Effect of domain subdivisions on alloy solidification

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A B S T R A C T

The sensible heat portion of thermal energy storage (TES) for concentrated solar power (CSP) can be achieved using off-eutectic materials. These materials have the advantage of storing in latent as well as sensible heat through a given temperature range. On the other hand, off-eutectic materials have the disadvantage of possibly experiencing segregation effects, most likely impairing their solidification. During solidification, macrosegregation can occur due to a number of possible causes such as density differences in the solid and liquid portions of the mixture/alloy, flows due to capillary forces, flows due to electromagnetic fields or forced stirring, etc. In some cases, macrosegregation can severely affect solidification. One possible means to limit this segregation is with porous media. In this study, the segregation of an off-eutectic material in a porous medium is studied. Pore sizes and porous medium thermal conductivity are varied, revealing the importance of various mechanisms affecting solidification. Smaller pore sizes and higher porous medium thermal conductivities are shown to improve segregation and solidification.

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1. Introduction

Thermal energy storage (TES) plays an essential role in renewable energy systems by reducing the mismatch between supply and demand and by improving the systems' performance and reliability. In fact, TES is the main competitive advantage of concentrated solar power (CSP) systems in comparison to other types of renewable energy, allowing dispatchable electricity generation and management of the solar resource intermittency. However, if CSP is an emerging system to meet greenhouse emission targets [1], substantial technological and cost reduction efforts are required. As a result, recent research is focusing on developing new, more cost-effective and energy efficient TES. Sensible heat storage is commonly used in solar energy applications. In particular, molten salts are mostly used in CSP plants, but the temperature cannot easily be increased past 565 °C due to degradation, limiting the energy density of the system. Latent heat TES based on phase change materials (PCM) is a very attractive solution because it can provide higher energy density storage per unit mass/volume at nearly isothermal conditions, which corresponds to the phase transition temperature of the storage material.

A wide range of compositions of salt mixtures and metal alloys are being investigated as potential PCM [2,3]. Often eutectic compositions are used as TES materials because they melt at a lower temperature than each of the mixture's constituents. Pramod et al. [4] have presented a review of possible phase change materials for low temperature heat storage applications. Eutectic materials change phase at a constant temperature, whereas off-eutectics change phase throughout a temperature range. Studies [5,6] show that multiple PCMs with different melting temperatures arranged in a cascade can perform better than a single PCM with a unique melting temperature. Using an off-eutectic composition can be similar to using a PCM cascade [6] in that they absorb/release latent heat through a temperature range or at various temperatures. The advantage is that the system will be composed of a single mixture, instead of multiple combinations of materials and containers. However, some drawbacks of off-eutectic mixtures include incongruent melting and segregation upon solidification.

Undesirable phenomena that appear during the PCM solid-liquid phase change include supercooling, phase segregation, corrosion, and lack of thermal stability [3,7]. Microsegregation appears as the various components coalesce and melt into the distinct phases that form during phase change. Macrosegregation is induced by four known forces: buoyancy force resulting from thermosolutal convection, solid movement force of sedimentation or floating, shrinkage force during volume contraction/expansion,

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and oxide-based inclusion flotation [8]. Macrosegregation typically appears due to a redistribution of the segregated elements in the mushy zone (or region where the phase change takes place), induced by variations of density that develop with temperature and concentration gradients [7]. This fluid flow induced by thermal and solutal natural convection are in a strongly non-linear coupling, especially if there are large disparities of diffusion scales of heat, momentum and mass (very low Prandtl numbers and high Lewis numbers). These phenomena have been extensively investigated in metallurgy [7,9,10] since macrosegregation is one of the major casting defects that appear. For TES applications the effect of segregation is also negative, inducing slower solidification and, thus, supplying insufficient heat to the heat transfer fluid during TES discharge. However, macrosegregation applied to TES systems has not yet been thoroughly investigated and will be particularly important in evaluating the phase change of off-eutectic materials.

