3. 2-D SIMULATION OF GASEOUS SPECIES CONCENTRATION PROFILES IN A HYPOTHETICAL RESERVOIR BASIN WITH REACTIVE STRATIFIED FLOW

This section brings together techniques previously developed in this thesis. The formulations previously described, where MDBC is applied as the outlet BC to momentum and species governing equations, are used to compute concentrations profiles for selected situations. Thus, Equation 105 is the basic equation that applies in the following simulation tests. It must be noted that, in these computations, flow velocities do not need to be calculated directly, its coupling to the concentration being provided by the stream function derivatives (Equation 105). It is also to point out that the vorticity transport equation encompasses the buoyant term (Equation 88) and also contributes to the coupling of concentration to the momentum transport.

3.1 Concentration Profile Simulations Tests

The computational code that was developed is provided with enough resources that make possible GQ integration of variable number of points and to generate meshes in two shapes. Nevertheless, to limit the risk of being redundant, this section restricts itself to results produced in discretized domains of 1800 regular triangular shape elements, where integrations were performed exclusively through GQ of seven points.

This mesh was chosen based upon experiments already made in Section 2. It was found that this refining can produce stable solutions within practical computing times, in face of the hardware available. The criteria already used in Section 1 (Equation 50) is also observed in order to obtain appropriate time stepping.

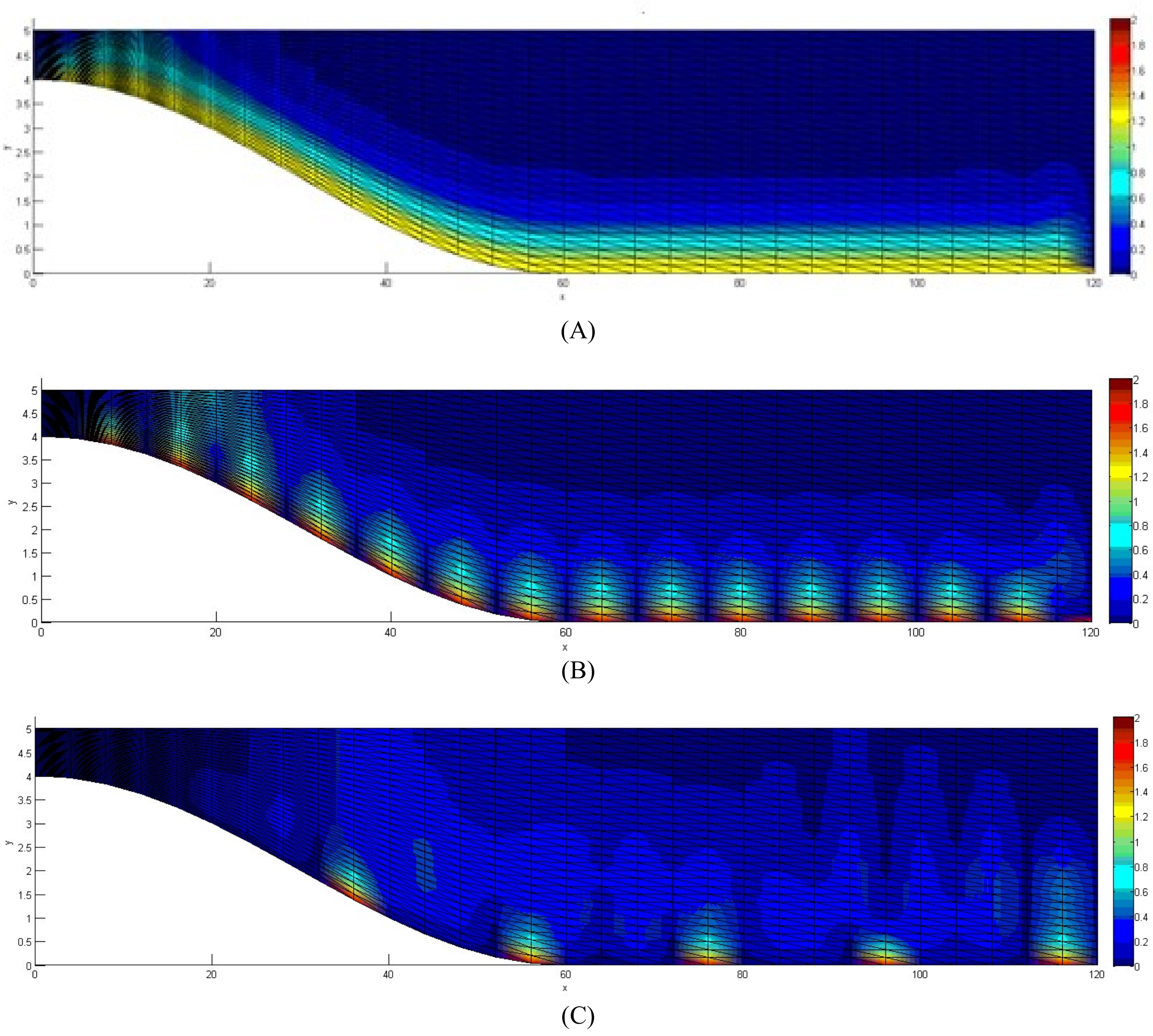
It is to note that, in huge reservoir basins, the time to detect notable changes of concentration transport under chemical reaction, flow and weather influence may be very large to be of interest of simulation testing. So, time is set arbitrarily, as if phenomena were occurring in an accelerated time scale.

