Calculation of Dendrite Settling Velocities Using a Porous Envelope

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The convective transport and gravitational settling of unattached equiaxed grains and dendrite fragments can cause macrosegregation and influence the structure of the equiaxed zone in a variety of solidification arrangements. An understanding of how the highly nonspherical geometry of the dendrite influences its settling and transport characteristics is needed to determine the motion of unattached dendrites and predict structure and segregation in castings. The empirical results of previous works have been used to develop a FORTRAN 77 computer program to calculate the settling velocity of various dendritic shapes and a number of other parameters of interest, such as the volume and surface area of the dendrite. Required inputs to the code are the physical properties of the system and some simple geometric parameters of the dendrite being considered, such as the average radius of the primary arm. The predicted settling velocities were on average within ± 5 pct of those measured for model dendrites and were consistent and in good agreement with three other experimental investigations. Future development of the code will attempt to overcome many of its present limitations by including particle-particle interactions and the effects of tertiary arms, for example.

I. INTRODUCTION

IT has been shown that the settling (or floating) of dendrites and equiaxed grains can cause severe macrosegregation in metal castings^[1-4] and that the formation of free, unattached grains and their movement is critical to the formation and structure of the equiaxed zone in a variety of solidification arrangements.^[5-8] An understanding of the settling characteristics of dendritic grains is needed to understand and predict this type of segregation and the development of the equiaxed zone. Attempts have been made to use Stokes' law to assist in the analysis of dendrite settling processes.^[8,9,10] However, since dendrites are highly nonspherical, the use of Stokes' law has yielded only rough estimates of dendrite velocities.

In a recent experimental study by Zakhem *et al.*,^[11] the effects of shape on the settling rate of model dendrites were examined. In this study, the low Reynolds number drag and settling speed ratio of equiaxed dendritic grains and dendrite fragments were determined. Plastic dendrite models patterned after the shapes of real dendrites observed in metallic alloys and metal analogs were constructed and tested in a large Stokes' flow facility. The size, shape, and density of these were varied so that the drag and terminal velocities of 34 different models undergoing free fall along their axis of symmetry were measured. It was concluded in this work that the interdendritic liquid of settling grains is effectively immobilized, and thus, the added surface area of secondary dendrite arms does not significantly add to the drag coefficient of the particle.

Ahuja et $al^{[12]}$ advanced this work through use of a conceptual envelope which (1) surrounds the dendrite, (2) is defined as a porous particle, and (3) is used to determine an effective density and sphericity for the particle. Figure 1 shows a typical shape of an equiaxed dendrite and two possible envelopes, one idealized. The nonspherical envelope contains both the solid dendrite and the interdendritic liquid. The fluid flow around the dendrite is mainly controlled by the nonspherical shape of the dendrite envelope, while the fluid flow through the dendrite is determined by the porosity and permeability of the dendrite. These two flows affect the drag force experienced by the dendrite and hence its settling velocity. In Ahuja et al., [12] relevant dimensionless parameters useful in quantifying the effects of the shape and porosity of dendrites on settling velocity were identified. In the present work, a model for the drag coefficient for a single dendrite (equiaxed and uniaxial) settling in an infinite medium is further developed. The experimental data of Zakhem et al.[11] is reanalyzed in view of the proposed model, and the results of the model compared with experiments.

These two articles^[11,12] represent a significant advancement in our ability to estimate the relative settling velocity of dendritic shapes. However, computation of the relevant geometric parameters needed to use these findings is cumbersome. This article presents: (1) a FORTRAN 77 computer program written to overcome the difficulties encountered in dendrite settling analyses, (2) an estimate of corrections for wall and inertial effects, and (3) a comparison of dendrite velocities measured and predicted using the new code. Additional complexities, such as forced and natural convection, particle interactions, dendrite and liquid density gradients, and dendrite orientation, are not considered. Only dendrites having either primary or primary and secondary arms are considered; the influence of tertiary arms has not been considered.

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Fig. 1—(a) Idealized envelope around an equiaxed dendrite. (b) Dendrite envelope used in the code.

