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Abstract

The main goal of this work is to numerically simulate convection phenomena in solid-liquid phase change processes and its application in the analysis of a thermal energy storage system with phase change materials.

First two chapters consist in the resolution of two well-known numerical problems used as an introduction to the governing equations of fluid flows and heat transfer. Here, the necessary tools for discretizing and solving these equations are briefly described.

Third chapter specifically deals with the problem of modelling solid-liquid phase change and its application into the simulation of a special thermal storage system.
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Report
Chapter 1

Driven Cavity problem

1.1 Introduction

The numerical resolution of the “Driven Cavity” problem is posed. It consists in solving the velocity (and pressure) field of a fluid in a square two-dimensional cavity with the top wall in motion, with a constant horizontal velocity. The nondimensional form of the problem is considered, thus the lengths of the walls, as well as the velocity of the upper wall, are equal to 1.

To determine the velocity field, the incompressible Navier-Stokes equations need to be solved numerically.

1.2 Domain discretization

The domain is divided in \( N_x \times N_y \) rectangles, with a node in the center of each one, where the pressure \( p \) is defined. The grids for the horizontal and vertical components of the velocity (\( u \) and \( v \)) are staggered with respect to the pressure, as proposed by Patankar (1980).

1.3 Discretization of the equations

Incompressible Navier-Stokes equations to be solved are:

Mass conservation equation:

\[
\nabla \cdot \vec{u} = 0
\]  

(1.1)

Momentum equation:

\[
\frac{\partial \vec{u}}{\partial t} = -(\vec{u} \cdot \nabla)\vec{u} + \frac{1}{Re} \Delta \vec{u} - \nabla p
\]  

(1.2)

Where the term of the left side of the equation is the transient term, the first of the right side is the advective-convective term (accounts for transport of momentum with the flow), the second of the right side is the diffusive term (accounts for the transfer of momentum due to the internal forces present in newtonian viscous fluids) and the last term of the right side is the pressure term.

These equations are discretized in space using the Finite Volume Method (FVM) (see Patankar (1980)) and in time using an explicit time scheme.
1.3.1 Time discretization

For the temporal discretization of the transient term, a central difference scheme is used for the time derivative. A fully explicit time integration scheme is used for convective and diffusive terms (2\textsuperscript{nd} order Adams-Bashforth). The pressure term and the divergence of the velocity in the continuity equation are treated implicitly. Thus:

\[
\frac{\vec{u}^{n+1} - \vec{u}^n}{\Delta t} = \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - \nabla p^{n+1}
\]  
(1.3)

\[\nabla \cdot \vec{u}^{n+1} = 0\]  
(1.4)

where \( R(\vec{u}^n) \) and \( R(\vec{u}^{n-1}) \) are the sum of the discretized convective and diffusive terms, evaluated at times \( n \) and \( n - 1 \).

1.3.2 Fractional Step Method

Velocity and pressure are coupled in Navier-Stokes equations. Therefore, some strategy has to be adopted to make the decoupling. The method adopted here for this purpose is the Fractional Step Method. It consists in calculating an intermediate velocity field \( \vec{u}^p \) from the momentum equation, not taking into account the pressure gradient, then calculating the pressure field from this intermediate velocity field (also called predictor velocity) - making use of the continuity equation - and finally calculating \( \vec{u}^{n+1} \). The resulting equations from the application of this method are the following:

\[\vec{u}^p = \vec{u}^n + \Delta t \left( \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) \right)\]  
(1.5)

\[\vec{u}^p = \vec{u}^{n+1} + \Delta t. \nabla p^{n+1} \rightarrow \nabla \cdot \vec{u}^p = \nabla \cdot \vec{u}^{n+1} + \Delta t(\nabla \cdot \nabla p^{n+1})\]  
\[\text{continuity} \rightarrow \Delta t \Delta p^{n+1} = \nabla \cdot \vec{u}^p\]  
(1.6)

\[\vec{u}^{n+1} = \vec{u}^p - \Delta t \nabla p^{n+1}\]  
(1.7)

And the algorithm to solve the problem is:

1. Evaluate \( R(\vec{u}^n) \)
2. Evaluate \( \vec{u}^p \) from equation (1.5)
3. Evaluate \( \nabla \cdot \vec{u}^p \) and solve equation (1.6)
4. Obtain the new velocity field with equation (1.7)

1.3.3 Space discretization scheme

Finite Volume Method is used for the spatial discretization of the equations (Patankar (1980)). This method consists in integrating the governing differential equations over discrete control volumes.
1.3. Discretization of the equations

Figure 1.1: Notation used for the position of the nodes, where the letters E, N, S, W recall from east, north, south and west positions with respect to the node being calculated (P). This notation is used either for pressure or velocities nodes. Lower-case is used to indicate the relative position of the faces.

**Diffusive term**

The diffusive term is treated as follows:

\[
1/V \int V \nabla^2 \vec{u} \, dV = 1/V \int A \nabla \vec{u} \cdot \hat{n} \, dA \approx 1/V \sum_f (\nabla \vec{u} \cdot \hat{n})_f A_f
\]  

(1.8)

where the divergence theorem has been used in the first equality. Sub-index \textit{f} indicates that the sum is performed over the surfaces of the control volume.

In a uniform 2D structured grid - taking the same notation for the nodes coordenates as in Patankar (1980) (see fig. 1.1) - this term can be expressed as follows for the horizontal velocity \((u)\):

\[
\sum_{f=e,w,n,s} (\nabla u \cdot \hat{n})_f A_f = \Delta y (\partial u_e/\partial x - \partial u_w/\partial x) + \Delta x (\partial u_n/\partial y - \partial u_s/\partial y)
\]  

(1.9)

where the derivatives evaluated at the faces can be further approximated as the difference between the values of the velocities at the adjacent nodes, as follows:

\[
\Delta y (\partial u_e/\partial x - \partial u_w/\partial x) + \Delta x (\partial u_n/\partial y - \partial u_s/\partial y) \approx \Delta y (u_E - u_P)/\Delta x - (u_P - u_W)/\Delta x + \Delta x (u_N - u_P)/\Delta y - (u_P - u_S)/\Delta y
\]

\[
\partial u_e/\partial x \approx u_E - u_P
\]  

(1.10)

\[
\partial u_w/\partial x \approx u_P - u_W
\]  

(1.11)

\[
\partial u_n/\partial y \approx u_N - u_P
\]  

(1.12)

\[
\partial u_s/\partial y \approx u_P - u_S
\]  

(1.13)

Dividing eq. (1.9) by \(V = \Delta x \Delta y\) and using eqs. (1.10) to (1.13), it results in:

\[
\nabla^2 \vec{u} \approx \frac{u_E + u_W - 2u_P}{\Delta x^2} + \frac{u_N + u_S - 2u_P}{\Delta y^2}
\]  

(1.14)
which is the same equation that would be obtained applying Finite Differences with the usual 2\(^{nd}\) order approximation of the second derivative:

\[
\frac{\partial^2 f}{\partial x^2} = \frac{f(x + \Delta x) + f(x - \Delta x) - 2f(x)}{(\Delta x)^2}
\]

Thus, eqs. (1.10) to (1.13) result in a 2\(^{nd}\) order approximation of the diffusive term. However, this approximation cannot be used in some of the nodes next to the boundaries, where either the value of \(f(x + \Delta x)\) or of \(f(x - \Delta x)\) do not exist. Therefore, if we want that the local approximation in the boundaries be of 2\(^{nd}\) order we should adopt the following expression in those nodes:

\[
\frac{\partial^2 f}{\partial x^2} = \frac{16}{\Delta x^2} f(x - \frac{\Delta x}{2}) - 5f(x) + 2f(x + \Delta x) - \frac{1}{5} f(x + 2\Delta x)
\]

(1.15)

Where \(\Delta x\) is the distance between nodes in the interior of the cavity and \(\frac{\Delta x}{2}\) is the distance between the boundary node and the one next to it, inside the cavity. Here \(f\) is either \(u\) or \(v\) and \(x\) may be the vertical or the horizontal direction.

As a result of the staggered grid, there is only need to calculate the first derivative in up and bottom walls (not in right and left walls) for the horizontal component of the velocity \(u\), and in right and left walls for the vertical component \(v\). This is where the previous approximation has been used.

**Convective term**

The application of the FVM for treating the convective term, working only with the horizontal component of the velocity (\(u\)), gives:

\[
\frac{1}{V} \int_V \nabla \cdot (u\vec{u}) \, dV = \frac{1}{A} \int_A u(\vec{u} \cdot \hat{n}) \, dA \approx \frac{1}{V} \sum_f [u(\vec{u} \cdot \hat{n})]_f A_f
\]

(1.16)

where - for convenience - the conservative form of the momentum equation has been used. Here again, divergence theorem has been used to derive the first equality.

In a uniform structured 2D grid, this equation yields:

\[
\frac{1}{V} \sum_{f=e,w,n,s} [u(\vec{u} \cdot \hat{n})]_f A_f = \frac{(u_e u_e - u_w u_w)}{\Delta x} + \frac{(u_n u_n - u_s u_s)}{\Delta y}
\]

(1.17)

Several schemes exist to approximate the velocities at the faces (Patankar (1980)). In this work, a symmetry preserving scheme (Verstappen and Veldman (2003)) has been adopted, by which the velocities at the faces are approximated as the mean value between adjacent velocities. It should be noted that this scheme is exactly the same as central difference scheme (CDS) for uniform grids. For example, horizontal velocities at the faces become:

\[
\begin{align*}
    u_e &= \frac{u_P + u_E}{2} \\
    u_w &= \frac{u_P + u_W}{2} \\
    u_n &= \frac{u_P + u_N}{2} \\
    u_s &= \frac{u_P + u_S}{2}
\end{align*}
\]
1.3. Discretization of the equations

Other approximation schemes taken from Patankar (1980) - as UPWIND, HYBRID and POWER LAW - have also been implemented in the generated computer code.

