



# Modeling mesoscopic solidification using dissipative particle dynamics



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## ABSTRACT

Dissipative particle dynamics with energy conversion (DPDe) is a simulation technique that has been used to model thermal transport characteristics and heat transfer at mesoscale. This study shows further development of the DPDe method capturing solid/liquid phase-change phenomena and its application to water freezing in a parallel-plate straight channel. In this work, the weighting functions of the random and dissipative forces are modeled as functions of temperature in order to correctly predict the temperature dependent properties of the fluid in a two-dimensional domain. An equation of state is incorporated in the model in order to model the solidification of water. Careful consideration is taken to couple the latent heat of the system to real world units, and the solidification predicted using this model is compared to a well known analytical solution. The developed model is employed to simulate the thermally developing flow in a parallel-plate channel with constant wall temperatures below the freezing point. A liquid pump is introduced along with a region initiating the liquid temperature in order to create the thermally developing flow. The investigations show that the fluid velocity has a small effect on the time it takes for the channel to freeze completely. The dominating factor will be the temperature of the solid walls in the domain. The simulations also show that when a higher wall temperature is applied, the solid/liquid interface will be rougher due to mesoscopic fluctuations of heat and momentum.

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## 1. Introduction

Dissipative Particle Dynamics (DPD) is a particle-based, mesh-free simulation method introduced by Hoogerbrugge and Koelman [1]. The method has been used extensively in simulations at the mesoscale, where the domains investigated are too large for molecular dynamics (MD) simulations to be efficient, but the materials are still not sufficiently homogeneous to justify a macro-scale continuum description. Polymers used in the membranes of fuel cells [2–4], red blood cells [5,6], and surfactants [7,8] are representative examples of DPD applications. In every time step of a DPD simulation, three types of interactions occur: (i) conservative repulsion caused by spatial arrangement and energetic interaction between the different particles, (ii) dissipative interaction caused by energy lost due to friction or viscosity within a particle, and (iii) random interactions stemming from the thermal motion of the

molecules within a DPD particle [9]. The dissipative and random interactions are linked together in order to satisfy the fluctuation–dissipation theorem and act as a thermostat to maintain a constant simulation temperature. The result is that although momentum is conserved, energy is not [10].

To be able to model thermal energy transport in mesoscopic systems, the dissipative particle dynamics with energy conservation (DPDe) was introduced by Español [10] and Avalos and Mackie [11]. The DPDe method has been used to study heat transfer by convection in several configurations [12–14], thermal conduction in nanoparticle suspensions [15–18], and ballistic-diffusive thermal conduction in thin films [19]. A comprehensive review of the current status of the DPDe method was recently published by Chaudhri and Lukes [20].

A challenge that should be taken into account for further enhancement of the DPDe method is to capture the phase-change phenomenon, a topic of significance at mesoscale. An example showing the importance of phase-change is the ice formation in the porous materials used in proton exchange membrane fuel cells (PEMFCs). Recent studies have shown crucial performance

