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SIMULATION OF LAMINAR DOUBLE DIFFUSION IN FLUID-SATURATED INERT POROUS MEDIA USING THE MULTIGRID METHOD

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Abstract. *The present work investigates the efficiency of Multigrid Method when applied to solve two-dimensional double difusion driven reactive flow transport problems in a fluid-saturaded inert porous media. . Numerical analysis is based on the finite volume discretization scheme applied to structure orthogonal regular meshes. Performance of the correction storage (CS) Multigrid Algorithm is compared for diferents Darcy number. Up to Four grids were used for both V- and W-cycles. Advantages in using more than one grid are discussed. Results further indicate an increase in computational effort for higher Da and an optimal number of relaxation sweeps for both V- and W-cycles.*

Keywords*. Numerical Modeling, Porous Media, Multigrid Method, Double Diffusion, Heat and Mass Transfer*

1. Introduction

The study of double-diffusive natural convection in porous media has many environmental and industrial applications, including grain storage and drying, petrochemical processes, oil and gas extraction, contaminant dispersion in underground water reservoirs and electrochemical processes, to mention a few applications (Mamou et al, 1995, Mohamad and Bennacer, 2002, Goyeau, Songbe and Gobin, 1996, Nithiarasu et al, 1996, Mamou et al, 1998, Bennacer et al, 2001, Bennacer, Beji and Mohamad, 2003). In most cases, numerical solutions are sought, which suffer from long computing time due to the intricate coupling among all variables involved. Usually, iterative methods are applied were individual equations are relaxed until overall residue histories are brought down to a pre-selected level.

Accordingly, it is known that convergence rates of most iterative solutions of single-grid calculations are greatest in the beginning of the process, slowing down as the iterative process goes on. Effects like those get more pronounced as the grid becomes finer. Large grid sizes, however, are often needed when resolving small recirculating regions or detecting high heat transfer spots. The reason for this hard-to-converge behavior is that iterative methods can efficiently smooth out only those Fourier error components of wavelengths smaller than or comparable to the grid size. In contrast, multigrid methods aim to cover a broader range of wavelengths through relaxation on more than one grid.

The number of iterations and convergence criterion in each step along consecutive grid levels visited by the algorithm determines the cycling strategy, usually a V- or W-cycle. Within each cycle, the intermediate solution is relaxed before (pre-) and after (post-smoothing) the transportation of values to coarser (restriction) or to finer (prolongation) grids (Brandt, 1977, Stüben & Trottenberg, 1982, Hackbusch, 1985).

Accordingly, Multigrid methods can be roughly classified into two major categories. In the CS formulation algebraic equations are solved for the corrections of the variables whereas, in the full approximation storage (FAS) scheme, the variables themselves are handled in all grid levels. It

has been pointed out in the literature that the application of the CS formulation is recommended for the solution of linear problems being the FAS formulation more suitable to non-linear cases (Brandt, 1977, Stüben & Trottenberg, 1982, Hackbusch, 1985). An exception to this rule seems to be the work of Jiang, et al, (1991), who reported predictions for the Navier-Stokes equations successfully applying the Multigrid CS formulation. In the literature, however, not too many attempts in solving non-linear problems with Multigrid linear operators are found.

Acknowledging the advantages of using multiple grids, Rabi and de Lemos (1998a) presented numerical computations applying this technique to recirculating flows in several geometries of engineering interest. There, the correction storage (CS) formulation was applied to non-linear problems. Later, Rabi and de Lemos (1998b) analyzed the effect of Peclet number and the use of different solution cycles when solving the temperature field within flows with a given velocity distribution. Optimal multigrid studies have also been conducted (Rabi and de Lemos, 2001, 2003). In all those cases, the advantages in using more than one grid in iterative solutions were confirmed. Furthermore, de Lemos & Mesquita, 1999, introduced the solution of the energy equation in their Multigrid algorithm. Temperature distribution was calculated solving the whole equation set together with the flow field as well as uncoupling the momentum and energy equations. A study on optimal relaxation parameters was there reported.

