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Résolution du problème de Stefan avec une méthode numérique sans maillage

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DEDICATION

This master degree dissertation is dedicated to every lover of knowledge and science who came before us and to those who will review our work after us,

To Palestine and all the martyrs of Al-Aqsa and the neighbourhood of Sheikh Jarrah

ملخّص

الهدف الرئيسي من هذه الدراسة هو استعمال أداة تعتمد على طريقة العناصر المنفصلة (DEM) وهي طريقة عددية غير متشابكة لحل مشكلة ستيفان. بعد الكشف عن محدودية ومشاكل هذه طريقة العناصر المنفصلة DEM الاصلية ، تم ربط الطريقة بتقنية المحتوى الحراري المعدلة وأثبتت أنها فعالة ودقيقة للغاية.

الكلمات الدالة: مشكلة ستيفان ، طريقة العناصر المنفصلة ، المحتوى الحراري ، تغير الطور

Résumé

L'objectif principal de cette étude est l’utilisation d'un outil basé sur la méthode des éléments discrets (DEM qui est une méthode numérique sans maillage) pour résoudre le problème de Stefan. Après avoir exposé les limites et les problèmes liés au DEM simple, la méthode a été couplée à une technique d'enthalpie modifiée qui s'est avérée très efficace et précise.

Mots clés : Problème de Stefan, Méthode des éléments discrets, Enthalpie, changement de phase

Abstract

The main objective of this study is the usage of a tool based on the Discrete Elements Method (DEM which is a meshless numerical method) to solve Stefan's problem. After exposing the limitations and the problems related to the simple DEM, the method was coupled with a modified enthalpy technique and proved to be very efficient and accurate.

Keywords: Stefan problem, Discrete elements method, Enthalpy, phase change

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LIST OF SYMBOLS

a_i	Thermal diffusivity	$[m^2/s]$
Bi	Number of Biot	
C_p	The specific heat of the particle	$[J/kg \cdot °C]$
D	Diameter	[m]
E_{ij}	The effective Young's modulus	
W	Interpolation function (smoothing function)	
ρ	the density	$[kg/m^3]$
Q_{ij}	The amount of heat	[J]
$r_{c,ij}$	The radius of the (circular) contact area between particles i and j.	[m]
i, j	Particle indices	
k	The thermal conductivity;	[W/m.K]
Λ_{ij}	The conductance between particles i and j	[W/m^2.K]
H	The Enthalpy	[J]
m_p	The mass of the particle;	[Kg]
C	real constant	
$\beta, \aleph$	constants	
λ	specific heat capacity	[J/Kg.K]
T_i, T_j	Particles temperature	[°C]
t	Time	[s]
$\frac{dT_i}{dt}$	The time derivative of the temperature	

GENERAL INTRODUCTION

INTRODUCTION

When a physical body which is at one single state: solid or liquid is subjected to a boundary condition above (or below) its melting temperature it changes its state. The change of state does not take place instantaneously on the entire body, but evolve gradually. The problem of tracking the time-dependent evolution of the solid fluid interface in the thermal phase change process is called Stefan's problem.

For few very simple theoretical cases the Stefan problem admits an analytical solution. For the remaining more realistic situations only numerical methods can be used.

This study is the continuation of the project initiated last year dealing with thermal problems by the meshless numerical method known as Discrete Elements Method (DEM).

The main objective of this study is to contribute to the development of a numerical modeling tool based on the Discrete Elements Method (initiated last year) augmented by the Enthalpy one to study the phase change problem of a pure material. The calculation tool developed by programming on Matlab is based on the adaptation of the DEM, which is a meshless numerical method, by the introduction of the Enthalpy technique. The adaptation is inspired from previous works using the Finite Differences Method also augmented by the Enthalpy technique.

Our study is organized in four chapters, in addition to a general introduction and conclusion. The 1st chapter is a Literature Review that situates the general context of the study, and the 2nd one presents the mathematical formulation of the Stefan problem. In the same chapter, the analytical solution which will be used for the validation thereafter is also given.

The 3rd chapter is devoted to the Enthalpy technique coupled with of Finite Differences Method. The novelty of the study comes in the last chapter the 4th.

In this chapter the DEM is first introduced, then its inability to deal with Stefan's problem without modification is shown. The modification of this meshless method is inspired from chapter 3 and allowed us to obtain results in agreement with those obtained analytically.

We conclude our work with a general conclusion that summarizes the main results and gives some perspectives for any future work in continuation of ours.

CHAPTER I
LITERATURE REVIEW

CHAPTER I : LITERATURE REVIEW

I.1. The problem definition of

A Stefan problem is a special kind of limit value problem for a partial differential equation with respect to the heat distribution in a phase changing medium. Since the scalable interface is unknown a priori, part of the solution is to determine the boundary. An example is heat diffusion during ice melting and when melting occurs the position of the ice boundary changes. The problem is referred to by some authors as the " free boundary value problem " because the limit of the domain is a priori unknown. **[1] [2] [3]**

In order to distinguish the case of a moving boundary (associated with a time-dependent problem) from the problem of the stationary boundary, some authors refer to the latter as "moving boundary problem". **[4]**

I.2. Historical notes

“The first known paper about diffusion of heat in a medium with a change of phase state was published by the French mathematicians Gabriel Lamé and Benoît Paul Émile Clapeyron in 1831”. **[5]**

The problem was to cool a liquid that fills the half-space $x > 0$ and to determine the thickness of the solid crust, with a constant boundary condition at $x = 0$. They found that the thickness of the crust is proportional to the square root of the hour, but no determination of the coefficient of proportionally was attached.

Almost 60 years later, in 1889, this question was taken up and asked more generally by the Austrian physicist and mathematician Joseph Stefan.**[6]**

Josef Stefan was born on March 24, 1835 in St. Peter near Klagenfurt in Austria and died a century ago on January 7, 1893. In 1853 he enrolled at the University of Vienna. Stefan became professor for higher mathematics and physics at his university in 1863, and three years later he was appointed director of the Institute for Experimental Physics founded by Doppler in 1850. Stefan was a brilliant experimenter and a valued teacher.

Stefan's most important work deals with thermal radiation (1879). He discovered that thermal radiation is proportional to the fourth power of absolute temperature. The theoretical

deduction for this relationship was given by Boltzmann in 1884 and resulted in what is now known as the Stefan-Boltzmann radiation law.

"Stefan published further experimental and theoretical works on the kinetic theory of heat: on heat conduction in fluids, on diffusion in fluids, on ice formation, and on evaporation. In these papers Stefan describes mathematical models for physical problems, containing an interface of which the position changes in time. Since Stefan gives the first detailed study of this type of problems, free or moving boundary problems are called Stefan problems. We note that the paper on ice formation in the polar seas is reprinted. Of the four papers published in 1889, this publication has drawn the most attention, as for the origin of the Stefan problem we note that a similar problem is already given. They determined the thickness of a solid crust generated by the cooling of a liquid globe. Furthermore, the mathematical solution was found by F. Neumann about 1860 and is known as the Neumann solution see Weber, 1901. **[7]**

I.3. Numerical methods

In recent years, these problems have led to significant research on numerical resolution methods. A wide range of numerical methods applied to Stefan's problems have been described with selected references from Crank's extensive book. **[8]**

I.3.1.Classical methods

i. The Finite Differences Method (FDM)

The finite difference method (FDM) replaces the area over which the independent variables of the PDE are defined with a finite grid (also known as mesh) of points to which the dependent variable is approximated. The partial derivatives of the PDE at each point on the grid are approximated from the neighbouring values using Taylor's theorem.

Let U(x) have n continuous derivatives over the interval (a, b). Then for a < $x_0, x_0 + h$<b,

$$U(x_0+h)=U(x_0)+hU_x(x_0)+h^2\frac{U_{xx}(x_0)}{2!}+...+h^2\frac{U_{n-1}(x_0)}{(n-1)!}+O(h^n) \qquad (I.1)$$

Where,

- $U_x=\frac{dU}{dx},U_{xx}=\frac{d^2U}{dx^2},...,U_{(n-1)}=\frac{d^{n-1}U}{dx^{n-1}}.U_x=\frac{dU}{dx},U_{xx}=\frac{d^2U}{dx^2},\dots,U_{(n-1)}=\frac{d^{n-1}U}{dx^{n-1}}.$
- $U_x(x_0)U_x(x_0)$ is the derivative of U with respect to x evaluated at x=x_0.
- $O(h^n)\ O(h^n)$ is an unknown error term defined in Appendix A.

In FDM we know the U-values at the grid points and would like to replace the partial derivatives in the PDE that we solve with approximations at these grid points. We do this by interpreting (I.1) in a different way. In FDM, x_0 and $x_0 + h$ are grid points and U(x_0)and $U(x_0 + h)$ are known. This allows us to reorganize equation (I.1) to get what are known as finite difference (FD) approximations of derivatives that have the notation $O(h^n)$ **.[9]**

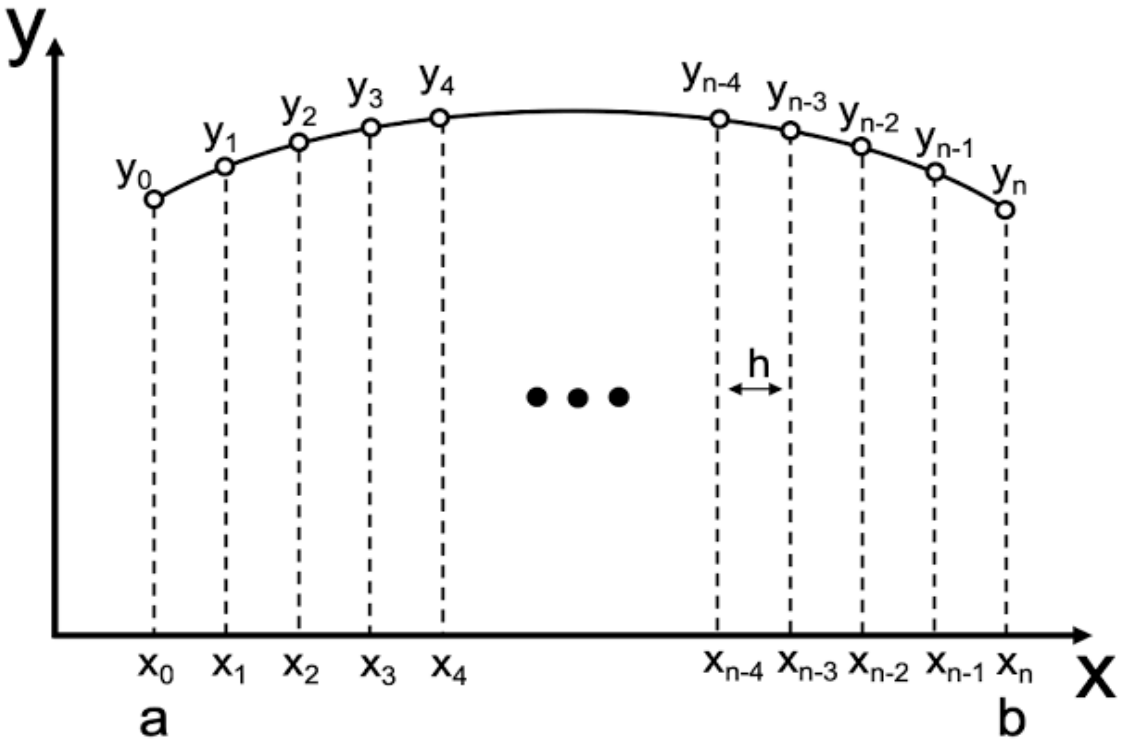

Figure I-1: simple example of FDM

ii. The Finite Volumes Method (FVM)

In the method of finite volume, some of the terms of the conservation equation are converted into area flows and evaluated on the areas with finite volume. The flow that enters a given volume is identical to the one that leaves the neighbouring volume. The FVM is strictly conservative. This inherent retention property of FVM makes it the preferred method for CFDs (computational fluid dynamics). Another important feature of FVM is that it can be formulated in physical space on unstructured polygonal meshes. After all, in FVM it is quite easy to implement a large number of boundary conditions non-invasively, since the unknown variables are evaluated at the gravity centres of the volume elements and not at their interfaces.

