Towards analytical solutions of the alloy solidification problem.

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Abstract.
In this paper, an analytical solution of alloy solidification problem is presented. We develop a special method to obtain an exact analytical solution for mushy zone problem. The main key of this method is a requirement that thermal diffusivity in the mushy zone to be constant. From such condition we obtain an ordinary differential equation for liquid fraction function. Thus the method can be examine as "a model" to achieve analytical solution of some unrealistic problems.

An example of solutions is presented: the noneutectic titanium-based alloy solidification. We provide the comparison of numerical simulation results with obtained exact solutions. It shown that very simple apparent capacity-based numerical scheme is provided a good agreement with exact positions of the solidus and liquidus isotherms, and with temperature profiles also.

Finally, some extensions of the method are outlined.

1. Introduction.
A general methodology of achieving analytical solutions of the alloy solidification problem is presented in this manuscript. There is an analytical solution for pure substance (Stefan’s problem) and few analytical and semi-analytical solutions for alloys [1, 2, 3]. We suggest a general methodology which can provide wide range solutions to test different numerical schemes [1, 2].

We consider the case when physical properties \( \Phi \) (density, heat capacity, or heat conductivity) in solid and in liquid are constant. Within mushy zone these properties and the enthalpy depend on temperature as follows (i.e. obey the lever rule):

\[
\Phi(T) = [1 - \lambda(T)] \Phi_s + \lambda(T) \Phi_l,
\]

where \( \Phi_s \) and \( \Phi_l \) are properties in solid and liquid, respectively, \( \lambda(T) \) is volumetric liquid fraction. Then we rewrite heat transfer equation in the full enthalpy term \( H(T) \). The key idea of the present work is the mushy heat diffusivity requirement to be constant.

\[
\alpha(T) = \frac{\kappa(T)}{dH(T)/dT} = \alpha_{sl} = \text{const},
\]

\( \alpha \) is heat diffusivity, \( \kappa \) is heat conductivity.
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where $\kappa(T)$ is heat conductivity. From this condition we can find liquid fraction $\lambda(T)$ by means of which we are able to linearize an initial energy conservation equation. Thus, the following methodology is

(i) To rewrite of the heat equation in the full enthalpy term.
(ii) To require of the thermal diffusivity to be constant in the solid, mushy and liquid zone.
(iii) Condition $\alpha(T) = \alpha_{sl} = \text{const}$ is ordinary differential equation for liquid fraction $\lambda = \lambda(T)$. Additionaly we require $\lambda(T_s) = 1$.
(iv) To solve this ODE and find $\lambda = \lambda(T, \alpha_{sl})$.
(v) To impose additional condition $\lambda(T_s, \alpha_{sl}) = \lambda_0$. For $\lambda_0 = 0$ we have noneutectic alloy, and for $\lambda_0 \neq 0$ – eutectic. From this condition we find $\alpha_{sl}$.
(vi) Now we have the heat equation with constant-peace coefficients and we can it solve easy.

It needs to note, that this problem cannot be solved with well defined (predefined) $\lambda(T)$ function, instead of the function $\lambda = \lambda(T)$ is determined from linearisation conditions.

2. The linearisation of the heat equation.

We will solve an energy conservation equation

$$\frac{\partial H}{\partial t} = \text{div} (k(T)\text{grad} T),$$

where full enthalpy $H$ is

$$H(T) = \rho(T) [1 - \lambda(T)] \int_0^T C_s(\zeta)d\zeta + \rho(T)\lambda(T) \int_0^T C_l(\zeta)d\zeta + \rho(T)\lambda(T)L,$$

where $C_s, C_l$ is specific heat in solid and in liquid, $L$ is latent heat of fusion, $\rho = \rho_s = \rho_l$ is density, which all are constants. We express the heat conductivity in the "mixture" form

