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### Numerical Simulation of Contaminants Transport in Confined Medium

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#### 1. General introduction

Multiplication of the human activities and their diversity in all the sectors of the life such as industry, agriculture, transport, etc... had , as consequences, the increase in traditional pollution and appearance of new types , which have in turns generated diseases. Some polluting products such as CO<sub>2</sub>, waste water, etc form already part of our everyday life. In addition to these generated products, other natural products release a permanent radioactivity in the air and the water that the human ones consume daily. The accumulation of the amounts generate damages, sometimes in the short term. It is thus significant to understand the mechanisms of transport and circulation of these contaminants in our space of life to be able to bring an effective solution.

In this work, we are interested in the simulation of the transport of two pollutants which cohabit with the human ones.

The first is the Radon gas resulting from the disintegration of Uranium and Thorium and emanating from geological layers. This gas is also present in the subsoil waters which we consume and in the air and building materials of our houses.

The second pollutant is the waste water or brine rejected in the ground following the industrial water treatment or the desalination of brackish and sea water.

In the simulation, the transport of the two contaminants is investigated in time and space.

The Radon gas is transported by the air inside the habitat by diffusion-convection, and recirculation zones (accumulation of the amounts) due to the confinement appear with time. The effect of the temperature is demonstrated.

In the case of the brine, transport is done by water through porous heterogonous and anisotropic layers. The residence time of the contaminant in each layer depends on the thermo-physical properties and the importance of the flow.

In these two cases, the flow is modelled by the Navier-Stokes equations coupled with the energy and species equations to take into account the temperature and the dose effects.

For simplification, only the two-dimensional flow is considered.

#### 2. Numerical method

These partial derivative equations need to be numerically solved. A panoply of methods is available in literature and CFD software makes it possible to simulate a large range of industrial problems. In order to reduce the number of nonlinear partial equations and

overcome the difficulties related to the pressure calculation, the stream function  $\psi$  and the vorticity function  $\Omega$  formulation is used with:

$$u = -\frac{\partial \Psi}{\partial y}, v = \frac{\partial \Psi}{\partial x}, \Omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$$

In our case, the equations are solved using a difference finite scheme based on a compact Hermetian method where the function and its first and second derivates are considered as unknowns. This method allows to reach a good accuracy: fourth order O (h<sup>4</sup>) for  $\psi$  and second order O (h<sup>2</sup>) for  $\Omega$ , T and C. The Alternate Direction Implicit technique (A.D.I) is used to integrate the parabolic equations. This scheme is well described in the literature and has been widely used for natural convection and recirculation flow and was proposed by (Loc & Daube, 1978) to solve the Navier-Stokes equations and by (Safi & Loc, 1994) to solve coupled problems. This procedure has the advantage that the resulting tri-diagonal matrix instead of a matrix with five occupied diagonals can easily be solved by factorization algorithm. Some difficulties were encountered in implementing the vortices boundary conditions. Different approximations were tested and the Padé approximation was employed to overcome the numerical instability (Safi & Loc, 1994). The convergence criterions were defined by the following relations:

$$MAX \left| \Psi_{ij}^{n+1/2} - \Psi_{ij}^{n} \right| + MAX \left| \Psi_{ij}^{n+1} - \Psi_{ij}^{n+1/2} \right| < \chi \qquad \text{for } \Psi$$
$$MAX \left| \left( \Omega, T, C \right)_{ij}^{n+1} - \left( \Omega, T, C \right)_{ij}^{n} \right| < \chi \qquad \text{for } \omega, \text{T and } C$$

 $\chi$  is equal to 10<sup>-6</sup> for the stream function  $\Psi$  and 10<sup>-4</sup> for the  $\Omega$ , T and C.

#### Nomenclature

A: Aspect ratio of the cavity= H/L c: Specific heat at constant pressure C: Dimensionless concentration D: Massic diffusivity D<sub>p</sub>: Massic diffusivity of porous media D<sub>T</sub>: Thermal diffusivity of solute concentration g: Gravitational acceleration H: Height of the cavity K: Permeability of porous media L: Reference width of the cavity Le: Lewis number Nu: Average Nusselt number Gr: Gradshof number Da=K/H<sup>2</sup>: Darcy number  $N = \alpha \Delta C_0 / \beta \Delta T_0$ : Floatability number Ra<sup>T</sup>= Gr Pr : Thermal Rayleigh number Ra<sup>s</sup>=NRa<sup>T</sup>: Solutal Rayleigh number