These properties have made the finite volume method very well suited for the numerical simulation of a wide variety of applications involving fluid flow and heat and mass transfer, and developments in the method have been closely linked to the advancement of CFD. From a limited potential that was originally limited to solving simple physics and geometry in structured lattices, the FVM is now able to handle all kinds of complex physics and applications. **[10]**

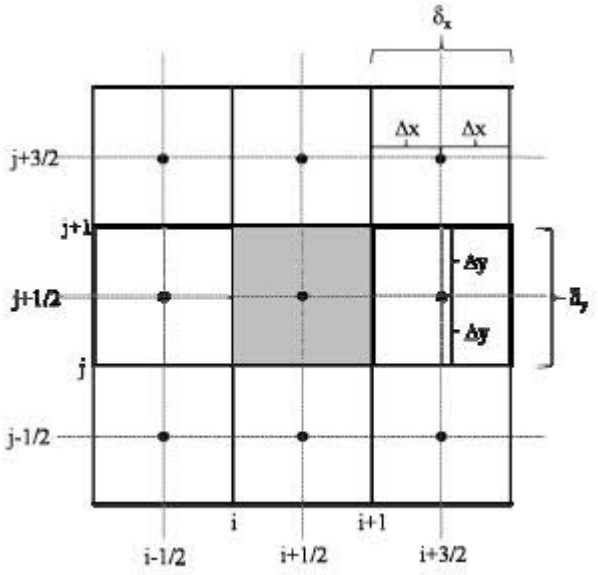

Figure I-2: Representation of the control volume.

iii. The Finite Elements Method (FEM)

The finite element approximation functions are determined as nodal values of a physical field of interest. A continuous physical problem is transformed into a discretized finite element problem with unknown node values. For a linear problem a system of linear algebraic equations has to be solved. Values within finite elements can be obtained using nodal values.

Two features of the GEF are noteworthy:

1) The piecewise approximation of physical fields on finite elements offers good precision even with simple approximation functions (by increasing the number of elements we can get any precision).

2) The locality of the approximation leads to sparse systems of equations for a discretized problem. This helps to solve problems with a very large number of unknown nodes. **[11]**

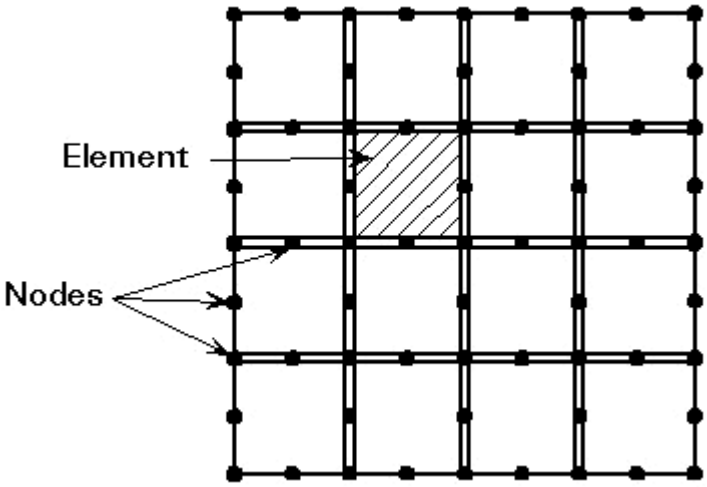

Figure I-3: Simple representation of FEM

I.3.2. Meshless methods

i. The Discrete Elements Method (DEM)

The discrete element method, initiated by P. Cundall and O. Strack **[12],** is one of the most powerful tools. DEM can simulate the movement of particles and the interaction between particles. Not only are the obvious geometric and material effects such as particle shape, non-linearity of the material, viscosity, friction, etc, considered, but various effects are also considered, the physical field of the environment or even the chemical reaction. **[13]**

The most fascinating and interesting mechanical problems are usually the hardest to solve. With today's computing capabilities, discrete problems can be solved even when a large number of components are involved. The numerical methods used to solve such problems are called discrete methods (DM).

In most cases, the problem should be broken down ad infinitum into infinitesimal components, resulting in local governance equations (usually differential) that involve infinite components. These problems are called "ongoing" problems. A continuous problem assumes that the material being examined is continuous and completely fills the space it occupies.

Because computer performance is limited, continuous problems can only be solved accurately using mathematical techniques, and mathematical techniques are generally limited to very simple situations. **[14]**

As an alternative to continuous methods (finite difference, volume and element), the discrete element method (DEM) was introduced in the 1970s, which is also known as the method for different elements and is booming today. The DEM offers the possibility to

numerically model the kinematic effects and dynamics of a large number of interacting particles. Today DEM is undoubtedly regarded as one of the numerical method tools in modelling many technical applications, such as:

• Granular flows,

• Powder mechanics,

• Rock mechanics,

• etc.

ii. The Smoothed Particle Hydrodynamic Method (SPH)

The reliability and stability of SPH simulations (as well as the stability of other numerical methods) can be compromised under certain circumstances by non-physical numerical fluctuations. This can be avoided by using additional digital stabilization terms (such as artificial viscosity, artificial loading, etc.). The SPH material models (the incompressible fluid model and the elastic solid model), which contain the stabilization terms, are implemented and applied to various test problems.

In the SPH formulation, the computation domain is discretized by a finite set of interpolation points (particles) with invariant coordinates in the material frame of reference. SPH particles represent a finite mass of the discretized continuum and contain information about all physical variables that are evaluated at their positions. Function values and their derivatives on a specific particle level are interpolated from function values on surrounding particles using the interpolation function (smoothing function) and its derivatives, respectively,

$$f_i = \sum_j \frac{m_j}{\rho_j} f_j W(|r_i - r_j|, h), \tag{I.2}$$

$$\nabla_i f_i = \sum_j \frac{m_j}{\rho_j} f_j \nabla_i W(|r_i - r_j|, h), \tag{I.3}$$

Where m is the mass, ρ is the density and W is the interpolation function (smoothing function) with a continuous derivative $\nabla_i W$ .The index i, j denotes the variables at the level of the particle i and j, respectively, and ∇_i denotes a derivative along r_i , which is the position vector.

The smoothing function W is defined in such a way that its value decreases monotonically with increasing distance between the particles. It has a compact support domain, the radius of which is defined by the smoothing length h. The smoothing function is normalized and in the borderline case the smoothing function becomes the Dirac delta function when the smoothing length goes to zero. **[15]**

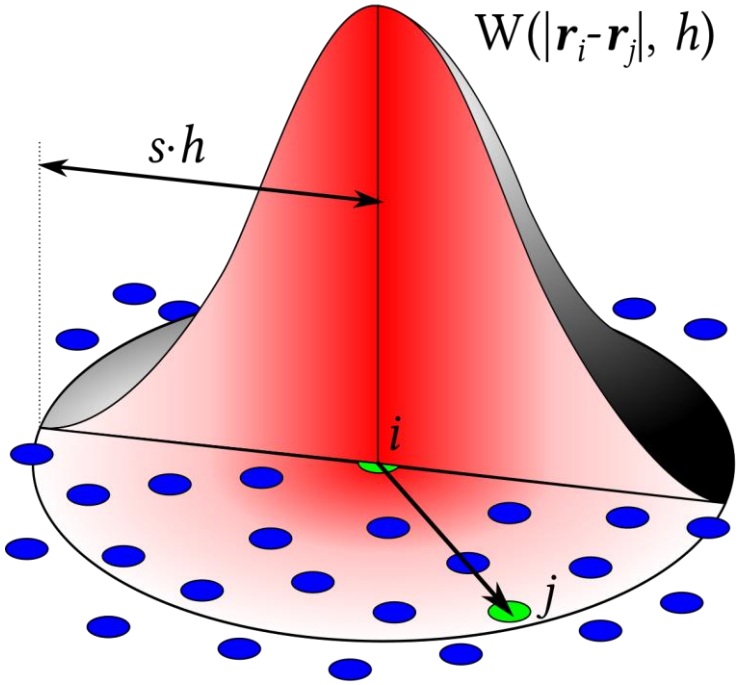

Figure I-4: SPH interpolation

CHAPTER II
MATHEMATICAL FORMULATION

CHAPTER II : MATHEMATICAL FORMULATION

In this chapter we will give the main aspects of the mathematical formulation behind the Stefan problem and its analytical as well as numerical solutions.

II.1. The hypotheses

To make the mathematical model sufficiently simple to be solved analytical we will make the following assumptions:

- The effects of natural convection in the liquid phase are neglected and the heat transfer is considered one-dimensional, i.e. the heat transfer occurs only in the direction normal to the surface
- It is assumed that the material has a defined melting point, which is to say that the phase change is isothermal
- It is assumed that the physical properties of the solid and fluid phases of the material are identical and constant over the entire temperature range, i.e. the volume change is neglected
- The chemical interactions in the liquid composition at the interface will be neglected.
- Constitutional supercooling will be neglected
- Since we are concentrating on solidifying a molten material with a cooling, the temperature gradients in the liquid will be positive, so that the latent heat generated at the interface dissipates through the solid. **[16]**

II.2. The transient heat equation in one homogeneous phase

The heat equation is an important partial differential equation (PDE) which describes the distribution of heat (or variation in temperature) in a given region over time.

The transient conduction problem can be treated in two ways: either by using the lumped capacity method by considering time as single independent variable, or by solving the partial differential equation directly which is in this case, a function of time and spatial coordinates. This second method is possible only for geometries of simple shapes (plates, cylinders, spheres, etc.). Taking the case of an infinite block, without internal heat sources ($Q \rightarrow 0$) and

where the temperature is uniform over two directions (y and z). So, the problem is one-dimensional (distribution along x only) and transient ($\partial / \partial t \neq 0$). **[17]**

In this case, the energy (heat) equation can be given by:

$$\frac{\partial T}{\partial t} = \frac{k}{\rho C}\frac{\partial^2 T}{\partial x^2} \tag{II.1}$$

By expressing the coefficient of thermal diffusivity by α = (k / ρ.C), equation (II.1) can be rewritten as the following form:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{II.2}$$

Assuming that the infinite block of thickness (2e) is initially at uniform temperature (T_i). At t = 0, the surfaces suddenly cool down to $T = T_1$.Introducing the variable: θ = T-T_1Equation (II.2) becomes:

$$\frac{\partial \theta}{\partial t} = \alpha \frac{\partial^2 \theta}{\partial x^2} \tag{II.3}$$

