ISSN 2176-5480

22nd International Congress of Mechanical Engineering (COBEM 2013)
November 3-7, 2013, Ribeirão Preto, SP, Brazil

OPTIMIZATION OF A MUSHY ZONE PARAMETER IN A SOLIDIFICATION MODEL

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Abstract. *This work deals with the particle swarm optimization of a mushy zone parameter present in a solidification model. The solidification model is based on the heat transfer equation employing the effective capacity method. The heat transfer equation is solved by a finite volumes method with an explicit scheme where the central differences interpolation function is adopted. The temperature profile and the thickness of the solidification layer are used to evaluate the numerical solution obtained with the optimum mushy zone parameter. Populations with different sizes are investigated to analyze the particle swarm performance.*

Keywords: *Solidification, Particle Swarm, Inverse Problems*

1. INTRODUCTION

The phase change that occurs from the liquid state to the solid state is called solidification. This phenomenon is present in nature and in industrial processes. In nature, it can be observed in ice formation and in the solidification of volcanic lava, while in industry, it is found in freezing, casting and welding (Tan *et al.*, 2011; Yajun *et al.*, 2013).

Because of its great importance in society, solidification processes have been widely studied. Experimental techniques and mathematical models have been developed to improve knowledge associated with the phenomenon under consideration (Bauer, 1993).

Among the mathematical approaches it can be singled the classical Stefan problem, which consists of a moving boundary problem. However, despite this problem has been studied since the XIX century, analytical solutions are available only for a few special situations. However, the contribution of these relevant solutions for understanding the solidification phenomena then is also important today, when these analytical solutions are widely used in validation and verification of numerical solutions.

The Stefan problem is based on the heat equation, where the phase change interface is a moving boundary, which is represented by a jump condition, that link sand the liquid domains. To avoid the complexity of this moving boundary problem, other mathematical models have been proposed, such as the method of apparent heat capacity and the effective heat capacity (Hashemi and Sliepcevich, 1967; Poirier and Salcudean, 1998; Mosaffa *et al.*, 2013). In these methods, the solidification problem is solved in a single domain, where a modified heat capacity takes into account the phase change phenomenon. In other words, these methods employ the heat transfer equation with variable themophysical properties for the liquid, for the solid and for the phase change regions, by using a modified heat capacity in a single domain (Hu and Argyropoulos, 1996).

The apparent and the effective heat capacity methods consider the existence of a mushy region, where liquid and solid are simultaneously present. This assumption is valid for solidification of mixtures, but for pure substances it is an approximation. Nevertheless, these methods facilitated the study of the solidification process in multidimensional geometries by using numerical methods with fixed meshes.

Developed initially by Eberhart and Kennedy (1995) as an alternative method for the genetic algorithm, the Particle Swarm Optimization - PSO is a stochastic optimization technique, where restrictions or parameters depend on random variables (Landim, 1991). The PSO is based on the social behavior of various species and tries to balance the individuality and sociability of the individuals in order to locate the optimum parameter of interest (Colaço *et al.*, 2006).

2. PHYSICAL PROBLEM AND MATHEMATICAL FORMULATION

The physical problem analyzed in this paper consists of a one-dimensional transient heat solidification problem. In the rectangular coordinates system initially, the entire medium is at a uniform temperature and only the liquid phase is

ISSN 2176-5480

present. Suddenly, a heat sink is applied at the origin of the system of coordinates (x=0) and thus a prescribed temperature is attained at this boundary. The material then starts to solidify at x=0 and a solidification front moves away from the origin. The physical properties of liquid and solid phases are assumed constant at each phase.