$$\kappa(T) = [1 - \lambda(T)] \kappa_s + \lambda(T)\kappa_l,$$

where $\kappa_s$ and $\kappa_l$ are constant heat conductivity in solid and liquid, respectively. Taking into account the expression

$$\text{grad} T = \frac{\text{grad} H}{\frac{\partial H}{\partial T}}$$

the Eq. (3) can be rewritten in the general form

$$\frac{\partial H}{\partial t} = \text{div} (\alpha(T)\text{grad} H),$$
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where \( \alpha(H) \) is thermal diffusivity, which defined as

\[
\alpha(T) = \frac{\kappa(T)}{dH(T)}.
\]  
(8)

If \( \kappa(T) \) and \( dH(T)/dT \) depend on temperature arbitrary manner then Equation (7) is nonlinear. To achieve an analitical solution we need to require the thermal diffusivity to be constant in all regions (solid, mushy and liquid).

\[
\alpha(T) = \begin{cases} 
\alpha_s = \text{const} & \text{for } T < T_s \\
\alpha_{sl} = \text{const} & \text{for } T_s \leq T \leq T_l \\
\alpha_l = \text{const} & \text{for } T > T_l
\end{cases}
\]  
(9)

In our case \( \alpha_s = \kappa_s \rho C_s \) and \( \alpha_l = \kappa_l / \rho C_l \) are constant by definition. For the derivation of mushy enthalpy (the apparent capacity \( \times \) density) we get:

\[
\frac{1}{\rho} \frac{dH(T)}{dT} = [1 - \lambda] C_s + \lambda C_l + [(C_l - C_s)T + L] \frac{d\lambda(T)}{dT}.
\]  
(10)

then from the mushy part of Eq. (9) we obtain an ordinal differential equation for \( \lambda(T) \)

\[
[1 + pT] \frac{d\lambda(T)}{dT} + a \lambda(T) + b = 0,
\]  
(11)

where we denote

\[
a = \frac{a_{sl} \rho (C_l - C_s) - (\kappa_l - \kappa_s)}{a_{sl} \rho L},
\]  
(12)

\[
b = \frac{a_{sl} \rho C_s - \kappa_s}{a_{sl} \rho L},
\]  
(13)

\[
p = \frac{C_l - C_s}{L}.
\]  
(14)

We require

\[
\lambda(T_l) = 1,
\]  
(15)

where \( T_l \) is a liquidus temperature. Solution of Eqs. (11) and (15) is

\[
\lambda(T) = -\frac{b}{a} + \frac{a + b}{a} \left( \frac{1 + pT_l}{1 + pT} \right)^\frac{b}{a}.
\]  
(16)

It needs to determine an additional condition for \( \lambda(T) \) function, namely to define the liquid fraction value at solidus temperature

\[
\lambda(T_s) = \begin{cases} 
0 & \text{for noneutectic alloy} \\
\lambda_0 & \text{for eutectic alloy}
\end{cases}
\]  
(17)

To obtain the analytical solution of Eq. (7) we need to solve Eq.(17) to find root \( a_{sl} \). Then we need to solve Eq. (7) with suitable initial and boundary conditions.
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The enthalpy of the system (4) we may design

\[ \frac{H(T)}{\rho} = \begin{cases} 
C_s T & \text{for } T < T_s \\
C_s T + \lambda(T) [(C_l - C_s)T + L] & \text{for } T_s \leq T \leq T_l \\
C_l T + L & \text{for } T > T_l
\end{cases} \tag{18} \]

In future we need the value \( dT/dH \):

\[ \frac{\rho dT}{dH} = \begin{cases} 
\frac{1}{C_s} & \text{for } T < T_s \\
\frac{1}{[1 - \lambda]C_s + \lambda C_l + [(C_l - C_s)T + L]} \frac{d\lambda}{dT} & \text{for } T_s \leq T \leq T_l \\
\frac{1}{C_l} & \text{for } T > T_l
\end{cases} \tag{19} \]