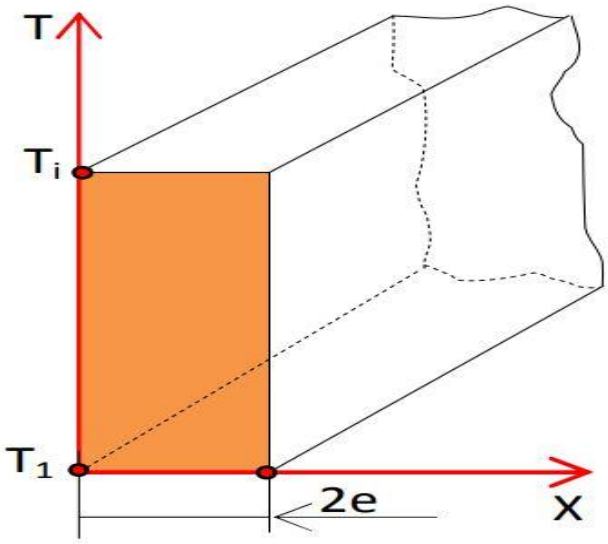

Figure II-1: Infinite plate

II.3. Equation classification (Parabolic)

II.3.1.Physical origin:

Parabolic equations govern "evolution" or "unsteady" problems involving the "diffusion" or "dissipation" mechanism. These problems are generally defined on a bounded spatial domain border on which the unknown is subject to boundary conditions of the same type as in elliptical (sometimes, however, themselves unsteady), The one-dimensional thermal conduction in transient state is governed by the equation parabolic and the following boundary and initial conditions:

A classic example is that of the calculation of the temperature T (x; t) during the time (t ≥0) in a homogeneous cylindrical bar, of constant section (0≤ x≤ a). The initial temperature of the bar is known:

$$T(x,0) = \theta_0(x) \qquad (0 \le x \le \alpha)\ T(x,0) = \theta_0(x) \qquad (0 \le x \le a)$$

Where θ_0(x) is not necessarily a continuous function. Moreover, from now on initial, one imposes conditions on the two ends of the bar; these can be for example Dirichlet conditions:

$$\forall t > 0:\ T(0,t) = T_0, T(a,t) = T1\ T(0,t) = T_0, T(\alpha,t) = T_1$$

The energy balance of the slice of bar located between the abscissas x and x + dx is expressed as follows: the internal energy variation (of the unit) is equal to the flux heat received (per unit of time):

$$\rho \delta x C \frac{\partial T}{\partial t} = q(x) - q(x + dx)$$

Fundamental models of mechanics:

(ρ : linear mass; C: specific heat capacity). Furthermore, the heat flow is expressed by Fourier's law:

$$q(x) = -k \frac{\partial T}{\partial x}$$

(k: thermal conductivity).

$$T_t = \alpha T_{xx}$$

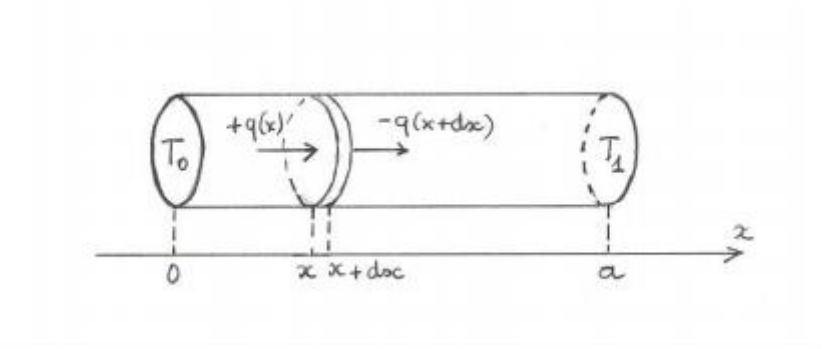

Figure II-2: Temperature problem in a homogeneous cylindrical bar

Where $\alpha = k/(\rho C) \succ 0$

II.3.2.Standard equation:

$$aU_{xx} + bU_{xy} + cY_{yy} + dU_x + eU_y + fU = g \qquad \text{(II.4)}$$

We consider equation (II.4), assuming here that we have:

$$b^2 - 4ac = 0$$

The equation

$$a\aleph^2 - b^2 + c = 0$$

Admits the double root b = (2a). By introducing the change of variables defined by

$$\begin{cases} e = y - \dfrac{b}{2a}x \\ n = y - \aleph x \\ \upsilon = ue^{-\alpha e \beta n} \end{cases}$$

(Where $\propto, \beta$ and $\aleph$ are suitably chosen real constants), the equation takes the form [**18**]:

$$\upsilon_e - \upsilon_{nn} + C\upsilon = h(e,n)\; v_e - v_{nn} + Cv = h(e,n)$$

II.4. Analytical solution in one dimension

On the surface of separation between the liquid and solid phase (it is the solid-liquid interface) marked by X (τ), the condition will be satisfied:

$$T_1 = T_2 = T_m \quad when \quad x = X(\tau) \tag{II.5}$$

When the interface moves a distance of dX, a quantity of heat L.ρ.dX per unit area is released, and will be carried by condition.

That implies:

$$k_1 \frac{\partial T_1}{\partial x} - k_2 \frac{\partial T_2}{\partial x} = L.\rho.\frac{dX}{d\tau} \tag{II.6}$$

temperatures T1 and T2 in solid and liquid regions must satisfy:

$$\frac{\partial^2 T_1}{\partial x^2} - \frac{1}{\alpha}\frac{\partial T_1}{\partial \tau} = 0 \tag{II.7}$$

$$\frac{\partial^2 T_2}{\partial x^2} - \frac{1}{\alpha}\frac{\partial T_2}{\partial \tau} = 0 \tag{II.8}$$

In addition to (II.5) (II.6) (II.7) and (II.8), there must be other fixed boundary conditions, which presents possible cases.

We will consider the following case:

Solidification of a molten material, initially at temperature T_0 with the surface $x = 0$ maintained at a temperature $T_{x=0}$ for all $\tau > 0$, and for a semi-infinite geometry (i.e. when $x \to \infty$) therefore:

$$T_2 \to T_0 \quad when \quad x \to \infty \tag{II.9}$$

$$T_1 = T_{x=0} \quad when \quad x = 0 \tag{II.10}$$

For an expression of the form:

$$\frac{\partial^2 U_1}{\partial x^2} - \frac{1}{\alpha}\frac{\partial U}{\partial \tau} = 0 \tag{**}$$

We have the particular solution:

$$U = \tau^{\frac{1}{2}} e^{-x^2/4\alpha\tau}$$

It has the following properties:

$$U \to 0 \quad \text{when } \tau \to 0 \text{ for } x \neq 0$$

$$U \to \infty \quad \text{when } \tau \to 0 \text{ if } x = 0$$

$$\int_{-\infty}^{\infty} U dx = 2(\pi\alpha)^{\frac{1}{2}}, \text{ for all } \tau \succ 0$$

It follows that $\int_0^x \tau^{\frac{1}{2}} e^{-x^2/4\alpha\tau} dx = 2\alpha^{\frac{1}{2}} \int_0^{x/2(\alpha\tau)^{\frac{1}{2}}} e^{-\xi^2} d\xi$ also satisfies the preceding differential equation (**).

II.4.1.The Error function $erf(x)$

The error function is defined as: $erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\xi^2} d\xi$. We will then have $A\,erf \frac{x}{2(\alpha\tau)^{\frac{1}{2}}}$ as a solution of the differential equation (**), where A is an arbitrary constant determined by the condition and initials.

The function is the complementary function of the function and: $\text{erfc}(x) = 1 - \text{erf}(x)$

So:

$$T_1 = A.erf \frac{x}{2(\alpha_1\tau)^{\frac{1}{2}}} \tag{II.11}$$

We will determine A by (II.7) and (II.10) and:

$$T_2 = T_0 - B.erfc \frac{x}{2(\alpha_2\tau)^{\frac{1}{2}}} \tag{II.12}$$

With B satisfying (II.8) and (II.9), then (2-10) implies:

$$A.erf \frac{x}{2(\alpha_1\tau)^{\frac{1}{2}}} = T_0 - B.erfc \frac{x}{2(\alpha_2\tau)^{\frac{1}{2}}} = T_m \tag{II.13}$$

The expression (II.13) must satisfy all the values of time, and therefore X must be proportional to $\tau^{\frac{1}{2}}$, this gives:

$$X = 2\lambda\left(\alpha_1\tau\right)^{\frac{1}{2}} \tag{II.14}$$

Where λ is a constant determined by condition (II.6). Using (II.11), (II.12), and (II.14) this will give:

$$k_1 A e^{-\lambda^2} - k_2 B\left(\frac{\alpha_1}{\alpha_2}\right)^{\frac{1}{2}} e^{\frac{\alpha_1\lambda^2}{\alpha_2}} = \lambda.L.\alpha_1.\rho.\pi^{\frac{1}{2}} \tag{II.15}$$

Or by using (II.13) and (II.14)

$$\frac{e^{-\lambda^2}}{erf\,\lambda} - \frac{k_2\sqrt{\alpha_1}\left(T_0 - T_m\right)e^{-\alpha_1\lambda^2/\alpha_2}}{k_1\sqrt{\alpha_2}\left(T_m - T_s\right)erfc\lambda\sqrt{\left(\alpha_1/\alpha_2\right)}} = \frac{\lambda.L.\sqrt{\pi}}{c_1.\left(T_m - T_s\right)} \tag{II.16}$$

After finding λ of (2-21), and can be written according to (II.11), (II.12), (II.13), and (II.14):

$$T_1 = \frac{\left(T_m - T_s\right)}{erf\,\lambda}.erf\left(\frac{x}{2\left(\alpha_1\tau\right)^{\frac{1}{2}}}\right) + T_s \tag{II.17}$$

$$T_2 = T_0 - \frac{\left(T_0 - T_m\right)}{erfc\left[\lambda\left(\alpha_1/\alpha_2\right)^{\frac{1}{2}}\right]}erfc\left(\frac{x}{2\sqrt{\left(\alpha_2\tau\right)}}\right) \tag{II.18}$$

The interface between the solid and the liquid phases position is given analytically by equation (II.14) but it needs the value of λ that has to be calculated numerically by solving equation (II.16).

A typical problem that is widely cited in the literature [25] is used to the validation part, then the demonstrate the different numerical methods studied in this work. The different parameters of the model are presented table III.1.

II.4.2. Results obtained by the non-modified Enthalpy Method

The enthalpy method is applied to the problem above. We can notice on Figure III 3 that the numerical solution oscillates around the analytical one. By increasing the space samples

(decreasing the space steps) the gap between the two curve decreases but the number of oscillations does the opposite. The solution at the middle node is represented in Figure II-3.

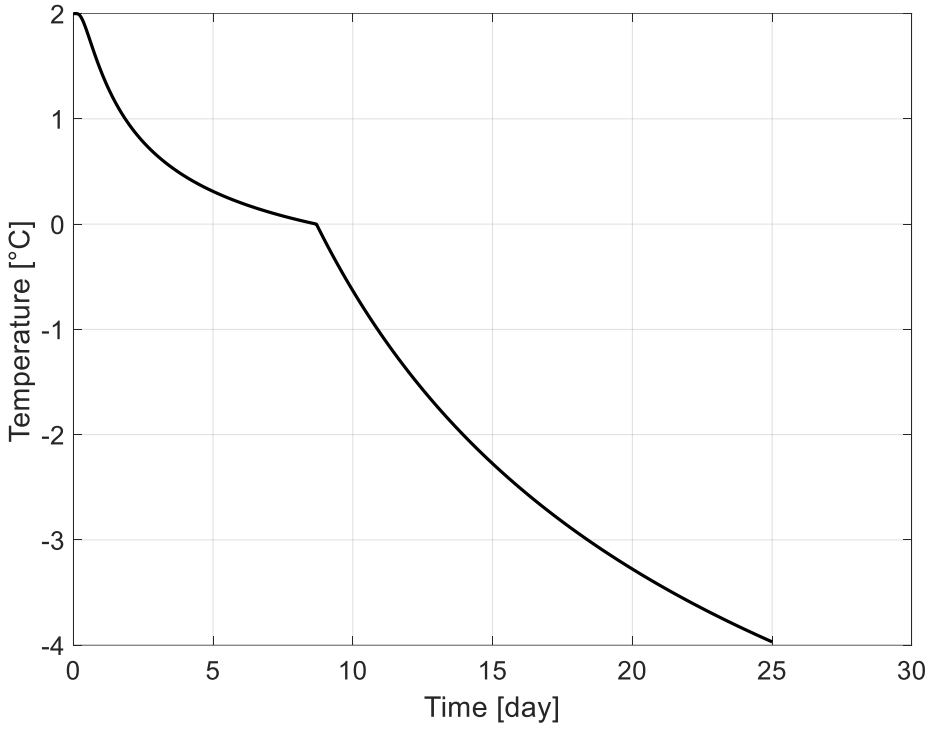

Figure II-3: Analytical temperature evolution at position x=0.5m

II.5. The enthalpy method

Numerical methods are often used to find solutions when it is difficult to find analytical ones because of the changing boundary conditions due to the moving boundaries.