In order to cope with general reservoir dynamics, the code simulates gas evolution from the bottom, as may be the case of a flooded terrain that was covered by vegetation which undergoes anaerobic decomposition. In order to simulate biomass depletion, the number of spots that generates gas is programmed to decrease with time, through conveniently formulated EBCs (Equation 107) in the code function applCC2 (Appendix B). Features of the code that simulates blowing wind on the reservoir surface and environmental driven loads are also explored.

3.1.1 No wind blowing on reservoir surface

For zero surface vorticity (ω_s), which means no wind blowing on reservoir surface (see Equations 75 to 78), Figure 33 shows outcomes for flow parameters such as arbitrarily equal two-dimensional diffusivity coefficients ($D_x = D_y = 0.5$), Re = 100 and decay coefficient of –0.5. It illustrates the two-dimensional transport of the gas and the dynamic of the biomass depletion, which shows reduction of the gas production area as time progresses, assuming there is no biomass renovation. The concentration profiles obtained indicate consumption of the reactive gas along the reservoir depth, its vertical and longitudinal transport due to diffusion and convection, and some bubbling at the surface.

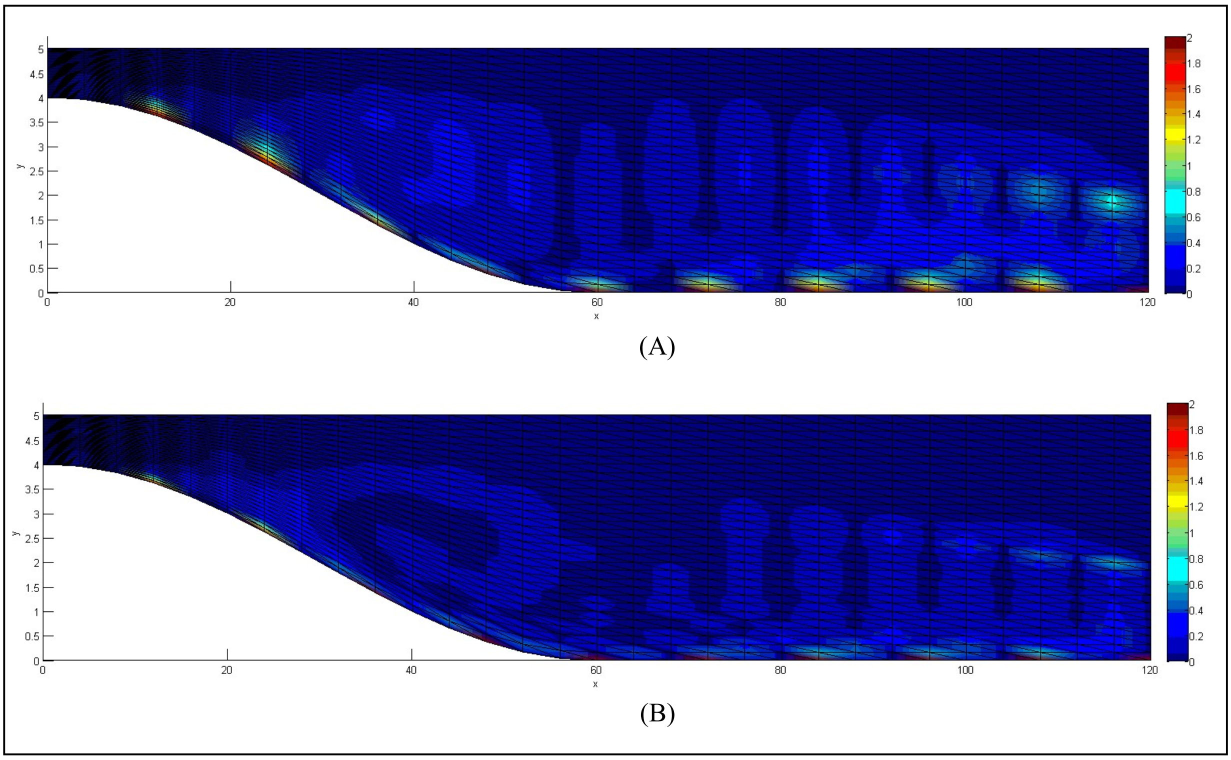
Figure 33 – Gas concentration profile computation for different time lapses (Re = 100)