The most basic heat exchangers for PCMs are typically tube and shell heat exchangers, where the heat transfer fluid (HTF) circulates within the tubes and exchanges heat with the storage material in the tank [11]. When the materials are not very conductive, it is common to add fins to the tubes in order to increase heat transfer [12]. As an extension to this, conductive enhancers and porous materials may be used when the thermal conductivity of the storage material is very low [13,14]. Although introduction of a porous medium can increase costs due to lower overall energy density for the same volume of composite material, the porous material enables the heat to quickly diffuse throughout the storage system, enabling a much improved discharge/charge time of the system. The porous material also has another effect on the solidification: it impedes the macrosegregation of the components of the mixture/alloy, improving the solidification characteristics. This phenomenon has been studied to a much lesser degree in the literature. This work focuses on this aspect of the porous medium, exploring the effect of the pore size and thermal conductivity in global segregation and solidification rates. As this work is purely numerical, some strong assumptions have been proposed to focus on specific phenomena and parameter influences. Microsegregation is not modeled here, and only macrosegregation is taken into account: the domain sizes associated with the validated references are similar to the current domain. At smaller scales it is understood that the importance of microsegregation effects should have an increasingly larger effect on solidification relative to macrosegregation effects. This effect is not however taken into account. Nonetheless, the results presented in this study can be used to evaluate pore sizes for limiting macrosegregation, which will most likely present the greatest difficulties for solidification in a solar thermal energy storage system, which can be several meters in diameter. Moreover, the porous medium is represented by an ideal skeleton made of only square, closed pores with a uniform size. Such a situation is useful to represent the phase change material solidification effects, coupled with thermal transfer of the porous medium. Obviously, even if it limits comparison with experimental processes, it supplies data for comparison and validation of numerical codes devoted to thermal energy storage. Moreover, the material properties are supposed to be constant, and the material aging and cyclability are not considered in the present work. Such a consideration introduces various parameters into the phase change material design, resulting in a loss of generality to other PCM systems that may have different geometries, heating rates, etc.

The present study uses a modified version of a CFD research home made code called Thétis to model the phase change of multicomponent materials. Navier–Stokes, energy and species transport equations are evaluated. Microsegregation is modeled through the use of the lever rule. The mushy zone is modeled with a modified permeability depending on a simplified dendritic arm spacing model [15]. The domain geometry is varied to model different pore sizes by placing domain subdivisions, creating square pores within the computational domain. The thermal conductivity of these subdivisions is also varied to explore the effect on segregation. The results indicate that the improvements on global solidification of PCM for TES can be significant. This study gives information on the way to form new compound materials TES.

2. Modeling

Heat storage and discharge is obtained by phase change of a binary alloy contained in a porous medium. Physically, such a foam is characterized by a distribution of more or less spherical pores with various sizes. To focus the analysis on the influence of the pores size and matrix conductivity, the present model is based on an ideal porous medium saturated in PCM, with a regular square shape pattern. A 2D configuration is retained to perform simulations.

2.1. Physical modeling

The phenomena in this study are based on interaction between three physical models: heat transfer, fluid flow, and species transport. First, the medium is submitted to a given cooling rate, involving heat transfer within the material. As the sample is considered large enough, buoyancy is effective. The liquid phase flows, whereas the solid phase is considered fixed (zero velocity). During the PCM phase change, the solute distribution evolves in space and time, as solutal convection is present. Thus, three main parameters must be computed in time and space at a macroscopic scale: temperature, velocity and solute fields.

The global movement is defined by the momentum equations, expressed in an incompressible form. The Boussinesq approximation [16,15] is used, considering a constant density ρ_0 in all phases, except in the gravity term, where the density depends on both temperature and liquid concentration: $\rho = \rho_0(1 - \beta_T(T - T_0) - \beta_C(C_l - C_0))$, where ρ is the density, ρ_0 is the reference density, β_T as the thermal expansion coefficient, T is the temperature, T_0 is the reference temperature at which ρ_0 is known, β_C is the solutal expansion coefficient, C_l is the liquid composition, and C_0 is the reference composition (also chosen as the initial condition). As the solid phase is assumed to be fixed, only the liquid part contributes to movement. The Grashof number for thermal buoyancy ($g\beta_T(T_s - T_\infty)L^3/\nu^2$ with g as the gravity constant, T_s as the temperature on the heated surface, T_∞ as the bulk temperature, L as the length of the heated surface, and ν as the kinematic viscosity) in the entire domain defined by the boundary and initial conditions in Section 2.3 and the constants in Table 1 is 0.97. This is a relatively small Grashof number, implying laminar flow due to thermal buoyancy. Likewise, the Grashof number for solutal convection ($g\beta_C(C_a - C_b)L^3/\nu^2$ with $C_a = C_{max} = 1$ as the maximum possible composition and $C_b = C_{min} = 0$ as the minimum possible composition) cannot exceed 0.40, also implying a laminar flow. These two Grashof numbers are in terms of the entire domain, and smaller subdivisions of the domain will have even smaller Grashof numbers. The undivided domain is shown to experience thermo-solutal convection due to buoyancy (see the preliminary validation of the code for a similar domain in [7]), and smaller subdivisions should reduce the Grashof number, having a significant effect on movement and thus solidification.

The governing equations have been proposed by Bellet et al. [17] in a numerical benchmark with the following assumptions, where **v** is the velocity vector, f_l is the liquid fraction, $\mathbf{v}_l$ is the liquid