The general method is the enthalpy method that introduces the enthalpy function. The flow state is automatically filled across the phase front, which is realized as a discontinuity in the enthalpy transition. There are many ways to track boundaries using the enthalpy method. Some researchers use a continuous tracing method that can only be applied to planar geometry or does not take geometry into consideration. Caldwell and Chan **[21]** also applied the enthalpy formula to Stephan's problem with cylindrical shape and obtained results that were in good agreement with the results obtained from other numerical methods. In **[22]** the author has developed an enthalpy method that makes it easy to track phase change. He applied this method to one-dimensional and two-dimensional problems in plane geometry.

Enthalpy method is one of the most common fixed-domain methods for solving the Stefan problem. The main advantage is that this method does not require explicit processing of the moving boundary. To enter the expression, we define the enthalpy function h as a function of temperature T. **[23]**

CHAPTER III
CLASSICAL NUMERICAL APPROACH

CHAPTER III : CLASSICAL NUMERICAL APPROACH

This chapter deals with the classical Finite Differences Method which is a cartesian mesh based numerical method. The objective of this chapter is to present the model from which we will inspire the Enthalpy technique and its algorithm modification integration. The same integration used in the literature on the Finite Differences Method will be adapted to the Discrete Elements one.

III.1. Finite differences method applied to 1D model of a pure medium

Most real mathematical problems do not have analytical solutions. However, they do have the real answers for each of the problems. To obtain these solutions we can use other methods such as graphical representations or numerical analysis. Numerical analysis is the mathematic method that also considers the accuracy of an approximation. The solution in partial differential equations arising in scientific and engineering problems is very important to conclude the study of a physical situation. In case of analytic solution of partial differential equation also, numerical values at different intervals of variables are required. Therefore, numerical solution of a problem is very useful and important.

In this study, we will use numerical analytical to solve the parabolic partial differential equations. Heat equation, diffusion problems are examples of parabolic equations. There are two methods in solving these problems which are explicit method and implicit method.

III.1.1.Explicit method:

Let the one-dimensional thermal conduction equation (for each phase)

$$\frac{\partial T_i}{\partial t} = \alpha_i \frac{\partial^2 T_i}{\partial x^2}$$

α_i : Thermal diffusivity

The derivatives which appear there are approximated by the derivatives with the finite differences

$$\frac{\partial T}{\partial t} = \frac{T_i^{k+1} - T_i^{k}}{\Delta t}$$

$$\frac{\partial T}{\partial x} = \frac{T_{i+1}^{k} - T_{i}^{k}}{\Delta x}$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\Delta x}\left(\frac{T_{i+1}^{k} - T_{i}^{k}}{\Delta x} - \frac{T_{i}^{k} - T_{i-1}^{k}}{\Delta x}\right) = \frac{T_{i+1}^{k} - 2T_{i}^{k} + T_{i-1}^{k}}{(\Delta x)^2}$$

The finite deference equation is then of the form:

$$\frac{T_{i}^{k+1} - T_{i}^{k}}{\Delta t} = \alpha \frac{T_{i+1}^{k} - 2T_{i}^{k} + T_{i-1}^{k}}{(\Delta x)^2}$$

And let $\lambda = \frac{\alpha \Delta t}{\Delta x^2}$

$$T_{i}^{k+1} - T_{i}^{k} = \lambda\left(T_{i+1}^{k} - 2T_{i}^{k} + T_{i-1}^{k}\right)$$

Or

$$T_{i}^{k+1} = \lambda T_{i+1}^{k} + (1 - 2\lambda)T_{i}^{k} + \lambda T_{i-1}^{k} \qquad \text{(III.1)}$$

To solve this equation, the temperature is calculated only for isolated points i = 1, 2, 3 …n, resting on the x-axis. We suppose then that at any moment the distribution of temperature in the interval between neighbouring points is linear. These points are usually called nodes of the spatial network.

The expression (III.1) must be considered as a system of algebraic equations of which the number n is equal to that of the unknown temperatures.

The indices k and k + 1 define the instant to which the temperature value corresponds.

T^{k} : the value of the temperature at a certain instant t

T^{k+1}: the value of the temperature at the instant t + Δt

Each of the finite difference equations contains a single temperature unknown T_i^{k+1}. This temperature appears in the node, after the flow of the small-time interval Δt.

We suppose then that the initial temperature in each node is $T_i^{\,k}$, for the calculation of the unknown temperature $T_i^{\,k+1}$, the system composed of n algebraic equations of the type (III.1) is resolved successively for each step-in time. The equation must then be solved as many times as there are steps in the calculation time interval.

When taking the first step in time, the system (III.1) is solved for the first time from the values of the initial temperatures which are taken from the initials conditions. In successive resolutions, the values of $T_i^{\,k}$ are taken from the previous time slice.

III.1.2.Implicit method:

To improve the precision of the resolution one must choose Δx small enough. The heat equation is then solved by resorting to finite difference equations implicit in the form:

$$\left(\frac{\partial T}{\partial t}\right)_i^{k+1} = \frac{T_i^{k+1} - T_i^k}{\Delta t}$$

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_i^{k+1} = \frac{T_{i+1}^k - 2T_i^k + T_{i-1}^k}{(\Delta x)^2}$$

By setting , $\lambda = \frac{\alpha \Delta t}{\Delta x^2}$ .the temperature at iteration n + 1 is given by:

$$T_i^k = (1+2\lambda)T_i^{k+1} - \lambda\left(T_{i+1}^{k+1} + T_{i-1}^{k+1}\right) \qquad \text{(III.2)}$$

We say that the systems (III.2) use the differences in time respectively in forward and backward (with respect to the instant t for which the differences are composed spatial).

The explicit and implicit finite difference schemes can be combined:

$$\frac{T_i^{\,k+1} - T_i^{\,k}}{\Delta t} = \alpha\left[\frac{T_{i+1}^{\,k+1} - 2T_i^{\,k+1} + T_{i-1}^{\,k+1}}{(\Delta x)^2}\sigma + (1-\sigma)\frac{T_{i+1}^{\,k} - 2T_i^{\,k} + T_{i-1}^{\,k}}{(\Delta x)^2}\right]$$

Then for σ = 0 we obtain a system of explicit finite difference equations; and for σ = 1 a system of implicit equations. **[24]**

III.1.3.Implementation of the Enthalpy method:

The Stephan's problem class that has analytic solutions is small. Numerical schemes on the basis of equation (II.2) require the phase change boundary, x = X (t), to be traced precisely. This necessity makes a large part of available digital graphs difficult to implement.

One way to get around this problem is to reformulate the equation as a function of enthalpy H, and latent heat. In this case, the Stefan equations reduce to a single equation

$$\rho \frac{\partial H}{\partial t} = k \frac{\partial^2 T}{\partial x^2}, \tag{III.3}$$

Where the conductivity k and density ρ are functions of the temperature and the temperature is related to the enthalpy via

$$T = \begin{cases} H/c & , H \le cT_m \\ T_m & , cT_m \le H \le cT_m + L \\ (H-L)/c & , H \ge cT_m + L \end{cases} \tag{III.4}$$

And it can be written

$$H(T) = \begin{cases} cT & T < T_m \\ cT + L & T > T_m \end{cases} \tag{III.5}$$

The advantages of this approach are:

(1) There are no conditions to be satisfied at x = X (t), the phase change boundary;

(2) It is not necessary to strictly follow the phase change boundary;

(3) It is not necessary to consider the areas on either side of x = X (t) separately, and

(4) It is easy to get into a “mushy” region, i.e. where the phase change occurs across a range of temperatures rather than a single point.

The representation of enthalpy formulation of the finite difference (explicit method) is given

$$H_i^{j+1} = H_i^j + \frac{k}{\rho}\eta\left(T_{i+1}^j - 2T_i^j + T_{i-1}^j\right) \tag{III.6}$$

Which when combined with equation (III.4) provides an algorithm to calculate the temperature history of a one-dimensional region. Further, the condition needed to ensure convergence is simply [25]:

$$\eta = \frac{\delta\tau}{\delta x^{2}} < \frac{\rho c}{2k}$$

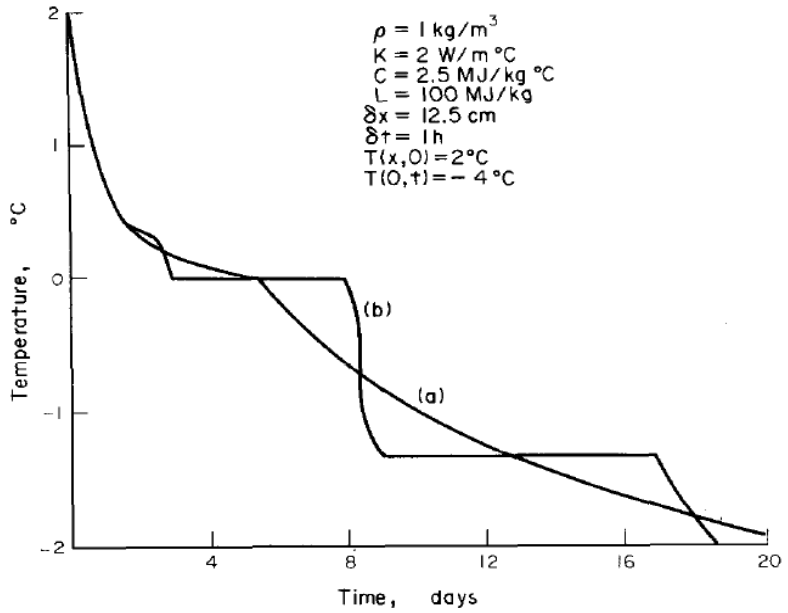

Figure III-1: Comparison of analytic [curve (a)] and enthalpy [curve (b)] solutions for the temperature history at z=25cm. [25]

III.2. Stability of the numerical schemes (explicit et implicit)

III.2.1.Stability of the system of explicit finite difference equations

For the resolution of a system of finite difference equations, the correct choice of Δt and Δx is decisive. Figure (III.2) visualizes the results of exact and numerical resolution of the problem of non-stationary thermal conduction for a plane wall divided between four-time intervals.

The comparison shows that the calculations with: $a\frac{\Delta t}{(\Delta x)^{2}} = \frac{1}{2}$ provide results perfectly satisfactory, while with $\lambda \succ \frac{1}{2}$ appears the phenomenon of instability.

