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On the analytical modelling of the initial ice growth in a supercooled liquid droplet

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ABSTRACT

Ice formation in metastable, super-cooled droplets, which are frequently found in the atmosphere, influences the appearance and characteristics of atmospheric clouds significantly, for example regarding precipitation. Its numerical investigation can provide deep insight into the underlying physical mechanisms and supports the deduction of models that describe these processes on the microscale; those models are required for a description of the macrophysical system. However, even the processes on the microscale span about four orders of magnitude. A semi-analytical sub-scale model based on similarity solutions is thus deduced in order to narrow the gap between the different scales describing the initially spherical ice growth in a super-cooled droplet, which can be reduced to a radially symmetric, but highly non-linear Stefan-type problem. All relevant physical effects, e.g. the reduction of the melting temperature, the expansion of the water phase due to the decrease of density upon solidification and high degrees of supercooling, are taken into account in contrast to classical approaches. The maximum relative error in terms of the freezing time, which is given explicitly as well as the temperature fields, is less than 10% at a degree of supercooling of 35 K and decreases rapidly as the ambient temperature increases.
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1. Introduction

One important aspect of freezing processes in nature is the formation of ice crystals in clouds in our atmosphere. According to [1,2], the ice formation determines the appearance of clouds, their dynamic behavior, stability and characteristics such as the amount, beginning and duration of precipitation. Cloud ice may exist, for example, at the top of cumulonimbus clouds and cirriform clouds, as pointed out in [3]. The ice particles form either by deposition of water vapor or by freezing of super-cooled liquid droplets [1,4].

The present paper focuses on the initial freezing of super-cooled droplets that are liquid at temperatures below their equilibrium melting point and thus exist in a metastable state [4,5]. Crystallization of super-cooled water will not start unless a solid ice cluster of critical size has been formed by nucleation [6]. Supercooled water nucleates homogeneously in the absence of foreign insoluble substances due to fluctuations in quantities such as density, pressure and temperature, which are caused by the perpetual formation and disintegration of small ice clusters. In contrast, heterogeneous nucleation is initiated by ice forming nuclei like aerosols at lower degrees of supercooling [7]. According to data on nucleation rates from literature [9] and the concentration of ice-forming nuclei per volume, the appearance of a second nucleus within the super-cooled droplet is very unlikely during the relevant time span. Furthermore, the ice growth of the initial nucleus impedes the formation of a second one due to the release of latent heat.

The significance of ice formation in super-cooled droplets, which are frequently found in the atmosphere [7], has already been stated in the year 1933 by T. Bergeron [8] who hypothesized that most heavy rainfall from super-cooled clouds requires the formation of ice. According to [9], global precipitation is predominantly produced by clouds containing an ice phase. However, knowledge about its formation still remains incomplete, as also stated in [10]. Understanding these processes on droplet scale and linking them to larger scales is of crucial necessity for weather and climate modeling [11] and has been an important field of research during the last decades. However, according to [12], cloud models lack detailed parameterizations for the ice initiation processes in cirrus clouds. In [2] the uncertainties in precipitation models that arise due to poor knowledge of the ice initiation processes in clouds and their implications for climate studies are mentioned. An improvement in the description of ice formation processes in clouds is demanded in [1]. They also emphasize the significance of numerical models in studying cloud processes due to limitations in experimental investigations. A contribution to finding answers

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Nomenclature

Latin characters

a	thermal diffusivity ($m^2\,s^{-1}$)
A_n, B_n	constants (–)
$C_1 - C_8$	constants (–)
$\bar{C}_3, \hat{C}_3, \tilde{C}_4$	constants (–)
c_i	specific heat capacity of ice ($J\,kg^{-1}\,K^{-1}$)
$c_{p,w}$	specific heat capacity of water at constant pressure ($J\,kg^{-1}\,K^{-1}$)
D_n, E_n	constants (–)
E_τ	maximum relative error in time (–)
g	specific free energy ($J\,kg^{-1}$)
k	thermal conductivity ($W\,m^{-1}\,K^{-1}$)
L	specific latent heat of fusion ($J\,kg^{-1}$)
r	radial coordinate (m)
R	radial ice-water interface position (m)
R_c	critical nucleus radius according to Eq. (1) (m)
R_d	reference droplet diameter (m)
$R_{d,\min}$	minimum droplet diameter (m)
$R_{\max}$	maximum size of the ice particle (m)
R_{stable}	radius defining the upper limit of spherical ice growth according to Eq. (2) (m)
$\dot{R}$	radial velocity of the ice-water interface ($m\,s^{-1}$)
St	Stefan number, $St = c_{p,w}(T_m - T_\infty)/L$ (–)
t	time or time span (s)
T	temperature (K)
ΔT	degree of supercooling (K)
T_m	standard melting temperature (K)
T_{GT}	reduced melting temperature due to a curved interface (K)
v	velocity of the water phase ($m\,s^{-1}$)
X	water-air interface position (m)
Z	transformed temperature gradient $Z = \zeta^2 d_\zeta \Theta_w^{ss,\Delta\rho}$ (–)