Mesquita & De Lemos, 2000a-b analyzed the influence of mesh size on convergence rates. They also investigated optimal values for several parameters used during the multigrid cycle, for different geometries. Further, Mesquita and de Lemos, 2003 considered a square cavity submitted to vertical temperature gradients and conducted a numerical study based on the convergence characteristics of multigrid solution. More recently, de Lemos and Tofaneli, 2004 presented a new formulation for turbulent heat and mass transport in permeable structures.

The present contribution extends the early work on CS Multigrid methods to the numerical solution of thermo-solutal natural convective flows in a porous media. More specifically, steady-state laminar flows in a square cavity, (height *H*, width *L*: aspect ratio $A = H / L$), totally filled with a porous material are calculated with up to 4 grids. A schematic of such configurations is show in Figure 1 horizontal temperature and concentration differences are specified between the vertical walls (T_C and C_C at the left wall, T_H and C_H at right wall) , and zero mass and heat fluxes are imposed at horizontal walls. All the boundaries are impermeable. The fluid is assumed to be Newtonian and to satisfy the Boussinesq approximation, the fluid is incompressible, laminar, 2D and in steady state. Further, the porous medium is supposed to be a isotropic, homogeneous and in a thermodynamical equilibrium with the fluid. The Soret and Dufour effects are assumed to be negligible. The controlling parameters are the Rayleigh number, $Ra_T = \dfrac{gb_T H \Delta TK}{n a_{eff}} = Gr_T \,\mathrm{Pr}\, Da$; the Darcy number, $Da = \dfrac{K}{H^2}$; the thermal Grashof number, $Gr_T = \dfrac{gb_T \Delta T H^3}{n^2}$; the salute Grashof number, $Gr_C = \dfrac{gb_C \Delta C H^3}{n^2}$; the Prandtl number, $\mathrm{Pr} = \dfrac{n}{a}$; the Schmidt number, $Sc = \dfrac{n}{D_\ell}$ and the Lewis number, $Le = \dfrac{Sc}{\mathrm{Pr}}$, where $a_{eff} = k_{eff} \big/ (rc_p)_f$. The particle diameter is given by $D_p = \sqrt{\dfrac{144(1-f^2)}{f^3}}$ and buoyancy ratio *N* is defined as $N = \dfrac{Gr_C}{Gr_T}$.

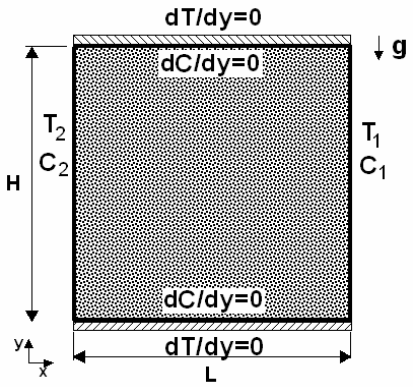


Figure 1 – The cavity under consideration.

2. mathematical Formulation and Numerics

The equations used are demonstrated in the work of Pedras and de Lemos, 2001, Pedras and de Lemos (2000) and de Lemos and Braga (2003). This work extends the development therein in order to include the buoyancy term in the governing equations.

Accordingly, the Boussinesq hypothesis can be written as,

$r = r_{ref}\left[1 - b_T\left(T - T_{ref}\right) - b_C\left(C - C_{ref}\right)\right]$. Substituting this term in the momentum equation, the buoyancy term reduces to,

$$r_{ref}\, g\left[b_T\left(T - T_{ref}\right) + b_C\left(C - C_{ref}\right)\right], \tag{1}$$

where, $\nabla p^* = \nabla p - r_{ref}\, g$ is a modified pressure gradient

Applying the volumetric average one has,

$$\left\langle r_{ref}\, g\left[b_T\left(T - T_{ref}\right) + b_C\left(C - C_{ref}\right)\right]\right\rangle^V = \frac{\Delta V_f}{\Delta V}\frac{1}{\Delta V_f}\int_{\Delta V_f} r\mathbf{g}\left[b_T\left(T - T_{ref}\right) + b_C\left(C - C_{ref}\right)\right]dV \tag{2}$$

