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Numerical calculation of the condensational growth of liquid particles in non-dilute and non-ideal media

F.J. Fernández [a,*,1], M.M. Prieto [a,1], J.M. Fernández-Díaz [b]

[a] Department of Energy, University of Oviedo, Campus de Viesques, 33204 Gijón, Spain
[b] Department of Physics, University of Oviedo, C/Calvo Sotelo, 33007 Oviedo, Spain

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ABSTRACT

Condensational growth in aerosols involves simultaneous heat and mass transfer between particles and their surrounding medium. There are several ways of modelling this phenomenon: dilute medium in the vapour species, ideal gas behaviour, ideal mixture, constant thermophysical properties, etc. Most of the solutions proposed for this problem are analytical, at the cost of simplifying many aspects of the phenomenon. This study develops a numerical method for the solution of the steady-state condensational growth of aerosol liquid particles submerged in a gaseous mixture of condensable vapour and inert (non-condensing) gas. Following the principles of the finite volume method, the mass and energy conservation and the droplet heat balance equations are discretized in a spherical mesh around the particle, obtaining their solution by means of a matrix procedure. Heat and mass are transferred satisfying the first-order phenomenological equations. Transport and thermophysical properties of the mixture can be calculated independently, avoiding other assumptions required in analytical procedures. In order to test the method, it was compared with two analytical solutions for the non-dilute condensational growth problem. One of these methods was applied as formulated in the literature, but the other was significantly improved, applying new factors to separate heat and mass transfer as functions of temperature and composition, respectively. The comparison was performed for four condensing substances (H_2O, R-134a, *n*-pentane and *n*-octane) with air as the inert gas. The results show good agreement under conditions for the ideal gas law, with differences in the case that deviates slightly from this behaviour.

1. Introduction

The interaction between liquid particles and their surrounding gaseous medium is a key aspect in the study of aerosols. Consisting of a continuous gas phase with a discrete liquid phase suspended within it, aerosols of this kind, also known as fogs, are very important in atmospheric physics, but can also be present in other systems. The term 'condensational growth' describes the process by means of which a droplet grows or shrinks due to the condensation or evaporation on its surface of the species that forms it.

The study of the condensational growth of aerosol particles can be addressed in various ways. Some authors use techniques based on the method of moments [1,2], while others use molecular kinetics [3,4]. If changes in droplet size or composition and/or in the bulk medium are expected to be very fast, non-steady state versions of the energy balance are proposed, with a simpler formulation of heat and mass transfer than in first-order transport equations [5–7]. Among the latter, the relative velocity between the medium and the particle is sometimes considered and the problem is studied in terms of convective heat and mass transfer, like studies in drug administration [8,9], particles in combustion engines [10] and other more general studies [11]. In other cases, purely diffusive heat and mass transfer are considered [12,13]. Non-steady particle growth caused by diffusive heat and mass transport between phases in gas–liquid contact devices with multiple species involved was studied by Schaber et al. [14–16].

Condensational growth of aerosols in atmospheric physics is usually based on the assumption of low vapour concentration (dilute medium). It is formulated in this way in benchmark books in this field [17,18] and is a frequent assumption in particles surrounded by moist air. There are many other situations in which the composition of the gaseous mixture can have a broad range, so the dilute assumption is not applicable.

The first theoretical basis of droplet growth under the dilute medium assumption was established by Maxwell [19], with heat

* Corresponding author. Tel.: +34 985182112; fax: +34 985182143.
E-mail addresses: javierfernandez@uniovi.es (F.J. Fernández), manuelap@uniovi.es (M.M. Prieto), julio@uniovi.es (J.M. Fernández-Díaz).
[1] Group associated with the Spanish Scientific Research Council (CSIC).