**Pressure equation**

The integration of eq. (1.6) results in:

\[
\frac{1}{V} \int V \Delta t \nabla \cdot (\nabla p^{n+1}) dV = \frac{1}{V} \int V \nabla \cdot (\vec{u}^p) dV \tag{1.22}
\]

Following the same line of reasoning that in previous sections, eq. (1.22) becomes:

\[
\frac{1}{V} \sum_f (\Delta t \nabla p^{n+1} \cdot \hat{n})_f A_f = \frac{1}{V} \sum_f (\vec{u}^p \cdot \hat{n})_f A_f \tag{1.23}
\]

Decomposing the sum of the left part of eq. (1.23) the same way as for the diffusive term it becomes:

\[
\frac{1}{V} \sum_{f=e,w,n,s} (\nabla p \cdot \hat{n})_f A_f = \frac{1}{\Delta x} (\frac{\partial p_e}{\partial x} - \frac{\partial p_w}{\partial x}) + \frac{1}{\Delta y} (\frac{\partial p_n}{\partial y} - \frac{\partial p_s}{\partial y}) \tag{1.24}
\]

At the boundaries, the following condition is applied:

\[
\nabla p \cdot \hat{n} = 0 \tag{1.25}
\]

and then, assuming that face \( e \) is boundary:

\[
(\Delta t \nabla p^{n+1} \cdot \hat{n})_e A_e = 0 \tag{1.26}
\]

and inner nodes adjacent to the boundaries are “decoupled” from boundary pressure nodes; i.e. the pressure inside the cavity does not depend on the pressure of the walls.

The term at the right side of eq. (1.23) is very similar to the discretized mass balance equation. Its expression in a 2D structured grid becomes:

\[
\frac{1}{V} \sum_{f=e,w,n,s} (\vec{u}^p \cdot \hat{n})_f A_f = \frac{(u^p_e - u^p_w)}{\Delta x} + \frac{(v^p_n - v^p_s)}{\Delta y} \tag{1.27}
\]

If a staggered grid is adopted for the velocity components with respect to the pressure nodes, there is no need for an extra approximation in the calculation of predictor velocities at the volume faces. The reason for this is that the integration of equation (1.22) is performed over control volumes centered at the pressure nodes and because of the staggered grid adoption, velocities nodes are placed exactly at the faces of these pressure-centered control volumes.

In the case of adopting a centered grid scheme, i.e. where velocity and pressure are calculated at the same points, some approximation has to be adopted in order to determine predictor velocities at the faces.
In this chapter, a staggered grid scheme is adopted.

With all these considerations, eq. (1.23) expressed for all inner nodes results in a system of linear equations of the kind:

\[
\hat{p}^{n+1} = a_E \hat{p}_E^n + a_N \hat{p}_N^n + a_S \hat{p}_S^n + a_W \hat{p}_W^n + a_P \hat{p}_P^n + b
\]

where \( \hat{p} = \Delta t p \) and:

\[
\begin{align*}
    a_E &= a_N = \frac{1}{\Delta x^2}; \\
    a_W &= a_S = \frac{1}{\Delta x^2}; \\
    a_P &= a_E + a_W + a_N + a_S \\
\end{align*}
\]

and

\[
b = \frac{(u^p_e - u^p_w)}{\Delta x} + \frac{(v^p_n - v^p_s)}{\Delta y}
\]

which has to be solved using some linear “solver”.

1.4 Solution of the equations

The objective is to calculate the velocity field in steady state with several values of \( \text{Re} \). To do this, the unsteady equations are solved several times until the steady state is reached at time \( t_{\text{steady}} \), for which there is no significant change in the variables. There is no difficulty in calculating \( u^p \) as eq. (1.5) is explicit.

To determine pressure values, the system of equations defined by eq. (1.28) has to be solved. For this problem, an iterative solver is used: the Gauss-Seidel method combined with TDMA (also called line-by-line method in Patankar (1980)).

1.5 Code verification

To verify that there are no mistakes in the code, specifically in the calculation of the convective and diffusive terms, a strategy similar to the method of manufactured solutions (MMS) is used (Roache (2002)).

The functions used to do the checking are the following:

\[
\begin{align*}
    u_a &= (1 - \cos 2\pi x) \sin 2\pi y \\
    v_a &= \sin 2\pi x (\cos 2\pi y - 1)
\end{align*}
\]

Here \( u_a \) is the horizontal component of the velocity and \( v_a \) the vertical component. These equations were derived from the continuity equation, searching for solutions of the kind of \( u_a(x, y) = f(x).g(y) \), with \( u_a = v_a = 0 \) in the boundaries. In fact, the value of \( u \) in the real velocity field is 1 in the upper wall, but as the values of the velocity are 0 in the other walls, there is a singularity in the upper corners of the cavity. This is why it does not exist a derivable function, solution of the continuity differential equation, that can take the boundary conditions of the real problem. For this reason, \( u = 0 \) is taken as a boundary condition at the upper wall.

As shown in fig. 1.2, both the convective and diffusive terms have a 2nd order behaviour, that is, the error is reduced four times if the number of nodes in each direction is doubled. It should be noted that the error is calculated as the maximum error encountered in the whole domain, including the nodes next to the boundaries. This means that the eq.(1.15) works as intended to.
1.6 Results and discussion

Fig. 1.2: Result of the verification of the computations of diffusive and convective terms. Comparison with 1st and 2nd order lines.

1.6 Results and discussion

Simulations have been run for Reynolds numbers 100, 400, 1000, 3200, 5000, 7500 and 10000. Figures 1.3 to 1.7 show some streamtraces of the final velocity fields for the different Re numbers and mesh sizes of 129 x 129. The expected vorticity increase with Re is observed.

Fig. 1.7 shows the velocity field for Re = 10000 at time t = 3000. At this time, steady state has not been reached, strictly speaking, because it is in a turbulent regime. For this reason, the calculation is stopped not by a convergence criterion but by an elapsed-time criterion, where time is calculated by adding time increases in every iteration. In this case t = 3000, which is a large number taking into consideration that for Re = 7500 the time elapsed until convergence is reached is around t = 415.

1.6.1 Simulation validation

To verify the correctness of the velocity fields obtained, comparison against benchmark (extracted from Guia and Guia (1988)) is performed. u benchmark values are available only for a vertical line passing through the center of the cavity, and v values available only for a horizontal line passing through the center. Figures 1.8 to 1.12 show the agreement between results and benchmark for some characteristic Reynolds numbers.

A fairly good agreement between benchmark and results is obtained. Maximum errors with respect to benchmark available data, are shown in tabular form in figure 1.14.

A slight deviation is observed in Re = 7500, probably due to the effect of “false diffusion” which becomes more evident as Re increases. As Re increases, the influence of diffusive term on the velocity field decreases, so the real diffusion is less significant with respect to convection, and therefore, with respect to “false diffusion” too. To correct this, further simulations should be performed with finer grids.
Figure 1.3: Streamlines of the solution for $Re = 100$.

Figure 1.4: Streamlines of the solution for $Re = 400$.

Agreement between benchmark and simulation results is not evaluated for $Re = 10000$ because convergence is not reached in this case, as mentioned before, because the fluid is in turbulent regime.
1.7 Conclusions

Simulations for the Driven Cavity problem with different Reynolds numbers have been successfully performed, applying an explicit Fractional Step Method using the Adams-Bashforth scheme for time integration and the symmetry preserving scheme for approximations in space.
An increase in vorticity is observed for higher $Re$, as was expected.

For $Re = 10000$ a steady state solution is not obtained as the fluid is in turbulent regime. In this case, time average should be done to determine when the “steady” turbulent state is reached.
1.7. Conclusions

Figure 1.9: Comparison of results for \( v \), \( Re = 100 \), with benchmark.

Figure 1.10: Comparison of results for \( u \), \( Re = 1000 \), with benchmark.
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Figure 1.11: Comparison of results for $v$, $Re = 1000$, with benchmark.

Figure 1.12: Comparison of results for $u$, $Re = 7500$, with benchmark.
1.7. Conclusions

Figure 1.13: Comparison of results for $v$, $Re = 7500$, with benchmark.

<table>
<thead>
<tr>
<th>$Re$</th>
<th>$u$</th>
<th>$v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>0.0049</td>
<td>0.0091</td>
</tr>
<tr>
<td>400</td>
<td>0.0021</td>
<td>0.0057</td>
</tr>
<tr>
<td>1000</td>
<td>0.0042</td>
<td>0.0149</td>
</tr>
<tr>
<td>3200</td>
<td>0.0180</td>
<td>0.0312</td>
</tr>
<tr>
<td>7500</td>
<td>0.0235</td>
<td>0.0274</td>
</tr>
</tbody>
</table>

Figure 1.14: Maximum errors of obtained solutions with respect to benchmark.
Chapter 2

Differentially Heated Cavity problem

2.1 Introduction

The numerical resolution of the “Differentially Heated Cavity” problem is posed. It consists in solving the velocity, pressure, and temperature fields of a fluid in a square two-dimensional cavity, where the lateral walls have constant temperatures $T_1$ and $T_2$ where $T_1 > T_2$. The nondimensional form of the problem is considered, in which Prandtl number ($Pr$) is set to 0.71 and the Rayleigh number ($Ra$) varies between $10^3$ and $10^6$.

To determine the velocity field, Navier-Stokes equations need to be solved numerically. Boussinesq approximation is adopted to account for the density variation effects on the gravity force.

2.2 Domain discretization

The domain is divided in $N_x \times N_y$ rectangles ($N_x = N_y$), with a node in the center of each one, where the pressure $p$ and the temperature $\phi$\(^1\) is calculated. The grids for the horizontal and vertical components of the velocity ($u$ and $v$) are staggered with respect to the pressure, as proposed by Patankar (1980).

2.3 Discretization of the equations

Non-dimensional Navier-Stokes equations with Boussinesq approximation to be solved:

\[
\nabla \cdot \vec{u} = 0 \quad (2.1)
\]

\[
\frac{\partial \vec{u}}{\partial t} = -(\vec{u} \cdot \nabla)\vec{u} + Pr\Delta \vec{u} - \nabla p + \vec{f} \quad (2.2)
\]

\[
\frac{\partial \phi}{\partial t} = -(\vec{u} \cdot \nabla)\phi + \Delta \phi \quad (2.3)
\]

\[
\vec{f} = 0 \cdot \hat{i} + RaPr\phi \cdot \hat{j} \quad (2.4)
\]

Here $\vec{f}$ is the buoyancy term introduced by the Boussinesq approximation. These equations are discretized using Finite Volume Method.

