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Sensitivity study for the mass transfer at a single droplet

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Abstract

The mass transfer between a single droplet and a surrounding fluid can be described mathematically solving the momentum and mass balances in both phases (conjugate problem). This study of dimensionless parameters shows how the process is influenced by changes in material properties and operating conditions.

The influence of the Reynolds number *Re* on the mass transfer is found to be small and to vanish for creeping flows. A sensitivity to the viscosity ratio μ^* exists only in a limited range. The influence of the Peclet number *Pe* can be approximated for small *Pe* by considering only the external problem and for high *Pe* by considering only the internal problem.

Keywords: Mass transfer; Droplet; Two phase flow; Moving boundaries; Computational fluid dynamics

1. Introduction

Unsteady mass transfer between fluid particles and a surrounding continuous fluid is fundamental for many technical applications, like bubble columns, airlift reactors, liquid/liquid extraction, etc. This transport process is influenced by the physical properties of the species, by the operating conditions and by the particle properties.

To model this system mathematically the momentum and mass balance equations have to be solved in both phases considering adequate boundary conditions and interfacial conditions including all relevant forces and the thermodynamic equilibrium. At present, this can not be done in the full complexity because of two reasons: Firstly, the physics of some phenomena is not yet understood qualitatively and quantitatively, which leads to difficulties in setting up a mathematical description [16]. This includes changes in surface tension and surface mobility caused by the mass transfer process or irregular time dependent particle shapes.

The second point is the huge numerical effort required for a sufficiently accurate solution of the balance equations even for a single particle. For a swarm of particles the computing time will be in the order of weeks, months, or longer. To deal with this situation the mathematical description used in this work is based on a couple of simplifications: Only a single spherical droplet is considered and all effects caused either by changes of surface tension (like Marangoni convection) or by changes in the physical properties of the phases are neglected. Here, both phases are liquid, but the same algorithm can be applied also for liquid/gas and gas/liquid systems using suitable parameter sets. Based on the knowledge gained from this investigation the influence of parameter variations can be judged and suitable models for more complex systems can be developed in a subsequent step.

In our setup we investigate the mass transfer of an additive from a droplet into an ambient continuous

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Nomenclature

A_i	area of interface, m^2
c	concentration, mol/m^3
D	diffusion coefficient, m^2/s
D^*	ratio of diffusion coefficients, –
d	diameter of the droplet, m
Fo	Fourier number, –
Fr	Froude number, –
$\vec{g}$	gravitational acceleration, m/s^2
k	mass transfer coefficient, m/s
m	distribution coefficient, –
$\dot{n}$	molar flux, mol/s
p	pressure, Pa
p'	reduced pressure, –
Pe	Peclet number, –
R	radius of the droplet, m
Re	Reynolds number, –
r	radial coordinate, m
r'	reduced radial coordinate, –
Re	Reynolds number, –
Sc	Schmidt number, –
Sh	Sherwood number, –
t	time, s
t'	reduced time, –
$\vec{v}$	velocity, m/s
$\vec{v}'$	reduced velocity, –
$\vec{v}_r$	relative velocity between the phases, m/s
Greek symbols	
μ	dynamic viscosity, kg/ms
μ^*	ratio of dynamic viscosities, –
ν	kinematic viscosity, m^2/s
ρ	density, kg/m^3
ρ^*	ratio of densities, –
ξ	averaged reduced concentration in the particle, –
ξ'	reduced concentration, –
Subscripts	
∞	far away from the droplet or after long time
0	initial
1	dispersed phase
2	continuous phase
i	interface

liquid phase. Mass transfer in the opposite direction can be described similarly. The initial additive concentration in the continuous phase is zero which is an easy but not restricting assumption since mass transfer and the Sherwood number used for its description depend only on concentration differences and not on absolute concentrations.

Mass transfer around a single droplet has been studied experimentally and numerically by a number of research groups during the last decades. The activities in this field served on the one hand to the validation of numerical methods by comparing the results to analytical solutions of limiting cases (e.g. [3]), and on the other hand they were used to validate models with respect to experimental data (e.g. [17]). In the first case good agreement was found up to Peclet numbers of 10^4 [12]. In the second case most simulations resulted in slower mass transfers than found in the corresponding experiments. Computations with advanced models describing the interfacial processes have not yet been presented. Simple models like those that involve an artificial increase of the diffusion coefficient D [5,6] are not investigated in this paper since the dependence of the modified diffusion coefficient D on material or flow properties is not known and thus the prediction reliability of such models is not higher compared to the basic model. However, since this paper gives mainly a parameter study in terms of dimensionless numbers the solution for such adapted models can be obtained by replacing the molecular diffusion coefficient by a modified one that is expressed in these dimensionless numbers.

There are a couple of parameters describing fluid properties of the two phases that influence the mass transfer between them. The influence of the ratio of these parameters can be studied. The goal of the present paper is not a general description of the influence of parameters on the system behavior but determination of the range in which a parameter has an influence and the one in which it can be varied without affecting the resulting asymptotic Sherwood number Sh_∞. Sh_∞ is a dimensionless measure for the mass transfer rate. The investigations will concentrate on the Reynolds number Re, the Peclet number Pe, and the viscosity ratio μ^*. From these, regions of stability against changes in the operating condition and of sensitivity to operating conditions can be derived. Correspondingly, ranges of parameters can be found in which changes of operating conditions do not influence Sh_∞ and ranges in which they do.

2. Model description

2.1. Velocity field

Under the assumptions discussed in Section 1 the velocity field $\vec{v}$ inside and outside the droplet can be considered to be stationary and independent of the