It should be note that some expressions with \( d\lambda/dT \) may be written in more simplified form versus \( \lambda \), for example:

\[ \frac{d\lambda}{dT} = -\frac{a\lambda + b}{1 + pT} = -\frac{a\lambda + b}{(C_l - C_s)T + L} L, \tag{20} \]

and the combination

\[ [(C_l - C_s)T + L] \frac{d\lambda}{dT} = -(a\lambda + b) L. \tag{21} \]

3. An analytical solution for enthalpy.

We will examine the simple problem

\[ \frac{\partial H}{\partial t} = \alpha(H) \frac{\partial H}{\partial x}, \tag{22} \]

\[ H(t = 0) = H(T_{\text{init}}), \tag{23} \]

\[ H|_{x=0} = H_{\text{out}} = H(T_{\text{out}}), \tag{24} \]

\[ H|_{x=\infty} = H_{\text{init}} = H(T_{\text{init}}). \tag{25} \]

The solution of these equations with constant-piece function \( \alpha(H) \) can be easy find [4]. To solve this equation we divide whole region \([0, \infty)\) into three subintervals \([0, X_s)\), \([X_s, X_l]\) and \((X_l, \infty)\) (\(X_s \) and \(X_l\) are solidus and liquidus positions, respectively). Moreover, we assume that (the similarity solution):

\[ X_s(t) = k_s \sqrt{t}, \quad X_l(t) = k_l \sqrt{t}, \tag{26} \]

where \(k_s\) and \(k_l\) are constants. Solutions on the subintervals are:

\[ H(x, t) = H_{\text{out}} + (H_s - H_{\text{out}}) \frac{\text{erf} \left( \frac{x}{2\sqrt{D_{\text{eff}}} t} \right)}{\text{erf} \left( \frac{k_s}{2\sqrt{D_{\text{eff}}}} \right)}, \quad x \in [0, X_s), \tag{27} \]
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\[ H(x, t) = \frac{(H_l - H_s) \text{erf} \left( \frac{x}{2\sqrt{\alpha_s}t} \right) + H_s \text{erf} \left( \frac{k_s}{2\sqrt{\alpha_s}} \right) - H_l \text{erf} \left( \frac{k_l}{2\sqrt{\alpha_s}} \right)}{\text{erf} \left( \frac{k_l}{2\sqrt{\alpha_s}} \right) - \text{erf} \left( \frac{k_s}{2\sqrt{\alpha_s}} \right)}, \quad x \in [X_s, X_l], \]  

(28)

\[ H(x, t) = H_{\text{init}} - (H_{\text{init}} - H_l) \frac{\text{erfc} \left( \frac{x}{2\sqrt{\alpha_l}} \right)}{\text{erfc} \left( \frac{k_l}{2\sqrt{\alpha_l}} \right)}, \quad x \in (X_l, \infty), \]  

(29)

where we defined

\[ H_s = H(T_s) = \rho C_s T_s, \]  

(30)

\[ H_l = H(T_l) = \rho (C_l T_l + L). \]  

(31)

By using the two conditions at the interfaces (the first one from which is Stefan’s condition at the solidus (eutectic) point):

\[ \alpha_s \frac{\partial H}{\partial x} \bigg|_{x=X_s-0} = \alpha_s \frac{\partial H}{\partial x} \bigg|_{x=X_s+0} + \rho \lambda_0 L \frac{dX_s(t)}{dt}, \]  

(32)

\[ \alpha_{sl} \frac{\partial H}{\partial x} \bigg|_{x=X_l-0} = \alpha_l \frac{\partial H}{\partial x} \bigg|_{x=X_l+0}, \]  