\(^1\phi = \frac{T - T_2}{T_1 - T_2} \) is the non-dimensional temperature
2.3.1 Time discretization

A fully explicit time integration scheme is used for convective and diffusive terms (Adams-Bashforth scheme). A fully implicit scheme is used for pressure and buoyancy terms in momentum equation and for the divergence of the velocity in the continuity equation. Transient term is discretized by adoption of a central difference scheme. Thus, the resulting equations are:

\[
\frac{\vec{u}^{n+1} - \vec{u}^n}{\Delta t} = \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - \vec{f}^{n+1}
\]

\[
\nabla \cdot \vec{u}^{n+1} = 0 \quad (2.5)
\]

\[
\frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{3}{2} R(\phi^n) - \frac{1}{2} R(\phi^{n-1})
\]

\[
\vec{f}^{n+1} = 0 \cdot \hat{i} + Ra Pr \phi^{n+1} \cdot \hat{j} \quad (2.6)
\]

where \( R(\vec{u}^n) \) (and \( R(\phi^n) \)) and \( R(\vec{u}^{n-1}) \) (and \( R(\phi^n) \)) are the sum of the convective and diffusive terms discretized, evaluated at \( n \) and \( n - 1 \).

2.3.2 Fractional Step Method

The method used here for decoupling velocity and pressure is the Fractional Step Method as explained in chapter 1. The resulting equations from the application of this method are the following:

\[
\vec{u}^p = \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) + \vec{f}^{n+1} \right] \quad (2.7)
\]

\[
\vec{u}^p = \vec{u}^{n+1} + \Delta t \nabla p^{n+1} \rightarrow \nabla \cdot \vec{u}^p = \nabla \cdot \vec{u}^{n+1} + \Delta t (\nabla \cdot \nabla p^{n+1})
\]

\[
\frac{\nabla \cdot \vec{u}^p}{\Delta t} \Delta p^{n+1} = \nabla \cdot \vec{u}^p \quad (2.8)
\]

\[
\vec{u}^{n+1} = \vec{u}^p - \Delta t \nabla p^{n+1} \quad (2.9)
\]

And the algorithm to solve the problem is:

1. Evaluate \( \phi^{n+1} \) from equation (2.7) and calculate \( \vec{f}^{n+1} \) from equation (2.8)
2. Evaluate \( R(\vec{u}^n) \)
3. Evaluate \( \vec{u}^p \) from equation (2.9)
4. Evaluate \( \nabla \cdot \vec{u}^p \) and solve equation (2.10)
5. Obtain the new velocity field with equation (2.11)

2.3.3 Discretization scheme

The same assumptions made in the resolution of the Driven Cavity problem (chapter 1) are adopted here.
2.4 Solution of the equations

The objective is to calculate the velocity field in steady state for several values of \( Ra \), and \( Pr = 0.71 \). To do this, the unsteady equations are solved several times until the steady state is reached at time \( t_{\text{steady}} \), for which there is no significant change in the variables. There is no difficulty in calculating \( u^p \) as eq. (2.9) is explicit.

Equation (2.10) is implicit, which means that it is necessary to solve a system of equations to reach the solution for \( p \). In this work an iterative method of solution is used: the Gauss-Seidel method combined with TDMA.

2.5 Code verification

The same code used for solving the Driven Cavity problem is used here with the needed implementations to solve the energy equation. Therefore, code verification of convective and diffusive operators has already been performed and verified.

2.6 Results and discussion

Simulations have been run for Rayleigh numbers \( 10^3, 10^4, 10^5 \) and \( 10^6 \), all with Prandtl number of 0.71. Figures 2.1 to 2.4 show some contour maps of the solutions obtained. The expected vorticity increase with \( Ra \) is observed.

2.6.1 Simulation verification

To verify the correctness of the velocity fields obtained, comparison against benchmark (De Vahl Davis (1983)) is performed (see table 2.1). The variables compared are:

1. \( u_{\text{max}} \): Maximum horizontal velocity in the vertical centerline.
2. \( v_{\text{max}} \): Maximum vertical velocity in the horizontal centerline.
3. \( Nu_{0,m} \): Average Nusselt number calculated at the left wall.
4. \( Nu_{\text{max}} \): Maximum local Nusselt number at the left wall.
5. \( Nu_{\text{min}} \): Minimum local Nusselt number at the left wall.
6. \( \psi_m \): Stream function evaluated at the center of the cavity.

The local Nusselt number at the left wall is calculated as:

\[
Nu_{0,m} = \int_0^1 \frac{\partial \phi}{\partial x} \bigg|_{x=0} dy
\]

The coordenates where the maximum and minimum values are located are also registered. \( N \) stands for the number of pressure nodes used in the simulation.

It must be pointed out that no interpolation has been made to calculate local variables, therefore slight differences between results and benchmark are expected, specially in the coordenates values.

A fairly good agreement between benchmark and results is obtained. Maximum errors with respect to the benchmark are shown in table 2.0(c). For \( Ra = 10^6 \) two set of results are shown, corresponding to two different mesh sizes. An increment on the accuracy with mesh density is observed.
Chapter 2. Differentially Heated Cavity problem

2.7 Conclusions

Simulations for the Differentially Heated Cavity problem with different Rayleigh numbers have been successfully performed, by the application of an explicit Fractional Step Method and using the Adams-Bashforth scheme for time integration and the CDS scheme for approximations in space. Results are very similar to the ones obtained by De Vahl Davis (1983).

Natural convection produced by temperature differences has been observed. An increase in vorticity is observed for higher $Ra$, as was expected.
2.7. Conclusions

(a) Horizontal velocity $u$

(b) Vertical velocity $v$

(c) Temperature $\phi$

(d) Stream function $\psi$

**Figure 2.2:** Contour maps for $Ra = 10^4$
Figure 2.3: Contour maps for $Ra = 10^5$
2.7. Conclusions

(a) Horizontal velocity $u$

(b) Vertical velocity $v$

(c) Temperature $\phi$

(d) Stream function $\psi$

Figure 2.4: Contour maps for $Ra = 10^6$
Chapter 2. Differentially Heated Cavity problem

(a) Benchmark results

<table>
<thead>
<tr>
<th>Ra</th>
<th>$T_{\text{ref}}$</th>
<th>$y$</th>
<th>$T_{\text{ref}}$</th>
<th>$y$</th>
<th>$\text{Nu}_{\text{ref}}$</th>
<th>$\text{Nu}_{\text{ref}}$</th>
<th>$\mu_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^3$</td>
<td>3.459</td>
<td>16.179</td>
<td>34.730</td>
<td>64.630</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$10^4$</td>
<td>3.687</td>
<td>19.617</td>
<td>68.590</td>
<td>219.360</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$10^5$</td>
<td>0.178</td>
<td>0.119</td>
<td>0.066</td>
<td>0.018</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$10^6$</td>
<td>1.117</td>
<td>2.258</td>
<td>1.609</td>
<td>8.017</td>
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</table>

(b) Simulation results

<table>
<thead>
<tr>
<th>Ra</th>
<th>$T_{\text{ref}}$</th>
<th>$y$</th>
<th>$T_{\text{ref}}$</th>
<th>$y$</th>
<th>$\text{Nu}_{\text{ref}}$</th>
<th>$\text{Nu}_{\text{ref}}$</th>
<th>$\mu_m$</th>
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<tr>
<td>$10^3$</td>
<td>3.643</td>
<td>15.969</td>
<td>34.033</td>
<td>63.040</td>
<td>63.123</td>
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<tr>
<td>$10^4$</td>
<td>3.657</td>
<td>19.273</td>
<td>68.373</td>
<td>214.706</td>
<td>217.371</td>
<td></td>
<td></td>
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<tr>
<td>$10^5$</td>
<td>0.180</td>
<td>0.113</td>
<td>0.069</td>
<td>0.014</td>
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<td></td>
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</tr>
<tr>
<td>$10^6$</td>
<td>1.121</td>
<td>2.262</td>
<td>1.638</td>
<td>8.866</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(c) Error percentages with respect to benchmark

<table>
<thead>
<tr>
<th>Ra</th>
<th>$%$</th>
<th>$y$</th>
<th>$%$</th>
<th>$y$</th>
<th>$\text{Nu}_{\text{ref}}$</th>
<th>$%$</th>
<th>$\text{Nu}_{\text{ref}}$</th>
<th>$%$</th>
<th>$\mu_m$</th>
<th>$%$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^3$</td>
<td>5.01%</td>
<td>-1.23%</td>
<td>-2.01%</td>
<td>-1.22%</td>
<td>-0.77%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$10^4$</td>
<td>-1.08%</td>
<td>-1.75%</td>
<td>-0.32%</td>
<td>-2.12%</td>
<td>-0.68%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$10^5$</td>
<td>-0.35%</td>
<td>0.64%</td>
<td>0.64%</td>
<td>0.77%</td>
<td>0.56%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$10^6$</td>
<td>0.55%</td>
<td>0.33%</td>
<td>0.96%</td>
<td>0.44%</td>
<td>-0.23%</td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

Table 2.1: Numerical results
Chapter 3

Solid-Liquid change of phase and simulation of a thermal energy storage system with phase change material (PCM)

3.1 Introduction

Thermal energy storage systems are an essential feature to make an efficient use of solar energy due to the inherent intermittence of this energy source. These systems allow making use of thermal energy - accumulated in hours of high solar radiation - in moments of lower solar radiation, reducing the mismatch between the supply and demand of the energy. Phase change materials (PCM) provide an effective way of accumulating thermal energy, due to their high capacity to store heat at a constant or near to constant temperature.

This chapter deals with the numerical simulation of thermal energy storage systems with PCM. Numerical simulations are a powerful tool for predicting the thermal behaviour of thermal systems, as well as for optimizing their design.

The system under study is a cylindrical container, filled with spheres containing paraffin wax (PCM) and water occupying the space left between the spheres. Two different processes are studied: charging and discharging. In charging mode, hot water coming from the solar field passes through the container, delivering energy to the PCM spheres. In the discharging mode, cold water from supply comes through, extracting the energy previously stored in the PCM and leaving the tank at a higher temperature.

Firstly, a simplified study similar to the presented by Felix Regin et al. (2009) and Bédérrecats et al. (2009) is developed, where assumptions of one dimensional fluid flow and heat transfer - in the flow and inside the spheres - are made. Results of liquid fraction, outlet temperature and accumulated energy are presented. Comparison against previous works is carried out.