Greek characters

Γ	adapted constant from similarity solution (–)
Γ^{ss}	constant from a similarity solution where $\Delta\rho \neq 0$ (–)
$\Gamma^{ss,\Delta\rho=0}$	constant from a similarity solution where $\Delta\rho = 0$ (–)
Δ	difference in a quantity between liquid water and ice (–)
η	coordinate, $\eta = \left(\tilde{r} - \tilde{R}\right)/\left(\tilde{X} - \tilde{R}\right)$ (–)
Θ	dimensionless temperature, $\Theta = (T - T_m)/(T_\infty - T_m)$ (–)
Ψ	transformed dimensionless temperature, $\Psi = \Theta\tilde{r}$ (–)
ρ	density ($kg\,m^{-3}$)
σ	interfacial energy between two phases ($N\,m^{-1}$)
τ	dimensionless time, $a_w t/R_d^2$ (–)
ξ	coordinate, $\xi = \tilde{r}/\tilde{R}$ (–)
ζ	coordinate, $\zeta = \tilde{r}/\tilde{R}$ (–)

Subscripts

0, ref	reference or initial value
i	ice phase
n	index of a sum
w	water phase
∞	ambient conditions

Superscripts

h	solution to a homogeneous problem
p	particular solution
$\sim$	dimensionless quantity
R, X	quantity is evaluated at the specified location

to some of these questions is Direct Numerical Simulation (DNS) of the ice formation in a super-cooled droplet. The size of a typical cloud droplet is in the order of micrometers, while the nucleus, which starts to grow inside this droplet, has a diameter of a few nanometers only. The resolution of at least four orders of magnitude in great detail is impossible today due to a limit in available computational power. We thus derive a semi-analytical sub-scale model that can be easily implemented into a numerical code and narrows the gap between the processes on nanometer and droplet scale. It represents the growth of a single initial ice particle in the droplet's center. Following the work of [13] this initial ice particle remains spherical up to a threshold radius because instabilities on the surface are damped. According to [14], cloud droplets with diameters in the order of micrometers are spherical, too. The problem that is referred to as Stefan problem can thus be reduced to a freezing problem with radial symmetry and is described in more detail in the following section. No exact solution to this problem seems to exist according to e.g. [15]. Approximate solutions to Stefan problem frequently found in literature ([16–21] and others) base on perturbation methods. The authors of the present paper also presented a solution to the moving ice-water interface in a super-cooled liquid droplet using perturbation methods [22]. In general, the accuracy of perturbation solutions decreases with an increase of the perturbation parameter. This parameter in Stefan type problems represents the supercooling. Perturbation methods are thus applicable only if the supercooling is low. Hence, the perturbation analysis in [22] has only been used as a starting solution to a subsequent iterative numerical scheme in order to reduce computational time.

The solution we suggest in the following can also be applied to ice growth in metastable droplets with very high supercooling. In contrast to other solutions presented in literature, it involves all physical aspects that are identified as relevant to the problem under consideration in Section 3. The solution is given explicitly in terms of a temperature field in ice and water as well as in terms of the freezing time. It can be thus implemented directly into any numerical code that is used for the simulation of the subsequent dendritic ice growth.

The mathematical formulation of the Stefan problem of interest is given in Section 2. In Section 4 we present an approximative analytical solution to the problem that accounts for all important physical effects as well as the results by means of temperature distribution in the ice and water phase and growth of the ice particle's interface, which are compared to a numerical reference solution.

2. Mathematical formulation and identification of the most important physical effects

Further growth of an ice nucleus in super-cooled water is energetically favorable once the critical cluster size R_c is exceeded which is characterized by the maximum in the specific Gibbs free energy g. Accounting for the thermodynamic equilibrium of both phases and using Gibbs fundamental equation to express the specific Gibbs free energy g in terms of temperature T, the critical cluster radius reads

$$R_c = \left(- \frac{2\sigma}{\rho_i \left(L\left(\frac{T_\infty}{T_m} - 1\right) + \left(c_{p,w} - c_i\right)\left(T_\infty \ln\left(\frac{T_\infty}{T_m}\right) + T_m - T_\infty\right)\right)} \right) \quad (1)$$

with surface tension σ, ice density ρ_i, specific latent heat of fusion L, specific heat capacity of ice c_i and of water at constant pressure $c_{p,w}$. The temperature T_m indicates the standard melting temperature and T_∞ the ambient temperature of the gas phase.

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