(33)

we derive the following two equations from which to evaluate \( k_s \) and \( k_l \):

\[ \frac{\sqrt{\alpha_s}(H_s - H_{\text{out}}) \exp \left( -\frac{k_s^2}{4\alpha_s} \right)}{\text{erf} \left( \frac{k_s}{2\sqrt{\alpha_s}} \right)} - \frac{\sqrt{\alpha_{sl}}(H_l - H_s) \exp \left( -\frac{k_s^2}{4\alpha_{sl}} \right)}{\text{erf} \left( \frac{k_l}{2\sqrt{\alpha_{sl}}} \right) - \text{erf} \left( \frac{k_s}{2\sqrt{\alpha_{sl}}} \right)} = \frac{\sqrt{\pi}}{2} \rho \lambda_0 L k_s, \]  

(34)

\[ \frac{\sqrt{\alpha_{sl}}(H_l - H_s) \exp \left( -\frac{k_l^2}{4\alpha_{sl}} \right)}{\text{erf} \left( \frac{k_l}{2\sqrt{\alpha_{sl}}} \right) - \text{erf} \left( \frac{k_s}{2\sqrt{\alpha_{sl}}} \right)} - \frac{\sqrt{\alpha_l}(H_{\text{init}} - H_l) \exp \left( -\frac{k_l^2}{4\alpha_l} \right)}{\text{erfc} \left( \frac{k_l}{2\sqrt{\alpha_l}} \right)} = 0. \]  

(35)

4. What we can get from the exact solution?

Usually we have numerical scheme which gives us the temperature, but not enthalpy. Below we write down formulas for temperature evaluation versus enthalpy and some other parameters.

4.1. Solidus and liquidus velocities.

From Eq. (26) we get the front velocities

\[ v_l(t) = \frac{dX_l(t)}{dt} = \frac{k_l}{2\sqrt{t}}, \quad v_s(t) = \frac{dX_s(t)}{dt} = \frac{k_s}{2\sqrt{t}}. \]  

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4.2. Temperature curves.

From Eq. (18) and Eqs. (27) - (29) we can easy to find:

In the solid \((x < k_s \sqrt{t})\):

\[
T(x, t) = \frac{1}{\rho C_s} \left[ H_{out} + (H_s - H_{out}) \frac{erf \left( \frac{x}{2\sqrt{\alpha_s t}} \right)}{erf \left( \frac{k_s}{2\sqrt{\alpha_s t}} \right)} \right].
\] (37)

In the mushy zone \((k_s \sqrt{t} \leq x \leq k_l \sqrt{t})\) we need to solve nonlinear equation to get \(T = T(x, t)\):

\[
C_s T + \lambda(T) [(C_l - C_s)T + L] = \frac{1}{\rho} \frac{(H_l - H_s)erf \left( \frac{x}{2\sqrt{\alpha_{st}}} \right) + H_s erf \left( \frac{k_l}{2\sqrt{\alpha_{st}}} \right) - H_l erf \left( \frac{k_s}{2\sqrt{\alpha_{st}}} \right)}{erf \left( \frac{k_l}{2\sqrt{\alpha_{st}}} \right) - erf \left( \frac{k_s}{2\sqrt{\alpha_{st}}} \right)}. \] (38)

In the liquid \((x > k_l \sqrt{t})\):

\[
T(x, t) = \frac{1}{\rho C_l} \left[ H_{init} - (H_{init} - H_l) \frac{erfc \left( \frac{x}{2\sqrt{\alpha_{lt}}} \right)}{erfc \left( \frac{k_l}{2\sqrt{\alpha_{lt}}} \right)} \right] - \frac{L}{C_l}. \] (39)

4.3. Temperature gradients.

From equation

\[
\frac{\partial T}{\partial x} = \frac{dT}{dH} \frac{\partial H}{\partial x}
\]
end from Eq. (19) easy to achive the expressions for temperature gradients:

\[
\frac{\partial T}{\partial x} = \begin{cases} 
\frac{1}{\rho C_s} \frac{\partial H}{\partial x} & \text{if } T < T_s \\
1 \frac{\partial H}{\partial x} & \text{if } T_s \leq T \leq T_l \\
\frac{1}{\rho C_l} \frac{\partial H}{\partial x} & \text{if } T > T_l
\end{cases}
\] (40)