Secondly, in order to account for natural convection inside the PCM spheres, detailed CFD simulations of the solid-liquid phase change are performed using the fixed-grid enthalpy-porosity model (Brent et al. (1988); Voller and Prakash (1987)). Verification and validation of the phase change modelling are performed against previous numerical and experimental results (Costa et al. (1991); Gau and Viskanta)
(1986)). The CFD code is used for modelling the PCM inside the spheres and it is coupled with the simple 1D model of the water, resulting in a more detailed model of the entire system. Simulations of the charging and discharging modes are performed and results obtained are compared against previous 1D analysis results.

The work described in this chapter has generated an article presented in the ISES Solar World Congress 2011 in Kassel, Germany (Galione et al. (2011)).

### 3.2 Simplified modelling (1D)

The mathematical formulation for the heat exchanging fluid (water in the cases studied here) is based on both mass and energy conservation equations. Simplifying assumptions are:

- One-dimensional fluid flow and temperature distribution (in the flow direction).
- Constant density ($\rho$) and specific heat ($C_p$).
- Heat conduction ($k$) in flow direction is not considered.
- Ambient losses are negligible.
- Negligible radiation transfer.

The equations are discretized using the Finite Volume Method as detailed below.

The cylindrical container is divided in $N_x$ equal parts in the axial direction, in which fluid temperature is considered uniform (see Figs. 1 and 2). The spheres are discretized in $N_r$ parts along the radial direction (Fig.2). As 1D conditions are assumed, all the spheres in the same section of container have the same temperature distributions. Therefore, only one sphere per section is simulated.

**Fluid temperature equations:**

$$\rho V_i C_p \frac{\partial T_i}{\partial t} = -\dot{m}C_p(T_{\text{out}}^i - T_{\text{in}}^i) - h_i A_{\text{sph},i}(T_i - T_{\text{cap,ext}}^i) \quad (3.1)$$

where:

$$h = \frac{kNu}{D_{\text{cap,ext}}} \quad (3.2)$$

and

$$Nu = 2.0 + 1.1Re^{0.6}Pr^{1/3} \quad \text{with } 15 < Re < 8500 \quad (Wakao et al. (1979)) \quad (3.3)$$

or,

$$Nu = 18.1Pr^{1/3} \quad \text{with } Re < 40 \quad (Vafai and Sozen (1990)) \quad (3.4)$$

Here, sub-index $i$ indicates the tank section where the temperature is being calculated, $T_{\text{out}}^i$ and $T_{\text{in}}^i$ are the temperatures of outgoing and ingoing flows from and into the tank control volume and $T_{\text{cap,ext}}^i$ the temperature of the PCM capsule.
3.2. Simplified modelling (1D)

external surface. $V_i$ is the volume of the tank section, $A_{sph}$ is the area of the external surface of the capsules contained in the section and $\dot{m}$ is the fluid mass flow. Here, Reynolds number is calculated using the superficial velocity:

$$Re = \frac{\dot{m} D_{cap,ext}}{\mu A}$$ (3.5)

where $A$ is the cross-sectional area of the tank.

As the ranges of validity of eqs. (3.3) and (3.4) are overlapped, two different values of $Nu$ could be obtained for the same $Re$; in which case, the highest of both has been considered.

Sphere temperature equations, inner nodes:

$$\frac{\partial H_{i,j}}{\partial t} = \left(kA \frac{\partial T}{\partial r}\right)_{i,j-1/2} - \left(kA \frac{\partial T}{\partial r}\right)_{i,j+1/2}$$ (3.6)

Where the sub indices $j - 1/2$ and $j + 1/2$ indicate the boundaries of the control volume $j$, near to the wall and to the center of the sphere, respectively. $A$ indicates the area of surface limiting adjacent control volumes of sphere and $r$ indicates the radial direction.

Sphere temperature equations, boundary node:

$$\frac{\partial H_{i,0}}{\partial t} = \frac{T_{f,i} - T_{f,0}}{R_{conv} + R_{cap}} - \left(kA \frac{\partial T}{\partial r}\right)_{i,1/2}$$ (3.7)

where $R_{conv} = \frac{1}{k_f A_{cap,ext}}$ and $R_{cond} = \frac{1}{4\pi k_{cap}} \left(\frac{1}{r_{cap,int}} - \frac{1}{r_{cap,ext}}\right)$. Sub-index $f$ indicate the fluid flow, and sub-indices $cap,ext$ and $cap,int$ indicate the external and internal surfaces of capsule, respectively.

To solve these equations, it is necessary to define a relation between enthalpy and temperature of the PCM. The material used as PCM in this work is paraffin wax, which has a range of phase change temperatures rather than a unique temperature.
Chapter 3. Solid-Liquid change of phase and simulation of a thermal energy storage system with phase change material (PCM)

(i.e. during heating there is an increase in temperature between the onset and the end of the melting process). Therefore, a function that relates enthalpy and temperature can be defined. Nevertheless, as a first approximation we are also interested in modelling the constant temperature phase change, because in the CFD simulations described in the next subsection this condition is assumed.

The enthalpy - temperature relation is defined by eqs. (3.10) to (3.10) for the constant temperature phase change and by eqs. (3.11) to (3.14) for the variable phase change temperature, similarly as in Felix Regin et al. (2009).

Constant phase change temperature:

\[ h = C_{ps} T, \quad T < T_{sl} \]  
\[ h = C_{ps} T + \epsilon L, \quad \text{with}\ \epsilon = \frac{h - h_s}{L}; \quad h_s < h < h_l; T = T_{sl} \]  
\[ h = C_{pl}(T - T_{sl}) + C_{ps}T_{sl} + L, \quad T > T_{sl} \]  

Where \( T_{sl} \) indicates the phase change temperature and \( \epsilon \) the liquid fraction.

Variable phase change temperature:

\[ h = C_{ps} T, \quad T < T_{sl} \]  
\[ h = C_{ps} T + \epsilon L, \quad \text{with}\ \epsilon = \frac{T - T_s}{T_l - T_s}; \quad T_s < T < T_{sl} \]  
\[ h = C_{pl}(T - T_{sl}) + C_{ps}T_{sl} + \epsilon L, \quad \text{with}\ \epsilon = \frac{T - T_s}{T_l - T_s}; \quad T_{sl} < T < T_l \]  
\[ h = C_{pl}(T - T_{sl}) + C_{ps}T_{sl} + L, \quad T > T_l \]  

Where \( T_{sl} \) indicates the temperature in the phase change range (\( T_s < T_{sl} < T_l \)) beyond which the material has a mostly liquid behavior, and below which it behaves mostly as solid.

Actually, in the 1D model, variable phase change formulation is used to simulate constant phase change by defining \( T_s \) and \( T_l \) very close to \( T_{sl} \). This strategy is adopted because 1D analysis was based on finding temperature values instead of enthalpy values, so there is a need to be able to identify every state with its temperature, which is not verified by the constant phase change formulation. However, for the detailed CFD analysis, the above indicated formulation is indeed used.

For the temporal discretization a 1st order fully implicit scheme is chosen. Furthermore, an upwind-like scheme is used to determine the temperatures of the flow entering and leaving each section. Thus, the temperature of the fluid entering each section of the tank becomes the same as the temperature of the fluid in the upstream section, and the leaving fluid temperature the same as the one of the present section. This scheme allows to adopt a step by step method to solve the entire tank, first solving the section where the inlet is placed (in the top or bottom of the tank), then the next section downstream, and so on advancing in the direction of the flow, without needing to iterate.

In each section, fluid and PCM temperatures have to be solved. The final matrix of coefficients derived from the system of equations in each container section has a tri-diagonal pattern, thus a TDMA algorithm is used to solve the linear system. This formulation is implemented in a simple computer code intended
to simulate the behavior in charging and discharging modes of the whole energy accumulation system. A simulation of 10 hours of operation takes only a few seconds of computations in a single conventional CPU core (here used: Intel Core i-5 2300 2.8GHz).

Current formulation includes the implicit assumption that there is no need to refine the container subdivisions further than one sphere’s diameter high; as it is considered that each sphere “sees” a uniform temperature of fluid. This constraint does not allow modelling a system with “big” spheres that make this assumption too coarse. However, as our intention was to simulate an efficient energy accumulation device, it is acceptable to think that the size of sphere used would be much smaller than the height of the tank, in order to maximize the relation of heat transfer area over volume of PCM.

Results presented in this work were obtained with $N_x = 24$ and $N_r = 12$. Some tests have been carried out with finer grids, and the results obtained were very close to the presented here, indicating acceptable grid independence.

### 3.3 Detailed modelling of the change of phase (2D - 3D)

When the PCM inside the spheres are changing phase, natural convection is produced due to the difference between solid and liquid densities and gravity action. To simulate this phenomenon, Navier-Stokes and energy equations are numerically solved. Some simplifying assumptions are made:

- Incompressible fluid.
- Boussinesq approximation (density is considered constant, except in the gravity forces term).
- Constant thermo-physical properties and equal between solid and liquid states.

Based on the above mentioned hypotheses and adopting the enthalpy-porosity model to account for the phase change phenomenon (Voller and Prakash (1987); Brent et al. (1988)), mass, momentum and energy equations can be written in the following form:

\[ \nabla \cdot \vec{u} = 0 \quad (3.15) \]
\[ \frac{\partial \rho \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = -\nabla P_d + \mu \nabla^2 \vec{u} - \rho g \beta (T - T_0) \hat{j} - S \vec{u} \quad (3.16) \]
\[ \frac{\partial h}{\partial t} + \nabla \cdot (\rho \vec{u} C_{pl} T) = -\nabla \cdot (k \nabla T) \quad (3.17) \]

Where the enthalpy $h$ includes both sensible and latent components. The source term $-S \vec{u}$ is introduced into the momentum equation to account for the presence of solid in the control volumes. Its final form depends on the porosity (or liquid fraction), as explained in Voller and Prakash (1987) and in Brent et al. (1988).

#### 3.3.1 Discussion about the form of the energy equation

In Brent et al. (1988) and Voller and Prakash (1987) the differential equation for the energy balance in the phase changing process is presented as:
Chapter 3. Solid-Liquid change of phase and simulation of a thermal energy storage system with phase change material (PCM)

\[
\frac{\partial h}{\partial t} + \nabla \cdot (\rho u h) = -\nabla \cdot (k \nabla T) \tag{3.18}
\]

This equation has a slight difference compared to (3.17): the advection-convection term. The transported property in (3.18) is total enthalpy (including latent), while in (3.17) only the sensible part of the enthalpy is considered to be transported by the flow.