By solving equation (III.1) in an explicit form with respect to the function unknown T_i^{k+1}, we get:

$$T_i^{k+1} = AT_{i+1}^k + BT_i^k + CT_{i-1}^k \quad \text{(III.7)}$$

Where $A = C = \lambda$ and $B = 1 - 2\lambda$. Moreover A + B + C = 1

To simplify the reasoning, let us admit that T> 0. In the general case, among the known values T_i^{k+1} .T_{i+1}^k andT_{i-1}^k there is a maximum value and a minimum value.

If we advance the hypothesis that T_{i+1}^k is the maximum value and T_{i-1}^k the value minimal, then by virtue of the fact that:

$$T_i^{k+1} = T_{i+1}^k - B\left(T_{i+1}^k - T_i^k\right) - C\left(T_{i+1}^k - T_{i+1}^{k-1}\right)$$

and

$$T_i^k = T_{i-1}^k + A\left(T_{i+1}^k - T_{i-1}^k\right) + B\left(T_i^k - T_{i-1}^k\right)$$

for positive A, B and C the value of the temperature T_{i+1}^k to be calculated by the resolution satisfies the inequality

$T_{i+1}^k > T_i^{k+1} > T_{i-1}^k$, and by suite is bounded in advance, from physical considerations, A and C cannot be less than zero; therefore, to exclude the infinite growth of T_i^{k+1} during their solution, it is necessary, by choosing Δt, to fulfil the following stability condition to the system finite difference equations:

$B = 1 - 2\lambda \geq 0$ or $\lambda \leq \frac{1}{2}$

$$B = 1 - 2a\frac{\Delta t}{(\Delta x)^2} \geq 0 \qquad \text{or} \qquad 2a\frac{\Delta t}{(\Delta x)^2} \geq \frac{1}{2}$$

$$\text{that is to say: } \Delta t_{atm} = 0.5\frac{(\Delta x)^2}{\alpha}$$

Where Δt_{atm} is the maximum admissible value of the step in time **[24].**

III.2.2.Stability of the system of implicit finite difference equations

$$V^{n+1} = A(\beta)^{-1} V^{n}$$

$$A(\beta) = I + \beta B, \qquad B = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \vdots \\ 0 & -1 & \ddots & \ddots & 0 \\ \vdots & 0 & \ddots & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix}$$

A (β) with strictly dominant diagonal

$$\delta = \min\left(|a_{ii}| - \sum_{j \neq i} |a_{ii}| \right) = 1 \succ 0$$

$$\Rightarrow \left\| A^{-1} \right\| \leq \delta^{-1} = 1$$

$$\Rightarrow \left\| A^{-n} \right\| \leq 1$$

$$\left\| V^{n} \right\|_{\infty} = \left\| A^{-n} V^{0} \right\|_{\infty} \leq \left\| V^{0} \right\|_{\infty} \text{ stable}$$

III.3. Validation of the numerical model

Where the water in the solid state (ice) is initially at its melting temperature, at the instant t = 0 the temperature of its surface at x = 0 is instantly raised to the temperature of 2°C, then kept constant. We take the following parameters corresponding to the water:

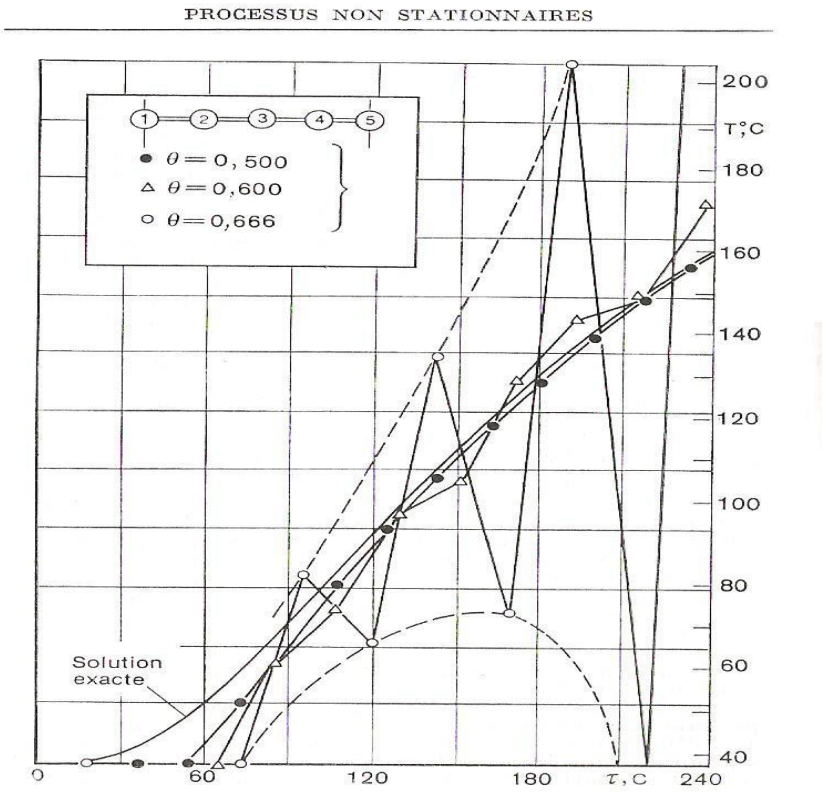

Figure III-2: Exact and numerical resolution of the thermal conduction problem not stationary for a flat wall.

III.3.1.Results obtained by the non-modified Enthalpy Method

The enthalpy method is applied to the problem above. We can notice on Figure III-3 that the numerical solution ocsillates around the analytical one. By increasing the space samples (decreasing the space steps) the gap between the two curve decreases but the number of ocsillations does the opposit.

Table III-1: Physical and numerical parameters of the studied model [25]

Parameter	Value
Solid temperature (°C)	0
Liquid temperature (°C)	2
Initial temperature (°C)	2
Solid thermal conductivity (W/(m K))	0.5
Liquid thermal Conductivity (W/(m K))	2
density of the particle(kg/m3)	1
Total time (day)	25
Time step (second)	781.25
Length (*m*)	1
Length step(*m*)	0.05
Specific heat (J/(kg K))	2.5e06

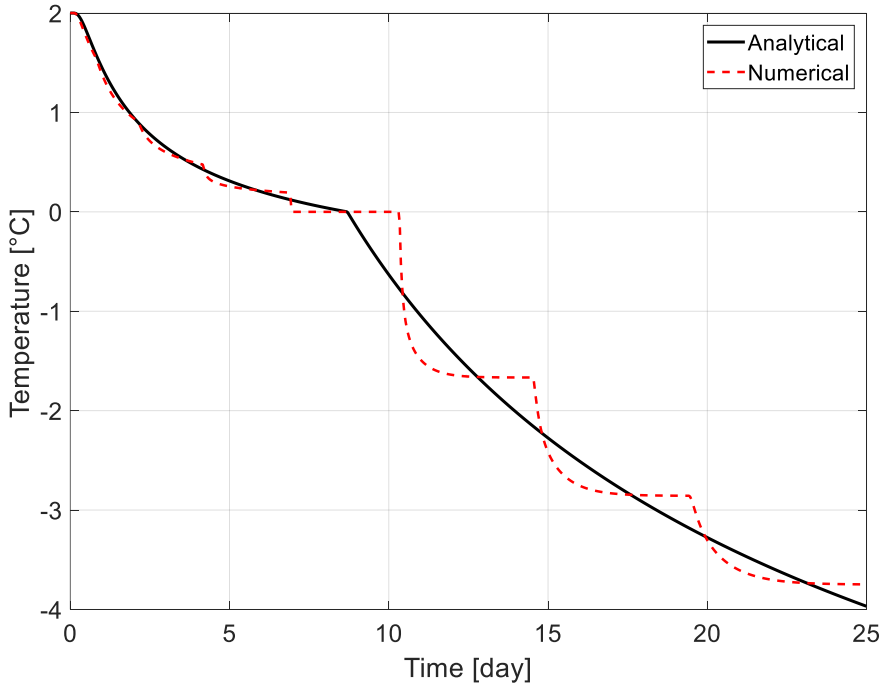

Figure III-3: Comparison between the analytical and the numerical (explicit) solutions for $x=0.5m$ with $\Delta x = 0.1m$ or 11 nodes in space.

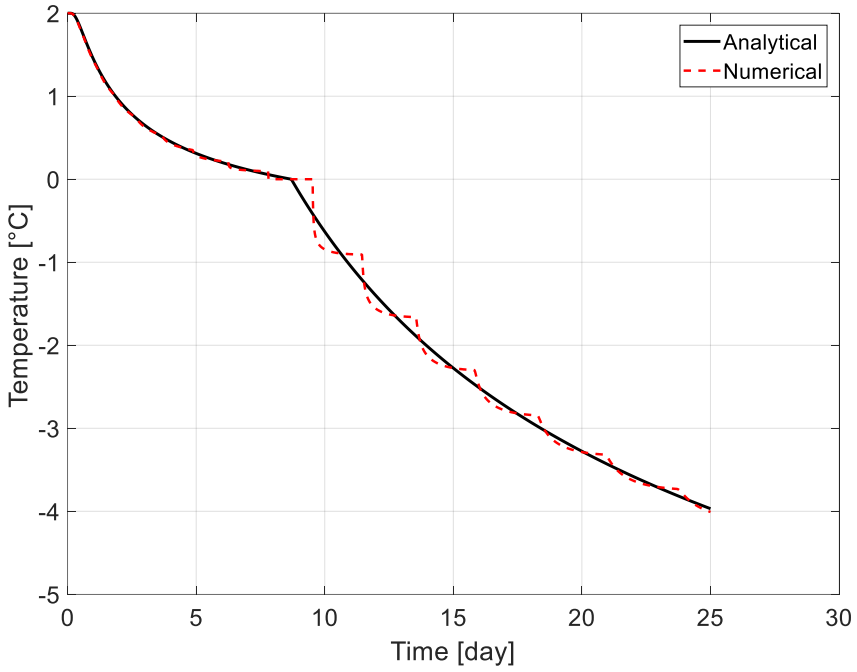

Figure III-4: Comparison between the analytical and the numerical (explicit) solutions for x=0.5m with $\Delta x = 0.05m$ *or 21 nodes in space.*

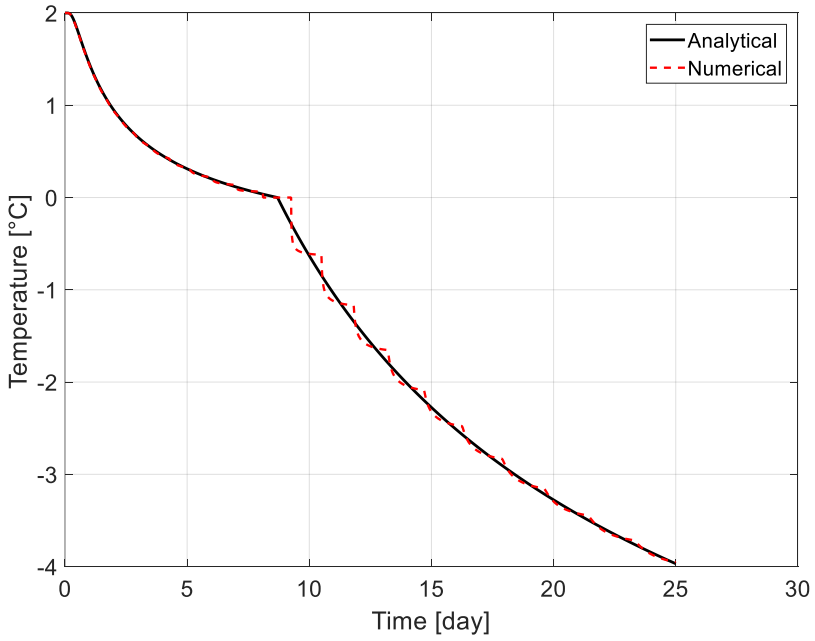

Figure III-5: Comparison between the analytical and the numerical (explicit) solutions for x=0.5m with $\Delta x = 0.033m$ *or 31 nodes in space.*

By analysing the three figures we can conclude that increasing the number of nodes doesn't eliminate the oscillations but only squeeze it. The solution of the problem is by reformulating the algorithms to treat the enthalpy differently.

