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Study of melting mechanism of a solid material in a liquid

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ABSTRACT

Experiments utilizing ice/water and frozen ethanol/water have been conducted as an analog physical model to study the factors influencing the melting of solids in liquid metals. A coupled thermal-composition-fluid flow mathematical model based on the commercial software package ANSYS CFX V12.1 has also been developed to analyze the experimental results and provide further insight into the factors influencing melting. The results of both the experimental measurements and numerical analyses reveal that thermal and compositional driven buoyancy flows and surface tension (Marangoni) flows, when present, can have a significant impact on solid melting behavior in a system where forced convection is not significant. The various flow drivers influence the development of the interfacial boundary layer and impact on heat and mass transfer. Thus application of empirical-based heat and mass transfer coefficients will be prone to error and may need to be modified depending on the particular aspects of the system under analysis.

1. Introduction

The melting/dissolution of solids in liquids is important in a number of metallurgical processes including copper, nickel and platinum group metal matte converting operations [1], steel making [2,3] and in the refining of titanium [4–6]. The phenomena of concern range from the melting/dissolution of alloy additions to the removal of deleterious constituents in refining operations and span situations in which the solid has a melting point higher than the liquid (dissolution) and lower (melting) and where either forced or natural convection is occurring. Past techniques applied to characterize the transport processes involved include experimental characterization [7–9], physical model based characterization [1,10] and more recently numerical model based characterization [5,6,11]. Early work under conditions of natural convection tended to involve the development of empirical correlations based on the appropriate dimensionless numbers. For example, in the case of heat transfer occurring across a boundary layer, correlations of the form:

$$\overline{Nu} = f(Gr, Pr) \tag{1}$$

have been employed, where $\overline{Nu}$ is the mean Nusselt number, Gr is the Grashof number and Pr is the Prandtl number. One example correlation, applicable for free convection in an enclosed space, is shown in Eq. (2) [12]:

$$\overline{Nu} = \frac{C(GrPr)^n}{(L/b)^m} \tag{2}$$

where L is the characteristic length and b is the plate spacing. C, m and n are fitting constants applicable for the system on which the measurements have been made.

Similarly for mass transfer, expressions for the Sherwood number (Sh) based on Grashof number (Gr) and Schmit number (Sc) of the form:

$$\overline{Sh} = g(Gr, Sc) \tag{3}$$

have been developed.

The tendency has been to assume that heat transfer controls the melting of solids with a lower melting point than the bulk liquid and mass transfer controls the dissolution of solids when the solid has a higher melting point. Close inspection of the body of work reveals that in most practical situations temperature and compositional gradients can exist at the particle/melt interface at various stages and therefore both heat and mass transport are occurring. Moreover, the transport mechanisms include both diffusion and advection, the latter being driven by the prevailing flow conditions that develop due to thermal and/or compositional buoyancy forces in proximity to the solid/liquid interface (when present). If one also considers the case of particles with a lower density than the melt that reside on the surface, then temperature and compositional

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gradients (when present) can also give rise to Marangoni or surface tension driven flows on the free surface, which have the potential to further influence the transport processes at the interface.

As a prelude to investigating Al-Ti solid melting in the liquid Ti system (which is an experimentally challenging system), work has been undertaken on a low-temperature analog system to provide data suitable for development and validation of a modeling framework. The ethanol/water system has been selected for several reasons: firstly, the solute (ethanol) has a lower melting point than the solvent (water) allowing solid ethanol to be introduced into a higher temperature liquid, which is analogous to solid Al-Ti material added into liquid Ti; secondly, ethanol has a lower density, which is analogous to Al-Ti in liquid Ti; thirdly, ethanol has a lower surface tension, again analogous to Al-Ti material in liquid Ti; fourthly, both are in the appropriate physical states at reasonable temperatures; and finally both are transparent, making direct observation possible.

In this study, a series of experiments were conducted to examine the effects of four flow drivers on mass and heat transport occurring at the interface of a solid in a liquid while in the process of melting under conditions of natural convection: (1) thermal buoyancy; (2) compositional buoyancy; (3) thermal Marangoni; and (4) compositional Marangoni. The empirical data generated from the system has been used to support development and validation of a CFD-based numerical model of the system. The model in turn, has been used to gain further insights into the role of the various transport processes involved in melting.

2. Methods

2.1. Experimental setup

Fig. 1a shows a schematic diagram of the experimental apparatus. It consists of a transparent cylindrical glass beaker 50 mm in radius containing water (the solvent) into which a solid sample (the solute) is introduced and held at a fixed position. The experiments were conducted in ambient air at 20 °C. Temperatures at two locations were measured by Type-T thermocouples: one, within the solute at the centerline at mid-height (TC1); and a second, near the wall of the cell, 5 mm from the top surface (TC2) – see Fig. 1a.