Therefore, the buoyancy term becomes,

$$r_{ref}\mathbf{g}f\left[b_{Tf}\left(\left\langle T\right\rangle^i - T_{ref}\right) + b_{C_f}\left(\left\langle C\right\rangle^i - C\right)\right] \tag{3}$$

Therefore, for steady laminar flow and making $r_{ref} = r$, the macroscopic equations for continuity, momentum and temperature take the form:

$$\nabla\cdot\mathbf{u}_D \tag{4}$$

$$r\left[\nabla\cdot\left(\frac{\mathbf{u}_D\mathbf{u}_D}{f}\right)\right] = -\nabla\left(f\left\langle p^*\right\rangle^i\right) + m\nabla^2\mathbf{u}_D - \left[\frac{mf}{K}\mathbf{u}_D + \frac{c_F f r|\mathbf{u}_D|\mathbf{u}_D}{\sqrt{K}}\right] + r\mathbf{g}f\left[b_{T_f}\left(\left\langle T\right\rangle^i - T_{ref}\right) + b_{C_f}\left(\left\langle C\right\rangle^i - C\right)\right] \tag{5}$$

$$\left(rc_p\right)_f\nabla\cdot\left(\mathbf{u}_D\left\langle T\right\rangle^i\right) = \nabla\cdot\left\{\left[k_f f + k_s(1-f)\right]\nabla\left\langle T\right\rangle^i\right\} \tag{6}$$

$$\nabla\cdot\left(u_D\left\langle C\right\rangle^i\right) = \nabla\cdot\left(D_\ell\nabla\left\langle C\right\rangle^i\right) \tag{7}$$

where Da is the Darcy velocity, r is the density of the fluid, p is the total pressure and m is the dynamic viscosity. The gravity acceleration vector is defined by $\boldsymbol{g}$. b_{T_f} is the macroscopic thermal expansion coefficient and b_{C_f} is the macroscopic solutal expansion coefficient. $\left\langle T\right\rangle^i$ and T_{ref} are the

macroscopic and the reference temperatures respectively. $\langle C \rangle^i$ and C_{ref} are the macroscopic and the reference mass concentration. The thermal conductivity for the fluid and solid are labeled k_f and k_s respectively. The diffusion coefficient of specie ℓ is D_ℓ. Finally, c_p is the specific heat and f is the porosity, K is the permeability and c_F is the Forchheimer coefficient.

2.1. Numerical Model

The solution domain is divide into a number of rectangular control volumes (CV), resulting in a structure orthogonal non-uniform mesh. Grid points are located according to a *cell-centered* scheme and velocities are store in a *collocated* arrangement (Patankar, 1980). A typical CV with its main dimensions and internodal distances is sketched in Figure 2 Writing equations (2)-(4) in terms of a general form φ

$$\frac{\partial}{\partial x}\left(rUj - \Gamma_j \frac{\partial j}{\partial x} \right) + \frac{\partial}{\partial y}\left(rVj - \Gamma_j \frac{\partial j}{\partial y} \right) = S_j \qquad \textbf{(8)}$$

where j stands for U, V, and P. Integrating the equation (8) over the control volume of Figure 2,

$$\int_d \left[\frac{\partial}{\partial x}(rUj) + \frac{\partial}{\partial y}(rVj) \right] dv = \int_{dV} \left[\frac{\partial}{\partial x}\left(\Gamma_j \frac{\partial j}{\partial x} \right) + \frac{\partial}{\partial y}\left(\Gamma_j \frac{\partial j}{\partial y} \right) \right] dv + \int_{dv} S_j \, dv \qquad \textbf{(9)}$$

Integration of the three terms in (9), namely: convection, diffusion and source, lead to a set of algebraic equations. These practices are described elsewhere (e.g. Patankar, 1980) and for this reason they not repeated here. In summary, convective terms are discretized using the upwind differencing scheme (UDS), diffusive fluxes make use of the central differencing scheme.

