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Simulation of Binary Mixture Freezing: Application to Seawater Desalination

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***Abstract*— The solidification of seawater allows, under certain conditions, the separation of its components and gives rise to a preferential migration movement of solutes. The quantity and the concentration of the products obtained depend on the mechanisms of separation which depend on different parameters and the applied boundary conditions. In this way, the freezing of saltwater (H_2O-NaCl mixture) makes it possible to obtain a saltier liquid phase called brine and a solid phase of ice becoming fresh water after melting. This process can be used in desalination. In this paper, we present numerical simulation results of seawater freezing in a rectangular enclosure of aspect ratio equal to 10. For a fixed temperature and concentration, the results depend strongly on boundary conditions of freezing. Three cases were studied:**

- ***Freezing from below***
- ***Freezing from above***
- ***Freezing from lateral sides***

The other sides were considered impermeable and adiabatic. The numerical simulation were based on Navier stokes, energy and species equations in transient flow. The FLUENT software was used to solve these equations using a bi-dimensional formulation and using a rectangular grid of 25*251 meshes.

The results presented in terms of temperature, velocity and concentration fields (fig. 1) shows that:

- ***A convection movement takes place since the beginning and influences the separation mechanism. This convection is more important in the case of freezing from above.***
- ***In this case, the concentration in brine increases from 35g/l to 72 g/l in 24 hours whereas it reaches only 65 g/l when freezing by the bottom, during the same duration. It means that freezing from above allows to have purest ice.***
- ***The freezing by the lateral sides is the most efficient process.***

Keywords: **Numerical simulation, Freezing, Desalination, Phase change, Seawater.**

I. INTRODUCTION

Nowadays our world is facing a shortage of fresh water **[1]**. Recoming to the seawater and renewable energies is the sustainable solution. Knowing that producing cold by solar energy is more economic than producing heat; desalination by freezing becomes more competitive **[2]**. This process was tested in the 50^{th}, and most of the literature on the subject dates back to the 1950s, '60s, and '70s **[3-6]** and given u for different reasons among other, the ignorance of saltwater mechanisms of solidification and especially the dynamic of the freezing front.
The mass and heat transfer in liquid mixture have been investigated theoretically **[7-8]** and by experiences **[9]**. The same studies were applied in metal alloys fusion-solidification **[10]**. Freezing was also used to separate the titanium-aluminium alloy.
In this paper we focus on understanding the mechanisms of heat, and species transfer, interface formation and its evolution in space and time under different boundary conditions.

II. MODELLING

We consider a reservoir filled with brine solution at a fixed concentration. The solution is cooled by one side whereas the other sides were considered thermally isolated and rigid. The solution was considered incompressible. The Boussinesq approximation was used and the Duffour effect was neglected. Only the laminar and bidimensional flow was considered.
Hence the flow is described by the following equations:

In liquid zone: Continuity
$$\frac{\partial \rho_l}{\partial t} + \nabla(\rho_l V_l) = 0$$

Momentum
$$\frac{\partial}{\partial t}(\rho_l V_l) + \nabla(\rho_l V_l V_l) = -\nabla p_l + \mu_l \nabla^2 V_l + \rho_l g$$

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Species $$\frac{\partial}{\partial t}(\rho_l C_{i,l}) + \nabla(\rho_l C_{i,l} V_l) = -\nabla J_{i,l}$$

Energy $$\frac{\partial}{\partial t}(\rho_l H_l) + \nabla\left[\rho_l H_l V_l + \sum_{i=a}^{b} H^i J_{i,l}\right] = -\nabla q_l + \rho_l Q_l$$

In solid zone: Continuity $$\frac{\partial \rho_s}{\partial t} = 0$$

Species $$\frac{\partial}{\partial t}(\rho_s C_{i,s}) = -\nabla J_{i,s}$$

Energy $$\frac{\partial}{\partial t}(\rho_s H_s) + \nabla\left[\sum_{i=a}^{b} H^i J_{i,s}\right] = -\nabla q_s + \rho_s Q_s$$

Instead considering separately the two phases: solid and liquid and the mushy layer (interface), we used the approach of a single domain including the both phases. The passage from one phase to another is done by expressing the physical properties in function of the liquid fraction. We can notice that the mushy layer was reduced to a plane interface (due to Fluent's restrictions). Therefore the resulting equations are:

- Continuity : $$\frac{\partial \rho_l}{\partial t} + \nabla(\rho_l V_l) = 0 \quad (1)$$
- Species : $$\frac{\partial}{\partial t}(\rho_l C_{i,l}) + \nabla(\rho_l C_{i,l} V_l) = -\nabla J_{i,l} \quad (2)$$
- Energy : $$\frac{\partial}{\partial t}(\rho_l H_l) + \nabla\left[\rho_l H_l V_l + H^i J_{i,l}\right] = -\nabla q_l + \rho_l Q_l \quad (3)$$
- Momentum : $$\frac{\partial}{\partial t}(\rho_l V_l) + \nabla(\rho_l V_l V_l) = -\nabla p_l + \mu_l \nabla^2 V_l + \rho_l g \quad (4)$$

The adimensional equations are :

$$\nabla V_l^* = 0$$

$$\frac{1}{\Pr^*}\left(\frac{\partial V^*}{\partial t} + V^* \nabla V^*\right) = -\frac{1}{\Pr}\nabla P^* + \nabla^2 V^* + Ra_T\left(T^* + \psi C^*\right)$$

$$\frac{\partial T^*}{\partial t} + V^* \nabla T^* = \nabla^2 T^*$$

$$\frac{\partial C^*}{\partial t} + V^* \nabla C^* = \frac{1}{Le}\left(\nabla^2 C^* - \nabla^2 T^*\right)$$

Initial and boundary conditions :

- At $t = 0s$ The flow is considered at rest $\vec{V} = 0$
  $T_0 = 298°K$ and $C_0 = 3.5\%$ $\forall\ x, \forall\ y$
- $$\left.\frac{\partial C}{\partial n}\right|_{x=0} = \left.\frac{\partial C}{\partial n}\right|_{x=L} = \left.\frac{\partial C}{\partial n}\right|_{y=0} = \left.\frac{\partial C}{\partial n}\right|_{y=l} = 0$$
- $$\left.\frac{\partial T}{\partial x}\right|_{x=0} = \left.\frac{\partial T}{\partial x}\right|_{x=L} = \left.\frac{\partial T}{\partial y}\right|_{y=l} = 0$$
- Later one of two sides will be cooled at T_f=260°K

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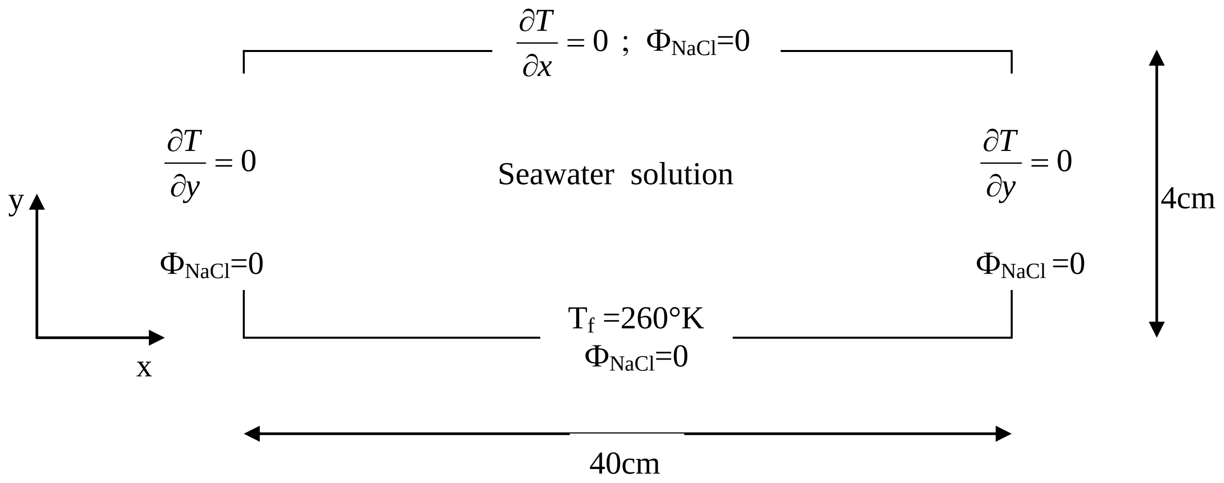

Fig.1. Studied Problem

III. NUMERICAL SIMULATION

A. Grid

The precedent set of equations was solved using the CFD FLUENT **[11]**. This industrial code uses the finite volume method to discretize the nonlinear partial derivative equations mentioned above. All the unknowns are calculated at the centers of the meshs and its values on the faces are rebuilt linearly by the interpolation model of Rhie and Chaw (1983). Diffusion terms are discretized by a second-order centered scheme. The velocity equation and the pressure one are coupled thanks to the SIMPLE algorithm. Spatial integration is accomplished by the Gauss Seidel iterative method.