For enthalpy gradients from Eqs. (27) - (29) we get

\[
\frac{\partial H}{\partial x} = \begin{cases} 
\frac{H_s - H_{out}}{erf \left( \frac{k_s}{2\sqrt{\alpha_{st}}} \right)} \cdot e^{-\frac{x^2}{4\alpha_{st}t}} & \text{if } H < H_s \\
\frac{H_l - H_s}{erf \left( \frac{k_l}{2\sqrt{\alpha_{st}}} \right) - erf \left( \frac{k_s}{2\sqrt{\alpha_{st}}} \right)} \cdot e^{-\frac{x^2}{4\alpha_{st}t}} & \text{if } H_s \leq H \leq H_l \\
\frac{H_{init} - H_l}{erfc \left( \frac{k_l}{2\sqrt{\alpha_{lt}}} \right)} \cdot e^{-\frac{x^2}{4\alpha_{lt}t}} & \text{if } H > H_l
\end{cases}
\] (41)
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Thus finally we have:

\[
\frac{\partial T}{\partial x} = \begin{cases} 
\frac{1}{\rho C_s} \cdot \frac{H_s - H_{out}}{\text{erf} \left( \frac{k_s}{\sqrt{2}\alpha_s} \right)} \cdot \frac{e^{-\frac{x^2}{4\alpha_s t}}}{\sqrt{\pi \alpha_s t}} & x < k_s \sqrt{t} \\
\frac{(H_l - H_s)}{\rho \left[ (1 - \lambda)C_s + \lambda C_l + [(C_l - C_s)T + L] \frac{\partial \lambda}{\partial T} \right]} \cdot \frac{e^{-\frac{x^2}{4\alpha_s t}}}{\sqrt{\pi \alpha_s t}} & k_s \sqrt{t} \leq x \leq k_l \sqrt{t} \\
\frac{1}{\rho C_l} \cdot \frac{H_{init} - H_l}{\text{erf} \left( \frac{k_l}{\sqrt{2}\alpha_l} \right)} \cdot \frac{e^{-\frac{x^2}{4\alpha_l t}}}{\sqrt{\pi \alpha_l t}} & x > k_l \sqrt{t}
\end{cases}
\]

There is a very interesting parameters as temperature gradient in liquid phase at the liquidus point \( G_l \). For it we can write down

\[
G_l(t) = \left. \frac{\partial T(x,t)}{\partial t} \right|_{x=X_l} = \frac{1}{\rho C_l} \cdot \frac{H_{init} - H_l}{\text{erf} \left( \frac{k_l}{\sqrt{2}\alpha_l} \right)} \cdot \frac{e^{-\frac{k_l^2}{4\alpha_l t}}}{\sqrt{\pi \alpha_l t}}
\]

This parameter controls the type of solidification microstructure.

4.4. Cooling rate.

As we can see \( G_l(t) \sim 1/\sqrt{t} \). Liquidus velocity (36) varies with time also as \( v_l(t) \sim 1/\sqrt{t} \), then cooling rate given by \( G_l v_l \sim 1/t \). It is easy to show that is so. The cooling rate is defined as

\[
\dot{T}(x,t) = \frac{\partial T(x,t)}{\partial t} = \frac{dT}{dT} \frac{dH}{dt} = \frac{dH}{dt} (44)
\]