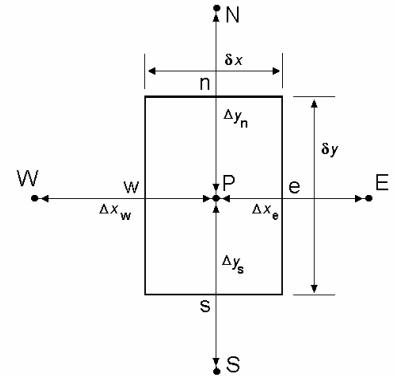


Figure 2 - Control Volume for discretization

Substitution of all approximate expressions for interface values and gradients into the integrated transport equation (9), gives the final discretization equation for grid node *P*

$$a_P j_P = a_E j_E + a_W j_W + a_N j_N + a_S j_S + b \qquad \textbf{(10)}$$

with the east face coefficient, for example, being define as

$$a_E = \max\left[-C_{e,0} \right] + D_e \qquad \textbf{(11)}$$

In (11) $D_e = {m_e d_y}/{\Delta x_e}$ and $C_e = (rU)_e d_y$ are the diffusive and convective fluxes at the CV east face, respectively, and

2.2. Multigrid Tecnique

Assembling equation (10) for each control volume of Figure 2 in the domain of Figure 1 defines a linear algebraic equation system of the form,

$$\mathbf{A}_k \mathbf{T}_k = \mathbf{b}_k \tag{12}$$

where $\mathbf{A}_k$ is the *matrix of coefficients*, $\mathbf{T}_k$ is the *vector of unknowns* and $\mathbf{b}_k$ is the vector accommodating source and extra terms. Subscript "k" refers to the grid level, with k=1 corresponding to the coarsest grid and k=M to the finest mesh.
defined as

As mentioned, multigrid is here implemented in a *correction storage* formulation (CS) in which one seeks coarse grid approximations for the *correction* defined as $d_k = \mathbf{T}_k - \mathbf{T}_k^*$ where $\mathbf{T}_k^*$ is an *intermediate value* resulting from a small number of iterations applied to (12). For a linear problem, one shows that δ_k is the solution of (Brandt, 1977, Stüben & Trottenberg, 1982, Hackbusch, 1985),

$$\mathbf{A}_k d_k = \mathbf{r}_k \tag{13}$$

where the *residue* is defined as

$$\mathbf{r}_k = \mathbf{b}_k - \mathbf{A}_k \mathbf{T}_k^* \tag{14}$$

Eq. (10) can be approximated by means of a coarse-grid equation,

$$\mathbf{A}_{k-1} d_{k-1} = \mathbf{r}_{k-1} \tag{15}$$

with the *restriction operator* I_k^{k-1} used to obtain

$$\mathbf{r}_{k-1} = I_k^{k-1} \mathbf{r}_k \tag{16}$$

The residue restriction is accomplished by summing up the residues corresponding to the four fine grid control volumes that compose the coarse grid cell. Thus, equation (16) can be rewritten as,

$$r_{k-1}^{I\,J} = r_k^{i\,j} + r_k^{i\,j+1} + r_k^{i+1\,j} + r_k^{i+1\,j+1} \tag{17}$$

Diffusive and convection coefficients in matrix $\mathbf{A}_k$ need also to be evaluated when changing grid level. Diffusive terms are recalculated since they depend upon neighbor grid node distances whereas coarse grid mass fluxes (*convective terms*) are simply added up at control volume faces. This operation is commonly found in the literature (Peric, et al, 1989, Hortmann et al, 1990).