III.3.2.The modified enthalpy method:

If the point of correspondence of the two curves can be predicted we can find an almost exact algorithm for the classic Stefan problem. As a first step towards such an algorithm, the enthalpy in the discretized region, which solidifies, must be re-interpreted.

Let us put i the point of the node in this region and ε_i its associated element. The total heat in the element ε_i at any time is approximated to $H_i \delta x$, where H_i is the enthalpy of the node and δx is the width of the element.

If in time t the solidification front is on the element ε_i and moves to ε_{i+1} the total heat in the element can be approximated to the sum of the heat in the solid and in the liquid of the element:

$$H_i \delta x = \left(cT_i S + \left(cT_i + L \right)\left(1 - S \right) \right).\delta x \qquad \text{(III.8)}$$

where S is the fraction of the element that is solid. When the solidification front reaches the node i, S will be equal to $\frac{1}{2}$ and $T_i = T_m$ equation (III.8) reduces to:

$$H_i = cT_m + L/2 \qquad \text{(III.9)}$$

Hence, wherever the nodal enthalpy H_i of the discretized region is, it is the sum of the sensible heat cT_m of the phase change and the $\frac{1}{2}$ latent heat associated with the phase change, the phase interface will be approximately on the node i.

The new algorithm

From the interpretation of the enthalpy given before, we will propose the algorithm for solving Stefan's problem as follows:

The enthalpy and a "working" temperature are calculated at each iteration over time by the explicit finite difference diagram given by equation (III.6) and the equation (III.5)

Anywhere the enthalpy at a node is such that at time $j+1$, $H_i^j > cT_m + L/2$ and $H_i^{j+1} < cT_m + L/2$ (for a solidification problem) the phase change limit has passed through the point $i\delta x$ (i.e. when: $H_i^j = cT_m + L/2$)

The time is:
$$\tau_i = (j + X)(\delta\tau) \tag{III.10}$$

Where X is estimated by a linear interpolation over time:

as:
$$X = \frac{L/2 + cT_m - H_i^j}{\left(H_i^{j+1} - H\right)} \tag{III.11}$$

At time τ_i the temperature in the node i is T_m, the temperature at the other points is easily estimated using linear interpolation:

$$T_i^{j+X} = X\left(T_i^{j+1} - T_i^j\right) + T_k \qquad k \neq i \tag{III.12}$$

In the case where the thermal properties differing between the solid and the liquid, the algorithm will be modified using the following finite difference scheme:

$$H_i^{j+1} = H_i^j + \rho\frac{\delta\tau}{\delta x^2}\left(K_{i-1}\left(T_{i-1}^j - T_i^j\right) - K_{i+1}\left(T_i^j - T_{i+1}^j\right)\right) \tag{III.13}$$

instead of equation (III.6). The new interpretation leads to the following enhancements:

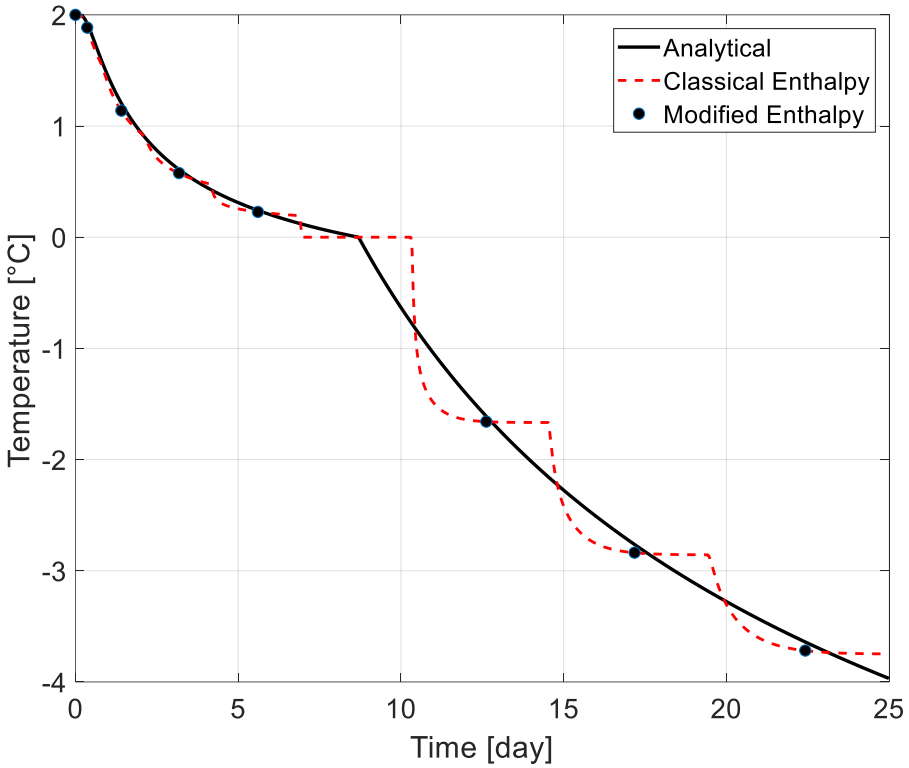

Figure III-6: Comparison between: the analytical, the original and the modified Enthalpy method solutions for x=0.5m with $\Delta x = 0.1m$ *or 11 nodes in space.*

In the Figure III-6 we can see clearly the dramatic enhancement of the solution. The modified enthalpy method reduces the number of samples to only those that corresponds to the two curves and eliminates the entire remaining incorrect samples.

Increasing the number of pace nodes makes the new algorithm perform better, which is clear in the following Figure III-7 and Figure III-8.

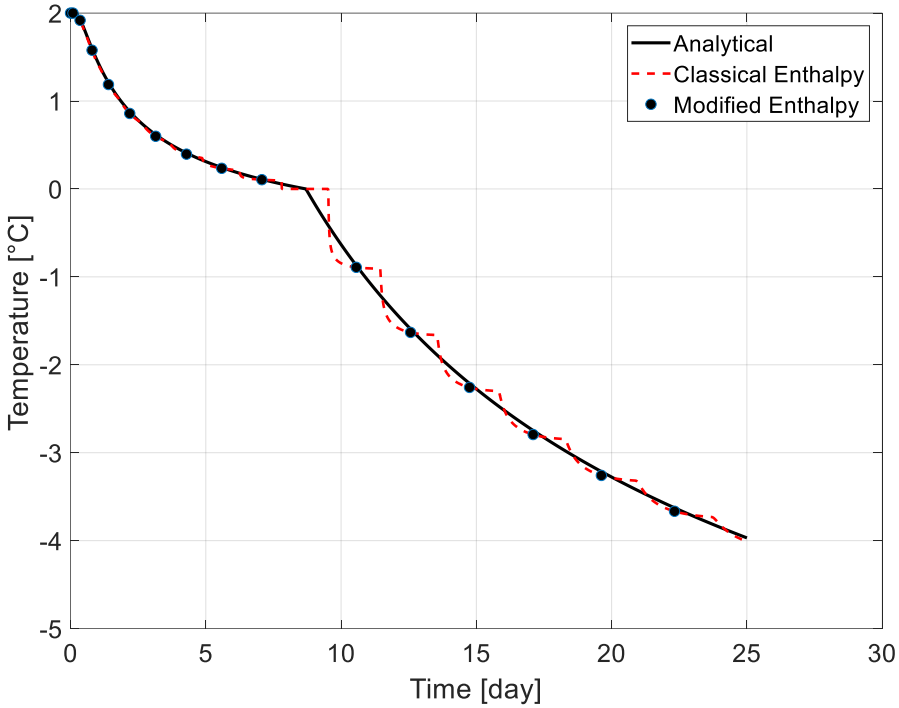

Figure III-7: Comparison between: the analytical, the original and the modified Enthalpy method solutions for x=0.5m with $\Delta x = 0.05m$ *or 21 nodes in space.*

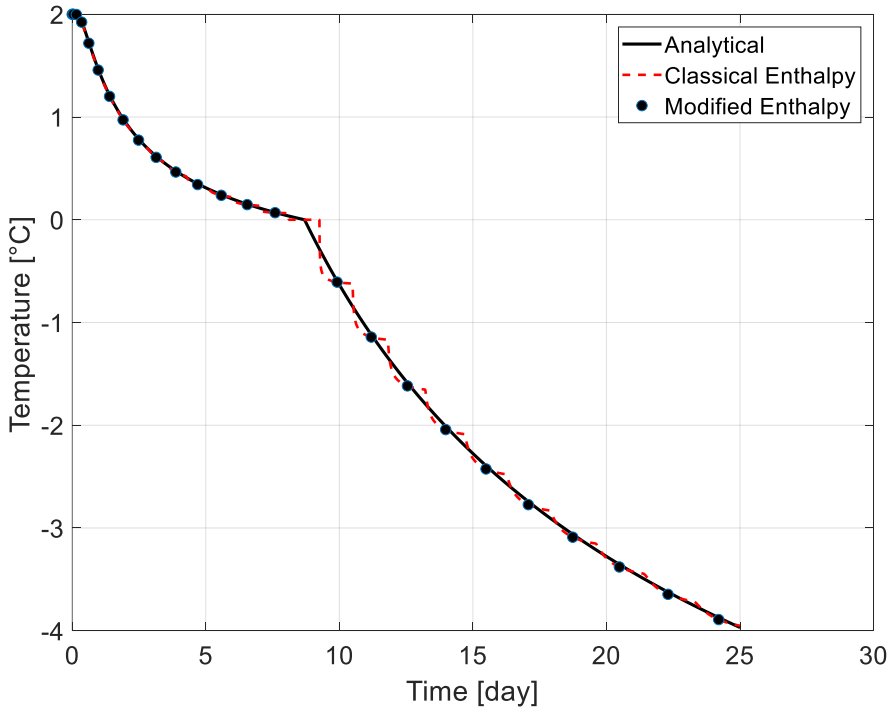

Figure III-8: Comparison between: the analytical, the original and the modified Enthalpy method solutions for x=0.5m with $\Delta x = 0.033m$ *or 31 nodes in space.*

CHAPTER IV
THE MESHLESS NUMERICAL APPROACH

CHAPTER IV : THE MESHLESS NUMERICAL APPROACH

IV.1. The discrete elements method applied to 1D model of a pure medium

In the context of the discrete element method this scenario is simplified to an interpenetration without deformation. The conductance between the two particles is defined as the amount of heat transported through the contact area under the influence of one unit of temperature difference in one unit of time (1s). In the case of contact between two spherical particles i and j of the same nature (same material) it is given by:

$$\Lambda_{ij} = 2\,k\,R_{c,ij} \qquad \text{(IV.1)}$$

With:

Λ_{ij} : The conductance between particles i and j ;

k : The thermal conductivity;

$R_{c,ij}$: The radius of the (circular) contact area between particles i and j.