For this problem, the thermophysical properties are given by:

$$\widetilde{k}(\mathrm{T}) = \begin{cases} k_{sol}(\mathrm{T}); & \mathrm{T} \leq \mathrm{T}_m - \Delta\mathrm{T} & - \text{ solid zone} \\ k_{ls}(\mathrm{T}) = k_{sol}(\mathrm{T}); & \mathrm{T}_m - \Delta\mathrm{T} < \mathrm{T} < \mathrm{T}_m + \Delta\mathrm{T} & - \text{ mushy zone} \\ k_{liq}(\mathrm{T}); & \mathrm{T} \geq \mathrm{T}_m + \Delta\mathrm{T} & - \text{ liquid zone} \end{cases} \tag{1}$$

$$\rho(\mathrm{T}) = \begin{cases} \rho_{sol}(\mathrm{T}); & \mathrm{T} < \mathrm{T}_m & - \text{ solid zone} \\ \rho_{liq}(\mathrm{T}); & \mathrm{T} \geq \mathrm{T}_m & - \text{ liquid zone} \end{cases} \tag{2}$$

$$C_{ap}(\mathrm{T}) = \begin{cases} C_{sol}(\mathrm{T}); & \mathrm{T} \leq \mathrm{T}_m - \Delta\mathrm{T} & - \text{ solid zone} \\ C_{ls}(\mathrm{T}); & \mathrm{T}_m - \Delta\mathrm{T} < \mathrm{T} < \mathrm{T}_m + \Delta\mathrm{T} & - \text{ mushy zone} \\ C_{liq}(\mathrm{T}); & \mathrm{T} \geq \mathrm{T}_m + \Delta\mathrm{T} & - \text{ liquid zone} \end{cases} \tag{3}$$

The specific heat per unit volume for the solid-liquid, respectively, as:

$$C_{sol} = \rho_{sol} c_p; \quad C_{liq} = \rho_{liq} c_p; \quad C_{ls} = \frac{\rho_{sol}\Delta\mathrm{H}}{\Delta\mathrm{T}} + \frac{C_{liq}(\mathrm{T}) + C_{sol}(\mathrm{T})}{2}. \tag{4}$$

where, ρ_{liq} is the density of the liquid, ρ_{sol} is the density of the solid, c_p is the specific heat, ΔH is the latent heat and ΔT is the mushy zone parameter.

The mathematical formulation for this physical problem can be written as

$$C_{ap}(\mathrm{T})\frac{\partial \mathrm{T}}{\partial \mathrm{t}} = \frac{\partial}{\partial \mathrm{x}}\left[\widetilde{k}\frac{\partial \mathrm{T}}{\partial \mathrm{x}}\right] \qquad 0 < \mathrm{x} < \mathrm{L} \qquad \mathrm{t} > 0 \tag{5}$$

$$\mathrm{T} = \mathrm{T}_0 \qquad 0 \leq \mathrm{x} \leq \mathrm{L} \qquad \mathrm{t} = 0 \tag{6}$$

$$\mathrm{T} = \mathrm{T}_w \qquad \mathrm{x} = 0 \qquad \mathrm{t} > 0 \tag{7}$$

$$\frac{\partial \mathrm{T}}{\partial \mathrm{x}} = 0 \qquad \mathrm{x} = \mathrm{L} \qquad \mathrm{t} > 0 \tag{8}$$

and T_0 is the uniform initial temperature, T_m is the melting temperature of the material, T_w the wall temperature at x = 0, C_{ap} is the apparent heat capacities and $\widetilde{k}$ is the thermal conductivity function.

3. Effective capacity method

Initially proposed by Poirier and Salcudean (1998) in an effort to improve the apparent capacity method, this technique assumes a temperature profile between the nodes. For the volume control method, the effective capacity is calculated based on the following into over one volume, where this work will be presented by:

$$C_{ef} = \frac{\left(\int C_{ap}\mathrm{dV}\right)}{\mathrm{V}} \tag{9}$$

where C_{ef}, C_{ap} and V are the effective heat capacity, heat capacity and apparent volume control, respectively.

In this fashion, by applying the effective capacity method to the problem described by Eqs (5) - (8), the following problem results

$$C_{ef}(\mathrm{T})\frac{\partial \mathrm{T}}{\partial \mathrm{t}} = \frac{\partial}{\partial \mathrm{x}}\left[\widetilde{k}\frac{\partial \mathrm{T}}{\partial \mathrm{x}}\right] \qquad 0 < \mathrm{x} < \mathrm{L} \qquad \mathrm{t} > 0 \tag{10}$$

$$\mathrm{T} = \mathrm{T}_0 \qquad 0 \leq \mathrm{x} \leq \mathrm{L} \qquad \mathrm{t} = 0 \tag{11}$$

$$\mathrm{T} = \mathrm{T}_w \qquad \mathrm{x} = 0 \qquad \mathrm{t} > 0 \tag{12}$$

$$\frac{\partial \mathrm{T}}{\partial \mathrm{x}} = 0 \qquad \mathrm{x} = \mathrm{L} \qquad \mathrm{t} > 0 \tag{13}$$

ISSN 2176-5480

4. Reference solution

In this paper, the model phase change model described above is compared to the problem of solidification in a Half-Space (Two-phase Problem), for which an analytical solution is present in Özişik (1993).