II. CODE DEVELOPMENT

Required inputs to the code are the dimensions of the dendrite and thermophysical properties of the alloy. The velocity of the settling dendrite, its Reynolds number, and other variables of interest, such as the dendrite volume, surface area, and settling speed ratio, are calculated. Stokes' law, corrected for geometric effects, wall blockage, and inertial effects, is used to estimate the dendrite terminal velocity, U_d , as shown in the following equation:

$$U_d = \frac{2}{9} \left(\frac{r^2 g \Delta \rho}{\mu} \right) \frac{K S_e}{K}$$
[1]

where g is the acceleration of gravity, $\Delta \rho$ is the difference in density between the envelope and liquid ($\Delta \rho = \varepsilon(\rho_{\text{solid}} - \rho_{\text{liquid}})$, ε is the solid volume fraction of the envelope), μ is liquid viscosity, and K is a correction factor for wall and inertial effects. The envelope equivalent radius, r, is defined as the radius of a sphere of volume equal to that of the dendrite envelope. The settling speed ratio, KS_e , is defined as

$$KS_e = \frac{U_s}{U_r}$$
[2]

where U_s is the Stokes settling velocity of the dendrite and U_r is the Stokes velocity of the reference sphere which is the envelope equivalent sphere. Note that the envelope equivalent sphere has the same volume and density as the envelope, and thus, an important input to the code is the number of secondary dendrite arms (and their radius) which is used to determine the solid fraction of the envelope and its density. A correction factor, K, to compensate for the effects of neighboring walls and inertial effects due to nonzero Reynolds numbers is defined as

$$K = \frac{U_s}{U_d}$$
[3]

The subscript e is used with the speed ratio, KS_e , to remind the reader that the reference speed is that of the envelope equivalent sphere and not the Stokes velocity of the equivalent sphere of the dendrite.

Ahuja et al.^[12] used the data of Zakhem et al.^[11] to

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develop the following empirical relationship for the settling speed ratio for equiaxed dendrites:

$$KS_e = 1.26 \log_{10} \left(\frac{\Psi}{0.163} \right)$$
$$\times \frac{2\beta^2 + 3(1 - \tanh(\beta)/\beta)}{2\beta^2(1 - \tanh(\beta)/\beta)}$$
[4]

in which the envelope sphericity, Ψ , is the ratio of the surface area of the envelope equivalent sphere to that of the envelope, A_e , as described by

$$\Psi = \frac{4\pi r^2}{A_e}$$
 [5]

and β is the normalized radius sensitive to the permeability, K_p , of the dendrite structure represented by

$$\beta = \frac{r}{\sqrt{K_p}}$$
[6]

The speed ratio KS_e is analogous to C_{ed} in Ahuja *et al.*^[12] The permeability is estimated using the Kozeny-Carman equation,^[13]

$$K_p = \frac{\left(1 - \varepsilon\right)^3}{5\left(A_d/V_e\right)^2}$$
[7]

where A_d is the surface area of the dendrite, V_e is the volume of the envelope, and ε is the solid volume fraction of the envelope. It should be noted that the numerical constants in Eq. [4] are slightly different from those in Reference 12 due to errors later corrected in Reference 11. Corrections to Zakhem *et al.*^[11] can be found in Reference 17.

A similar relation among KS_e , Ψ , and β can be found using data from Zakhem *et al.*^[11] for uniaxial dendrites (a single primary arm) as expressed by

$$KS_e = 1.06 \log_{10} \left(\frac{\Psi}{0.113} \right)$$
$$\times \frac{2\beta^2 + 3(1 - \tanh(\beta)/\beta)}{2\beta^2(1 - \tanh(\beta)/\beta)}$$
[8]

The first term (containing Ψ) in Eqs. [4] and [8] accounts for the nonspherical shape of the dendrite and envelope and is calibrated using the settling data of dendrites without secondary arms from Zakhem *et al.*^[11] The second term (containing β) in Eqs. [4] and [8] accounts for the effect of the permeability of the envelope and is based on the analytical work of Neal *et al.*^[18] where β is based on the envelope volume-equivalent radius, *r*.

III. DENDRITE ENVELOPE

In an effort to develop a shape parameter consistent with changes in a speed ratio (KS_e) , the dendrite envelope was introduced.^[12] One possibility of an appropriate envelope is shown in Figure 1(*a*), formed by smoothly joining the tips of the primary and secondary arms. It has been shown that a similar, yet simplified, envelope

is effective at relating sphericity and permeability to settling speed ratio.^[12] Three different envelopes were examined in the development of this work and all vielded good results. The envelope shown in Figure 1(b) yielded the best results and is used in the code for equiaxed dendrites with secondary arms. For uniaxial dendrites, an envelope consisting of two pyramids having a common base is used, the tips of the pyramids coinciding with the tip and base of the primary arm of the uniaxial dendrite. The envelope collapses to coincide with the primary arms for dendrites with no secondary arms; thus, in this case, $\varepsilon = 1$. The envelope used in this work (Figure 1(b)) for equiaxed dendrites is different from the envelope used by Ahuja et al.^[12] and is more form fitting to the dendrite; thus, less liquid is contained in the envelope, resulting in a greater solid volume fraction (higher ε). The average angle between the primary arm and the tips of the secondary arms defines the pyramid angle, θ , and the tips of the secondary arms are at the corners of the pyramid. The secondary arm was formerly parallel to the side of the pyramid.^[12] The volume and surface area of the dendrite can be estimated using Appendix B of Zakhem *et al.*^[11,17] The volumes and surface areas of the dendrite and envelope are then used to determine Ψ , β , and in turn KS_{e} .