\[
\frac{\partial T}{\partial t} = \begin{cases} 
\frac{1}{\rho C_s} \cdot \frac{H_s - H_{out}}{\text{erf} \left( \frac{k_s}{\sqrt{2}\alpha_s} \right)} \cdot \frac{\alpha_s x e^{-\frac{x^2}{4\alpha_s t}}}{2\sqrt{\pi}(\alpha_s t)^{3/2}} & x < k_s \sqrt{t} \\
\frac{(H_l - H_s)}{\rho \left[ (1 - \lambda)C_s + \lambda C_l + [(C_l - C_s)T + L] \frac{\partial \lambda}{\partial T} \right]} \cdot \frac{\alpha_s x e^{-\frac{x^2}{4\alpha_s t}}}{2\sqrt{\pi}(\alpha_s t)^{3/2}} & k_s \sqrt{t} \leq x \leq k_l \sqrt{t} \\
\frac{1}{\rho C_l} \cdot \frac{H_{init} - H_l}{\text{erf} \left( \frac{k_l}{\sqrt{2}\alpha_l} \right)} \cdot \frac{\alpha_l x e^{-\frac{x^2}{4\alpha_l t}}}{2\sqrt{\pi}(\alpha_l t)^{3/2}} & x > k_l \sqrt{t}
\end{cases}
\]

Thus, cooling rate at the liquidus point is given by

\[
\dot{T}_l = \dot{T} \bigg|_{x=X_l+0} = -\frac{1}{\rho C_l} \cdot \frac{H_{init} - H_l}{\text{erf} \left( \frac{k_l}{\sqrt{2}\alpha_l} \right)} \cdot \frac{k_l e^{-\frac{k_l^2}{4\alpha_l t}}}{2\sqrt{\pi \alpha_l t}} \sim \frac{1}{t} \tag{46}
\]

The value \( \dot{T}_l \) is very important, because it defines secondary arm dendrite spacing [7]. The another important expression is \( G_l^{-1/2} v_l^{-1/4} \), which defines primary arm dendrite spacing [8]. From Eqs. (36) and (43) we can show that primary arm spacing varies versus time like \( \sim t^{3/8} \). However, as it’s very known, after some critical gradient and velocity at the liquidus point will be take a place columnar to equiaxed transition [9].
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4.5. Local solidification time

For directional solidification, the local solidification time \( t_{ls} \) can be estimated from the following equation:

\[
t_{ls}(x) = \left[ \frac{1}{k_s^2} - \frac{1}{k_l^2} \right] x^2,
\]

(47)

where quadratic increasing with \( x \) of \( t_{ls} \) we have, because the mushy zone length increases versus \( x \) and solidus/liquidus velocities decrease. The local solidification time controls the some segregation processes in the mushy zone.

5. Numerical scheme.

We will solve heat transfer equation

\[
\rho C(T) \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( \kappa(T) \frac{\partial T}{\partial x} \right)
\]

(48)

which concerns with Eq. (23). Here \( \kappa(T) \) edfined by Eq. (5) and mushy heat capacity (so-called apparent capacity):

\[
C(T) = [1 - \lambda(T)] C_s + \lambda(T) C_l + [(C_l - C_s) T + L] \frac{d\lambda(T)}{dT}.
\]

(49)

The first, we draw the grid with spatial step \( h = x_{i+1} - x_i \), where \( i = 0, 1, ..., N \). The second, integrating the Eq. (48) over the \( x \in [(i - \frac{1}{2})h, (i + \frac{1}{2})h] \) we can write heat balance equation as follows

\[
\rho C(T_i) \frac{\partial T_i}{\partial t} h = \left( \kappa(T) \frac{\partial T}{\partial x} \right)_{x=(i+\frac{1}{2})h} \approx \kappa_{i+\frac{1}{2}} T_{i+1} - \frac{T_i - T_{i-1}}{h}.
\]

(50)