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Nomenclature

c	Mole concentration
c_p	Specific heat capacity at constant p
D_g	Binary diffusion coefficient
D_T	Thermal diffusion coefficient
d_c	Collision diameter
E	Energy
$F_T,\ F_M$	Factors of dependence in eqs. with separated variables
G	Geometrical factor in mesh definition
$\hat{g}$	Molar Gibbs free energy
h	Specific enthalpy
IT_T	Energy conservation indep. terms
IT_Y	Continuity independent terms
i	Cell counter
j	Mass flux
$\hat{j}$	Mole flux
$K_1,\ K_2$	Factors for linear law in
Kn	Knudsen number
K_t	Ratio of diffusivities
k	Thermal conductivity
M	Molecular Mass
m	Mass
$\dot{m}$	Mass flow rate
N	Number of moles
N_C	Number of mesh cells
n_m	Molecular concentration
p	Pressure
$\dot{Q}$	Heat transfer rate
q	eat flux
R_p	Particle radius
R_U	Ideal gas universal const.
r	Radial position
S	Saturation ratio
T	Temperature
t	Time
U_σ	Energy change by surface tension
$\vec{u}_r$	Unitary radial vector
V	Volume
v	Velocity
$\hat{v}$	Specific molar volume
y	Gas phase mole fraction

Greek Symbols

ΔH_{fg}	Specific latent heat of condensation
$\Gamma_T,\ \Theta_T,\ \Omega_T$	Energy conservation matrix terms
$\Gamma_Y,\ \Theta_Y,\ \Omega_Y$	Continuity matrix terms
α_t	Thermal diffusion factor
$\alpha_T,\ \alpha_M$	Mass and heat accommodation coeffs.
$\beta_T,\ \beta_M$	Factors for non-continuum regime
$\theta_X,\ \theta_T$	Factors for heat transfer eq.
λ	Mean Free Path
μ	Dynamic viscosity
$\xi_X,\ \xi_T$	Factors for mass transfer eq.
ρ	Density
σ_{lg}	Liquid–gas surface tension
τ_T	Factor for heat transfer eq.
φ	Fugacity coefficient

Subscripts

b	bulk
g	gas mixture
in	inert gas
l	liquid
p	particle
sat	saturation
v	vapour

and mass transport described by Fourier's law of heat conduction and Fick's law of diffusion, respectively, considering a motionless droplet within the uniform medium following a steady state process.

The more general first-order transport equations in Wagner [20] formulate condensational growth considering simultaneous heat and mass transfer, Stefan-flow, thermal diffusion and the Dufour effect around the droplet. Researchers have applied different hypotheses to obtain analytical solutions of these first-order transport equations over time. Wagner [20] assumed a zeroth-order (Fourier and Fick's laws) diffusion problem to obtain a solution. Kulmala and Vesala [21] and Heidenreich [22] assumed a relationship between concentration and temperature fields based on a pure diffusion conception of the problem (although Heidenreich [22] also provided a more complex option). The well-known solution of Barrett and Clement [23] starts from the transport equations without thermal diffusion or the Dufour effect and includes radiative heat exchange on the droplet surface.

An important simplification in analytical methods arises from the way they address the formulation of thermophysical properties, together with the equation of state defining the behaviour of the state variables. The problem is defined by the fields of temperature and composition of the gas mixture around the droplet, so the value of thermophysical properties should be obtained as a function of these variables. Difficult to formulate heat and mass transport properties are also needed. For example, Wagner [20] and Kulmala and Vesala [21] consider the exponential temperature dependence of the diffusion coefficient, while Heidenreich [22] calculates thermal conductivity as a function of temperature and composition. In these cases, the ideal gas equation of state is implicit in the solutions.

When the composition and temperature profiles around the droplet are considered to remain stationary for the solution of the heat and mass transfer, the process can also be considered as stationary. This is a common approach in condensational growth that can be applied when the relaxation time for temperature and composition profiles [18] is much shorter than the time taken by significant changes in the boundary conditions [24,25]. Known as the quasi-steady state approach, it is assumed in classical studies like Wagner [20], Heidenreich [22] and Kulmala and Vesala [21]. It is also assumed in studies dealing with binary condensational growth like in Kulmala et al. [26], whose analytical solution was recently applied by Davies et al. [25], and in others related to simulation of the behaviour of cloud condensation nuclei counters [27,28] in which condensational growth is calculated via the theory of diffusional growth [18].

During a study of aerosols in condensers of pure substances mixed with inert gas, the need arose for an accurate tool to calculate the heat and mass exchange between continuum and discrete phases. Inside a condenser, the assumption of the vapour being the minority species is not applicable; it could even be the main species. Obtaining one solution of the first-order phenomenological equations in Wagner [20] as precise as possible became the objective that has given rise to this paper. A numerical method based on the finite volume method (FVM) has been developed to achieve this aim, resulting in a highly flexible and precise procedure. The