Numerical Simulation of Contaminants Transport in Confined Medium

Pe= RePr : Peclet number Pr: Prandlt number Re: Reynolds number R<sub>i</sub>: Richardson number R<sub>d</sub>: effective Mass diffusivity ratio,  $R_d = \varepsilon + (1-\varepsilon)Rd_p$ Rd<sub>p</sub>: Mass diffusivity ratio R<sub>v</sub>: effective Viscosity ratio,  $R_v = v_e / v_e$ , where  $v_e = f(v_e) = v f(\varepsilon)$ t: dimensionless time t<sub>0</sub>: reference time t\*: dimensional time (u,v) : dimensionless velocity (x,y): dimensionless coordinate system **Greek Letters** α: Mass expansion coefficient β: Thermal expansion coefficient  $\Delta C$ : Concentration difference, C<sup>\*</sup>-C<sub>2</sub><sup>\*</sup>  $\Delta C_{ref}^*$ : Reference concentration difference,  $C_1^*$ - $C_2^*$  $\Delta \psi$ : Laplacien of stream function ε : Porosity v : Kinematic viscosity v<sub>e</sub>: Effective cinematic viscosity  $\psi$  : Stream function  $\Omega$ : Vorticity=  $\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$ Subscripts

e: Effective p: Refers to porous media

#### First example: The indoor diffusion-convection of the radon gas

#### 1. Introduction

Among the sources of natural radioactivity to which the man is exposed, is the radon gas emanating from the disintegration of Uranium and Thorium and other rocks. This gas is present in all the atmosphere under the effect of meteorology and in most the ground water. Owing to the fact that it emanates from the rocks, most of the applied and fundamental studies concentrated on its transport through these rocks considered as porous body (Durani & LLic, 1997; Tomozo & al, 2008).

Research on fine scales concerning multiphase transport to determine the coefficient of emanation of this gas starting from the rocks was carried out (Nielson & Rogers, 1994).

Few works related to the direct effect of the temperature on the diffusion or the convection of this gas especially in closed mediums like the dwelling or the factory exist whereas the principal producers of phosphate, significant source of radon emanation, are located in North Africa where the solar radiation exceeds sometimes  $1000W/m^2$ . Over more, the settlements of the workmen of the mines which were built last century around these mines

and with the stones coming from the same site are transformed into villages and cities cohabiting the phosphate and the radon.

In this study we choose the radon 222 whose half life time is only of 3.8 days in order to simulate the physical process during disintegration of this gas.

#### 2. Physical model

We consider a parallelepiped room whose walls are uniform including the ground and the ceiling. This symmetry of boundary conditions allows to consider only one vertical medium plane (X, Y, Z=1/2).

We consider a source of radon(S), placed at the middle of X to an H/3 height (Fig.1) and at constant concentration C.

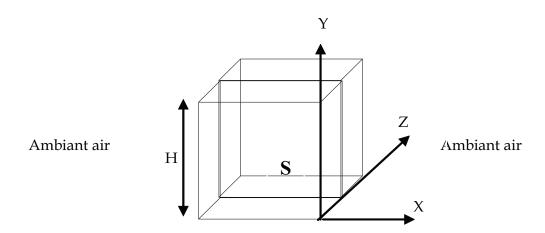
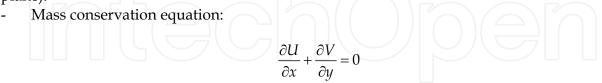


Fig. 1. Geometrical configuration of the physical model

Taking into account the thermo physical properties of radon, we can consider that it moves with the air at the same velocity and with the same properties especially viscosity but at a different concentration. For better determination of the temperature effect, only the natural convection is thus considered. The effect of the climate is limited to the temperature of the outer jacket of the habitat.

Thus the transport equations are written in a two dimensional geometry (vertical medium plane):



- Momentum equation:

$$\rho \frac{\partial U}{\partial t} + \rho (\vec{U} \nabla) \vec{U} = -\nabla p + \mu \nabla^2 \vec{U} + \rho \vec{g}$$

- Energy equation

$$\rho c \frac{\partial T}{\partial t} + \left(\frac{\partial UT}{\partial x} + \frac{\partial VT}{\partial y}\right) = \lambda \nabla^2 T$$

Concentration Equation:

$$\frac{\partial c}{\partial t} + \left(\frac{\partial Uc}{\partial x} + \frac{\partial Vc}{\partial y}\right) = \nabla (D\nabla c) - \lambda c + \lambda c^{\text{source}}$$

Where:

C is the Radon concentration expressed as radioactivity (Bq/m<sup>3</sup>),  $\left(\frac{\partial Uc}{\partial x} + \frac{\partial Vc}{\partial y}\right)$  is the advection term,  $\nabla(D\nabla c)$  is the diffusion term,  $-\lambda c$  is the decay term,  $\lambda c^{source}$  is the source term, and  $\lambda = \frac{\ln 2}{T_{c}^{(1/2)}}$  is the radon decay constant (1/s).