Once the coarse grid approximation for the correction d_{k-1} has been calculated, the *prolongation* operator I_{k-1}^k takes it back to the fine grid as

$$d_k = I_{k-1}^k d_{k-1} \tag{18}$$

In order to update the intermediate value

$$\mathbf{T}_k = \mathbf{T}_k^* + d_k \tag{19}$$

Figure 3 illustrates a 4-grid iteration scheme for both the *V*- and *W*-cycles where the different operations are: *s=smoothing*, *r=restriction*, *cg=coarsest grid iteration* and *p=prolongation*. Also, the number of domain sweeps before and after grid change is denoted by ν^{pre} and ν^{post}, respectively. In addition, at the coarsest k level (k=1), the grid is swept ν^{cg} times by the error smoothing operator.

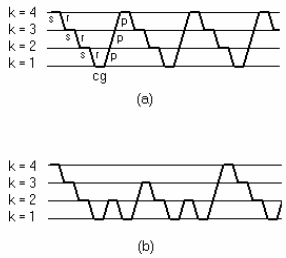


Figure 3 – Sequence of operations in a 4-grid iteration: (a) *V*-cycle; (b) *W*-cycle

3. Results and Discussion

The computer code developed was run on a IBM PC machine with two Pentium 1GHz processor. Grid independence studies were conducted such that the solutions presented herein are essentially grid independent. For *V*-cycle, pre- and post-smoothing iterations were accomplished via Gauss-Seidel algorithm while, at coarsest-grid, the TDMA method has been applied (Patankar, 1980). Also, cases in Figure 1 were run with the finest grid having size 66x66. Figure 4 shows the mesh used for the solution of the problem.

The residue is normalized and calculated according to

$$R_j = \sqrt{\sum_{ij} \left(R_{ij}^2\right)} \qquad \textbf{(20)}$$

with $R_{ij} = A_P j_P - \left(\sum_{nb} A_{nb} - j_{nb} \right)$.

where ij identifies a given control volume on the finest grid and nb refers to its neighboring control volumes.

The following figure show residue histories for the square cavity filled with porous material case, using four grids and following the *V*-cycle (see Figure 3). The solution follows a segregated approach in the sense that the temperature and mass concentration are always relaxed after the flow field, within the multigrid cycle.

Figures 5, 6 and 7 show residue histories for the buoyancy ratio *N* equal to 2, 3 and 10, respectively. One can readily notice for the *V* cycle that an increase in the buoyancy ratio does not affect the convergence rate. The figures also indicate the advantage in using more grids, for all cases presented here.

Figures 8 and 9 show the influence of the buoyancy ratio *N* on the flow, temperature and concentration patterns for Ra = 100, Le = 100 and Da = 10^{-7}. By inspecting the flow structure for low N, it may be seen that the whole enclosure is affected by the flow. For higher N, the opposite occurs. This modification of the flow structure has a direct visible consequence on the concentration field, leading possibly to vertical stratification. Although this transition towards a more solute dominated regime is barely visible, the results herein are comparable to the ones presented by Goyeau et al, 1996.