In pure solid and liquid phases there is no difference at taking any of both energy equations. This is because in the solid phase there is no enthalpy transport and in the liquid phase only differences in sensible enthalpy are needed to be accounted for, as only one phase is involved. However, in the regions (or control volumes) where both liquid and solid phases are present (i.e. interface nodes), the volume integration of both formulations give different results.

As the interface will not be infinitesimal in our simulations, due to the adopted numerical model, there will be control volumes that will contain the interface and where the fluid part will have a velocity different from zero. Furthermore, mass and energy will be entering and leaving these “interface” control volumes, and these interactions will be produced between liquid and interface nodes and also between different interface nodes. Thus, discretized momentum and energy equations will have non-zero advective terms in these control volumes (see section 3.3.3 below).

Regarding the energy equation, if we chose to evaluate its convective term taking the total enthalpy \( h \) as the transported property, then we would be transporting a variable that depends on the liquid fraction of the involved nodes (see eq. (3.9)); i.e. we would be transporting a “mean value” of the enthalpy of the solid and liquid phases of the involved control volumes. This is not right, as only the liquid phase is transported from one node to the other (assuming that the solid is fixed with respect to the grid). Therefore, only the enthalpy of the liquid phase is advected, and so, only differences in the sensible enthalpy of the liquid phase have to be included in the convective term.

In our simulations, notable differences have been observed by the adoption of total or liquid sensible enthalpy in coarse grids, although they tend to vanish as the grid is refined. It should be noted that these differences are produced by the discretization of the equations and by the fact that in one control volume both solid and liquid phases are present. This does not mean that eq. (3.18) is wrong; it is a differential equation and so can only be strictly applied to infinitesimally small volumes.

### 3.3.2 Nondimensionalization of the equations

To minimize the number of parameters on which the problem depends, nondimensionalization of the equations is carried out. The resulting dimensionless equations is shown in eqs. (3.19) to (3.24).

If \( L \) is a characteristic length and \( T_1 \) and \( T_0 \) characteristic temperatures of the problem:

\[
\mathbf{r} = (x, y, z) \implies \mathbf{r}^* = (x^*, y^*, z^*) \quad \text{(dimensionless position vector)}
\]

\[
\mathbf{u} = (u, v, w) \implies \mathbf{u}^* = (u^*, v^*, w^*) \quad \text{(dimensionless velocity)}
\]

and

\[
\mathbf{r}^* = \frac{\mathbf{r}}{L}; \quad t^* = \frac{t}{L^2}; \quad \phi = \frac{T - T_0}{T_1 - T_0}; \quad h^* = \frac{h}{C_p(T_1 - T_0)}
\]

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\[ \vec{u}^* = \vec{u}_L \alpha; \quad P_d^* = \frac{P_d L^2}{\rho \alpha^2}; \quad \nabla^* = L\nabla \]

and we obtain:

\[ \nabla^* \cdot \vec{u}^* = 0 \] (3.19)

\[ \frac{\partial \vec{u}^*}{\partial t^*} + (\vec{u}^* \cdot \nabla^*) \vec{u}^* = -\nabla^* P_d^* + Pr(\nabla^*)^2 \vec{u}^* - RaPr\phi j - S^* \vec{u}^* \] (3.20)

\[ \frac{\partial h^*}{\partial t^*} + \nabla^* \cdot (\vec{u}^* \phi) = -\nabla^* \cdot (\nabla^* \phi) \] (3.21)

where: \( Pr = \frac{\mu}{\rho \alpha}; \quad Ra = \frac{\rho g\beta \alpha L^3 (T_1 - T_0)}{\mu \alpha}; \quad S^* = \frac{L^2}{\alpha} S \)

Nondimensionalizing enthalpy-temperature relations (3.8) to (3.10) they remain:

\[ h^* = \phi + \frac{T_0}{T_1 - T_0}, \quad \phi < \phi_{sl} \] (3.22)

\[ h^* = f \frac{St e}{\phi_{sl}} + \frac{T_0}{T_1 - T_0}, \quad \phi = \phi_{sl} \] (3.23)

\[ h^* = \phi + Ste^{-1} + \frac{T_0}{T_1 - T_0}, \quad \phi > \phi_{sl} \] (3.24)

where:

\[ Ste = \frac{C_p(T_1 - T_0)}{L} \]

where either \( T_1 \) or \( T_0 \) are taken as the phase change temperature.

Therefore, the parameters of the problem are reduced to: \( Pr, Ra, Ste, S^* \), besides the ones that could arise from nondimensionalizing the boundary conditions.

The adoption of the fixed grid enthalpy-porosity method simplifies considerably the problem of placing the solid-liquid interface, as it is determined by the volume fraction \( \epsilon \). The control volumes or nodes of the mesh that have a value of \( \epsilon \) between 0 and 1 contain part of the interface. This procedure has the advantage of not having to solve more equations to find the interface and that the mesh does not have to be modified to follow the interface as in the interface tracking methods. However, it has the disadvantage of not being able of exactly determining the position of the interface.

3.3.3 Time discretization of the equations

We proceed to discretize the governing equations the same way as in previous chapters. The time scheme adopted here is an explicit 2nd order Adams-Bashforth scheme. To decouple pressure and velocity from the momentum equations we use the previously mentioned Fractional Step Method. From now on we assume that the equations are dimensionless and suppress the * for simplicity.

\[ \nabla \cdot \vec{u}^{n+1} = 0 \] (3.25)
Chapter 3. Solid-Liquid change of phase and simulation of a thermal energy storage system with phase change material (PCM)

\[
\frac{\bar{u}^{n+1} - \bar{u}^n}{\Delta t} = \frac{3}{2} R(\bar{u}^n) - \frac{1}{2} R(\bar{u}^{n-1}) - \nabla p^{n+1} - \tilde{f}^{n+1} \tag{3.26}
\]

\[
\frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{3}{2} R(\phi^n) - \frac{1}{2} R(\phi^{n-1}) \tag{3.27}
\]

where:

\[
\tilde{f}^{n+1} = S^* \bar{u}^{n+1} + RaPr \phi^{n+1} \cdot \hat{j} \tag{3.28}
\]

And applying the Fractional Step Method:

\[
\bar{u}^p = \bar{u}^n + \Delta t \left[ \frac{3}{2} R(\bar{u}^n) - \frac{1}{2} R(\bar{u}^{n-1}) - RaPr \phi^{n+1} - S \bar{u}^{n+1} \right] \tag{3.29}
\]

\[
\bar{u}^{n+1} = \bar{u}^p - \Delta t \nabla p^{n+1} \tag{3.30}
\]

\[
\Delta t \Delta p^{n+1} = \nabla \cdot \bar{u}^p \tag{3.31}
\]

The difference between this formulation and the one presented in chapter 2 is the form of source term vector \( \tilde{f} \). Here it has the additional term \( S \bar{u}^{n+1} \). This difference is important because it makes the predictor velocity \( \bar{u}^p \) depend on \( \bar{u}^{n+1} \), so the problem ceases to be fully explicit and we cannot calculate \( \bar{u}^p \) from the previous velocity fields. Expressing this source term using \( \bar{u}^n \) instead of \( \bar{u}^{n+1} \) is not an option because it would make the system unstable, as explained next.

The source term coefficient \( S \) is positive and - as indicated in Brent et al. (1988), Voller and Prakash (1987) and Costa et al. (1991) - it depends on the liquid fraction of the control volume, tending to infinity as \( \epsilon \) tends to zero. In the differential momentum equations, this makes the velocity near solid control volumes tend to zero. However, in the discretized equations, if an explicit time scheme is used, it results in an equation where the new velocity depends on the last velocity times \( \Delta t \) multiplied by a factor tending to infinity. Thus, the time step adopted to make the system stable would have to be infinitesimal. This can be more clearly seen by working with a simplified differential equation of the type:

\[
\frac{\partial u}{\partial t} = -Su \quad \text{where} \quad S > 0
\]

and watching what happens when \( S \to \infty \). The solution of this equation is:

\[
u(t) = u_0 e^{-S(t-t_0)} \quad \text{with} \quad u(t_0) = u_0 \]

It can be seen that

\[ S \to \infty \implies u(t) \to 0 \quad \text{and} \quad u_0 > 0 \quad \implies \quad u(t) > 0 \quad \forall t \]

Discretizing the differential equation using an explicit time scheme, it results in:

\[
u^{n+1} = u^n - \Delta t Su^n
\]
To keep the restriction of not crossing the zero limit, the time step $\Delta t$ has to be limited:
\[
u^n > 0 \implies \nu^{n+1} > 0 \implies \nu^n(1 - \Delta tS) > 0 \implies \Delta t < \frac{1}{S}
\]
Then,
\[S \rightarrow \infty \implies \Delta t \rightarrow 0\]

Therefore, the explicit formulation is unstable. To overcome this problem we adopt the following strategy.

The final form of the source term coefficient ($S$) depends on the approximation adopted for the behavior of the flow in the “mushy zone” (where mixed solid and liquid states are present). However, in the case of constant phase change temperature, the solid-liquid interface should be of infinitesimal width (Brent et al. (1988)) (although it cannot be thinner than the width of one control volume in our simulations); therefore, the formulation used for the source term is not very important in a physical sense, as long as it manages to bring the velocity to zero in mostly solid control volumes and to vanish if the volume contains pure liquid. Taking this into account, we modify the source term in our formulation making it depend on the predictor velocity instead of the actual velocity, which simplifies our problem. The resulting equation for the predictor velocity becomes the following:

\[
\begin{align*}
\vec{u}^p &= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} - S\vec{u}^p \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} - S\vec{u}^p \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} - S\vec{u}^p \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} \right] \\
&= \vec{u}^n + \Delta t \left[ \frac{3}{2} R(\vec{u}^n) - \frac{1}{2} R(\vec{u}^{n-1}) - RaPr\phi^{n+1} \right]
\end{align*}
\]
(3.32)

Then, if $S \rightarrow \infty$, $u^p \rightarrow 0$ and $\nabla \cdot u^p \rightarrow 0$. Thus, from (3.31):
\[
\Delta t \Delta p^{n+1} = 0 \quad (3.33)
\]

The solution of the system determined by (3.33) is a constant pressure field. Then, from (3.30):
\[
\vec{u}^{n+1} = 0 \quad (3.34)
\]

which is what we were looking for.