We notice that the concentration is not directly related to the temperature because we neglected the Dufour effect. However the two parameters are dependent each from the other through the velocity.

As mentioned above, streamline function  $\Psi$  and vorticity function  $\Omega$  were used to replace velocity components U, V and the pressure P.

To generalize this study independently of dimensions and time (by applying physical simulation), the transport equations inside the habitat are written in the following dimensionless form:

$$\Delta \Psi = \Omega \tag{1}$$

$$\frac{\partial\Omega}{\partial t} + \left(\frac{\partial u\Omega}{\partial x} + \frac{\partial v\Omega}{\partial y}\right) = \frac{\Pr}{R_t} \Delta\Omega + \frac{\Pr Ra^T}{R_t^2} \left(\frac{\partial T}{\partial x} - N\frac{\partial C}{\partial x}\right)$$
(2)

$$\frac{\partial T}{\partial t} + \left(\frac{\partial uT}{\partial x} + \frac{\partial vT}{\partial y}\right) = \frac{\nabla^2 T}{R_t}$$
(3)

$$\frac{\partial C}{\partial t} + \left(\frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y}\right) = \frac{\nabla^2 C}{R_t Le} - \ln 2C + \ln 2\frac{C^{source}}{\Delta C_0}$$
(4)

The boundary conditions on the walls were fixed as following:

- C=0 which means that the walls from where radon can exit towards outside remains at the low concentration,
- u=v=0 ; due to the adherence ,
- $\Psi$ =0 expresses conservation the flow rate inside the habitat ( there's no momentum change with the outside), and  $\Omega$  is calculated using Padé approximation.

Consequently, the phenomenon of diffusion-convection of radon depends on of the following dimensionless parameters:

- Lewis number  $Le=D_T/D_0$
- Prandlt number Pr=v/D<sub>T</sub>
- Thermal Rayleigh number  $Ra^T = \frac{\beta g \Delta T_0 H^3}{\nu D_0}$  with  $\Delta T_0 = 10$  K( temperature difference to

which natural convection is due)

- Floatability number :  $N=\alpha\Delta C_0/\beta\Delta T_0$ 

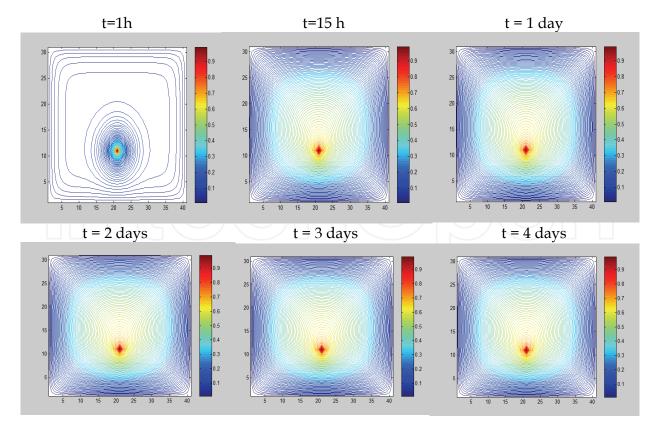
With:

-  $R_t = \frac{t_o}{T_{vie}^{(1/2)}}$  with  $T_{vie}^{(1/2)} = 4$  days (half life time of the radon gaz), and -  $t_0 = \frac{H^2}{D_T} = \frac{3^2}{410^{-6}} = 2.2510^6 s = 26.04$  days

#### 3. Results

Numerical simulation was carried out in a square cavity with a uniform grid of 41x31 nodes. Physical parameters were limited to the above values of  $\Delta C$  and  $\Delta T$ . Consequently we obtain: Pr=2.5, Le=0.221, Ra<sup>T</sup>=2.027 10<sup>11</sup>, N= 0.5510<sup>-23</sup>, R<sub>t</sub>=6.51. Notice that C=1000Bq/m<sup>3</sup> is considered as amount of alert in all the countries. The amounts maxima authorized are 150 Bq/m<sup>3</sup> in U.S.A and 400 in E.U.

In this study, different boundary conditions were considered.



#### 3.1 Isothermal diffusion of radon

Fig. 2. Iso-concentration lines of radon gas diffusion

We considered the case of a body source located at the middle of the room at 1m from the floor of the house (H/3). This source released a constant intensity of radon towards the rest of the room space including the walls, the floor and the roof. The whole system was considered at the same temperature. The numerical results are expressed in terms of iso-contours of concentration (Fig.2) which illustrate the different steps of the transfer inside the room.

