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Three-Dimensional Numerical Investigation of Constrained Melting of N-Octadecane in a Spherical Enclosure

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Extended Abstract

The study of heat transport and flow inside macro-encapsulated phase change materials is crucial to understand and improve latent heat thermal energy storages. In recent years, several researchers have utilized computational fluid dynamics (CFD) for the investigation of phase change materials in spherical enclosures. In an effort to reduce the computational cost, the assumption of two-dimensional axisymmetric flow has been commonly made (e.g. [1], [2] and [3]).

The focus of this study was to investigate the validity of this assumption for solid-liquid phase change problems with free convection. The computations were carried out on two-dimensional (2D) and three-dimensional (3D) grids and the results were compared and analyzed with respect to experimental results [4].

In the experiments, a glass sphere with a wall thickness of 1.5 mm and an inner radius of 50.83 mm, completely filled with sub-cooled n-octadecane, was immersed in a water bath at 40 °C. An acrylic tube was placed in the center of the sphere, restraining the solid from sinking down to the bottom of sphere.

The continuity, momentum and energy equations were solved by an open source finite volume method CFD code, OpenFOAM®. The phase change was modeled by a source update based enthalpy approach [5]. Temperature-dependent density variations were taken into account by a Bousinessq approximation source term added to the momentum equation. A Carman-Kozeny equation source term in the momentum equation was utilized to smoothly reduce the cell values for velocity with decreasing liquid volume fraction. The pressure-velocity coupling was accomplished by the PISO (pressure implicit with splitting of operator) algorithm. A Robin boundary condition was utilized to model convective heat transfer from the water bath to the glass capsule and heat conduction through the glass capsule. The no-slip effect of the acrylic tube was mimicked by a large Carman-Kozeny coefficient. Structured quadrilateral/hexahedral grids with O-H topology were created via the utility blockMesh. A grid dependence study with 2D meshes indicated that a minimal cell size of 0.3 mm is required to achieve grid convergence in terms of global liquid volume fraction. For the 3D calculations, grid convergence was assumed for the equivalent cell size, resulting in a mesh of 7,000,000 cells.

Compared to the experimental results, the temporal progression of the phase boundary was inaccurately predicted by the 2D computations, while the 3D simulations showed good agreement. Furthermore, unexpected velocity fields with alternating flow directions between the inner sphere wall and the bottom surface of the solid were obtained, resulting in alternating low and high temperature streams in this region. These effects could not be observed for the 3D computations. The 2D axisymmetric domain forced the fluid to recirculate at the symmetry axis, leading to an accumulation near the symmetry axis and maximal flow velocities that were up to 70% higher than those obtained from the 3D simulations. Consequently, disturbed temperature distributions and phase boundaries resulted. The computations carried out in the full

spherical domain showed distinctly three-dimensional convection flow patterns and their effect on the characteristic surface structure of the solid.

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