Tags: (A) – Time elapsed = 1.0; (B) – Time elapsed = 2.5; (C) – Time elapsed = 4.0.

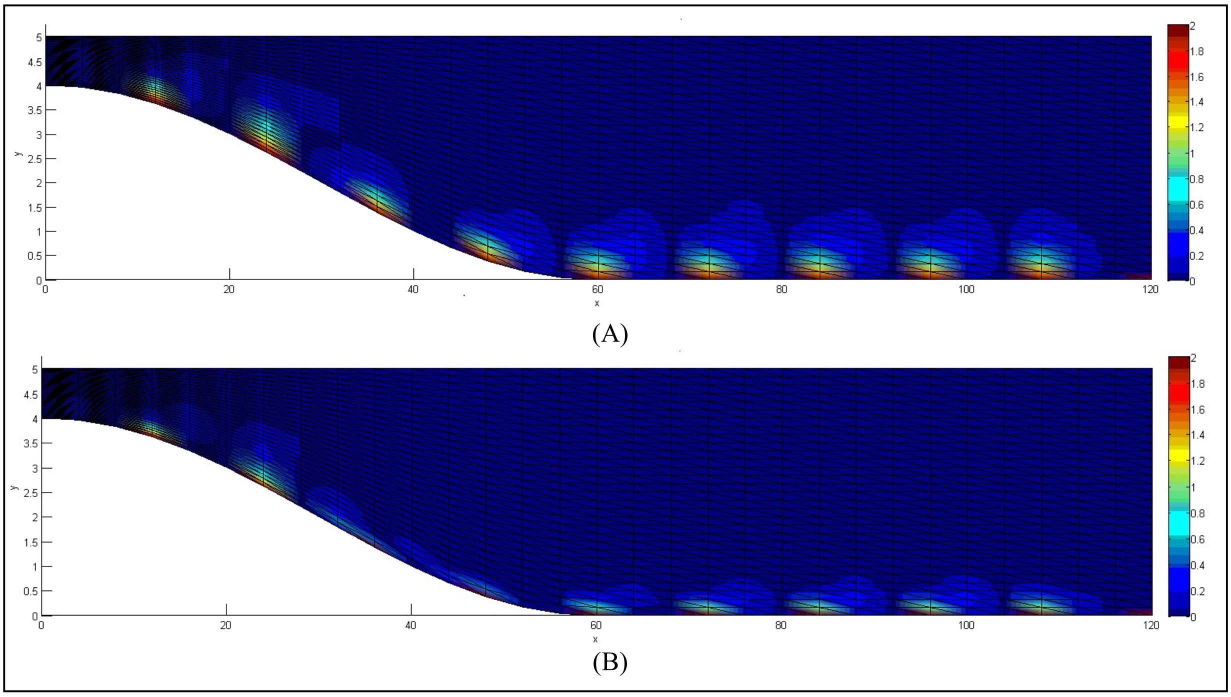
Figures 34 A and B illustrate the effect of smaller diffusivity coefficients for the same flow pattern (Re = 100) and for the same decay rate of – 0.5. As it can be noted, in spite of the greater elapsed time, simulation foresees larger gas depletion due to oxidation because smaller diffusivity naturally implies in longer residence time of the reactant in the medium. In Figure 36 B, besides the chemical reaction, the longitudinal velocity component couples to longitudinal diffusional transport, because D_x is greater than D_y, flattening the concentration profile. This may imply in non-reacted gas ejection from the reservoir to the outside, what is observed in actual cases (LIMA et al., 2008). As a consequence, in both figures, the amount of gas to bubble at the surface is reduced consistently.