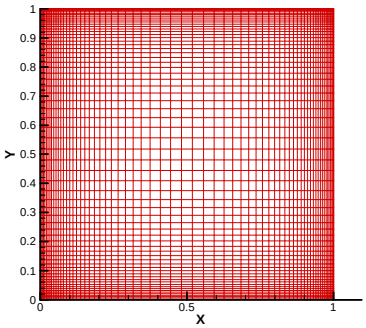
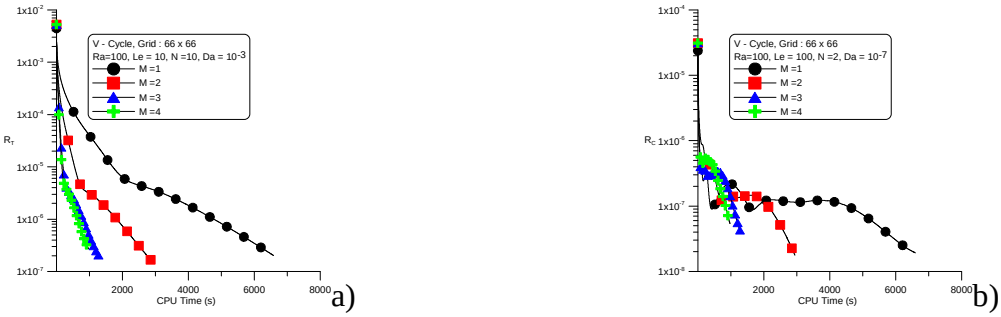
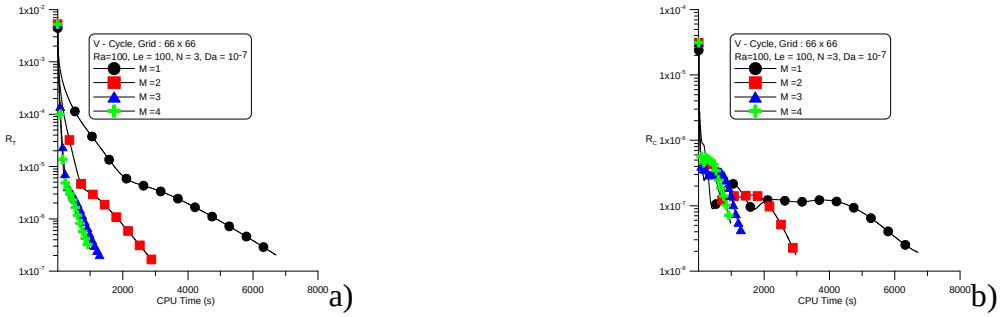


Figure 4 – Algebraically generated grid.



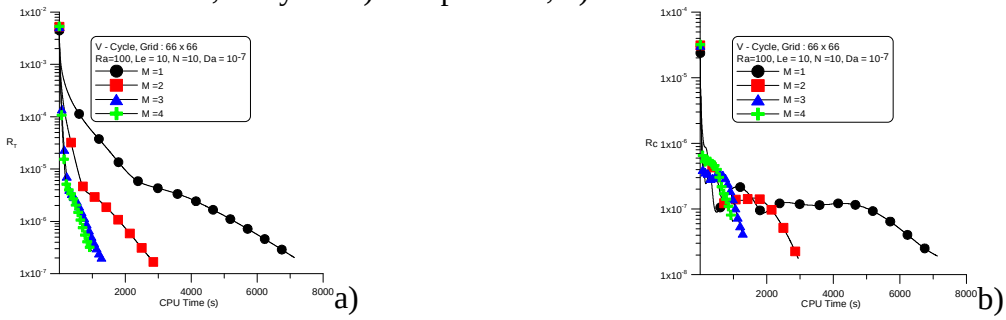
a) b)

Figure 5 - Residue history for square filled with porous material Ra = 100, Le = 100, Da = 10^{-7}, N=2, *V*-Cycle: a) Temperature; b) Mass concentration



a) b)

Figure 6 - Residue history for square filled with porous material Ra = 100, Le = 100, Da = 10^{-7}, N=3, *V*-Cycle: a) Temperature; b) Mass concentration



a) b)

Figure 7 - Residue history for square filled with porous material Ra = 100, Le = 10, Da = 10^{-7}, N=10, *V*-Cycle: a) Temperature; b) Mass concentration