At time $t = 0$, liquid at a uniform temperature T_0 that is higher than the melting temperature T_m of the solid phase is confined to a half-space $x > 0$. The boundary surface at $x = 0$ is lowered to a temperature T_w below T_m and maintained at that temperature for times $t > 0$. As a result, the solidification starts at the surface $x = 0$ and the solid-liquid interface moves in the positive x direction. This problem is a two-phase problem because the temperatures are unknown in both the solid and liquid phases (Özişik, 1993). This problem is more general than the on considered in the previous examples: its solution is known as *Neumann's solution*.

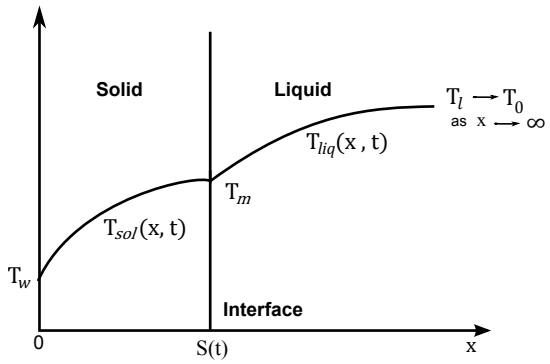

Figure 1. Solidification in a half-space.Two-phase problem. (Özişik, 1993)

4.1 Phase change analytical solution

According to Özişik (1993), the analytical solution for the temperature distribution in the solid-liquid region is given by:

$$T_{sol}(x,t) = T_w + (T_m - T_w)\left(\frac{erf\left(\frac{x}{2\sqrt{\alpha_{sol}t}}\right)}{erf(\lambda)}\right) \tag{14}$$

$$T_{liq}(x,t) = T_0 + (T_m - T_0)\left(\frac{erfc\left(\frac{x}{2\sqrt{\alpha_{liq}t}}\right)}{erfc\left(\lambda\sqrt{\frac{\alpha_{sol}}{\alpha_{liq}}}\right)}\right) \tag{15}$$

where the eigenvalues λ and the solidification front S(t) are given by

$$\frac{e^{-\lambda^2}}{erf(\lambda)} + \frac{k_{liq}}{k_{sol}}\sqrt{\frac{\alpha_{sol}}{\alpha_{liq}}}\frac{T_m - T_0}{T_m - T_w}\frac{e^{-\lambda^2(\alpha_{sol}/\alpha_{liq})}}{erfc\left[\lambda\sqrt{(\alpha_{sol}/\alpha_{liq})}\right]} = \frac{\lambda\Delta H\sqrt{\pi}}{c_{psol}(T_m - T_w)} \tag{16}$$

$$S(t) = 2\lambda\sqrt{(\alpha_{sol}t)} \tag{17}$$

In the above equations, T_0 is the uniform initial temperature, T_m is the melting temperature of the material, ΔH is the latent heat of solidification of the material, ρ is the density, k is the thermal conductivity, α is the thermal diffusivity, T is the temperature and the subscripts sol and liq refer to the solid and liquid phases, respectively.

ISSN 2176-5480

5. PSO mathematical formulation

In PSO each particle is assumed to have a capacity for individual learning and a learning capability based on the experience of the population.