Figure 34 – Gas concentration profile for different diffusion coefficients (Re =100; time elapsed = 5.0.)



Tags: (A) $D_x = D_y = 0.1$; (B) $D_x = 0.1$; $D_y = 0.01$.

Figure 35 – Gas concentration profile for $k = -2.0$ (Re = 100)



Tags: (A) $D_x = D_y = 0.5$; Time elapsed = 4.0; (B) $D_x = D_y = 0.1$; Time elapsed = 5.0.

Figures 35 A and B, by their turn, illustrate the effect of larger reaction rate ($k = -2.0$) for the same flow conditions of Figures 33 C and 34 A, respectively. As expected, it is shown that larger consumption of the reactive gas and its concentration is restricted to lower depths. However, it is expected that, after a considerable time, the gas may eventually reach the surface, if there is still decomposing biomass substrate, what is depicted by Figure 36.

Figure 36 – Gas concentration profile for $k = -2.0$ and elapsed time = 20 (Re = 100; $D_x = D_y = 0.5$).

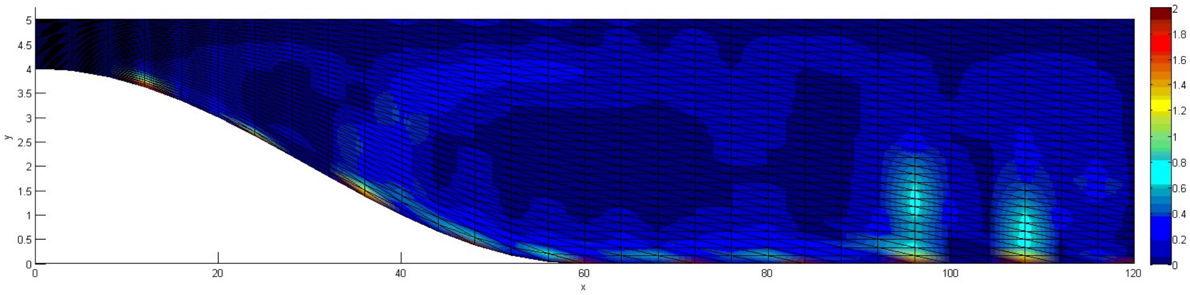
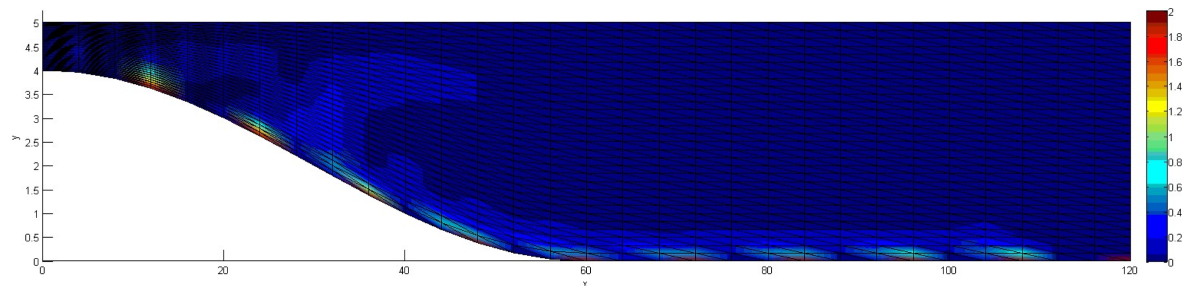
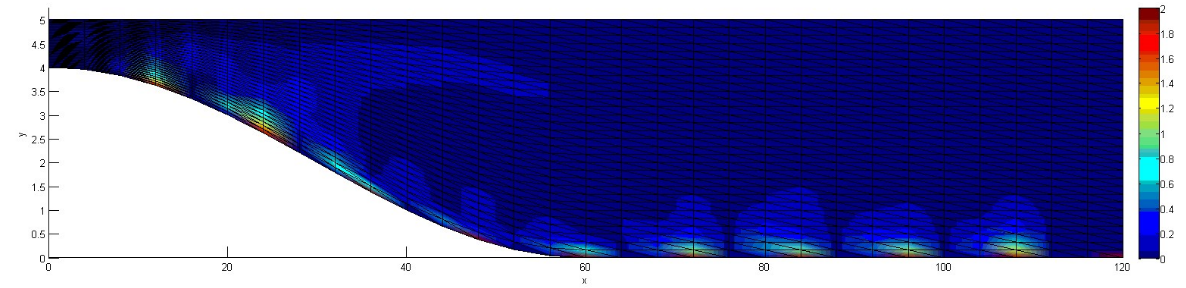


