Numerical investigation drag coefficient of micro-encapsulated roughened PCM particles in laminar flow

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Abstract. Phase Change Materials (PCM) have received considerable attention in recent years in many thermal energy storage applications, due to the isothermal phase change process and large storage capacities. This study deals with the hypothetical structure of micro encapsulated phase change materials of matrix type and the particle’s surface roughness influence on its laminar drag coefficient. The investigation has been performed by numerical simulation using commercially available software. Results show that the drag coefficient decreases as particles’ surface roughness increases, even at low Reynolds numbers.

1. Introduction

Phase Change Materials (PCM) are substances, which have the ability to absorb and release large amounts of heat energy, by melting and solidification, under almost constant temperature. This feature makes them suitable for applications of thermal comfort in buildings, thermal protection, cooling, air conditioning, solar heating systems, etc, gathering the interest of several research teams worldwide, especially in the last decade.

One of the production techniques used to avoid loss of material and to reduce any interaction (beyond heat) with the environment, while also controlling the volume change during the phase change process, is that of encapsulation. PCM particles are surrounded by a continuous membrane of inorganic or polymeric material, resulting in a capsule in the size range of 10⁻⁶-10⁻³m. These capsules may have spherical, tubular, oval or irregular shape and their internal morphology may be polynuclear, mononuclear or matrix. The encapsulated type is used either in the form of a powder or dispersed in fluids. In the latter case, problems may occur, such as the increase of the fluid viscosity (with impact on pumping), the reduced resistance to deformation, with consequent breakage and subcooling, etc. The recent production of nano-capsules promises to resolve some of these problems [1, 2].

Although the phase change materials’ melting and solidification processes have been studied macroscopically both experimentally and computationally, thermofluidic phenomena have not been studied, until now, at the level of micro (nano) capsules [3].
Encapsulated PCM production may be performed by various physical, chemical and physico-chemical methods. In the case of spray dryers, PCM capsules are produced in matrix and polynuclear type. The nature and possible periodicity of the microstructure of the outer surface is unknown, [4].

For the computational investigation of the drag coefficient of a nano capsule PCM, a realistic and precise geometry of the outer surface of the particle needs to be simulated. Due to the very small size of the capsule, the surface stresses are expected to play a crucial role in the formation of the stereo structure.

2. Problem Description

The scope of this work is to determine the drag coefficient of particles of different surface roughness at low Reynolds numbers and to investigate any possible relationship between these quantities.

The simulation is based on PCM particles produced by the substances [5], paraffin wax (as phase change material) and polyethylene (as matrix material), during evaporation of organic solvent heptane, in a spray dryer. The ratio of PCM to matrix is varied from 2:1 up to 1:1 by weight, converted to volume ratio using the density of the relative substances.

Since the repetitive spatial geometry of the produced encapsulated PCM particles in a spray dryer is unknown, a hypothesis is made, that these may be in the form of (a) the Weaire-Phelan structure and (b) a Cartesian one, as illustrated in Figure 1.

![Figure 1: (a) Weaire – Phelan structure (b) Cartesian structure](image)

Both geometries have been generated in the commercial software Gambit by Ansys, spatially repeated and then intersected with spheres of various diameters, in order to obtain particles with different roughness. The resulting outer surface cavities represent empty space, i.e. without phase change material, framed by rigid polyethylene, during production in the spray dryer. The final particles generated are illustrated in Figure 2.
**Figure 2:** (a) Weaire – Phelan rough particle (b) Cartesian rough particle

The mean diameter, \( D_m = 2r_m \), of each generated particle has been defined as the one that splits the total volume \( V_{\text{rough}} \) of peaks and voids, of the outer particle surface, into two equal parts. The roughness, \( \varepsilon \), is then calculated using the following formula, as defined in ISO 25178-2 standard [6]:

\[
\varepsilon = \frac{V_{\text{rough}}}{4\pi r_m^2}
\]

(1)

The relative roughness of each particle is determined as \( \varepsilon/D_m \).

3. **Numerical Details**

A 3D flow field of adequate dimensions 20D x 20D x 20D has been introduced, so as to avoid blockage effects. The particle center is at 5D from the inlet in the X direction.

The flow field has been meshed using mostly hexahedral cells of various sizes, whilst the cube surrounding the spherical particle has been meshed using unstructured tetrahedral cells. The overall mesh varied from 2.1M up to 12M grid cells for the particles under investigation. In order to improve solution accuracy, grid refinement was applied to the area around the particle, where the velocity and pressure gradients are expected to be more pronounced. Correspondingly, larger grid cells were located near the sides of the flow field. Figure 3 illustrates the mesh generated for the particles.

**Figure 3:** Computational grid in YX and YZ planes. Flow is always in the +X direction

Boundary conditions for the computational investigation were a prescribed uniform velocity \( (U) \) at the inlet corresponding to \( Re = U D_m/\nu = 4 \), a constant gradient outlet and symmetry conditions on all other sides of the computational domain. All the computations were performed assuming steady state conditions and incompressible air flow, whilst a second-order discretisation scheme was used.
To check whether the solution was dependent on the grid created, the mesh was refined in all planes resulting in a higher number of cells and the flow field for this grid was calculated as well. The difference between the two solutions was negligible. Indicatively, a 55% increase on the overall grid size, resulted in a 0.012% change of the drag coefficient.

Convergence of the numerical solution was monitored by means of continuity residuals, the net imbalance between incoming and outgoing flow rates, as well as the drag coefficient stabilisation.

4. Numerical Results

The predicted drag coefficient, $c_d$, at Re=4, is presented in Table 1 together with the calculated mean diameter of each particle, its relative roughness $\varepsilon/D_m$, and ratio of total particle surface ($A_t$) per smooth sphere surface, $A_{sphere}$ (based on mean diameter for all particles).

| $D_m$ ($\times 10^{-6}$) | $\varepsilon/D_m$ | $A_{total}$ | $A_{sphere}$ | $A_{t}/A_s$ | $c_d$ |
|--------------------------|-------------------|-------------|--------------|--------------|------|
| 3.044                    | 0.132             | 14698.5647  | 2914.04061   | 5.04         | 7.14 |
| 3.681                    | 0.092             | 14134.5194  | 4256.2279    | 3.32         | 7.56 |
| 3.28                     | 0.073             | 9383.65012  | 3378.86189   | 2.78         | 7.50 |
| 4.337                    | 0.064             | 16137.3082  | 5909.63639   | 2.73         | 7.66 |
| 2.917                    | 0.055             | 43488.0416  | 10695.7379   | 4.07         | 7.69 |
| 2.726                    | 0.052             | 23073.4912  | 9334.94573   | 2.47         | 7.87 |
| 3.139                    | 0.042             | 32522.9769  | 12380.4706   | 2.63         | 7.92 |
| 3.8                      | 0                | 3378.861888 | 3378.861888  | 1            | 8.67 |

The drag coefficient results, at Re=4, are plotted versus roughness as illustrated in Figure 4.

**Figure 4**: Drag coefficient computation results plot

The results show that the drag coefficient of rough particles is lower than the one for the smooth sphere ($c_d=8.67$). Moreover, the drag coefficient decreases as the particle’s roughness is increased.
5. Conclusions
Although, it is considered that roughness does not influence the drag coefficient in laminar flow [7], according to the computational results, the particles' roughness affects the drag coefficient, even at low Reynolds numbers.

Further investigation can be made at lower values of roughness, as well as at different Reynolds numbers in order to verify the range of the observed behavior. A further parametric analysis could be made by investigating the effects of different PCM to matrix ratios. A future work will include the thermal response of the particles as a function of time.

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