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At t=1 hour, the concentration is still located in the vicinity of the source.

At t=5h, the gas occupied the whole of the room with a maximum concentration around the source. We still have a diffusion transfer.

At t=15h, over than 50% of the space had a higher concentration, and a weak recirculation zones appear in the vicinity of the walls. This phenomena announces the beginning of the convective movement.

Since t=15 h to t=4 days, the recirculation zones extended slowly from the wall region towards the rest of the room and concentration tends to be uniform in a large region. This mixing convective movement is very weak and a quasi steady state is reached.

#### 3.2 Temperature effect

Temperature may occur in three ways (a) double diffusion phenomena, (b) transport by natural convection (c) and transport by forced convection.

In the present study, two geometrical configurations are considered.

#### 3.2.1 Lateral thermal gradient

This configuration simulates the difference of temperature between two walls (East-West or North –South) due to, for example, heating by solar radiation.

Results are represented by the isotherm and iso-concentration contours (Fig.3).

At t=1 hour, heat is transferred to the colder wall in a vertical front way. The most important thermal layer remains against the hot wall. The parallel vertical isotherms indicate that the transfer is occurring by pure diffusion. As a consequence, the radon is smoothly diffused in all the directions and the maximum concentration is found to be around the source.

At t=15h, the temperature front continue to move towards the cold wall and a recirculation zone appears entraining the gas in a rotational movement.

At t=1 day, the thermal front reaches 1/4 of the distance between the two lateral walls.

During the remaining three days, and due to natural convection, temperature and concentration continue to be transported inside at low velocities but faster than in the isothermal case.

#### 3.2.2 Vertical gradient

This configuration simulates the temperature difference between the floor and the roof. Such a gradient occurs, for example at noontime due to heating by vertical solar radiation or by heating from below during the cold season. The last case was investigated.

Results are represented by the isotherm and iso-concentration contours (Fig.4).

At t=1 hour, thermal front moves faster that in the previous cases. This is due to the buoyancy effect and to the fact that lateral walls were taken adiabatic. The concentration is spread faster but still in closed contours indicating the diffusion regime.

At t=5h, the temperature front reaches the cold side and recirculation zones appeared against the walls as in the precedent case at t=15h. We deduced that the transfer in this case is accelerated by about 10 hours.

At t=1 day, a quasi-linear thermal stratification appeared, such a phenomena is not advised for habitants and simultaneously the recirculation zones decreased in density.

Since that time and until t=4 days, temperature and concentration continue to spread slowly. A quasi state regime with weak vortices oscillating in density settles.

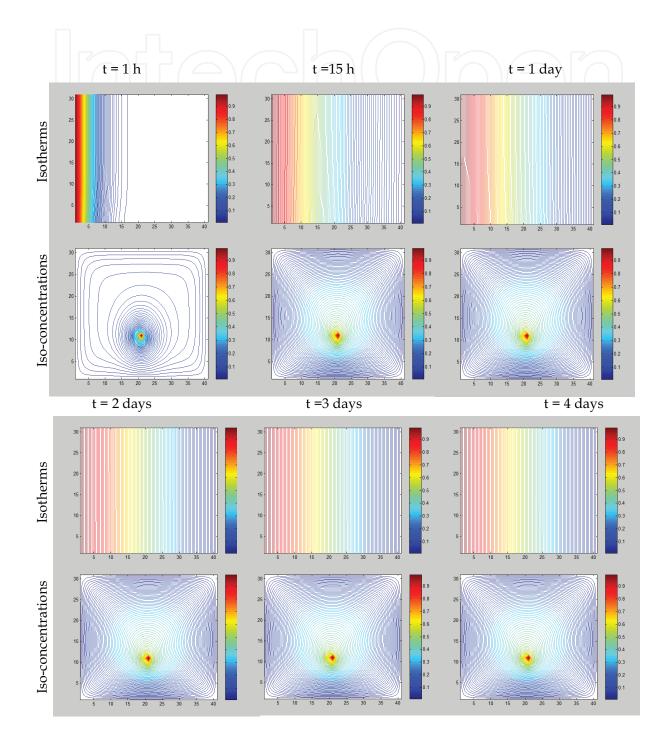
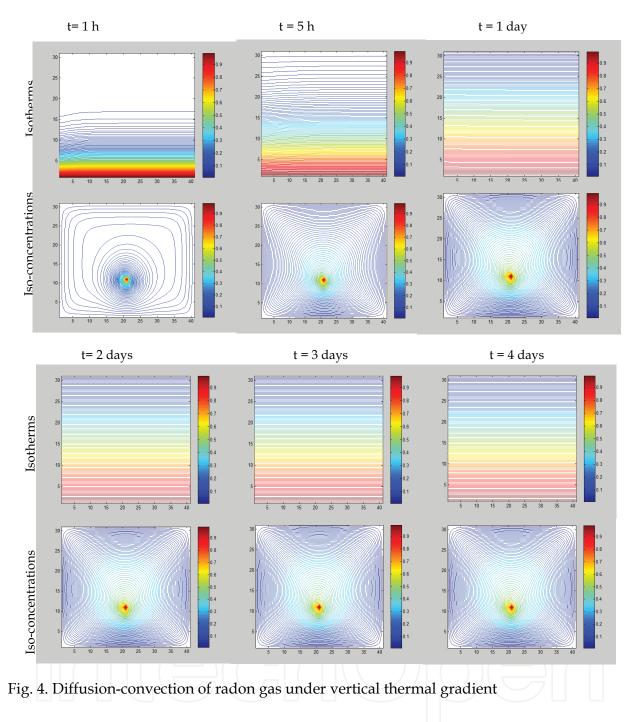