Furthermore, the usage of an explicit time scheme allows us to explicitly set the velocity in the solid nodes to zero, not needing to solve momentum equation in these nodes as with the implicit schemes used by Costa et al. (1991), Voller and Prakash (1987) and Brent et al. (1988).

In Costa et al. (1991), Brent et al. (1988), the form of $S$ was obtained by assuming that the “mushy zone” should be treated as a porous material. However - as we have previously mentioned - in constant phase change temperature materials we could take “any” expression that fulfill the requirements of vanishing in liquid nodes and of bringing velocity down to zero in near solid ones.
Then, taking into account stability issues Brent et al. (1988) we look for an expression of $S$ that make the evolution of $u^p$ with $\epsilon$ smoothly. More specifically, we adopt a linear variation of $u^p$ with $\epsilon$. That is:

$$S = \frac{1}{\epsilon} - 1 \implies u^p = \epsilon \{\bar{u}^n + \Delta t \left[ \frac{3}{2} R(\bar{u}^n) - \frac{1}{2} R(\bar{u}^{n-1}) - Ra Pr \phi^{n+1} \right] \}$$

### 3.3.4 Some considerations regarding the convective and diffusive terms of the momentum equations

The fact of having control volumes where both solid and liquid phases are present, has some implications on the discretization of the diffusive and convective terms of the momentum equations.

As mentioned above, the use of an explicit time scheme allows to “turn off” the velocity in the solid nodes without needing to “solve” the momentum equations in these control volumes. However, as the interface nodes do have velocities associated to the liquid part in them, momentum equations have to be solved in these control volumes.

In a 2D structured grid - taking the same notation for the nodes coordinates as in Patankar (1980) (see fig. 1.1)- this term can be expressed by eq. (1.9).

At the interface nodes, some of its faces could be limiting with purely solid control volumes (see fig. 3.2). In these cases the resulting approximation of the derivative is:

$$\frac{\partial u_e}{\partial x} \approx \frac{u_E - u_P}{\Delta x} = \frac{0 - u_P}{\Delta x} = -\frac{u_P}{\Delta x} \quad \text{if face } e \text{ limits with solid}$$

$$\frac{\partial u_w}{\partial x} \approx \frac{u_P - u_W}{\Delta x} = \frac{u_P - 0}{\Delta x} = \frac{u_P}{\Delta x} \quad \text{if face } w \text{ limits with solid}$$

$$\frac{\partial u_n}{\partial y} \approx \frac{u_N - u_P}{\Delta y} = \frac{0 - u_P}{\Delta y} = -\frac{u_P}{\Delta y} \quad \text{if face } n \text{ limits with solid}$$

$$\frac{\partial u_s}{\partial y} \approx \frac{u_P - u_S}{\Delta y} = \frac{u_P - 0}{\Delta y} = \frac{u_P}{\Delta y} \quad \text{if face } s \text{ limits with solid}$$

However, we know that the velocities over the faces themselves should be zero, as no flow can go throw the solid and because of the no-slip condition. Thus, a better approximation of the derivatives of the velocities at these faces is:

$$\frac{\partial u_e}{\partial x} \approx \frac{u_E - u_P}{\Delta x} = \frac{2(0 - u_P)}{2\Delta x} = -\frac{2u_P}{\Delta x} \quad \text{if face } e \text{ limits with solid}$$

$$\frac{\partial u_w}{\partial x} \approx \frac{u_P - u_W}{\Delta x} = \frac{2u_P - 0}{2\Delta x} = \frac{2u_P}{\Delta x} \quad \text{if face } w \text{ limits with solid}$$

$$\frac{\partial u_n}{\partial y} \approx \frac{u_N - u_P}{\Delta y} = \frac{2(0 - u_P)}{2\Delta y} = -\frac{2u_P}{\Delta y} \quad \text{if face } n \text{ limits with solid}$$

$$\frac{\partial u_s}{\partial y} \approx \frac{u_P - u_S}{\Delta y} = \frac{2u_P - 0}{2\Delta y} = \frac{2u_P}{\Delta y} \quad \text{if face } s \text{ limits with solid}$$

Fig. 3.2 show two sketches of part of a grid, where the three “phases” are present - liquid, solid and interface - in which the faces where the modifications of the diffusive term have to be implemented are indicated.
3.3. Detailed modelling of the change of phase (2D - 3D)

(a) Staggered. The velocity nodes that are placed in faces shared by interface and solid control volumes (associated to pressure nodes) are set to zero (crossed out).

(b) Centered

Figure 3.2: Scheme of a structured mesh of a part of a system having liquid, interface and solid phases for staggered and centered schemes. The black bold line indicates an hypothetical form of the interface line. Black dots indicate the pressure nodes, where also the liquid fraction is defined. Pressure control volumes are coloured by its state: red - liquid, green - interface, blue - solid. Red arrows indicate the velocity nodes where the diffusive and convective terms are modified, for its associated control volumes (indicated by the fine dashed boxes) share one or more faces with pure solid nodes. Red circles indicate these faces.

The convective term should also be modified in the nodes adjacent to pure solid control volumes. Normally, using a symmetry preserving scheme (Verstappen and Veldman (2003)), face velocities are evaluated as the mean value of neighbouring nodes:

\[
    u_e = \frac{u_P + u_E}{2} ; \quad u_w = \frac{u_P + u_W}{2} ; \quad u_n = \frac{u_P + u_N}{2} ; \quad u_s = \frac{u_P + u_S}{2}
\]

But in solid-neighbouring nodes, this formulation would lead to values different from zero in the faces shared with the pure solid zone. Then, at these faces, the zero velocity condition is explicitly imposed (see fig. 3.2).

3.3.5 Treatment of the pressure in the solid phase

The pressure is only needed to be solved inside the fluid phase, as finding the tensional state of the solid is not necessary for our purposes. However, as our system of equations is defined for the entire mesh, we need to solve the pressure equation (3.31) for all the nodes - including the solid ones.

The discretized equations for the fluid phase and for the interface are eqs. (1.23). We define then the equations in the solid nodes by setting trivial equations of the form:

\[ p_s = b_s \]

41
where the sub-index $s$ indicates that this is done for each of the solid nodes. $b_s$ can be any value that we choose, for example, zero.

Furthermore, we need to decouple the pressure nodes belonging to the solid from the ones belonging to the fluid and to the interface. In other words, between interface and solid (or liquid and solid in some cases) we apply the same condition applied for the boundaries where fluid is in contact with solid, i.e. the derivative of the pressure with respect to the normal of the boundary equals zero (eq. (1.25)).

Assuming that face $e$ is in contact with a solid control volume, we impose:

$$\frac{\partial p_e}{\partial x} = 0$$

and eq.(1.24) becomes:

$$\frac{1}{V} \sum_{f=e,w,n,s} (\nabla p \cdot \hat{n})_f A_f = \frac{1}{\Delta x}(-\frac{\partial p_w}{\partial x}) + \frac{1}{\Delta y} \left( \frac{\partial p_n}{\partial y} - \frac{\partial p_s}{\partial y} \right)$$

Where the node $P$ is decoupled from node $E$ (solid node).

### 3.3.6 Verification and validation of the modelling of the change of phase

The solid-liquid phase change modelling was both implemented into the previously developed code (in the resolution of Driven and Differentially Heated Cavity problems) and into a CFD code called TermoFluids (Lehmkuhl et al. (2009)), which was developed by TERMOFLUIDS S.L. (a spin off of the Technological Center of Heat Transfer of the Universitat Politècnica de Catalunya (CTTC - UPC)) intended to work with unstructured meshes and parallel computing.

To verify and validate the behaviour of these new phase change modelling tools, experimental and numerical results found in the bibliography were used.

**Gallium melting**

Firstly, a case of Gallium melting in a rectangular cavity (Gau and Viskanta (1986); Costa et al. (1991); Vidal (2007)) was simulated. The problem is 2D and consists of a rectangular cavity of aspect ratio $A_r = 0.5$ filled with Gallium in solid state. Top and bottom walls are adiabatic, while left and right walls are set to uniform temperatures. Initially, all the system is at a temperature slightly below the phase change. Suddenly, the left wall temperature is increased above the phase change and heat starts to enter the cavity, melting the Gallium. Natural convection is observed and the phase change interface starts to be deformed from its initial vertical-line shape.

The parameters of the problem are the following:

- Aspect ratio $A_r = 0.5$, $H(\text{height}) = 0.0445m$;
- $\rho = 6093 \text{ kg m}^{-3}$, $k = 32 \text{ W m}^{-1} \text{ K}^{-1}$, $C_p = 381.5 \text{ J kg}^{-1} \text{ K}^{-1}$;
- $Ra = 2.1E5$, $Pr = 0.0216$, $Ste = 0.0419$
3.3. Detailed modelling of the change of phase (2D - 3D)

Figure 3.3: Temperature contours and solid-liquid interface position of the melting gallium in the rectangular cavity, at time $t = 6$ min. The dots indicate the location of the interface obtained experimentally by Gau and Viskanta (1986).

Figure 3.4: Temperature contours and solid-liquid interface position of the melting gallium in the rectangular cavity, at time $t = 17$ min. The dots indicate the location of the interface obtained experimentally by Gau and Viskanta (1986).

Figure 3.5: Evolution of $NuRa^{-0.25}$ with dimensionless time $\tau = FoSt.eA^2$ (as in Gau and Viskanta (1986)). GV Exp: experimental results from Gau and Viskanta (1986). MC Num: Numerical results from Costa et al. (1991).

- Initial temperature of 28.3°C, hot wall temperature of 38°C and phase change temperature of 29.78°C.
Figures 3.3 and 3.4 show the interface position as well as temperature contours and fig. 3.5 shows a correlation between $NuRa^{-0.25}$ and dimensionless time $\tau$ as in Gau and Viskanta (1986). Results obtained are very similar to previous numerical ones from Costa et al. (1991) and very close to experimental ones, as it is shown in the above figures. Some causes of discrepancy between numerical and experimental results might be found in the facts that in the experimental setup the configuration is not exactly 2D (presence of front and back walls) and that left wall temperature does not reach its final value until some time has passed.