Each particle i of a given population *P* in a n-dimensional space has a velocity v_i^k and position x_{i^k}, updated in accordance with the Eqs. (18) and (19).

$$\mathrm{v}_i^{k+1} = \omega \mathrm{v}_i^k + c_1 r_{1i}(\mathbf{p_i} - \mathrm{x}_i^k) + c_2 r_{2i}(\mathbf{p_g} - \mathrm{x}_i^k) \tag{18}$$

$$\mathrm{x}_i^{k+1} = \mathrm{x}_i^k + \mathrm{v}_i^{k+1} \tag{19}$$

where
$i = 1, 2, ..., P$
x_i is i-th vector of individual parameters
$\mathrm{v}_i = 0$, for $k = 0$
r_{1i} e r_{2i} are random numbers between 0 and 1
$\mathbf{p_i}$ is the best value found for the vector x_i
$\mathbf{p_g}$ is the best value found for the entire population
$0 < \omega < 1$ inertial constant
$1 < c_1, c_2 < 2$ constants

In Eq. (18), the second term on the right hand side represents the individuality and the third term the sociability. The first term on the right-hand side represents the inertia of the particles and, in general, must be decreased as the iterative process runs. In this equation, the vector $\mathbf{p_i}$ represents the best value ever found for the ith component vector of parameters x_i during the iterative process. Thus, the individuality term involves the comparison between the current value of the i-th individual x_i with its best value in the past. The vector pg is the best value ever found for the entire population of parameters (not only the i-th individual). Thus the sociability term compares x_i with the best value of the entire population in the past.

Figure 2 shows the iterative procedure for the Particle Swarm Method.

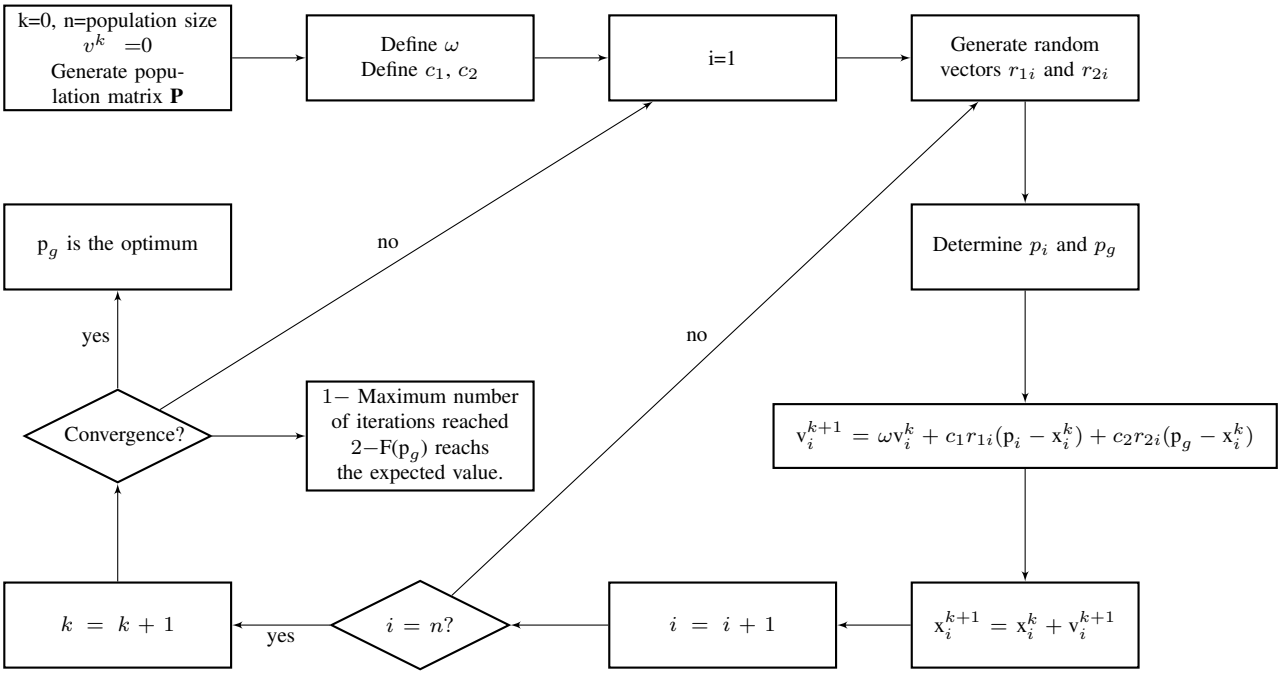

Figure 2. Iterative procedure for the Particle Swarm Method, (Colaço *et al.*, 2006).

