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Penetration of molten silicon into a bed of fines ☆

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ABSTRACT

During the casting process of silicon the mould must be buffered from the high temperatures of the molten silicon to prevent the mould melting and this is typically done by the operators laying down a layer of crushed silicon particles (fines) prior to pouring of the molten silicon. It is useful for operators to know how deep they should make the layer the fines so as to adequately separate the molten silicon from the mould. In this paper, we consider a model for the penetration of molten silicon into the pre-laid layer of silicon fines, which provides a predictive tool for estimating the necessary depth of fines in order to prevent the molten silicon touching the mould. The mathematical model developed here considers the flow of molten silicon as a Darcy flow and solidification due to heat flow as a one-phase Stefan problem. We are able to find a numerical solutions to this model, and from this we are able to extract data regarding the penetration depth of the molten silicon into the fines before solidification occurs. Our model and numerical solution can been seen as a first step toward understanding this important part of the casting process for silicon.

1. Introduction

It is known from the literature on solidification of pure silicon and silicon alloys that the cooling rate and mould structure will influence the microstructure of the obtained solid; see [1,2]. To prevent the mould melting during the casting of silicon, operators typically lay down a layer of crushed silicon fines prior to pouring of the molten silicon so as to buffer the mould from the high temperatures of the molten silicon. It is useful for operators to know how deep they should lay the fines so as to adequately separate the molten silicon from the mould. Therefore, in the present paper we construct a mathematical model to predict the depth of penetration of molten silicon into the fines layer which is laid down on the mould surface before pouring of the hot liquid melt. This could provide a useful tool for operators to know how deep they should lay their fines so as to separate the molten silicon from the mould, particularly since it is known that interactions with the fines can modify the microstructure obtained from that which might be expected from simply considering the rate of cooling [3]. There is also interest in expanding the understanding of silicon fines behaviour such as applications in the solar energy sector [4,5].

The basic approach taken here is to assume that the fines act as a solid porous material and that the molten silicon then travels through the pore structure until it cools and solidifies. The aim is to determine the movement of the molten silicon and in particular the distance that the molten silicon travels into the porous structure. In practical situations the molten silicon is only just above its melting temperature so melting of the porous structure can be neglected but the initially cold porous structure causes the molten silicon to solidify as it flows and thereby slow the flow down. Furthermore it is anticipated that the flow into the pores can be assumed to have a sharp interface between those pores that are filled with silicon and those that have yet to be filled. This will enable a saturated model of the flow to be used. Similar problems have been studied in relation to the percolation of water through snow [6-9]. The main difference is that in those situations the fluid flow typically includes non-saturated effects and, more importantly, the snow is only just below freezing and is insufficiently cold to completely freeze the water and close the pores. In contrast, here the fines are initially cold enough to allow the latent heat from the molten silicon to be completely removed and hence solidify the entire system.

The remainder of the paper is as follows. In Section 2, we shall outline the formulation and geometry of the fines problem. Then, in Section 3, we cast the relevant physical problem in terms of a Stefan problem. In Section 4, we give a type of similarity solution for the Stefan problem. From this solution, we are able to extract the salient features of the problem, in order to determine the penetration depth of molten silicon into the fines before solidification occurs. We discuss the results in Section 5, and mention possible directions for

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future work including the extension to more complicated scenarios that may arise in practical applications.

2. Formulation

To allow analytical progress and simple insight to be gained the porous material made by the fines will be assumed to be approximated by a series of isolated cuts in a solid silicon material and furthermore that problem will be taken to be two dimensional so the holes can be considered as channels. These channels will be taken to be long and thin, corresponding to a layer of fines that is many particles thick.

Consider the idealised geometry and the notation set out in Fig. 1. The molten silicon enters a narrow channel with the walls representing the fines made of solid silicon. Because the liquid is typically only just above the melting point assume that the liquid is at the solidification temperature, T_m, and that the solid is initially at air temperature, T_a. The molten silicon will flow into the channel due to the pressure created by overlying pool of static molten silicon which we shall assume gives a known pressure p_0 at the inlet of the channel. There is a free surface between the liquid fluid and the underlying air that moves down the channel. The details of the free surface will be complicated by the wetting of the solid silicon by the liquid silicon but here we shall simply assume that this surface is horizontal and at atmospheric p_a (we assume the air can easily escape from the region).

