



A novel multi-dimensional model for solidification process with supercooling



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ABSTRACT

It is well known that many materials do not solidify at their nominal phase-change temperature. Rather, nucleation occurs in them at a lower temperature. This phenomenon is usually termed “supercooling” or “subcooling” in the literature. Understanding, prediction and, if possible, prevention, or at least reduction, of supercooling are very important specifically to latent heat thermal energy storage (LHTES) systems, because the temperature differences in them must be small in order to achieve higher efficiency.

In the present study, a novel mathematical model of solidification with supercooling and heat transfer is developed. For the first time, it is multidimensional in space. The model encompasses all possible stages of the process, namely, single-phase liquid cooling from the initial state to the nucleation temperature, kinetic nucleation accompanied by a rapid temperature rise to the nominal phase-change temperature, regular solidification and finally cooling of the solid phase. The kinetic solidification speed, based on the activation energy, is temperature- and, as a result, time-dependent. The model ensures a smooth, physically meaningful transition from the kinetic to regular solidification. Local and overall energy balance preservation at all stages of the process is ensured.

The model is based on the enthalpy formulation, resolved using an in-house numerical code based on finite volumes. For the single phase cooling, it is validated using the well-known solutions from the literature. The model is then compared to experimental results of solidification of supercooled gallium in a vertical cylindrical mold. Accordingly, heat transfer in the mold is also included. It is shown that the model reflects the experimental results fairly well, in particular when predicting temperatures at various locations inside the material. Also, physically sound solidification patterns are obtained.

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1. Introduction

1.1. General considerations

Regular solidification is the process in which a matter in liquid state is first cooled to its phase-change temperature, and then begins to solidify while releasing its latent heat. The release of latent heat and continuation of the cooling process keep the system at a constant temperature. On the contrary, in the presence of supercooling, sometimes referred to in the literature as subcooling or undercooling of the liquid, solidification does not take place at the nominal phase-change temperature. Instead, the liquid phase continues to cool below that temperature (Fig. 1b). However, there it becomes thermodynamically unstable and thus a small amount of energy can initiate the solidification process, accompa-

nied by a sharp increase in the temperature due to the spontaneously released latent heat. This stage is known as the kinetic solidification. The difference between the nominal solidification temperature and the nucleation temperature, i.e. the actual temperature at which solidification begins, is called “the degree of supercooling (or subcooling).”

Glicksman [1] states that the relation between enthalpy and temperature of a supercooled liquid is the same as the relation used for non-supercooled liquids. Even though the latent heat is released, it is used to bring the system temperature up to the solidification temperature, and the warming of the liquid is balanced by creation of the solid, i.e. a phase with lower enthalpy. Energy considerations concerning the nucleation theory have been presented in many books dealing with solidification from the metallurgy point of view [2–5]. Research and development of latent heat thermal energy storage (LHTES) systems have caused new interest in the phenomenon. In these systems, the need to lower the cooling temperature in order to initiate solidification of the phase change

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Nomenclature

B	wall thickness, m
c_p	specific heat, kJ/(kg K)
d	molecular diameter, pm
G	Gibbs energy, kJ
h	mass specific enthalpy, kJ/kg
h_p	Planck's constant, $m^2 \text{ kg/s}$
H	cylinder height, m
J_0	zero-order Bessel function
J_1	first-order Bessel function
k	thermal conductivity, W/(m K)
k_B	Boltzmann's constant, $m^2 \cdot \text{kg}/(s^2 \text{ K})$
L	latent heat per unit mass, kJ/kg
N	number of cells undergoing temperature change
p	state of PCM parameter
Q	heat, kJ
r	radial coordinate, m
R	cylinder radius, m
R_{th}	thermal resistance, K/W
SF	solid fraction
t	time, s
T	temperature, °C
V	solidification speed, m/s
x	Cartesian coordinate, m
z	axial coordinate, m

Greek letters

α	thermal diffusivity, m^2/s
δT	half of phase change temperature range, °C

Δ	difference
ζ	conductivity parameter, W/(m K)
λ	eigenvalue, radial direction
ρ	density, kg/m^3
τ	integration variable
ϕ	solid–liquid ratio
ω	eigenvalue, axial direction

Subscripts

a	activation
env	environment
i	cell index in the radial direction
$init$	initial
j	cell index in the axial direction
l	liquid
m	melting
max	maximal
n	time step index
nuc	nucleation
PCM	PCM filled cells
s	solid
u	line index, axial direction
w	line index, radial direction
$wall$	wall

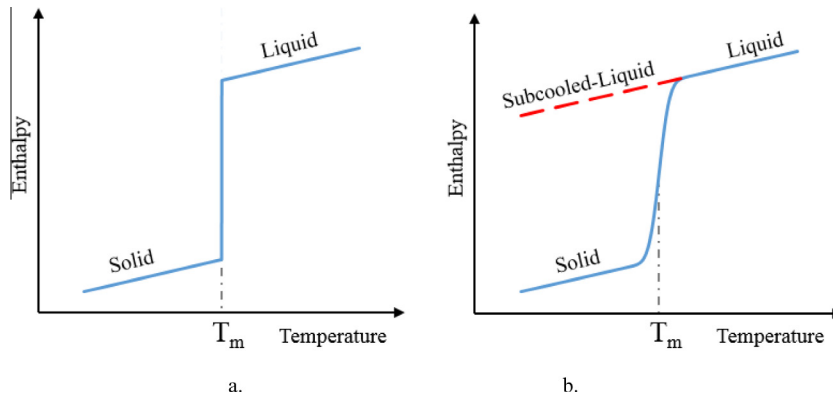


Fig. 1. (a) Enthalpy temperature relation used for the enthalpy method. (b) Enthalpy temperature relations used in this work.

material (PCM) in the presence of supercooling is highly undesirable: unlike metallurgy, the temperature differences in LHTEs must be small. Lowering the cooling temperature in order to “contain” supercooling in the system would definitely lead to a lower efficiency. Thus, even for a minor degree of supercooling the performance of the system might be impaired. For instance, Zhang and Niu [6] investigated the effect of supercooling on a full-scale microencapsulated slurry storage system that was used to cool a room. It was concluded that for the given system, the latent heat transition was not entirely completed due to supercooling in the microcapsules, raising the need for a lower temperature for the solidification of the PCM, which would lower the coefficient of performance (COP) of an electrically-driven cooling system or reduce utilization hours for natural cooling sources.

1.2. Experimental works

Studies on the subject of supercooling are abundant. Bigg [7] investigated supercooling in water drops, which were not in a contact with any solid surface that might initiate nucleation. The results indicate that the larger the drop volume and the lower the cooling rate, the higher the mean nucleation temperature. Saito et al. [8] studied the effect of the cooling surface on the solidification of water. Five kinds of plates, each with different surface roughness, were used as cooling surfaces. The experimental outcomes showed that for rougher surfaces, nucleation commenced at higher temperatures. Saito et al. [8] also presented a probability-of-nucleation function based on the surface roughness and cooling rate. Okawa et al. [9] looked at the effect of the surface

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