The left part of this equation we express as

\[
\rho C(T_i) \frac{\partial T_i}{\partial t} \approx \rho C(T_i^n) \frac{T_{i+1}^{n+1} - T_i^n}{\tau},
\]

where \( n \) is time index, \( \tau \) is time step. Thus the Eq. (48) we can write down in the discrete form as

\[
\left[ \frac{\tau \kappa_{i-1}}{h^2} \right] T_{i-1}^{n+1} - \left[ \tau h^2 \left( \kappa_{i-\frac{1}{2}} + \kappa_{i+\frac{1}{2}} \right) + \rho C_i \right] T_i^{n+1} + \left[ \frac{\tau \kappa_{i+\frac{1}{2}}}{h^2} \right] T_{i+1}^{n+1} = -\rho C_i T_i^n,
\]

(51)

where [10]

\[
\kappa_{i-\frac{1}{2}} = \frac{2\kappa_{i-1}\kappa_i}{\kappa_{i-1} + \kappa_i}, \quad \kappa_{i+\frac{1}{2}} = \frac{2\kappa_i\kappa_{i+1}}{\kappa_i + \kappa_{i+1}}.
\]

We note, that \( C_i \) etc are calculated at time \( t_n \), i.e.

\[
C_i = C(T_i^n), \quad \kappa_{i-1} = \kappa(T_{i-1}^n) \quad etc.
\]
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Boundary conditions are

\[ T_0 = T_{out}, \quad T_N = T_{init}. \]  

(52)

Because the Eq. (51) is tri-diagonal linear system, then its solving is trivial and we do not discuss this issue here.

6. Binary alloy solidification: numerical treatment.

In this section we consider the solidification of noneutectic titanium-based alloy, which we can treat as pseudo-binary alloy. Physical properties of titanium alloy VT3-1 (Ti-6.5Al-2.5Mo-1.5Cr-0.5Fe-0.3Si) are present in the Table 1. These parameters we are used for numerical simulation of liquid pool profiles during vacuum arc remelting process [5].

| Parameter | Value   |
|-----------|---------|
| \( C_s \) | 600 J/kg K |
| \( C_l \) | 1200 J/kg K |
| \( \kappa_s \) | 10 W/m K |
| \( \kappa_l \) | 35 W/m K |
| \( \rho \) | 4500 kg/m³ |
| \( L \) | \( 3.55 \times 10^5 \) J/kg |
| \( T_s \) | 1550 °C |
| \( T_l \) | 1620 °C |
| \( T_m \) | 1668 °C |

Table 1. Properties of the VT3-1 alloy.

A solution of the Eq. (17) with \( \lambda_0 = 0 \) is \( a_{sl} = 2.26891 \times 10^{-7} \) m²/s. Figure 1 shows the temperature dependence of the liquid fraction. Additionaly Figure 1 shows the function

\[ \lambda_t(T) = 1 - \frac{T_m - T_S}{T_l - T_s} \cdot \frac{T_l - T}{T_m - T}, \]  

(53)

which we used for VT3-1 alloy [5]. The difference between \( \lambda_T \) and \( \lambda_t(T) \) is small, then we have nearly realistic problem. If \( g(T) \) approximated with a power function [6]

\[ \lambda_n = \left( \frac{T - T_s}{T_l - T_s} \right)^n, \]

then we get \( n \approx 1.5 \). To test very simple numerical apparent capacity-based method we carried out simulations with following parameters: \( a_s = 3.7037 \times 10^{-6} \) m²/s, \( a_l = 6.48148 \times 10^{-6} \) m²/s, \( T_{out} = 800 °C, T_{init} = 1650 °C, H_{out} = 2.16 \times 10^9 \) J/m³, \( H_{init} = 10.5057 \times 10^9 \) J/m³, \( H_s = 4.185 \times 10^9 \) J/m³, \( H_l = 10.3455 \times 10^9 \) J/m³.

\( \lambda_n = \left( \frac{T - T_s}{T_l - T_s} \right)^n \)

Solutions of Eqs. (34)-(35) are \( k_s = 0.00134109 \) m/s⁰.⁰, \( k_l = 0.00206009 \) m/s⁰.⁰. The numerical model parameters are chosen as: length of domain \( d = 0.5 \) m, nodes number \( N = 500 \), time step \( \tau = 0.1 \) s. A numerical model can provide excellent
Towards analytical solutions of the alloy solidification problem.