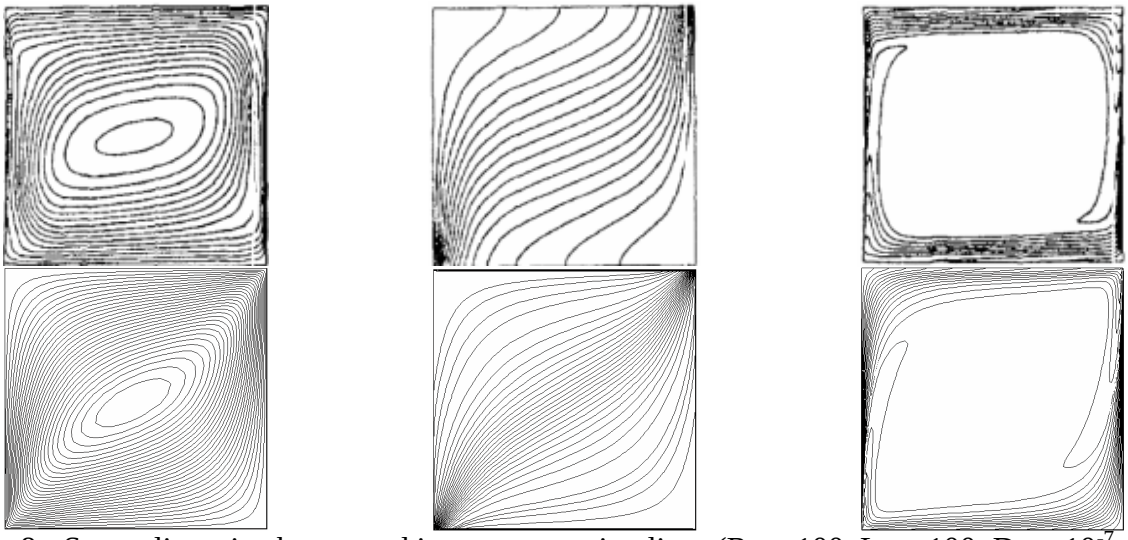


Figure 8 - Streamlines, isotherms and iso-concentration lines (Ra = 100, Le = 100; Da = 10^{-7}, N=2) Goyeau et al, 1996 (top) and presents results (bottom).

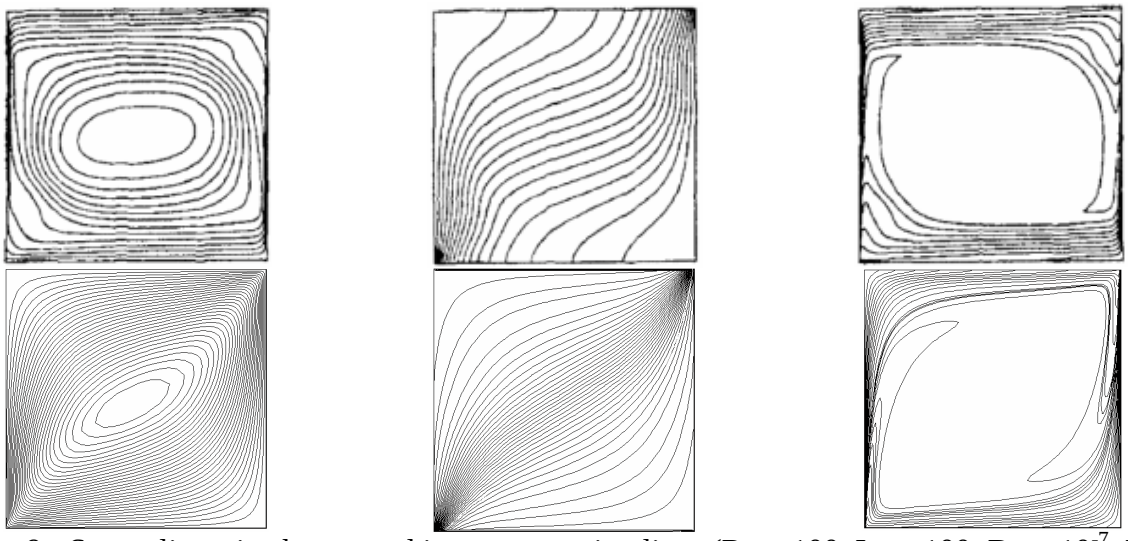


Figure 9 - Streamlines, isotherms and isoconcentration lines (Ra = 100, Le = 100; Da = 10^{-7}, N=3) Goyeau et al, 1996 (top) and presents results (bottom).

4. Acknowledgement

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