Fig. 3. Diffusion-convection of radon gas under lateral thermal gradient



#### 4. Conclusion

A numerical simulation of the transport of radon gas concentration, temperature and momentum in a room has been investigated numerically.

These simulations, allow us to predict the space-time evolution of the concentration, the temperature and the streamline fields. In the present work, although the source dose is important, the transport is influenced especially by the thermal buoyancy effect.

The results show that:

1. thermal natural convection, makes the transport of radon gas faster due to the air movement,

- 2. this acceleration is more important when a vertical gradient is applied to the room opposite walls.
- 3. by changing the concentration, we concluded that the dose variation doesn't affect the flow behaviour significantly.
- 4. The intrusion of radon from outside through windows will be investigate as well as the ventilation of the habitat.

## Second example: Flow and concentration transport through saturated porous layers

#### 1. Introduction

Some people still imagine, like one century ago, that the oceans and the ground are infinitely large to contain all the solid pollutants and liquids which they produce.

This false belief brought the inhabitants of the coast to discharge their contaminants in the sea and those of the remote zones to throw their contaminants at free surface or to bury them basement.

Last century, the Americain manufacturers of textile, oil and mines, poured, without any concern, million m<sup>3</sup> of waste water coming from dyeing, hydrocarbons and the factories of washing of the mines. Today the consequences are catastrophic as in Texas where: contamination of the tablecloths, desertification and lack of drinking water recall to the order. In California, due to an excess in desalting brackish tablecloths and to discharging the very concentrated brine into the soil; salty small-lakes appeared in under ground contaminating any form of life. These catastrophes gave birth for a certain regulation on the rejections.

Today, with the appearance of other essential activities for the human ones, pollution took other forms. Being limited only to the sector of water, source of the life, two forms of pollution are generated: the waste water and the brine resulting from desalination. To face the water shortage, many countries are recurring more and more to brackish and sea water desalination.

In the case of desalination of sea water, the brine is rejected on the coast with a salinity able to be four times initial salinity, with chemicals resulting from the pre-treatment and sometimes (thermal desalination) with an increase in temperature of + 10K. It results destruction of the phone and the flora. It is currently the case with the countries of the gulf and the Canary Islands. In the remote zones, R.O technique is usually used to desalt ground water at a salinity varying from 3 to 6 g/l. The desalt water is used to supply fresh water to the local population and to irrigate greenhouses, while the concentrated brine is released in the environment or injected into the ground water quality is degrading.

The waste water which constitutes the second source of water after that of the seas constitutes also the second form of pollution. It is rejected after treatment in the coast or into the ground. Even in the best cases where water is treated secondary, bacteria and especially viruses persist and are transported in the receiving mediums to proliferate unless this water undergoes a very expensive tertiary treatment which is not obligatory in any country. This water is more dangerous than the brines because it transports with it several types of chemicals and in significant amounts. In coastal regions which receive the two thirds of the world population, certain regulations impose the use of the emissary to discharge the contaminated water far from the coast. This solution is very expensive and when it is applied, it is not optimized because one badly knows the mechanisms of diffusion and dispersion of water in the sea. In addition, the interaction near field-far - field (coastbroad) is still badly known. This requires the establishment of accurate models and of largescale digital simulations. In the remote zones, the situation is more complicated because the receiving medium is not transparent and the in situ experiments are very expensive and hazardous. The prediction by the digital simulation, after characterizations of the medium and the waste water, makes it possible to approximate the residence time of these contaminants and to reduce the in situ experiments.