The volume, V_e , and surface area, A_e , of the equiaxed dendrite envelope are determined by dividing the envelope into six pyramids having square bases and a center volume having six square surfaces (coinciding with the bases of the pyramids) and eight equilateral triangular surfaces and are equal to

$$V_e = s^2 h_1 + (5/6)s^3$$
 [9a]

$$A_e = (6\sqrt{2})s\sqrt{(h_1)^2 + \frac{s^2}{8} + (\sqrt{3})s^2} \qquad [10a]$$

where $s = L \tan \theta / (1 + \tan \theta)$, $h_1 = L/2(1 + \tan \theta)$, L is the primary arm length, and θ is the angle between the primary arm and a straight line connecting the tips of the secondary arms.

For the envelope around a single primary arm with secondary arms, the envelope volume and surface area are

$$V_e = \frac{2}{3}h^2(b_1 + b_2)$$
 [9b]

$$A_e = (2\sqrt{2})h\left(\sqrt{(b_1)^2 + \frac{h^2}{2}} + \sqrt{(b_2)^2 + \frac{h^2}{2}}\right) \quad [10b]$$

where $h = (L\tan\varphi)/(1 + \tan\varphi/\tan\theta)$, $b_1 = L/(\tan\theta/\tan\varphi + 1)$, $b_2 = L/(\tan\varphi/\tan\theta + 1)$, and φ is the angle between the primary arm and the tips of the secondary arms from the base of the uniaxial dendrite.^[19]

IV. WALL BLOCKAGE AND INERTIAL CORRECTION

Estimates of wall blockage and inertial effects are needed, because the influence region associated with low Reynolds number flow is typically very large, and if very large grains are expected, higher velocities and nonzero Reynolds numbers can result in substantial inertial effects. Zakhem *et al.*^[11] used the correction procedures developed by Lasso and Weidman^[14] to estimate wall blockage and inertial correction factors for model dendrites. These correction procedures were used to develop a generalized relation for determining wall and inertial correction estimates. Only advancements to procedures detailed in References 11 and 14 are discussed here. These correction factors assume the particle to be settling along the centerline of a container with a circular or square cross section. A wall correction factor, K_w , is estimated using the following Taylor series adapted to Table III of Wakiya:^[15]

$$K_{w} = 1.0011 + 1.5395b + 1.8171b^{2} + 14.637b^{3}$$

- 0.0021644f + 0.83207bf + 1.0405b^{2}f
+ 3.8916 × 10^{-4}f^{2} - 0.089787bf^{2}
- 1.4334 × 10^{-5}f^{3} [11]

where f is the spheroid fineness ratio equal to L/w and b is an intermediate blockage ratio equal to w/W. The maximum height of the dendrite is L, w is the maximum dendrite width perpendicular to flow, and W is the characteristic width of the surroundings. If the surroundings are square, W is equal to the length of the side plus 10.6 pct.^[14] This wall correction is used to determine a sphere blockage ratio, B, through use of the following equation adapted to Table I of Sutterby^[16] at Re = 0:

$$B = 0.471425(K_w - 1) - 0.416166(K_w - 1)^2 + 0.258812(K_w - 1)^3$$
[12]

The equivalent Reynolds number, Re, of a sphere having the same drag as the test object is estimated through use of the following definition of Reynolds number and Stokes' law:

$$\operatorname{Re} \equiv \frac{\rho_l dU_e}{\mu} = \frac{d^3 \rho_l \Delta \rho g}{18 \mu^2 K_e}$$
[13]

where d = 2r, U_e is the velocity of the envelope equivalent sphere, and K_e is a wall and inertial correction factor for the envelope equivalent sphere (K_e is found using an iteration process as described in Sutterby,^[16] with B = d/W). The sphere blockage ratio, B from Eq. [12], and the equivalent Reynolds number, Re, are used in the following Taylor series adapted to Sutterby's^[16] Table I to give the combined inertial and wall correction factor, K, for the dendrite:

K = 1 + 0.14334Re - 0.0011212Re²

$$-0.0091635 \text{Re}^3 + 0.0025419 \text{Re}^4$$

- $-0.00020383 \text{Re}^5 + 1.5798 B$
- $-2.8517 \text{Re}B + 1.3261 \text{Re}^2B 0.200 \text{Re}^3B$
- $+ 0.0049145 \text{Re}^4 B + 23.046 B^2 + 8.8877 \text{Re} B^2$
- $-7.3132 \text{Re}^2 B^2 + 1.1035 \text{Re}^3 B^2$
- $-266.09B^3 + 48.076ReB^3$
- $-3.0625 \text{Re}^2 B^3 + 2025.9 B^4$
- $-122.36 \text{Re}B^4 5942.7B^5$ [14]

Table I. Measured NH₄Cl Equiaxed Dendrite Settling Rates, U_m ^{8,20} and Calculated Settling Rates, U_d

Dendrite Width (10^{-2} m)	$\frac{U_m}{(10^{-2} \text{ m/s})}$	U_d (10 ⁻² m/s)	$\frac{U_d - U_m}{U_m}$
0.08[8]	0.16	0.161	0.006
0.11 ^[8]	0.22	0.304	0.38
0.2[20]	1	1.06	0.06

This gives an estimate of K defined in Eq. [3] and used in Eq. [1] to find the terminal velocity of the dendrite, U_d . The high order terms of Eq. [14] are needed because of the complexity of the relationship among K, Re, and B. At constant B, the relation between K and Re goes from a power law (Eq. [15]) at lower B values, to linear at intermediate B values, and finally to exponential at higher B values.

V. EXAMINATION OF CODE RESULTS

Figure 2 shows the dendrite settling velocities calculated and the model dendrite velocities measured by Zakhem *et al.*^[11] The average difference between the calculated and measured velocities is ± 5 pct. This is considered to be excellent agreement, especially since wall and inertial corrections in these cases sometimes exceeded 20 pct and velocity is very sensitive to the densities of the solid and liquid. For example, for the lower density dendrite models used in the study, a 2 pct error in solid density would result in a 30 pct error in $\Delta \rho$ and settling velocity.

In a previous study, evidence of dendrite settling in eutectic Pb-Sn was found.^[4] By calculating velocities for Pb-Sn dendrites in a eutectic melt, we can determine if velocities predicted by the code are consistent with these previous findings. Several micrographs of the fragmented dendritic structure^[4] provide the geometric values needed in the code. Cooling curves show that during



Fig. 2—Dendrite settling velocity calculated by the code vs measured model dendrite settling velocity from Ref. 11, in units of 10^{-2} m/s.

"quench," solidification takes place over a span of approximately 30 seconds (Ingot No. 6). A dendrite settling velocity of 8.8×10^{-4} m/s was determined, using the following conditions: $\Delta \rho = 2.2$ g/cc, $\mu = 2.1 \times$ 10^{-3} kg/ms, primary arm length = 0.01×10^{-2} m, arm diameter = 0.0018×10^{-2} m, crucible diameter = 1×10^{-2} m 10^{-2} m, and a simple equiaxed shape with no secondary arms. de Groh's^[4] Ingot No. 6 shows Pb dendrites distributed throughout the bottom half of the 2.6 \times 10^{-2} -m-tall sample. For a dendrite to settle from the top to the center of the ingot (or from the center to the bottom), a settling distance of 1.3×10^{-2} m, an elapsed time of about 15 seconds (one half of the total solidification time) is required. This seems entirely feasible given the predicted velocity and shows the code to be consistent with these results in Pb-Sn.

Jang and Hellawell^[8] measured the NH₄Cl equiaxed dendrite settling rates shown in Table I. The physical properties and geometric parameters of these settling dendrites can be drawn from Reference 8, thus allowing use of the code. Using a micrograph of a typical NH₄Cl dendrite (Figure 7(a) of Reference 8), the geometric parameters were determined by proportioning the parameters of the example dendrite. The proportionality, P, used was the ratio of the dendrite widths, $P = W_d/W_e$, where W_d is the width of dendrite whose velocity was measured and W_e is that of the example dendrite (in Figure 7(a) of Reference 8). Table II shows the physical properties and geometric parameters used in the code. The agreement between the code and the measured velocities shown in Table I is considered excellent. The difference between the measured and calculated velocities can be fully accounted for by particle-particle interactions and the uncertainties in the measured velocity and dendrite width. Since only one or two significant figures are given for the measured NH₄Cl dendrite velocities and widths^[8] and no estimate of accuracy presented, it is implied that accuracies are in the range of ± 10 pct for both the velocities and widths. A 10 pct uncertainty in width alone translates to 20 pct uncertainty in velocity due to the r^2 term in Stokes' law. It should also be noted that the estimated accuracy of the dendrite dimensions determined from the micrograph is ± 5 pct.