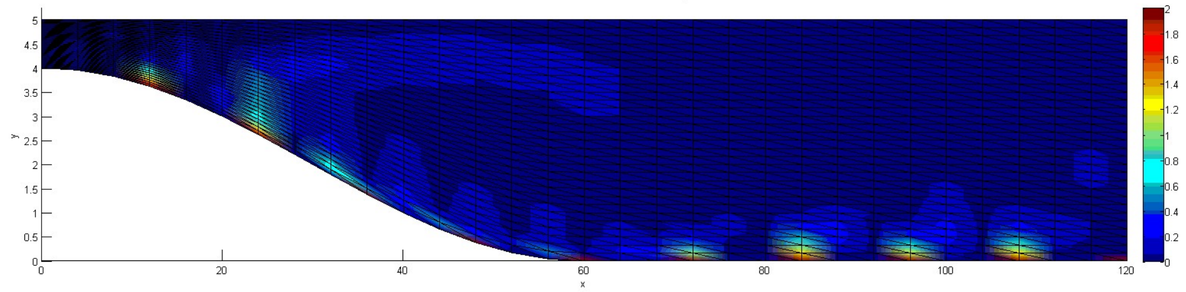
Figure 37 – Gas concentration profile for various Re ($D_x = D_y = 0.5$; $k = -1.0$; time elapsed = 10.0).



(A)



(B)



(C)

Tags: (A) – Re = 100; (B) – Re = 500; (C) – Re = 1000.

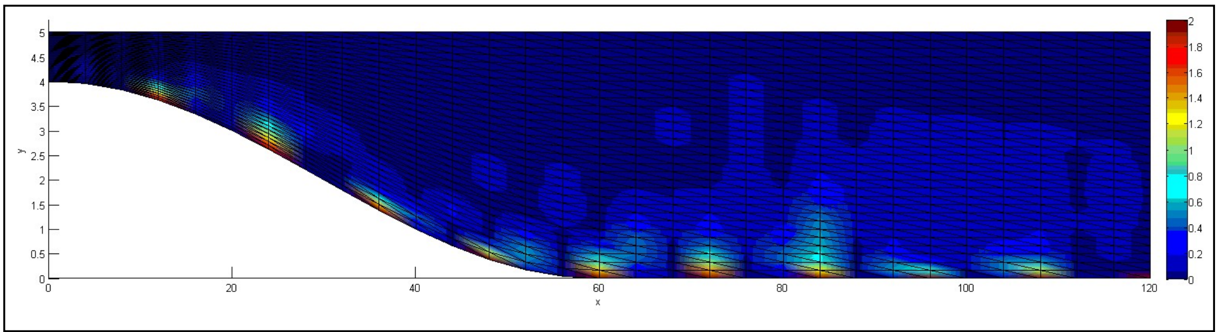
Figures 37 A, B and C, above, illustrate the effect of changing the flow pattern by varying Re. The figures depict variable concentration distribution and species mixing which seem to increase with increasing Re, as it would be expected. The results of these figures were obtained for the same diffusivity coefficients, decay parameters and elapsed times.

3.1.2 Wind blowing on reservoir surface

As shown in the preceding section, wind blowing on the water surface is supposed to change the value of the corresponding boundary vorticity, implying in modification of the flow velocity profile (see again, for instance, Equations 75 to 78). As expected, the simulation shows that the concentration profile also is influenced.