Different mesh densities have been used, and results show that a mesh density of 80x40 is enough to obtain quite accurate results at later times. However, with this mesh, a true converged solution is not yet obtained. This is concluded by the fact that by further grid refinement, notable differences with the results obtained with the 80x40 grid - at the initial moments of the simulation - are observed. These differences consist in a multicellular behaviour of the fluid part, not observed in the experimental results presented by Gau and Viskanta (1986). This aspect is taken into account in the next section, where the melting of pure tin is simulated.

**Melting of pure tin**

This problem is very similar to the one of gallium melting and is based on the experimental work of Wolff and Viskanta (1987). A square cavity is filled with tin, initially at solid state at the phase change temperature. Suddenly, the left wall is heated to a uniform higher temperature and the tin starts to melt from the left to the right walls. Top and bottom walls are adiabatic, while the right wall stays at the phase change temperature.

As the solid temperature cannot rise above the phase change temperature and the right wall is maintained constant, the solid is isothermal at every moment. Taking advantage of this fact, the simulations are run only over a portion of the whole cavity, since the objective is not to simulate the entire melting process but only the first 1000 - 2000 seconds.

The parameters of the problem - taken from Hannoun et al. (2003) - are the following:

- Aspect ratio $A_r = 1$, $H(height) = 0.1m$;
- $\rho = 7500 \text{ kg m}^{-3}$, $k = 60 \text{ W m}^{-1} \text{ K}^{-1}$, $C_p = 200 \text{ J kg}^{-1} \text{ K}^{-1}$;
- $Ra = 2.25E5$, $Pr = 0.04$, $Ste = 0.01$
- Initial temperature of 505 K, hot wall temperature of 508 K and phase change temperature of 505 K.

Figure 3.6 show the results obtained after 200, 450 and 1000 seconds. Most notorious differences are observed at 200 seconds between 100x100 and 400x400 meshes, although they are much more subtle than the obtained by Hannoun et al. (2003). Simulations with 200x200 and 400x400 meshes are very similar between them at all moments shown. For simulations at 450 and 1000 seconds, the three mesh densities give almost the same results.

Hannoun et al. (2003) presents several simulations of the problem using diverse numerical schemes (upwind, centered and hybrid) and the same mesh densities as the adopted in this work. They obtain quite different results between different numerical schemes and also between different meshes, specially at the 200 s results.
3.3. Detailed modelling of the change of phase (2D - 3D)

(a) Mesh: 100 x 100

(b) Mesh: 200 x 200

(c) Mesh: 400 x 400

Figure 3.6: Tin melting at times: 200 s (left column), 450 s (center column) and 1000 s (right column); with different grid densities. Red region: liquid. Green region: interface. Blue region: solid. Contours show streamlines, coloured by velocity magnitude. The images show a portion of the total cavity of 0.06 m x 0.1 m.
Chapter 3. Solid-Liquid change of phase and simulation of a thermal energy storage system with phase change material (PCM)

All our results are close to at least some of the obtained by Hannoun et al. (2003). In general, it could be said that they are most comparable to the presented by Hannoun et al. (2003) using an upwind scheme with a mesh of 400x400.

As stated in Hannoun et al. (2003), numerical solutions deviate considerably from experimental results obtained by Wolff and Viskanta (1987), as in the latter, apparently there is no multicellular behaviour like the obtained in the numerical simulations. They also observe that the results obtained with coarser grids are closer to experimental than the grid-converged simulations.

Evidently there is a problem, either with the mathematical model or with the experimental procedure not being able to meet the assumptions. However, overall behaviour is indeed similar between the experiments and the numerical modelling, and the results become more similar at more advanced time instants. Therefore, it is assumed here that the mathematical model is acceptable for our purposes.

Spherical capsules filled with N-Octadecane

Another case study used to validate the CFD phase change model is the melting of N-octadecane encapsulated in a sphere, as in Tan (2008) and Tan et al. (2009). A spherical capsule is filled with this material and taken to a temperature 1°C below the phase change. Suddenly, the capsule shell is heated and maintained at a constant temperature. Again, the phenomenon is assumed to be 2D. Parameters of the problem are:

- $D = 0.10166 \, m$ (diameter of sphere);
- $\rho = 772 \, kg \, m^{-3}$, $k = 0.1505 \, W \, m^{-1} \, K^{-1}$, $C_p = 2330 \, J \, kg^{-1} \, K^{-1}$;
- $Ra = 3.307E7$, $Pr = 59.76$, $Ste = 0.112913$
- Initial temperature of 27.2°C, hot wall temperature of 40°C and phase change temperature of 28.2°C.

The mesh used to discretize the domain is unstructured, and the simulations were carried out using TermoFluids (Lehmkuhl et al. (2009)), with the addition of the solid-liquid phase change modelling tools. The time scheme used is not exactly 2nd order Adams-Bashforth, but a similar one that takes into account an estimation of the eigenvalues of the transition function and finds an optimal one-leg 2nd order explicit scheme (for further details see Trias and Lehmkuhl (2011)).

Figure 3.7: Results of experiment and numerical simulation of the melting N-Octadecane in a spherical capsule, performed by Tan et al. (2009), at 40 and at 80 min.
3.4. Coupling of the models of the fluid flow (1D) and the PCM (CFD)

![Figure 3.8: Our results. Left half of the spheres show velocity vectors and enthalpy map. Right half of the spheres show temperature contours and map](image)

Fig. 3.7 shows two photographs of the experimental evolution of the phase change at different moments extracted from Tan (2008) and some results of the simulations performed by Tan et al. (2009). Fig. 3.8 shows some graphical results obtained by the present work. The mesh used in our simulations was designed to have similar quantity of nodes - between 7600 and 7700 cells - as the one used by Tan et al. (2009). There is an agreement in the overall behavior of the system, although a faster melting is encountered in numerical results from both authors, compared to experimental. However, it can be seen that the results presented here seem to be closer to experimental than the presented by Tan et al. (2009).

As in the gallium melting case, the faster melting obtained by the numerical simulations might be explained by the fact that a sudden rise of the temperature of the capsule shell is assumed, while in the experimental setup there is a natural delay in this temperature increase.

3.4 Coupling of the models of the fluid flow (1D) and the PCM (CFD)

To simulate the entire system (container with water and PCM spheres), detailed CFD was used to simulate the spheres - assuming 2D behavior - and coupled with the simple water flow 1D model previously described.

The tank was subdivided into 24 sections ($N_x = 24$) along the vertical direction, each one of them resulting to be a thin cylinder of area $A$ and height $\Delta x = \frac{H}{N_x}$. As in the simple 1D model, only one sphere is simulated in each division, assuming that all the spheres in a section have the same behaviour.

The algorithm adopted to solve the problem is the following:

1. Set initial conditions for the whole system (fluid and PCM spheres).

2. Calculate next time step in all inner nodes (not boundary nodes) of the sphere.
   As an explicit scheme is adopted, boundary nodes at the new time step are not needed at this point.
3. Calculate the heat transferred through the wall of the capsule associated to each section of the tank \((Q_i)\), making a global energy balance of the sphere:

\[
Q_i = \sum_j \rho V_{j,i} (h_{j,i}^{n+1} - h_{j,i}^n)
\]  

(3.35)

where the subindex \(i\) indicates the tank section, \(j\) indicates the inner nodes and \(n\) and \(n + 1\) the time steps. This calculation does not need the values in the boundary nodes at the new time step because these nodes do not have an associated volume but only a surface.

4. Calculate the temperature of the fluid flow in each section of container, making an energy balance using previously calculated heat transferred to (or from) the PCM sphere. The equation used for this task is eq. (3.1), but instead of calculating the heat transferred to the capsules, previously calculated value is used; then:

\[
\rho V_i C_p \frac{\partial T_i}{\partial t} = -m C_p (T_{out,i} - T_{in,i}) - Q_i
\]  

(3.36)

This equation is discretized using a backwards Euler 1st order explicit scheme. At this point, a heat transfer coefficient \(U\) can be calculated, using the following equation:

\[
U_i = \frac{1}{\frac{A_{cap, int}}{h_{ext,i}} + R_{cond}}
\]  

(3.37)

where \(R_{cond} = \frac{e_{cap} D_{cap, ext}}{k D_{cap, int}}\) is the thermal resistance of the capsule shell. Here, \(A_{cap, int}\) and \(A_{cap, ext}\) are the inner and outer surfaces of the capsule shell, \(h_{ext,i}\) the fluid heat transfer coefficient calculated by eq. (3.2).

5. With the obtained fluid temperatures and heat transfer coefficients for each section, boundary temperatures for the capsules are calculated for the next time step using the next formula:

\[
T_{b,j,i} = \frac{\left(\frac{k_{PCM}}{d_{j,i}}\right) T_{j,i} + UT_{f,i}}{\frac{k_{PCM}}{d_{j,i}} + U_i}
\]  

(3.38)

which has been derived by making an energy balance at the boundary. \(d_{j,i}\) is the distance between the center of the control volume (inner node) associated with the \(j^{th}\) boundary section and its boundary surface. The term \(\left(\frac{k_{PCM}}{d_{j,i}}\right) T_{j,i}\) accounts for the heat conduction resistance between the boundary and the inner node.

6. Go back to step 2

Each sphere was simulated using a 2D mesh of a slice, divided into 547 control volumes (see Fig. 3.9(a)). Some tests were made to check the mesh density suitability, simulating one sphere with a mesh of 1774 control volumes (Fig. 3.9(b)) with the same boundary conditions as the sphere of the first subdivision of the tank. The obtained results, although not exactly equivalent, were sufficiently close.
3.5. Results and discussion

(normally less than 5% of discrepancy in local liquid fraction and less than 1% in local fluid temperature).

Given the size of the problem (24 spheres divided into 547 control volumes each) several computers working in parallel were needed to solve it in a reasonable time. After some previous testing, it was concluded that with the available resources (a cluster of AMD Opteron Barcelona 2.1 GHz nodes of 8 cores each, connected through an Infiniband network 4X-DDR 20Gb/s), the best strategy was to group each sphere into one cluster node, so as the network latency would not affect their resolution, i.e. the resolution of the pressure equation (3.31) (which demands most of the time) would not be parallelized between different cluster nodes needing to communicate through the network. Communication between nodes were only needed for the interchanging of fluid flow temperatures of adjacent tank sections.