Some people use the phenomenon of Riverbank to filter their liquid pollutants. The Germans used this process to recover the permeate in the water of the Rheine river. This process cannot be an effective solution for all the types of waste water. Its efficiency depends on several parameters. The Riverbank filtration represents a natural process to use in first stage in the water treatment. This process is always in direct contact by the contamination of the organic, inorganic substances, viruses polluting and bacteria which can modify the quality of drinking water (Sontheimer, 1980; Jacobs et al, 1988; Magee et al, 1991; Matsunga et al, 1993). Contaminant transport in Riverbank filtration has been investigated by several researchers using different model. A kinetic model was proposed (Song & Yavuz, 2002) to simulate this phenomenon in the presence of dissolved organic matter and bacteria. This model can help to understand the behaviour of contaminants in riverbank filtration.

As a first step towards the design of an efficient system, we investigated a *numerical simulation* of brine discharge. The soil is simulated by *stratified porous layers* of different thickness and geological properties (porosity, permeability, etc...). The discharge is assumed to be at the surface in vertic direction. The mechanism of flow transport and concentration becomes strongly coupled and the prediction of its behaviour depends on the accuracy of the numerical scheme. Christophe Filder et al (2001) have already studied numerically the behaviour of a panache resulting from an injection located in a heterogeneous vertical porous medium of two superimposed layers of the same thickness and different permeabilities.

#### 2. Physical model equations

The system should be represented by a stack of 5 layers with different interface boundary layers (Fig.1).

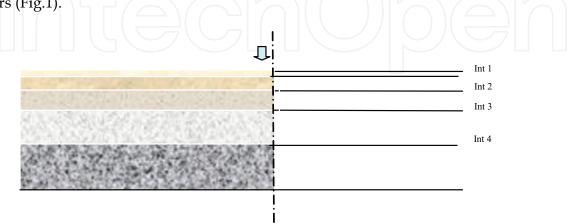


Fig. 1. Physical Model

The flow in such a configuration is three dimensional and need long time computing. As a first step for further complicated flows, we make the following assumptions (which could in fact be realistic):

- 1. The layers are homogeneous but different each from the other.
- 2. The bottom and the surface are permeable.
- 3. The liquid waste at high concentration is still considered as Newtonian fluid.
- 4. Geological layers are represented by porous media, we assume isotropic.

With assumptions, the flow could be considered two dimensional and Boussinesq approximation is valid. Hence the transfer phenomenon is described by Navier-Stokes and concentration equations including the Darcy-Brinkman-Forchheimer formulation.

To reduce the number of unknowns and overcome the resolution of the presence equation, the streamline and vorticity formulation is used as in the first example.

The consequent set of dimensionless equations is:

$$\Delta \Psi = \Omega \tag{1}$$

$$\frac{1}{\varepsilon}\frac{\partial\Omega}{\partial t} + \frac{1}{\varepsilon^2}\left(\frac{\partial u\Omega}{\partial x} + \frac{\partial v\Omega}{\partial y}\right) = \frac{R_v}{\text{Re}}\Delta\Omega + \left(\frac{\Omega}{\text{Re}\,Da} + \frac{b}{Da^{1/2}}\left(\frac{\partial|u|v}{\partial x} - \frac{\partial|u|u}{\partial u}\right)\right) - Ri\left(\frac{\partial C}{\partial x}\right)$$
(2)

$$\varepsilon \frac{\partial C}{\partial t} + \left(\frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y}\right) = \frac{Rd}{LePe} \Delta C \tag{3}$$

The following parameters were defined to obtain the dimensionless above equations:

$$(u,v) = \left(\frac{U^*}{V_1^*}, \frac{V^*}{V_1^*}\right), \ (x,y) = \left(\frac{X^*}{H}, \frac{Y^*}{H}\right), \ C = \frac{C^* - C_2^*}{\Delta C_{ref}}$$
(4)

and 
$$t = \frac{t^*}{t_0}$$
 where  $t_0 = \frac{H}{V_1^*}$  (5)

The Forchheimer coefficient b was taken equal to  $0.55\sqrt{Da}$  (Hwa-Chong Tien & Kwang\_Sheng Chiang, 2001).

It results that the flow depends on the following dimensionless parameters:

$$Da = \frac{K}{H^2}$$
$$Re = \frac{V_1 H}{\upsilon}$$
$$Gr = \frac{g\alpha\Delta C_{ref}^* H^3}{\upsilon^2}$$
$$Ri = \frac{Gr}{Re^2}$$

$$\Pr = \frac{\upsilon}{D_T}$$

Pe=RePr

$$Le = \frac{D_T}{D}$$

Da, b and  $\varepsilon$  depend mostly on the porous matrix structure and are influenced by the properties of the solid and fluid. However,  $R_d$  and  $R_v$  are functions of both the solid and fluid thermo physical properties, and may also be governed by the hydrodynamic and thermal dispersion. The variation in  $R_d$  and  $R_v$  is not still fully understood. Those two parameters has been considered in this study as constant equal to 1 as considered by most of authors.