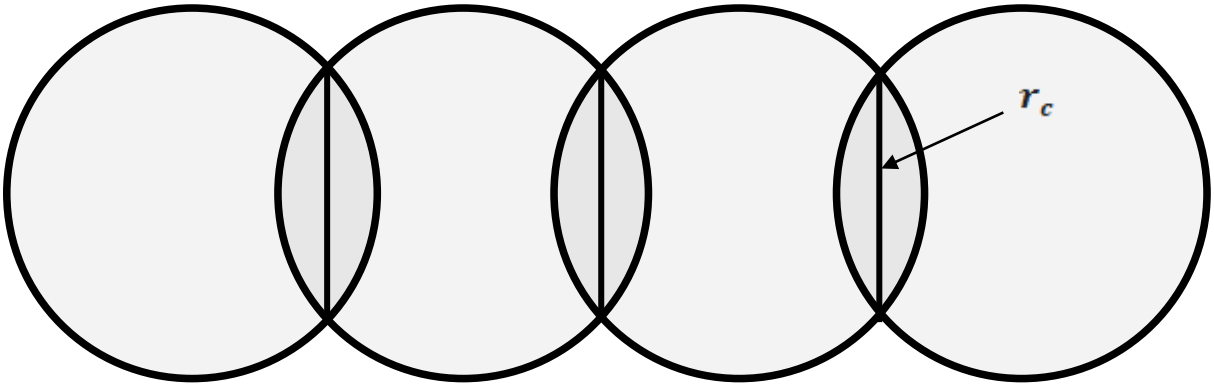

Figure IV-1: Schematic of discrete elements method applied to 1D model of a pure medium

The contact radius is given by: $R_{c,ij} = DE = \sqrt{R^2 - \frac{L_i^2}{4}}$

The area becomes: $a = \pi r^2 = \pi DE^2 = \pi\left(R^2 - \frac{L_i^2}{4}\right)$

We suppose that the particles have the same radius, and their number N_p is fixed (input data):

The total length: $$L = \sum_{i=1}^{N_p} L_i$$

Where, L_i is the distance between each consecutive particles. The distance between the centres of each consecutive pair of particles is given then by:

$$L_i = \frac{L}{\left(N_p - 1\right)}$$

If we suppose that all the particles have the same radius, and the number of particles N_p is an input value for the calculations, the minimum value of the particle radii is then:

$$R_{\min} = \frac{L}{2\left(N_p - 1\right)}$$

Bellow this value there will be no contact between the particles and no heat transfer. If we suppose also that the radius of the contact area is an input value, the radius of the particles will be given by:

$$R = \sqrt{R_{c,ij}^2 + \frac{L_i^2}{4}}$$

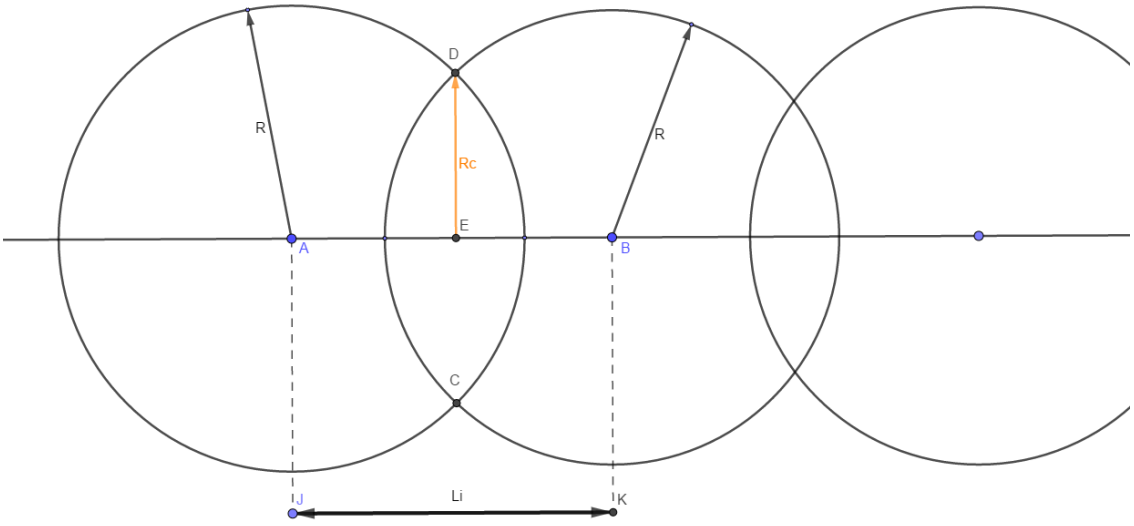

Figure IV-2: Details of the of discrete elements in 1D

The amount of heat transferred from particle j to particle i through the contact area in one second is:

$$\dot{Q}_{ij} = \Lambda_{ij}\left(T_j - T_i\right) \tag{IV.2}$$

With:

T_i : The temperature of particle i ;

T_j : The temperature of particle j.

Since the amount of heat is a scalar quantity (which can be positive or negative) if the i particle is in contact with N_p particles; the total amount of heat per unit of time $\dot{Q}_i^T$ will be:

$$\dot{Q}_i^T = \sum_{j=1}^{N_p} \dot{Q}_{ij} = \sum_{j=1}^{N_p} \Lambda_{ij}\left(T_j - T_i\right) \tag{IV.3}$$

And the relation with temperature will be given by the following differential equation:

$$\frac{\partial T_i}{\partial t} = \frac{1}{c_p m_p}\dot{Q}_i^T = \frac{1}{c_p m_p}\sum_{j=1}^{N_p} \dot{Q}_{ij} \tag{IV.4}$$

With:

c_p : The specific heat of the particle;

m_p : The mass of the particle;

$\frac{\partial T_i}{\partial t}$: The time derivative of the temperature.

The time derivative can be approximated by finite differences as follows:

$$\frac{\partial T_i}{\partial t} \approx \frac{T_i^{k+1} - T_i^k}{\Delta t} \tag{IV.5}$$

And the differential equation can be approximated as:

$$\frac{T_i^{k+1} - T_i^k}{\Delta t} \approx \frac{1}{c_p m_p}\sum_{j=1}^{N_p} \dot{Q}_{ij}^k \tag{IV.6}$$

Thus, the temperature of particle i at the new instant T_i^{k+1} can be calculated explicitly as a function of the temperature values of the same particle and its neighbours at the previous instant:

$$T_i^{k+1} \approx T_i^k + \frac{\Delta t}{c_p m_p} \sum_{j=1}^{N_p} \dot{Q}_{ij}^k \qquad \text{(IV.7)}$$

IV.2. Results:

One of the most important parameters of this method is the overlap size between each pair of particles in contact. This overlap is directly related to the contact radius R_c which is studied in the following section.

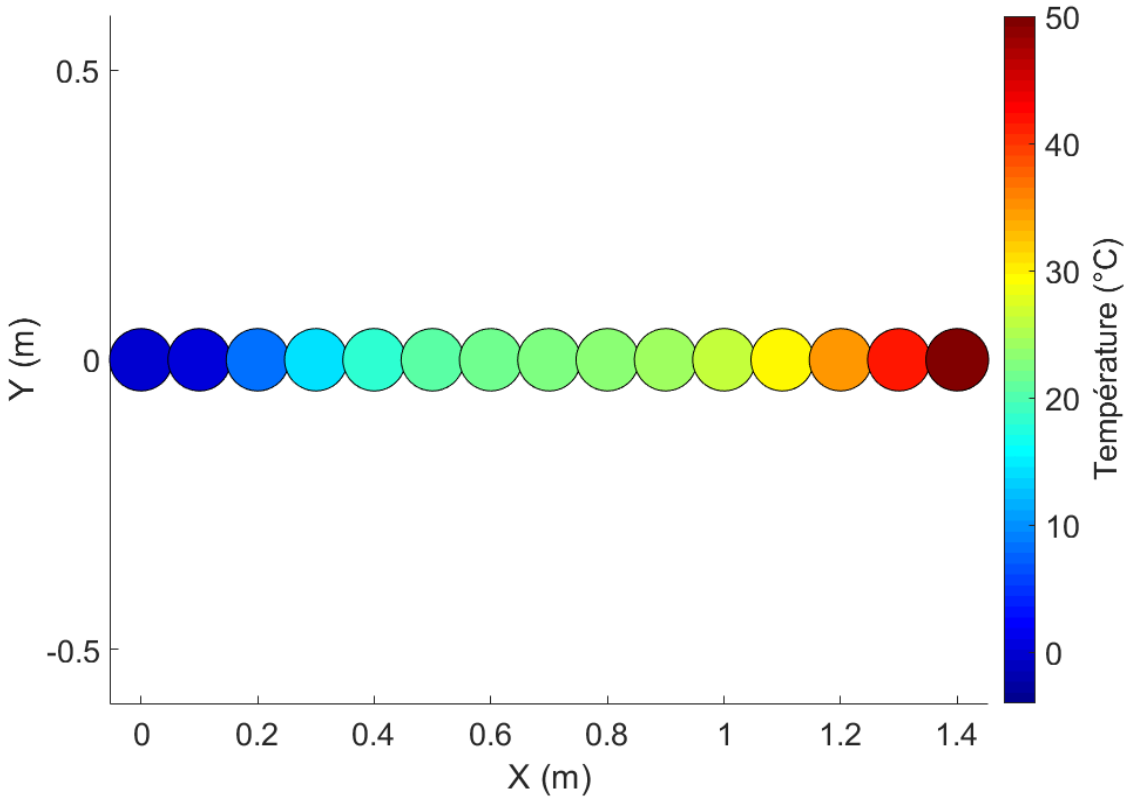

Figure IV-3: Temperature distribution on the discrete particles

The Discrete element method is based, as we've seen earlier, on particles (2D circular ones) rather than connected nodes.

One of the most important parameters of this method is the overlap size between each pair of particles in contact.

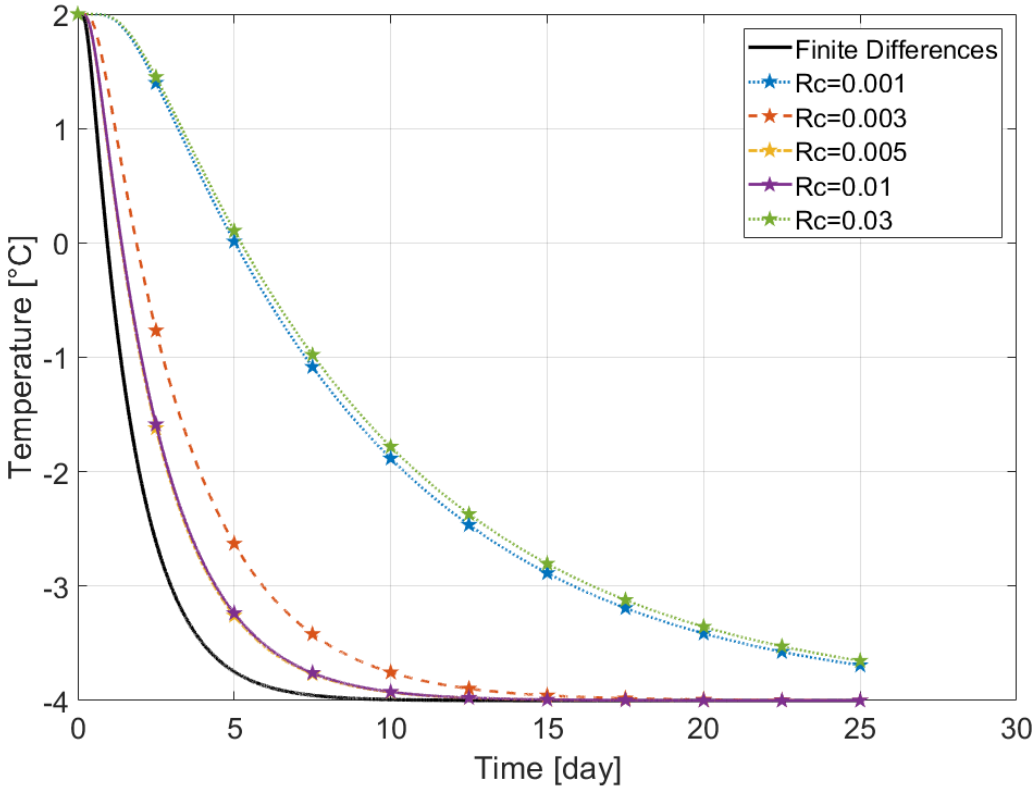

Figure IV-4: The influence of the contact radius size on the temperature evolution

In the Figure IV-4 that represents the monophase (without phase changing) temperature profile, we can see that the influence of contact radius is not clear. Confronting the results of the finite differences (or analytical) method to those of the Discrete element ones we can notice that there is an optimum value for the overlap size for a given number of particles. In this case Rc=0.01m and 0.005 with 21 nodes gives the closest result. Rc=0.01 and Number nodes N=21 will be adopted for the rest DEM analysis.