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6. Optimization procedure and results

The optimization procedure for the parameter ΔT consists of minimizing the difference between the position of the solidification front obtained by the analytical solution and the Neumann numerical solution proposal.

Eq. (20) presents the analytical solution for the position of the solidification front, while Eq. (21) defines the objective function for the optimization problem.

$$\mathrm{S(t)_{analical}} = 2\lambda\sqrt{(\alpha_{sol}\mathrm{t})} \tag{20}$$

The objective function, Eq. (21), is proposed based on the sum of the square differences between the analytical and numerical solutions.

$$\overline{\mathrm{F}} = \sum_{1}^{n}[\mathrm{S(t)_{analitycal}} - \mathrm{S(t)_{numerical}}]^2 \tag{21}$$

where n is the number of points along of the time.

The position of the solidification front was chosen because it depends only on the magnitude of time in constant to the temperature profile which depends on time and space. This feature facilitates the numerical implementation. The evaluation time is truncated to 70% of the total estimated time for solidification.

Random values between 1K and 10K are generated for the parameter ΔT, corresponding to the initial state of each particle. Populations were evaluated with 10, 30 and 50 particles.

Table 1 presents the optimal values obtained for ΔT, for three different amounts of particles. The number of individuals in the population is indicated in parentheses on the first column of the table. With 50 particles, as expected, the method minimized the objective function with the a minimum number os iterations, i.e., 121 iterations, but the computational time spent was the highest. This observation is confirmed by the analysis of Fig. 3, where the objective function is minimized over for this case.

Table 1. Effects of the number of particles on the optimal solution

Number of Particles	CPU(s)time	ΔT (K)	Objective Function	Iterations
$\mathrm{PSO}_{(10)}$	10705.52	3.55996119	0.13403172	168
$\mathrm{PSO}_{(30)}$	37277.47	3.55993432	0.13403156	195
$\mathrm{PSO}_{(50)}$	38629.23	3.55448620	0.13403026	121

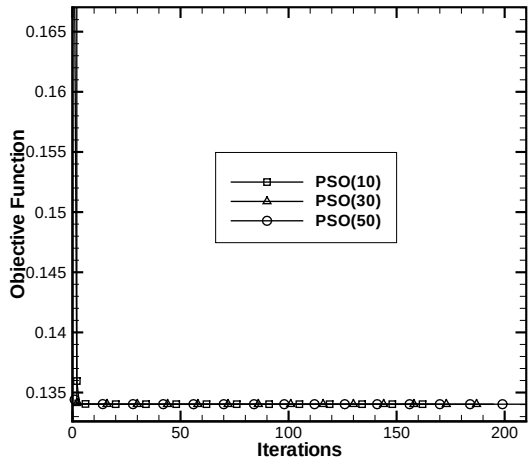

Figure 3. Evolution of the objective function for several iterations (10, 30 and 50 particles)

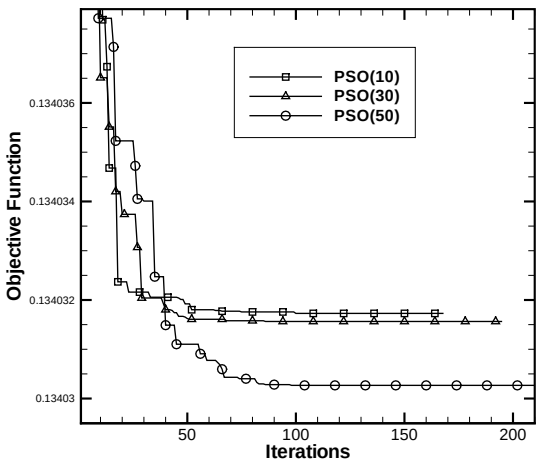

Figure 4. Micro Evolution of the objective function

ISSN 2176-5480

Table 2 shows the results for the solidification front at three different times. It is noted that for the evaluation of the position of the solidification front, the ΔT obtained with the $PSO_{(10)}$ provides satisfactory results. Therefore, the $PSO_{(10)}$ can be used in future studies aimed at evaluating the solidification front.