#### 3. Results and discussion

Numerical simulations are investigated for a rectangular cavity with 5 m deep and 200 m large hence the aspect ratio is equal to 40. The porosity, The Darcy number and the thickness (from top to bottom) of each layer are respectively equal to: (0.8, 0.3210<sup>-7</sup>, 0.6m);

(0.7,0.2810<sup>-7</sup>,0.8m); (0.6, 0.2410<sup>-7</sup>, 1m); (0.5; 0.210<sup>-7</sup>,1.2m); and (0.4, 0.1610<sup>-7</sup>, 1.4m).

The waste was injected vertically at the mid plane through a nozzle of 0.20m diameter and the exit was set along the horizontal boundaries.

Due to the symmetry of the geometry only the mid-domain is considered so the waste injection became located at the top corner and the aspect ratio is reduced to 10. As a waste water, we considered a brine rejected by a small thermal desalination plant producing  $1m^3/h$  fresh water at conversion rate of 20% (the maximum reached by thermal technology).

To ensure good accurate a grid of 1001x51 nodes was chosen and a convergence criteria was satisfied by the two following relations:

$$MAX \left| (\Omega, C)_{ij}^{n+1} - (\Omega, C)_{ij}^{n} \right| < 10^{-3} \qquad MAX \left| \Psi_{ij}^{n+1/2} - \Psi_{ij}^{n} \right| + MAX \left| \Psi_{ij}^{n+1} - \Psi_{ij}^{n+1/2} \right| < 10^{-6}$$

where n denotes the number of time increments and the residue 10<sup>-3</sup> was taken for  $\Omega$ ,  $\Psi$ , and C.

In order to achieve real time simulations, the set of equations was solved in transient regime. This required small time steps to ensure numerical stability and good convergence. The flow was simulated for 7 days, indeed calculation required a long time computing.

The transport phenomena was simulated for: Reynolds number Re=50, Prandlt number Pr=5, Lewis number Le=78.55, and Schmidt number Sc = 770.

Results of the computations are presented in the form of contours plots of stream function and concentration at different times for an aspect ratio equal to 10.

It was found (Fig.2) that:

- In the beginning, small vortices appear in the entrance and the exit, the most area of the system is of laminar flow with parallel streamlines. The concentration is located in the vicinity of the inlet. The parallel contours indicate that the transfer is due to diffusion.

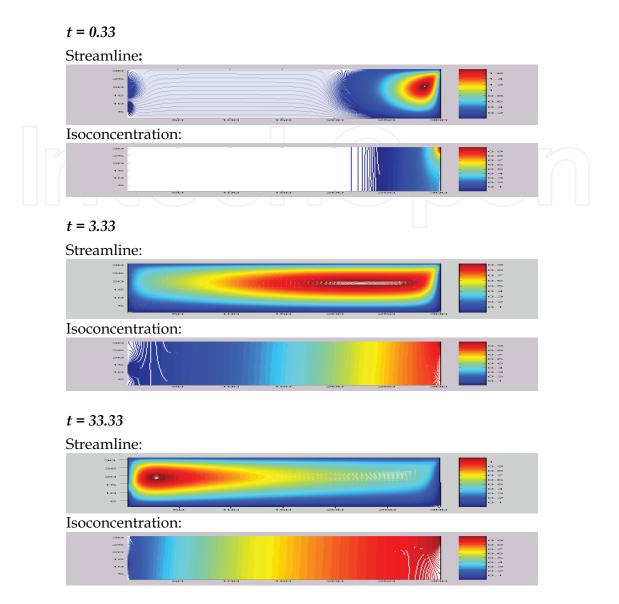
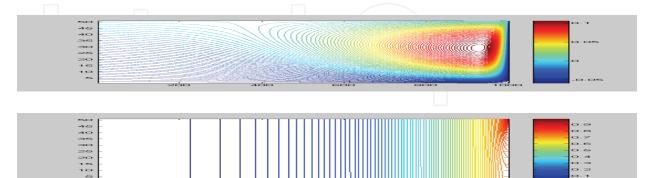


Fig. 2. Streamlines and Iso-concentrations evolution for A=10, Re=50, Ri=8  $10^{+4}$ , Pr=5 Le=78.75

- After some time, the vortex near the entry extended in the horizontal direction and a recirculation zone took place inducing the acceleration of the diffusion of concentration. At the same time the vortices at the exit grew and form a single vortex moving in the opposite direction of the main flow. This movement announced the development of a convection regime.
- As far as time increases, the recirculation zone extend towards the exit and hence, due to the presence of the backward movement, a chain of vortices took place increasing the dissipation of concentration.
- At t=33,33, a single cell occupied the whole system with a small outflow rate whereas the concentration continue to spread over the whole surface in a weak manner expressing the diffusion regime of concentration. This is due probably to the value of Richardson number which is much greater than 1 (threshold of appearance of the stratification).