In this work, simulation was applied to a cavity of 40*4 cm filled with seawater at 35g/l of salt. A 251*24 regular meshes were created by the GAMBIT software (Fig. 2). The studies case is characterized by the following dimensionless parameters:

$$\Pr = 7.23$$
$$Le = 111.7$$
$$Ra_{th} = 8.34 * 10^{6}$$
$$Ra_{sol} = 1.23 * 10^{13}$$
$$Gr_{th} = 1.13 * 10^{6}$$
$$Gr_{sol} = 1.52 * 10^{10}$$

Three physical cases were investigated: freezing by above, by the bottom and by the later sides. The results are presented in terms of temperature, concentration and velocity iso-contours via time evolution.

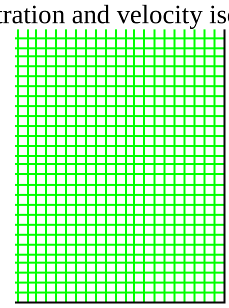

Fig.2. Grid used

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B. Discussion

In the three cases, a convection movement takes place since the beginning and influences the separation mechanism.
As shown in Fig.3, the isotherms in freezing from below remain linear during solidification. During the first minutes of solidification, the interface progresses in a plane way. The convection starts then develops by the appearance of gradient of concentration in the rejected solution.
Thermal and mass gradients are in the same direction and way that the gravity. This can explain that in this case, and after 24h of freezing, salt concentration in ice remains to 7g/l experimentally.

Freezing from above shows more important convection movement. In this case, the thermal and solutal gradients are in opposite direction and constitute a natural source of hydrodynamic instability.
Convective rollers settle in the solution and make go up the hottest solution towards the higher cold wall. This water cools and falls down to the bottom accelerating the movement. The velocity field shows that the vortices coaless with time to be bigger mixing, consequently, the mixture and accelerate the process. In this case, the concentration decreases from 35g/l to 1g/l in 24 hours. This value is near the standards of WHO **[1]** (World Health Organization) applied to drinking water.

Freezing from lateral sides shows symmetrical fields of temperatures, velocities and concentrations that's why we limit presentation at only the half of the cavity. A large vortex starts against the cold side and speeds toward the hot one. The center of this vortex is located in the center line of the cavity. Comparently, the temperature front moves in the same direction but in parallel to the freezing side. This profile expresses, usually, the diffusion phenomena. All occurs like if the convective movement is less strong than the diffusion one. In fact, the ice appearing against the cold side progress in the horizontal direction pushing the movement towards the opposite side. Hence, a vertical stratification of temperature and density (ice) takes place until the freezing of the whole mixture.
In this case, the concentration decreases from 35g/l to only 0.5g/l in 24 hours which is conform to the standards of WHO cited above and can be considered as efficient method to produce drinking water.

III. CONCLUSION

In this study, the effect of initial and boundary conditions is proved and help in the choice of the adequate configuration when applied to phase separation process especially in seawater desalination. Freezing from below seems to be the less performed. Freezing from above and from the side are competitive and he choice will be in function of the industrial applications.

APPENDIX

T : Temperature (°K)
φ : Density (kg/m^3)
p_l : Pressure in liquid phase
V_l : Velocity (m/s)
$C_{i,l}$: Concentration of solute i (g/l)
$J_{i,l}$: Massic diffusion fluxes
H_l : Enthalpy (J)
q_l : Thermal diffusion fluxes
$\Pr$: Prandtl Number (ν / α)
Le : Lewis Number (α / D)

$$Ra_{th} = \frac{\varphi g \Delta T l^3}{\nu \alpha}$$: Thermal Rayleigh Number

$$Ra_{sol} = \frac{\varphi g \Delta C l^3}{\nu \alpha}$$: Solutal Rayleigh Number

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$Gr_{th} = \dfrac{\beta_T g l^3 \Delta T \rho^2}{\mu^2}$: Thermal Grash of Number

$Gr_{sol} = \dfrac{\beta_{sol} g l^3 \Delta C \rho^2}{\mu^2}$: Solutal Grash of Number