Changing the Rc leads to a change in the heat flux through each particle from its neighbor particles. This influences every aspect of the calculation. The importance of this parameter is crucial to a successful agreement during the validation.

IV.3. Validation of the meshless numerical model

The DEM alone proved to be insufficient to model the phase change and solve the Stefan Problem, see Figure IV-5. The novelty of our work is the implementation of the Enthalpy technique to the Discrete Element Method to overcome this situation.

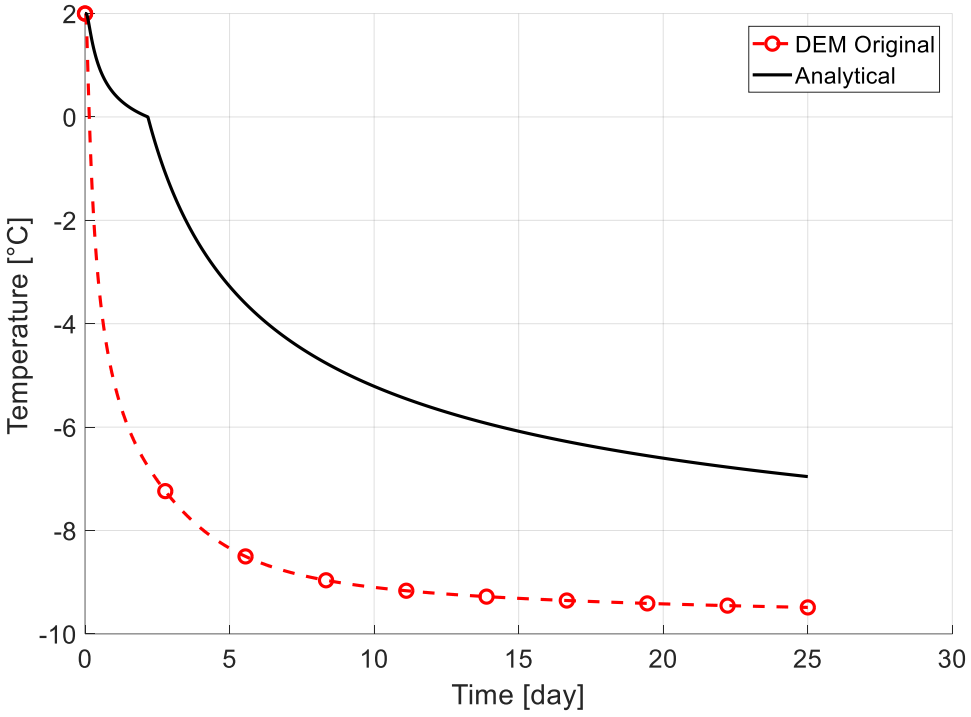

Figure IV-5: DEM without modification and analytical temperature profiles at the (x=0.25m) point and Rc=0.01

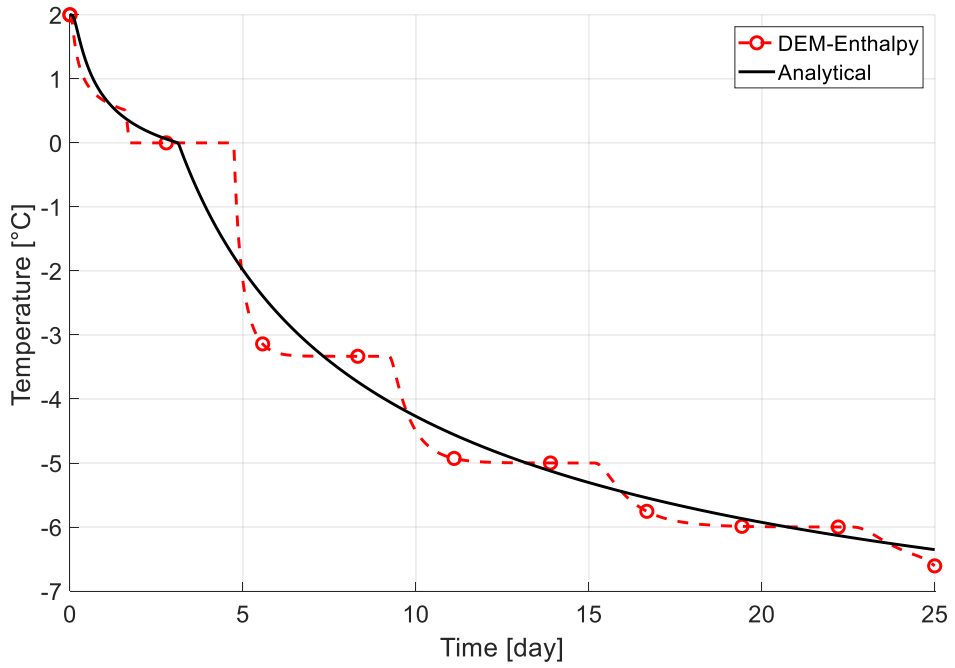

Figure IV-6: DEM-Enthalpy and analytical temperature profiles at the (x=0.25m) point and rc=0.01

Unfortunately, the original enthalpy method showed the same zigzagging behaviour of the solution (see Figure IV-6).

Applying the modified enthalpy algorithm to the discrete element method proved to be as efficient as in the finite difference method (see Figure IV-7). Which leads to the very accurate prediction of the phase interface position evolution shown in the following Figure IV-8.

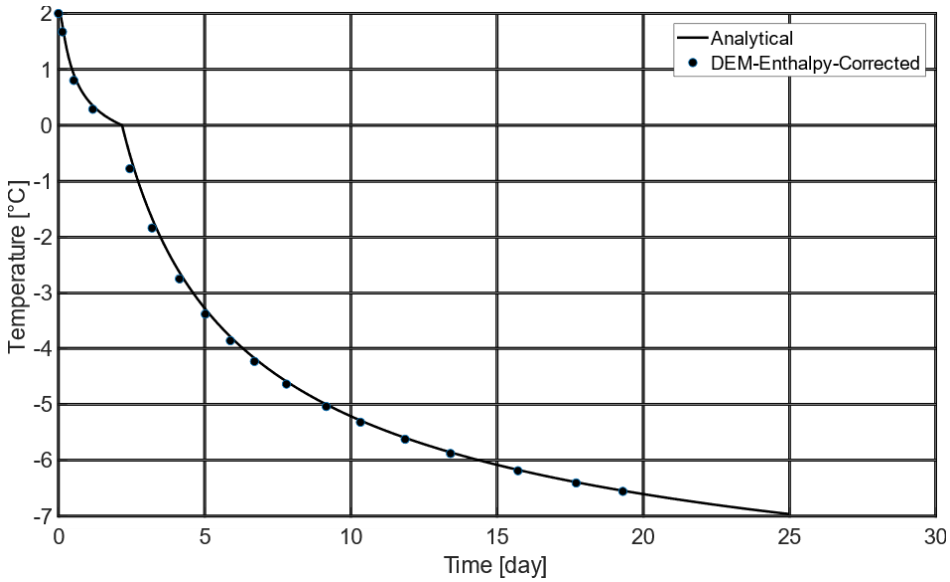

Figure IV-7: DEM-Enthalpy modified algorithm analytical temperature profiles (x=0.25m) point and rc=0.01

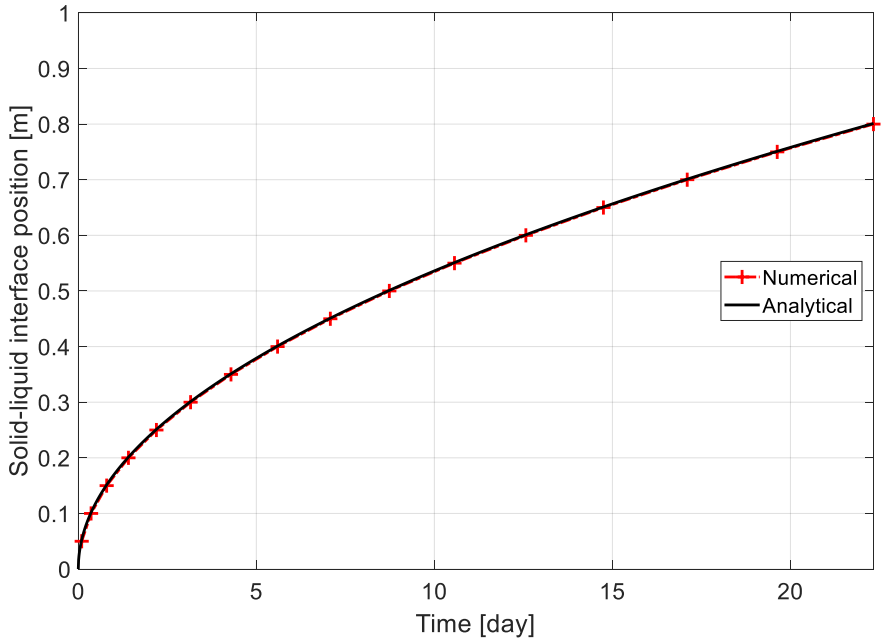

Figure IV-8: Simple representation of particles of DEM method at the (x=0.25m) point and rc=0.01

GENERAL CONCLUSION

GENERAL CONCLUSION

The main objective of our study being the development of a calculation tool based on the Discrete Elements Method (DEM) which is a meshless numerical method to solve Stefan's problem we have started by presenting its mathematical formulation with the analytical related solution. The validation is done by comparing the temperature profile as well as the temporal evolution curve of the position of the Liquid-Solid interface. Obtaining the analytical solution is made possible mainly by the fact that the problem is 1 dimensional and that the material considered is pure.

Then, we have discussed the Enthalpy method and its modified algorithm applied to the finite difference method.

The simple Discrete element method cannot model the phase change without modification. When the method is modified by introducing the enthalpy technique the Discrete element method suffers from the same problems encountered when using the finite differences method, which are:

- The stability of the time discretization scheme (explicit or implicit)
- And the oscillation of the numerical solution around the exact one

After showing the problems encountered with the application of the DEM alone, this method was coupled with the modified Enthalpy technique to predict the temperature profiles and the position curve of the interface between the Liquid-Solid phases, which makes the novelty of this study. The introduction of the modified algorithm to the enthalpy method enhances the DEM performances in the same way it does to the finite difference method.

For a logical future work, we propose to anyone who wants to flow up on this study to:

1. Introduce the kinematic of the particles
2. Mix the DEM with SPH to simulate the molten particles
3. And to expand the dimensions to 2nd or 3ed

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