Final set-up consisted in dividing the mesh of each sphere into two parts, leaving each cluster node in charge of calculating four spheres and tank sections. Hence, a total of 6 cluster nodes (or 48 cores) were necessary to calculate the whole system.

![Figure 3.9: Meshes used for the numerical simulations of the PCM inside the capsules](image)

This more detailed model of the system is much more costly in terms of computational requirements than the previous 1D model. Charging mode was more demanding than discharging, taking around 4 days of computations to simulate 5 hours of operation.

3.5 Results and discussion

In this section, the results of simulating the charging and discharging modes of operation of the thermal energy accumulation system are presented. Following parameters were used in both modes:
• Container dimensions: $H = 1.5 \text{ m}$ (height), $D = 1.0 \text{ m}$ (diameter);

• Capsules dimensions: $\phi_{ext} = 0.04 \text{ m}$ (outer diameter), $w = 0.0004 \text{ m}$ (capsule thickness);

• Paraffin wax as PCM. Thermo-chemical properties in Table 3.1.

• Capsules material: stainless steel.

• Water flow $\dot{m} = 0.0796 \text{ kg s}^{-1}$.

Table 3.1: Thermo-physical properties of paraffin wax used as PCM

<table>
<thead>
<tr>
<th>$\rho$ ($\frac{\text{kg}}{\text{m}^3}$)</th>
<th>$C_{ps}$ ($\frac{\text{J}}{\text{kg K}}$)</th>
<th>$C_{pl}$ ($\frac{\text{J}}{\text{kg K}}$)</th>
<th>$k_s$ ($\frac{\text{W}}{\text{m K}}$)</th>
<th>$k_l$ ($\frac{\text{W}}{\text{m K}}$)</th>
<th>$L$ ($\frac{\text{J}}{\text{kg}}$)</th>
<th>$\beta$ ($\frac{\text{K}}{\text{K}}$)</th>
<th>$\mu$ ($\frac{\text{Ns}}{\text{m}}$)</th>
<th>$T_{sl}$ (°C)</th>
<th>$T_s$ (°C)</th>
<th>$T_l$ (°C)</th>
</tr>
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<tr>
<td>850</td>
<td>2000</td>
<td>2150</td>
<td>0.24</td>
<td>0.22</td>
<td>190</td>
<td>9.1E-4</td>
<td>4.42E-3</td>
<td>59.9</td>
<td>52.9</td>
<td>61.6</td>
</tr>
</tbody>
</table>

3.5.1 Charging mode

In charging mode, the whole system is initially at a uniform temperature of 50°C, and a water flow at 70°C starts entering the tank through the top. Spheres, which were initially at solid state, start to receive heat and eventually to melt.

Fig. 3.10 shows a detail of the liquid flow, enthalpy and temperature maps of a representative sphere in the first section of tank in charging mode, simulated with the CFD model, with the mesh shown in fig. 3.9(b). Natural convection phenomenon is clearly identified.

Figure 3.10: Detail of the first sphere in the tank, in charging mode, at time = 40 min, simulated with the mesh showed in fig. 3.9(b). Left half shows the enthalpy map and velocity vectors, while right half shows the temperature map and contours.

An ascending flow is induced by the higher temperature of the fluid at the capsule shell, arriving to the top of the sphere and then descending to come into contact with the solid part. The liquid flow transfers some of its heat to the solid, getting cooler and descending along the solid boundary.

As the temperature of the capsule is higher than the inner temperature also at the bottom of the sphere, another ascending flow is generated here, with an
opposite spinning sense to the one of the main flow. This flow produces a high heat transfer rate locally, accelerating the melting process at the bottom and deforming the initially spherical shape of the solid portion.

The resulting temperature map and solid shape are appreciably different from the concentric ones that would be obtained if the convection were not present.

It should be noted that, in this work, forces acting on the solid have not been considered. These tend to bring the solid portion down to the bottom of the capsule at some moment of the melting, as shown by Tan (2008), deviating its evolution from the described by our model. These effects should be considered in future works.

In fig. 3.11, all 24 spherical capsules can be observed at time = 220 min. It can be observed that only a few capsules are changing phase.

![Figure 3.11: Representative capsules of the 24 container sections at time = 220 min, coloured by enthalpy values. Left: the whole 24 section capsules. Right: detail of the capsules changing phase.](image)

The numerical results of the simulations of the whole system (tank + capsules) are shown in figs. 3.12 to 3.15, where simplified analysis for constant and variable phase change temperature, as well as detailed constant phase change temperature are included.

Comparing simplified and detailed models for the constant phase change temperature case, it is observed that the differences are rather marginal, especially in the evolution of the global liquid fraction (fig. 3.12(b)), where almost no differences are encountered. However, looking at the evolution of the outlet fluid temperature (fig. 3.13) and at the local liquid fraction over time (figs. 3.14 and 3.15), some discrepancies are revealed, although not very pronounced. From these observations it is concluded that for this case of study the convection is not a very important phenomenon in a global sense, although its effects of enhancing the heat transfer are
Chapter 3. Solid-Liquid change of phase and simulation of a thermal energy storage system with phase change material (PCM)


Figure 3.14: Charging mode. Liquid fraction vs. distance from the top. S.C.: Simple, constant phase change model. D.C.: Detailed const. ph. ch. model.

noticeable at some scale.

However, when comparison is made between constant and variable phase change,
3.5. Results and discussion

Figure 3.15: Charging mode. Liquid fraction vs. distance from the top. S.V.: Simple, variable ph. ch. model.

Quite pronounced differences are observed. Figs. 3.12 and 3.13 reveal that the effectiveness of the heat accumulation system is enhanced significantly by the variable phase change temperature. Phase change starts before than in the constant temperature case (at 52.9°C instead of at 59.9°C) causing an earlier increase in the heat transfer rate (see figs. 3.14 and 3.15), and thus a faster lowering of the water temperature. This is due to the higher thermal inertia of the mixed solid-liquid phase state than that of the pure solid phase. These observations are in concordance with Felix Regin et al. (2009); although results are not the same, which is probably due to the differences in the assumptions adopted in both analyses.

3.5.2 Discharging mode

Discharging mode is characterized by an initial state of uniform temperature of 70°C of the whole system, and a water flow entering at 50°C from the bottom of the container. The PCM, initially in the liquid state, starts to release heat though the capsule shell and eventually to solidify.

In this case, the detailed simulations show that although natural convection is indeed produced, it does not have a strong effect on interface shapes nor on temperature distributions, which are almost exactly concentric to the spherical capsule shell.

Chapter 3. Solid-Liquid change of phase and simulation of a thermal energy storage system with phase change material (PCM)


Figure 3.18: Discharging mode. Liquid fraction vs. distance from the bottom. S.C.: Simple, constant phase change model. D.C.: Detailed const. ph. ch. model.

Figure 3.19: Discharging mode. Liquid fraction vs. distance from the top. S.V.: Simple, variable ph. ch. model.

Figs. 3.16 to 3.19 show the numerical results obtained by the different simulations. It is observed that in this case there are almost no deviations between results from different models. This is most likely due to the fact that solidification starting temperature is very similar between constant temperature (59.9°C) and variable temperature phase change (61.6°C) cases, making almost negligible the
difference in solidification onset moments and thus in heat transfer rates. Results obtained with the detailed model are even closer to the simple 1D analysis than in charging mode. This agrees with the previous observations regarding detailed simulations.

3.6 Conclusions

Simple 1D analysis, as well as a more detailed one including CFD calculations for the PCM have been performed in order to simulate the performance of a thermal energy accumulation system.

Fixed grid enthalpy-porosity model of the solid-liquid phase change has been successfully implemented in a parallel unstructured CFD code. Simulations were verified and validated against numerical and experimental data found in the bibliography.

Natural convection produced in the melting of the PCM inside spherical capsules has been observed to have noticeable effects on the solid-liquid interface shape and on the temperatures distribution. However, for the cases studied in this paper, simple-1D and detailed models considering a constant phase change temperature give very similar results for the whole system. This would indicate that natural convection is not a determinant phenomenon of the global behaviour of this system in these cases. However, it should be noted that convection could have significant effects under other operation conditions.

On the other hand, remarkable differences in the global system performance have been observed indeed between the simulations considering constant and variable phase change temperature. Better results were obtained in the variable phase change temperature case. Future work should be carried out in performing CFD calculations taking into account this physical characteristic of the PCM.

Future work should also consider the mobility of the solid parts.
Conclusions
Chapter 4

Conclusions

In this work, the governing equations of fluid flow and heat transfer have been numerically solved. Firstly, two standard problems have been treated with an own developed code, verified and validated against benchmark. Lastly, the solid-liquid phase change phenomenon has been implemented both in the previously developed computer code and in TermoFluids - a computer program designed to solve fluid flow and heat and mass transfer problems using unstructured meshes and parallel computing - and used to analyse the behaviour of a thermal storage system consisting of a cylindrical container filled with a phase change material contained in spherical capsules.

This last task involved the study of the formulation needed for modelling the phase change phenomenon, the deepening in the numerical methods applied, as well as an intense training on computer programming - including parallel computing and solver programming.

The thermal storage system has been modelled by two methods, a one-dimensional approach - in which several simplifying assumptions have been adopted - as well as a hybrid 1D/2D approach, in which several of the previously made assumptions of the behaviour of the PCM were eliminated. In the latter, the detailed CFD modelling of the phase change has been coupled with the one-dimensional analysis of the fluid flow through the tank. In the “pure” one-dimensional approach, the solid-liquid phase change has been modelled using two different assumptions with respect to the temperature at which it occurs. Both constant temperature and linearly variable temperature processes have been studied and compared.

The computer codes derived from this work can be used for the analysis of systems in which the solid-liquid phase change can play an important role, such as in solar heating systems, thermosolar generation plants and construction materials containing PCMs.

Future work should consist in eliminating some of the simplifying assumptions adopted in the modelling of the phase change. For example, expansion (or contraction) as a result of density changes should be taken into account, as well as the possibility to model the change of phase at variable temperature and the motion of the solid parts.

Furthermore, coupling of turbulence and solid-liquid phase change modelling should be carried out.
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