Figure 1. Liquid fraction versus temperature for noneutectic alloy. On the Figure: analytical – for \( \lambda(T) \), VT3-1 for \( \lambda_t(T) \).

agreement with obtained analytical solution. The results obtained are in a Figure 2: movement of both the solidus and the liquidus front (26). We used linear interpolation between \( T_i \) and \( T_{i+1} \) for estimating position of the fronts, whereas \( T_{s,l} \in [T_i, T_{i+1}] \).

Figure 2. Comparison of the apparent capacity-based numerical method with the analytical solution as applied to the solidification of VT3-1 titanium alloy. Figure: solidus and liquidus position versus time.

The errors in the positions of solidus/liquidus

\[
\epsilon_x(t) = \frac{X_{\text{num}}(t) - X_{\text{exact}}(t)}{X_{\text{exact}}(t)} \cdot 100\%
\]

are presented in the Figure 5. Moreover Figure 4 shows the temperature profiles after 20 and 500 seconds under the same numerical conditions.
Towards analytical solutions of the alloy solidification problem.

Figure 3. Solidus/liquidus front position errors versus time.

Figure 4. Temperature curves at 20 and 500 seconds.

Figure 5. Temperature curves errors at 20 and 500 seconds.
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Figure 5 shows temperature profiles errors defined by

\[ \varepsilon_T(x) = \frac{T_{\text{num}}(x) - T_{\text{exact}}(x)}{T_{\text{exact}}(x)} \cdot 100\%. \]

We would like to underline that the purpose of this work is to achieve the exact analytical solution on alloy solidification. Due to this, advantages and disadvantages different numerical algorithms can be done in future. Due to this, we don’t study the process of solidification of Ti-6.5Al-2.5Mo-1.5Cr-0.5Fe-0.3Si alloy, but only use the thermo-physical properties of this alloy to show as the model works.

7. Conclusions.

In this paper, analytical solution of alloy solidification problem is presented. We developed a special method to obtain an exact analytical solution for mushy zone problem. The main requirement of the method is thermal diffusivity to be constant in the mushy zone. Due to such condition ordinary differential equation for liquid fraction function is achieved. Thus the present method can be examined as "a model" way to get analytical solution of some unrealistic problems.

An example of solutions is given – the noneutectic titanium-based alloy solidification. We provide the comparison of the simple numerical simulation results with obtained exact solutions. We show that very our numerical apparent capacity-based scheme provides a good agreement with exact solutions for solidus/liquidus position and for temperatures profiles in different moments of solidification time.

Once again we would like to underline that the main goal of this paper to provide the benchmark for binary alloy solidification problem, but not in the analysis of used numerical scheme.

If predefined \( \lambda(T) \) function is to be examined, we can use another suggestions. For example, we can require to heat conductivity (from experiment, e.g.) to be proportional to the apparent capacity, i.e.

\[ \kappa(T) = a_{sl} \rho \left( C_s + (C_l - C_s)\lambda(T) + [(C_l - C_s)T + L] \frac{d\lambda(T)}{dT} \right). \]

Or, for the second example, we require to apparent capacity (from experiment) to be proportional to mushy heat conductivity, i.e.

\[ \frac{dH(T)}{dT} = \frac{\kappa_s + (\kappa_l - \kappa_s)\lambda(T)}{a_{sl}}. \]

Moreover, we may use the Bäcklund’s transformation [11] to make mushy heat equation linearisation. In this case we get nonlinear condition

\[ \frac{H^2(T)\lambda(T)}{\frac{dH(T)}{dT}} = \text{const.} \]

These linearization methods will provide us with some additional analytical solutions of alloy solidification problem.
Towards analytical solutions of the alloy solidification problem.

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