International Communications in Heat and Mass Transfer 79 (2016) 135–139

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ichmt

On the local mass transfer rates around arbitrary shaped particles calculated by X-ray computed microtomography: Prospective for a novel experimental technique

M. Santini [a,*], S. Fest-Santini [b], P. Foltyn [c]

[a] Department of Engineering and Applied Sciences, University of Bergamo, Viale Marconi 5, 24044 Dalmine, BG, Italy
[b] Department of Management, Information and Production Engineering, University of Bergamo, Viale Marconi 5, 24044 Dalmine, BG, Italy
[c] Faculty of Aerospace Engineering and Geodesy, University of Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany

ARTICLE INFO

Available online 15 November 2016

Keywords:
Local mass transfer coefficient
MicroCT
Free convention
Gaussian curvature
Sphere

ABSTRACT

The present manuscript presents the application of X-ray computed microtomography (microCT) as a non-intrusive technique to calculate the local and global mass transfer rates around arbitrary shaped particles. The technique is validated on the case of mass transfer around a spherical particle in free convection. A review of available experimental and numerical investigations for spherical particle is reported in comparison to the obtained results. The 3-dimensionality of the microCT approach allows the calculation of the local curvature. The correlation between local curvature and mass transfer rate is, therefore, made experimentally feasible for arbitrary shaped particles.

1. Introduction

The mass transfer in free convection from a particle to a surrounding fluid was mostly studied experimentally by dissolution in stagnant liquids of uniform temperature and monitoring the variation of the shape by the evaluation of 2-dimensional images [1–3] or by electrochemical methods (adding a supporting electrolyte) and correlating the current to the local mass transfer coefficient [4]. Such measurement principles implied a series of drawbacks: the first technique is limited by the 2-dimensional image distortions, differences in refractive indices, assumption of axial symmetry while the latter by the limitations in choosing of the supporting anode and the challenging controls of the flow regime for the electrochemical method.

The present manuscript introduces a non-invasive, high-resolution measurement method to determine local and global mass transfer coefficients of arbitrary shaped particles, based on the X-ray computed microtomography (microCT) technique. Further, this 3-dimensional approach enables the estimation of local curvatures and allows their correlation to local mass transfer rates.

Experimental and numerical investigations of spherically shaped bodies in free convection have been presented by different authors on the heat and mass transfer natural phenomena [1–11] and analogy between both was presumed. The "classical" experiment of mass transfer around a solid spherical particle has been chosen for the validation of the present technique.

Nowadays, experimental investigations are still highly demanded foreseeing the possibility to investigate properly this natural phenomenon that occurs in a multitude of applications, and for developing new predictive models because the analytical solution for arbitrary shaped particles does not exist. Despite that, the last formal experimental paper was in the late seventies of the past century, supposed due to the complexity and the limitations of the available techniques.

2. Experimental method

The experimental investigations of the mass transfer for spherically shaped fluids are challenging due to the attitude of the latter to change their shape, alongside a non-equilibrium boundary condition.

The analogy between the sublimation and the evaporation ensures a possibility for the experimental study of mass transfer using solid particles, with the undoubted advantage of shape stability and consistency during the phase change.

Anyway, the sublimation process should not to be too fast, allowing the microCT scan of the particle to be completed (in quasi steady-state condition), and either not too long for limiting the effects of instabilities of the boundary conditions during the sublimation.

---

[*] Corresponding author.
E-mail address: maurizio.santini@unibg.it (M. Santini).

http://dx.doi.org/10.1016/j.icheatmasstransfer.2016.11.001

Nomenclature

d	diameter [m]
D	diffusion coefficient [m^2/s]
K_G	Gaussian curvature [m^{-2}]
l_{ch}	characteristic length [m]
M_m	molar weight [kg/kmol]
p_{sub}	sublimation pressure [Pa]
P	atmospheric pressure [Pa]
R	radius [m]
T	temperature [K]
β	mass transfer coefficient [m/s]
ν	kinematic viscosity [m^2/s]
θ	polar angle [°]

Dimensionless numbers

Gr	Grashof number $Gr = \frac{l_{ch}^3}{\upsilon^2} g \frac{p_{sub}}{P}\left(\frac{M_{m,Camphor}}{M_{m,air}} - 1\right)$
Ra	Rayleigh number $Ra = Gr\,Sc$
Sc	Schmidt number $Sc = \nu/D$
Sh	Sherwood number $Sh = \beta\, l_{ch}/D$

Thus, the selection of the sublimating material constitutes the key to success within these experiments. It must be well known in its thermo-chemical properties allowing a prospectively theoretical analysis with a reasonable certainty.