It means that for a high concentration, Reynolds should be important to avoid stratification and to create forced convection in order to dissipate the brine quickly.

In order to reduce the computing time and especially to overcome the interface conditions, a second study was carried out to replace the 5 layers by a single one but at equivalent properties. The results showed a good agreement between the two models. Hence, one may use the equivalent model to save time and memory during computation.



Streamlines and Iso-concentrations for a one equivalent layer after 1 day

#### 4. Conclusion

The flow and concentration transport through saturated porous layers was investigated numerically using a numerical approach which considers the whole components as one domain to overcome the boundary conditions at the interfaces. The Naviers- Stockes equations and Darcy-Brinkman-Forcheimer formulation were used for modelling the transfer in each component going from the fluid to the porous media by changing the thermo physical properties of porous layers. The transient study of the flow allows to understand the evolution of the physical phenomena and thus the mechanism of transport.

In this physical problem we notice that some of the recirculation zones which appear could constitute stagnation region and increase the residence time, so we should increase the Reynolds number. Moreover, for a quick approximation, one can replace a stack of layers by only one equivalent layer having equivalent properties gaining by consequent much computing time.

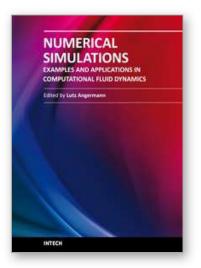
Further investigations with small Ri values will be achieved.

#### 5. References

- Chritophe, F.; Constantin, O. & Michel, B. (2001). Infiltration d'une solution saline dans un milieu poreux hétérogène en présence d'un gradient hydraulique, *XV*<sup>ème</sup> Congrés Français de Mécanique, Nancy, Spetembre 2001.
- Durrani, S.A. & Ilic, R. (1997). Radon Measurements by Etched Track Detectors: *Applications in Radiation Protection, Earth Sci. Environ*. (World Scientific, Singapore).
- Hwa-Chong, T. & Kwang- Sheng, C. (1999). Non Dary flow and heat transfer in a porous insulation with infiltration and natural convection, *J. of Marine Scien technology*, 7., 2., (125-131).

- Jacobs, L.A.; Von Gunten, H.R.; Keil, R. & Kusly, M. (1988). Geochemical changes along a river-groundwater infiltration flow path: Glattfelden, Switzerland. *Geochimica et Cosmochimica Acta*, 52, 11, (November 1988), (2693-2706)
- Nielson,K.K & Rogers, V.C. (1994). A sensitive effluent method for measuring radon gas emanation from low-emanating materials, *Nucl. Instrum. Methods Phys. Res.*, A353, (519–523).
- Magee, B.R.; Lion, L.W. & Lemley, A.T. (1991). Transport of dissolved organic macromolecules and their effect on the transport of phenanthrene in porous media, *Environ. Sci. technol.*, 25, (324-331).
- Matsunga, T.; Karametaxas, G.; Von Gunten, H.R. & Lichtner, P.C. (1993). Redox chemistry of iron and manganes minerals in river recharged aquifers: a model interpretation of a column experiment, *Geochim.Cosmochim.Acta*, 57, (1691-1704).
- Safi, M.J & Loc, T.P. (1994). Development of thermal stratification in two-dimensional cavity: a numerical study, *In.J. Heat Mass Transfer*, 37, 14, (2017-2024).
- Song-Bae, K. & Yavuz, C.M. (2002). Contaminant transport in riverbank filtration in the presence of dissolved organic matter and bacteria: a kinetic approch, *Journal of hydrology*, 266, (269-283).
- Sontheimer, H. (1980). Experience with riverbank filtration along the Rhine River. J. AWWA, 72, 7, (386-390).
- Sazaki,T.; Gunji,Y. & Iida,T. (2008) Theoretical Basis for Measuring Small Radon Diffusion Coefficients for a Radium-Bearing Porous Material Generated by Precipitation of Iron (III) Hydroxide. Journal of nuclear science and technology, 45, 7, (647–652).
- Loc, T.P. & Daube, O. (1978). A combined second and fourth order method for the numerical solution of steady and unsteady navier-Stokes equations, *International Conference on numerical Methods in Laminar and turbulent flow*, Swansea .





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