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Nomenclature	
$A$	Strength of conductive heat transfer
$a$	Strength of the conservative force
$C_v$	Specific heat at constant volume, $\text{J kg}^{-1} \text{K}^{-1}$
$D$	Diffusivity, $\text{m}^2 \text{s}^{-1}$
DPD	Dissipative particle dynamics
DPDe	Dissipative particle dynamics with energy conservation
$e$	Unit vector
$f$	Force, N
$h_{sf}$	Latent heat, $\text{J kg}^{-1}$
$K$	Proportionality constant
$k_b$	Boltzmann constant
$L$	Spatial length, m
$m$	Mass, kg
MD	Molecular dynamics
$n_{dim}$	Number of dimensions
$P$	Pressure, Pa
PEMFC	Proton exchange membrane fuel cell
Pr	Prandtl number ( $\nu\alpha^{-1}$ )
$Q$	Heat flux, $\text{W m}^{-2}$
$r$	Inter-particle distance
$r_c$	Cutoff-radius
$R$	Radius, m
Sc	Schmidt number ( $\nu D^{-1}$ )
$T$	Temperature, K
$T_{fr}$	Freezing temperature, K
$t$	Time, s
$t_{cl}$	Closing time, s
$v$	Velocity vector
$Y$	Position of interface, m
$\alpha$	Thermal diffusivity, $\text{m}^2 \text{s}^{-1}$
$\beta$	Ratio between fluid and solid density
$\gamma$	Dissipative strength
$\epsilon$	Internal energy, $\text{J kg}^{-1}$
$\zeta, \zeta^e$	Random numbers with zero mean and unit variance
$\kappa$	Strength of conductive heat flux
$\kappa_0$	Heat friction coefficient
$\lambda$	Thermal conductivity, $\text{W m}^{-1} \text{K}^{-1}$
$\nu$	Kinematic viscosity, $\text{m}^2 \text{s}^{-1}$
$\rho$	DPDe Density
$\sigma$	Strength of random interactions
$\omega$	Weighting function
<b>Subscripts</b>	
$C$	Cold
$ext$	External
$i, j$	Indices
$s, f$	Solid, fluid
$x, y$	Direction
<b>Superscripts</b>	
$C$	Conservative
$D$	Dissipative
$HC$	Conductive heat
$HR$	Random heat
$HV$	Viscous heat
$n_e$	Exponential of dissipative weighting function
$R$	Random
$\Re$	Real

degradation and mechanical damage of the materials caused by the ice formation during PEMFC operations [21]. The phase-change also has a significant impact for the manufacturing society. Three-dimensional additive manufacturing devices have been rapidly developed. The resolution with good surface finish of these devices is highly related to the liquid transport phenomena involving liquid–solid phase transition [22]. Therefore, further development of the phase-change model in the DPDe method will enhance its applicability to address the current scientific and engineering challenges. Another challenge in using the DPDe method is to correctly predict the behavior of simple fluids such as water or glycerin. In the standard DPDe method, the viscosity of the simulated fluid is directly proportional to the temperature of the fluid. However, for simple fluids, the opposite is true. Recently, Li et al. [23] proposed an improvement to the DPDe-model where the temperature dependent properties of simple fluids can be correctly predicted by incorporating a temperature dependence in the weighting function of the dissipative and random forces. Their improvement is also applied in this paper, together with an equation of state proposed by Willemsen et al. [24] that allows the modeling of phase-change between solid and liquid in the simulation domain.

The objective of this paper is to combine the proposed temperature dependent DPDe model for simple fluids [23] with the equation of state for solid/liquid interaction [24] into a model that can not only correctly predict the thermophysical properties of a simple fluid, but also the phase-change between liquid and solid state. Water is chosen as the working fluid, and careful consideration is taken to validate that the model behaves similar to water in

the investigated range of temperatures with regard to diffusivity, viscosity, heat transfer, and rate of phase-change to the solid state. The length, heat capacity, and latent heat of the simulation are linked to the real world units via physically justified equations. The paper also covers an application of the proposed model: the simultaneous fluid flow and freezing of water in a parallel plate channel with constant sub-zero wall temperatures. This set of simulations can be useful in studies of, e.g., the behavior of microfluidic phase-change valves [25]. In order to study forced convection using the DPDe method, a liquid pump [26,27] is introduced into the simulation domain.

## 2. Methodology

### 2.1. Governing equations

The DPD method is a mesh-free, particle-based method where the different particles in the simulation domain interact with one another through a set of distance and velocity dependent forces [9]. The time evolution of the simulated system is governed by Newton's second law:

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_{j \neq i} (\mathbf{f}_{ij}^C + \mathbf{f}_{ij}^D + \mathbf{f}_{ij}^R) + \mathbf{f}_{ext} \quad (1)$$

$\mathbf{f}^C$ ,  $\mathbf{f}^D$ , and  $\mathbf{f}^R$  are the forces acting between the particles in the simulation, namely conservative, dissipative, and random forces, respectively.  $\mathbf{f}_{ext}$  is an external force that can be used to induce a

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