There are a small number of practical chemicals offering these requirements – among them dry ice, camphor and naphthalene. Experiences of casting and sintering of the latter two for sublimation studies were presented by Charwat [12]. Here, camphor was chosen as the particle material. Camphor has by an anisotropic crystalline structure, and its properties are given in Table 1.

To determine the classical dimensionless numbers of free convection mass transfer (*Sh*, *Gr* and *Sc*), thermos-physical properties were needed. The variation of sublimation pressure with temperature was calculated from the Antoine equation [11]. The diffusivity of camphor in air at 0 °C and ambient pressure was specified by Presser [11] and its temperature dependency was assumed proportional to $T^{1.75}$.

Camphor spheres were produced by casting in molds designed and developed for this experiment, see Fig. 1. The mold walls were polished, which was reported to yield the growth of long, radially distributed crystals [12]. With fast heating and slow cooling of the cast, a recrystallization of the particle surface was achieved avoiding pronounced non-uniformities.

During the developing of the experiments, the macroscopic effects of the sublimation on the particles were considered: an important factor is relying on the stability of the particle position, during the phase change process of several hours. Attempts were made to cast directly a central stem on the particle itself, but its stiffness has suffered due to its sublimation, and moreover its limited height was affecting the free flow. Best results were obtained by fixing the particle on a thin graphite pin through the lower pole.

Table 1
Camphor thermo-chemical properties.

Properties	
Formula	$C_{10}H_{16}O$
Molar weight	152.23 kg/kmol
Crystal form	Hexagonal
Density (solid)	990 kg/m^3
Normal boiling temperature	204 °C
Normal melting temperature	176–177 °C
Heat of sublimation	244.76 kJ/kg
Heat capacity (solid)	1.86 kJ/(kg K)
Thermal conductivity (solid)	0.402 W/(m K)

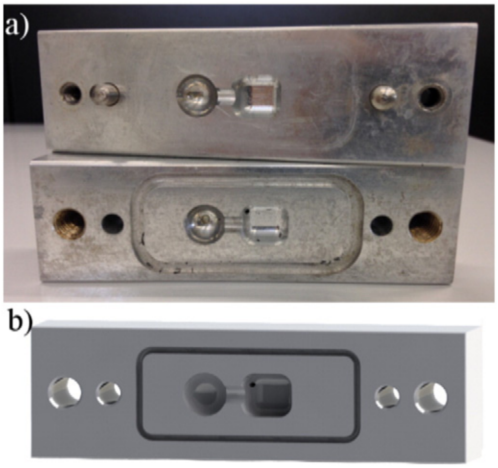

Fig. 1. a) The 2 halves of the mold, b) the CAD model.

To determine the sublimation rate, the microCT measuring technique was applied. To allow the quantification of the volume reduction of the spherical particle, the latter was scanned at different times. To avoid the undesired sublimation during the microCT scans, the camphor was enclosured into a climatic chamber. Such an approach was already successfully applied during the microCT scans of comparably fast-evaporating water and glycerol droplets [13–15]. The investigated particles were slowly rotated by small angular steps during the scanning, acquiring a multitude of 2-dimensional radiographies in the order of several thousands, in relation to the desired reconstruction resolution and the dimension of the particle itself. Fig. 2a) shows a radiographic image of a camphor sphere, and Fig. 2b) visualizes the difference of two radiographies, at the same angular position, due to the sublimation within 20 h.

The projections were collected for a complete rotation (360°) of the particle and reconstructed using standard filtered back-projection algorithms. The volume reconstruction was computed by the commercial software VGStudio MAX®. Further information concerning the microCT principles and the prototype facility at the University of Bergamo are reported in [13].

The reconstructed volume contains, beside the camphor sphere, also the sample holder (graphite pin) and the surrounding air. These different materials were needed to be segmented. The required thresholds were estimated from the global volumetric intensity histogram. Each material attenuates differently the filtered X-rays, if the energy range is properly chosen, and features a characteristic peak in the histogram, see Fig. 3. In this experimental configuration the midpoint between adjacent peaks corresponds to their separating value.

Fig. 2c) illustrates the 3-dimesional reconstructed volume of the camphor sphere (from 1200 projections over a full rotation) with a resolution of 7.50 μm voxel; acquired at 45 kV @ 40 μA with 800 ms of integration time. Digitalised datasets are discrete, and the surface shape cannot be analytically described making the computation of curvatures complicated. Meshes are defined at discrete vertices. Instead, the curvature is based upon derivates which are themselves defined as limit function and describe how the surface behaves in a local region around the vertex. Curvature calculation methods can be divided into two main categories: surface fitting and discrete methods. The surface fitting method is applied in combination with a pre-filtering algorithm to the digitalised volume.