, two example scenarios are presented in order to show the behavior of the model for fluid drops that are in contact with a solid surface.

At first a drop on a plane hydrophobic surface is considered. The result of the numerical computation can bee seen in Fig. 2. The input parameters are given in Table 1. Using Young's equation ($\cos(\Theta) = \frac{\gamma_{SG}-\gamma_{SL}}{\gamma_{GL}}$) the analytic contact angle for the given surface tensions is $\Theta \approx 150°$. The contact angle of the numerical simulation corresponds well with this analytic contact angle. As expected, there remains an area of contact between the liquid and the solid surface. The next example is a drop sitting on spikes with hydrophobic properties. Again, the input parameters can be found in Table 1. The three plots in Fig. 3 show the evolution at different times t. The full runtime is given by T. The computation is initialized with a drop whose lower edge is below the height of the spikes as one can see in the first plot which shows the phase field at $t = 0.3\%T$. As the computation evolves the drop is traveling upwards and is thereby reducing its contact area with the solid surface ($t = 33.2\%T$). At the final state of the solution ($t = T$) it is evident that unlike in the case of a drop sitting on a plane surface the drop sitting on spikes is barely in contact with the solid surface. This drop behavior mimics the self-cleaning properties of artificial as well as natural surfaces like the one of the lotus flower. Both examples provide plausible results which recommends the model for further development.

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References

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