Ahuja^[20] has recently measured NH₄Cl equiaxed dendrite settling velocities. The dimensional parameters for a dendrite were determined and are listed in Table II. The difficulty with this data is that at the larger sizes studied, the resulting Reynolds numbers are quite high, in the range of 10 to 60. Correction factors used in the code are based on data up to Re = 4. For comparison purposes, Sutterby's^[16] correction factors were extrapolated to Re = 14 (the Reynolds number of the 2 × 10^{-3} m tall equiaxed dendrite listed in Tables I and II). The nonlinear data, at constant blockage ratio, were adapted to the simple power curve as expressed by

$$K = 1 + 0.15 \,\mathrm{Re}^{0.7}$$
[15]

having a coefficient of determination^[21] of 0.993. The estimated accuracy of the measured dendrite settling velocity of 1×10^{-2} m/s listed in Table I is ±20 pct, based on the scatter of velocity measurements. The main cause of scatter in the measured velocities is believed to

	Physical Property	From Micrograph	$Dendrite^{[8]}$ Width = $8 \times 10^{-4} \text{ m}$	Dendrite ^[8] Width = 1.1×10^{-3} m	Dendrite ^[20] Width = 2×10^{-3} m
$\frac{1}{\rho_{\text{solid, kg/m}_{3}}}\rho_{\text{liquid, kg/m}}$ $[\mu], \text{ kg/m/s}$	$ \frac{1.53 \times 10^{3}}{1.08 \times 10^{3}} $ $ \frac{1.03 \times 10^{-3}}{1.03 \times 10^{-3}} $				
P Primary arm length tip to tip, m radius, m envelope pyramid angle, degrees Secondary arm number of sets (total	1.05 × 10	$1 \\ 1.4 \times 10^{-3} \\ 2.2 \times 10^{-5} \\ 16 \text{ deg}$	$0.566 \\ 8.0 \times 10^{-4} \\ 1.2 \times 10^{-5} \\ 16 \text{ deg}$	$0.778 1.1 \times 10^{-3} 1.7 \times 10^{-5} 16 deg$	$N/A 2 \times 10^{-3} 3.8 \times 10^{-5} 39 deg$
pairs) average length tip to tip, m radius, m		$\begin{array}{c} 60 \\ 1.6 \times 10^{-4} \\ 1.1 \times 10^{-5} \end{array}$	$\begin{array}{r} 36\\ 9.0 \times 10^{-5}\\ 6.2 \times 10^{-6} \end{array}$	$\begin{array}{c} 48\\ 1.2 \times 10^{-4}\\ 8.6 \times 10^{-6} \end{array}$	$ \begin{array}{r} 72 \\ 5 \times 10^{-4} \\ 1.3 \times 10^{-5} \end{array} $

Table II. Physical Properties of NH_4Cl-H_2O , Geometric Parameters from Micrograph of NH_4Cl Dendrite (Figure 7(a) of Reference 8), and of the Settling NH_4Cl Dendrites of References 8 and 20

be due to variations in solid volume fraction within the dendrites. The accurate measure of the dendrite dimensions (*i.e.*, secondary dendrite arm spacing and diameter) is also believed to be a major factor in limiting the accuracy of code predictions. Another factor which may influence settling speed is off axis tilting of the free dendrite. Off axis settling is the subject of a study presently under investigation by the authors. The 6 pct difference between the results of the code and the experiments is again considered excellent and is well within the uncertainties of the experiments and the physical parameters used in the code.

VI. CONCLUSIONS

A FORTRAN 77 computer program developed to calculate the velocity of a settling dendrite in a quiescent bath yields a good estimate of the volume, surface area, and velocity of various dendritic shapes. The use of the concept of an envelope around the dendrite enables the calculation of an effective sphericity. The use of the empirical relationships determining velocity, sphericity, and envelope permeability appears valid, as do the wall and inertial correction factors presented. At this time, the code does not account for gradients in composition or density, particle-particle interactions, tertiary dendrite arms, or the possible influences of off axis (tilted) dendrite settling. These limitations may be overcome with further code development in conjunction with laboratory testing. A copy of the current program may be obtained from de Groh.

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