Take z as the vertical coordinate (pointing down the channel) and x as the horizontal coordinate. The channel entrance is at $z = 0$ and there is a the free surface between the molten silicon and the air in the channel which is assumed to be a horizontal surface given by $z = Z(t)$. By symmetry we only need to consider one half of the channel so take $x = 0$ to be the solid wall and $x = a$ to be the channel centreline. Furthermore, we neglect the finite horizontal size of the particles and assume that the solid extends to minus infinity in x. The liquid will solidify, resulting in an interface between solid and liquid which we denote by $x = s(t, z)$.

To study the problem assume first that the movement of the liquid down the channel is known so that $Z(t)$ is given (and more importantly that the inverse $Z^{-1}(z)$ is known) and so only heat flow need be examined. We will subsequently derive a model for $Z(t)$ by considering the fluid flow. Hence we start by examining the heat dynamics of the silicon and particularly the movement of the interface $x = s(t, z)$.

3. The heat flow problem

For simplicity it has been assumed that the molten silicon is very close to the melting temperature, T_m and the silicon is very pure. In such a case it is not necessary to consider any complicated phase diagram behaviour so there will be a sharp interface as the material solidifies and only the latent heat of solidification and the diffusion of heat in the solid need to be accounted for. We use Fourier's law for the heat flux and conservation of energy to justify the use of the heat diffusion equation (see [10] for details). This is a free boundary problem (in particular it is a one-phase Stefan problem) where the phase boundary, which separates the solid silicon from the molten silicon, must be found as part of the problem. At the phase boundary the temperature of the silicon will be at the melting temperature and the interface moves according to the Stefan condition which can be derived from an argument of conservation of energy (see [11] for details). The problem is symmetric about the line $x = a$, so we expect a phase boundary to emerge from each wall of the narrow channel. Hence we need only consider one half of the channel, and therefore only one phase boundary. Without loss of generality, we shall consider the region $x \in (-\infty, a]$ and let the position of the phase boundary be denoted $x = s(t, z)$.

Table 1
List of dimensional parameter values provided by Elkem.

Constant	Typical value	Units
T_{pot}	323	K
T_m	1683	K
T_0	1700	K
T_a	293	K
d	0.03–0.1	m
ρ	2533	kg/m^3
L	1798060	J/kg
k_s	43	W/mK
k_l	23.5	W/mK
c_s	970	J/kg K
c_l	970	J/kg K
h	0.02	m
a	0.002	m
p_a	101325	kg/ms^2
g	9.8	m/s^2
μ	0.02	kg/ms

The heat flow in the solid is governed by the two-dimensional heat equation

$$\rho c_p \frac{\partial T}{\partial t} = k\nabla^2 T, \tag{1}$$

where ρ, c_p, and k are the density, specific heat capacity and thermal conductivity of the material respectively, which are all taken to be constant. In the narrow channel, however, the diffusion distance is much shorter than the channel length so that the heat flow in the solid is approximately governed by the one-dimensional heat equation

$$\rho c_p T_t = kT_{xx}. \tag{2}$$

One consequence of this one-dimensional heat flow approximation is that at any particular position down the channel, z, for times before the interface arrives, $t < Z^{-1}(z)$, the temperature will remain at its initial state and there is no solidification so that $s(t, z) = 0$. Therefore the heat flow at any position z only needs to considered $t \geq Z^{-1}(z)$.

At the phase boundary the temperature must equal the melting temperature, so

$$T(s(t, z), z, t) = T_m. \tag{3}$$

We have taken the density to be the same in both the liquid and the solid as the density of silicon only varies by about 2% at this transition. A list of the values of the various constants can be found in Table 1.

To change phase, the latent heat, L, of the silicon must be removed. The 'Stefan condition' (see [11]) dictates that the latent heat required to move the interface must be removed by the difference between the heat fluxes at either side of the solidification front. Considering that the temperature is constant (at melting temperature) in the liquid region, then we get

$$\rho L \frac{\partial s}{\partial t} = k \frac{\partial T}{\partial x}, \tag{4}$$

at $x = s(z, t)$.

To solve this problem consider the following scalings for each variable:

$$t = \frac{\rho L a^2}{k_l (T_m - T_a)} \hat{t}, \quad x = a\hat{x}, \quad T = T_m + (T_m - T_a)\hat{T}. \tag{5}$$

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