To allow for a broad range of conditions to be explored, both frozen ethanol and frozen water (ice) were used as the solute, facilitating measurements to be conducted with and without the compositional drivers of flow present, respectively. In addition, the solid solute was introduced into the solvent in two configurations, as shown in Fig. 2. In the fully immersed configuration, Fig. 2a, Marangoni forces are eliminated from the solid/liquid interface, leaving predominately buoyancy forces, whereas in the partially immersed condition, Fig. 2b, Marangoni forces are present in proximity to the solid/liquid interface at the junction of the three phases, solid, liquid and air. Four sets of experiments were conducted, as listed in Table 1. Note: reference is also made in Table 1 to the state of the flow driver as being either on (present) or off (absent) in proximity to the solid/liquid interface in the experiment.

Fixing the samples allowed for reproducible conditions to be maintained during the experiments. The configurations used allow for buoyancy driven flows to fully develop resulting in natural convection conditions. Marangoni driven flows on the other hand are only present in proximity to the solid interface for the period of time solid is present at the free surface of the liquid – e.g. in the case of the partially immersed ice experiments, rapid melting at the free surface of the liquid limited the time solid was present at the free surface. Conditions in which a solid of lower density is free to float and remains at the surface would allow for Marangoni driven flow to remain present at the solid liquid interface for the duration of melting.

Since both solvent and solute in the study are transparent, dyes were used to differentiate them. An organic-soluble blue dye (insoluble in water) was used to distinguish ethanol from water, whereas a water-soluble yellow dye was used in the solute when water was both the solute and solvent. The use of dyes allowed some aspects of the basic fluid low pattern to be ascertained and also the solid/liquid interface to be visually emphasized.

The experimental methodology was as follows: the cylindrical beaker was filled to a height of 60 mm with distilled water (solvent) at 45–50°C. The solute sample with an embedded thermocouple and support (made from wood) was then prepared by solidifying in liquid nitrogen. Once solidified, the frozen solute sample was removed and inserted into the solvent. In the case of the ethanol experiments, the solute was immediately immersed whereas in the case of ice, the sample was allowed to warm until a temperature of approximately −10°C was recorded on the solute thermocouple. Temperature and video data were then recorded using a data acquisition system.

2.2. Numerical model

To support analysis of the experimental data and ultimately to develop a framework for modeling the melting of solids in titanium refining, a CFD model describing the experiments was developed. In order to comprehensively describe the melting process, the numerical model necessarily incorporates the significant phenomena affecting heat, mass and momentum transport including compositional and thermal buoyancy, compositional and thermal Marangoni forces, Darcy damping flow and melting (phase change). A multi-component model was employed as two components (solute and solvent) are involved. The modeling was performed using a commercial CFD package - ANSYS CFX V12.1.

2.2.1. Computational domain

Given that the geometry of the physical model is circumferentially symmetric, a pie-shaped domain representing a 5° slice has been adopted for the computational domain. *Note: CFX does not permit the use of a 2-D axisymmetric model, hence the need for a 3-D 5° slice.* The domain is shown in Fig. 1b and includes the water (solvent), shaded light grey, and solid (solute), shaded blue, as presented in Fig. 1a. The solute is differentiated from the solvent by virtue of a different set of initial conditions and material properties. In addition, the free surface of the liquid (solvent) and the solid (solute) are assumed to be flat.

To generate the mesh, a vertical face of the domain was first discretized into a 0.5 × 0.5 mm grid, which was then rotated 5° about the centerline of symmetry. A single layer of elements was used in the circumferential direction. At the domain centerline, the resulting layer of triangular prism elements is of poor quality and was removed yielding a mesh comprised of 11,662 hexahedra elements containing 23,760 nodes. A sensitivity analysis to mesh size in the axial and radial directions was conducted by running cases with grids of 0.25 × 0.25 mm, 1.0 × 1.0 mm and 1.5 × 1.5 mm and comparing the results to the base-case 0.5 × 0.5 mm. For the example problem run, the predicted melting times where 79, 82, 97 and 109 s, in order of increasing grid size. Model execution times were approximately 250, 25, 9 and 4 hrs, also in order of increasing grid size. The base case grid of 0.5 × 0.5 mm was found to be a reasonable compromise between accuracy and execution time.

2.2.2. Model equations

The governing equations solved are the standard ones describing continuity, momentum and energy conservation for an incompressible fluid and are given by Eqs. (4)–(6), respectively.