$x^* = x/L \quad y^* = y/H$: A dimensional length and width

$V^* = \dfrac{V}{a/H}$: A dimensional velocity

$P^* = \dfrac{P}{\rho_0 a^2 / H^2}$: A dimensional pressure

$T^* = \dfrac{T - T_0}{T_0 - T_f}$: A dimensional temperature

$C^* = \dfrac{C - C_0}{C_0 - C_f}$: A dimensional concentration

$\psi = -\dfrac{\beta_T}{\beta_C}\dfrac{D_T}{D_C} C_0 (1 - C_0)$: Seapartion ratio

Subscripts:
l : liquid
s : solid
0 : Initial state
f : final state

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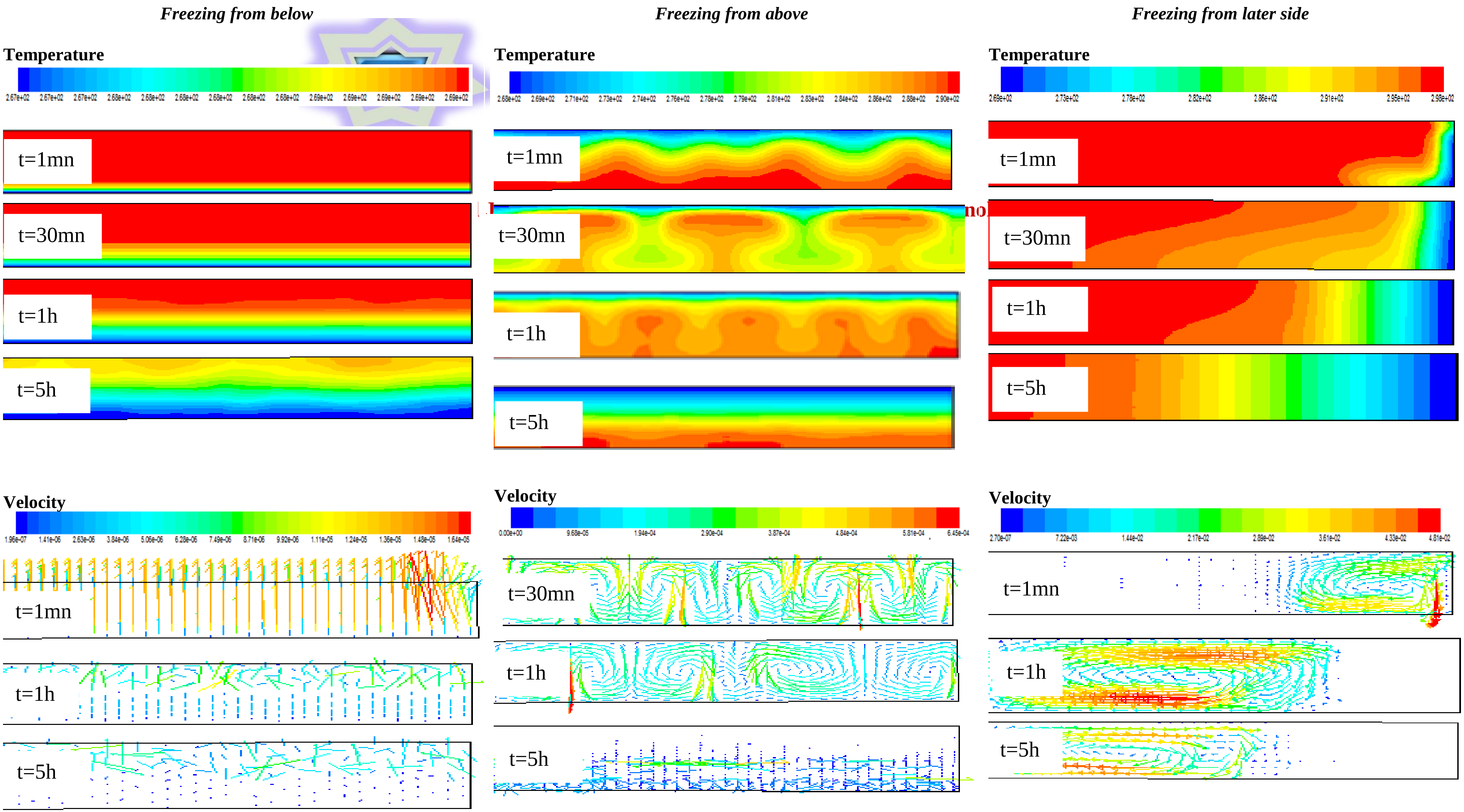

Fig.3. Numerical results of freezing simulation with different boundary conditions