Table 2. Deviations between $S_{analytical}$ and $S_{numerical}$ with optimal ΔT

Number of particles	time(s)	Numerical	Analytical	Relative error (%)
$PSO_{(10)}$	87340	0.107297	0.108114	0.755026
	436730	0.242574	0.241785	0.337337
	611420	0.290639	0.286052	1.603686
$PSO_{(30)}$	87340	0.107297	0.108114	0.755080
	436730	0.242574	0.241785	0.337328
	611420	0.290639	0.286052	1.603664
$PSO_{(50)}$	87340	0.107298	0.108114	0.754284
	436730	0.242577	0.241785	0.338563
	611420	0.290634	0.286052	1.601887

The curves shown in Figs. 5 and 6 refer to the $PSO_{(10)}$. Figure 5 shows the evolution of the position of the solidification front along time until 70% of the total time of solidification.

Figure 6 displays a comparison among numerical and analytical temperature profiles for select times as a function os axid position, as function of time. It is observed that for the temperature field, the results for the mushy zone show a deviation from the analytical solution used for comparison does not have this region.

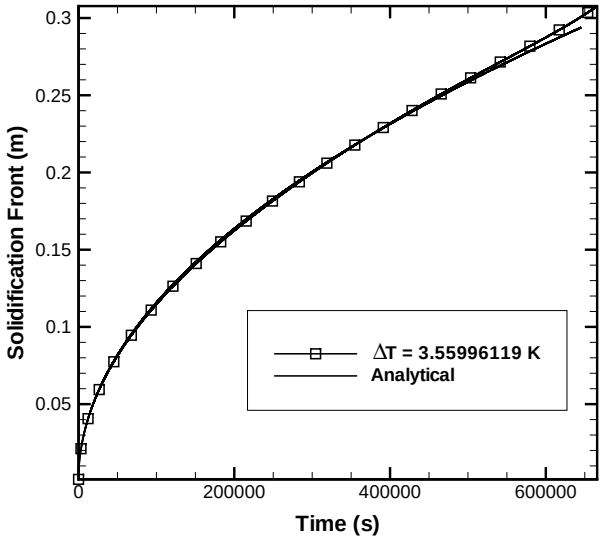

Figure 5. Evolution of the solidification front obtained with the ΔT optimal

ISSN 2176-5480

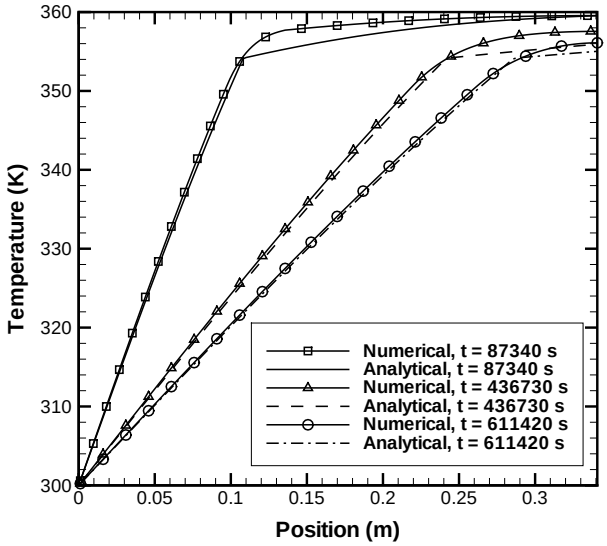

Figure 6. Temperature profile obtained with the ΔT optimal

7. CONCLUSIONS

The present work has determined the mushy zone parameter used in the effective heat capacity method by using an optimization procedure based on the particle swarm algorithm. In this optimization, the differences between the numerical solution and the reference analytical solution were minimized.

The results have shown that the optimum mushy zone parameter employed in the effective heat capacity method furnished a numerical solution with negligible discrepancies in relation to the analytical solution of the solidification front. Moreover, the almost linear temperature field in the solid zone was well represented by the numerical solution. However, divergences between the analytical and the numerical solutions were observed in the mushy zone and in the liquid zone.

The particle swarm performance was evaluated in relation to the numbers of the particles in the population. Populations with 10, 30 and 50 particles were compared and the results showed that, for the proposed problem and considering the populations studied, the numbers of the particles did not change significantly the temperature field and the minimum value of the objective function.

8. ACKNOWLEDGEMENTS

The authors would like to thank the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) for the financial support for this work.

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