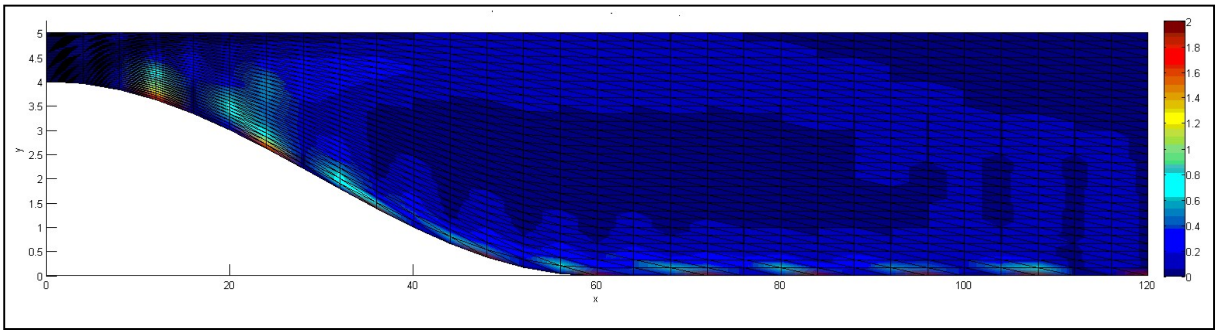
Figure 38 is the outcome for a simulation where flow parameters are similar to those of Figure 37 B. Nevertheless, wind blowing tangentially on the water surface, in the opposite direction of the longitudinal flow, is simulated by imposing a vorticity boundary value of 1.0 (ω_s). It is observed that the concentration profile changes, moving nearest to the bottom at first and showing a tendency to resurface at the reservoir last half, what is in accordance with the velocity profile depicted by Figures 21 and 28.

Figure 38 – Gas concentration profile for wind blowing on the reservoir surface (ω_s = 1.0).



In Figure 39, it is depicted a simulation where the wind blows in the same direction as the longitudinal flow, which is here achieved by imposing a vorticity boundary value of – 1.0 (ω_s). Other flow parameters are the same as those of Figure 39 C. It is observed that the gas shows a tendency of spraying and mixing along the reservoir length, mainly at smaller depths, transported by the higher flow velocities of the surface, what is in accordance with the velocity profile depicted by Figure 29.

Figure 39 – Gas concentration profile for wind blowing on the reservoir surface (ω_s = – 1.0).



3.1.3 Cyclic environmental effects simulation

Figure 40 depicts a simulation where the inflow changes under the influence of a seasonal effect, in a similar case to that depicted in Figure 23, where the flow inlet parameters (Table 3) are multiplied by (1+cos$m\pi$t). For this outcome, it was assumed no wind blowing at the surface and the flow parameters are: 2-D diffusion coefficients equal to 0.5; reaction term equal to – 1.0 and an arbitrary time limit of 20. Stressing again the difficulty to figure out the dynamic of these periodic changes in a static figure, we observe that the concentration profile assumes a form that is likely to be under influence of velocity profile variation (see Figure 23).

Figure 40 – Gas concentration profile for cyclic inflow variation (Re = 100).

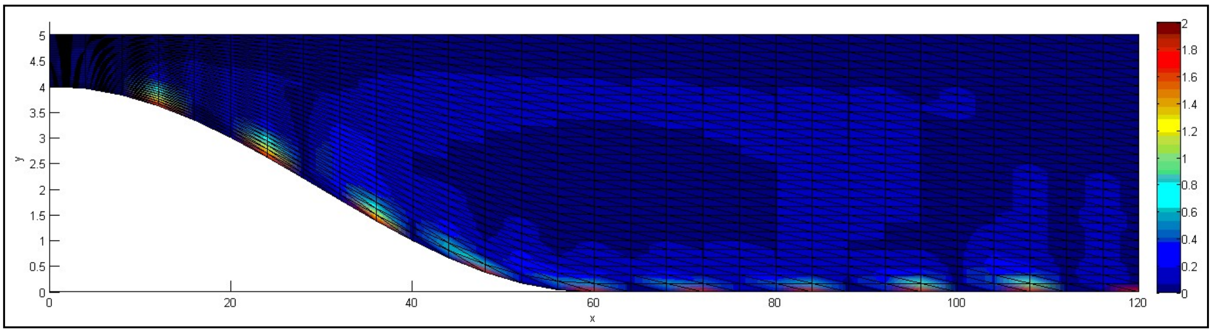
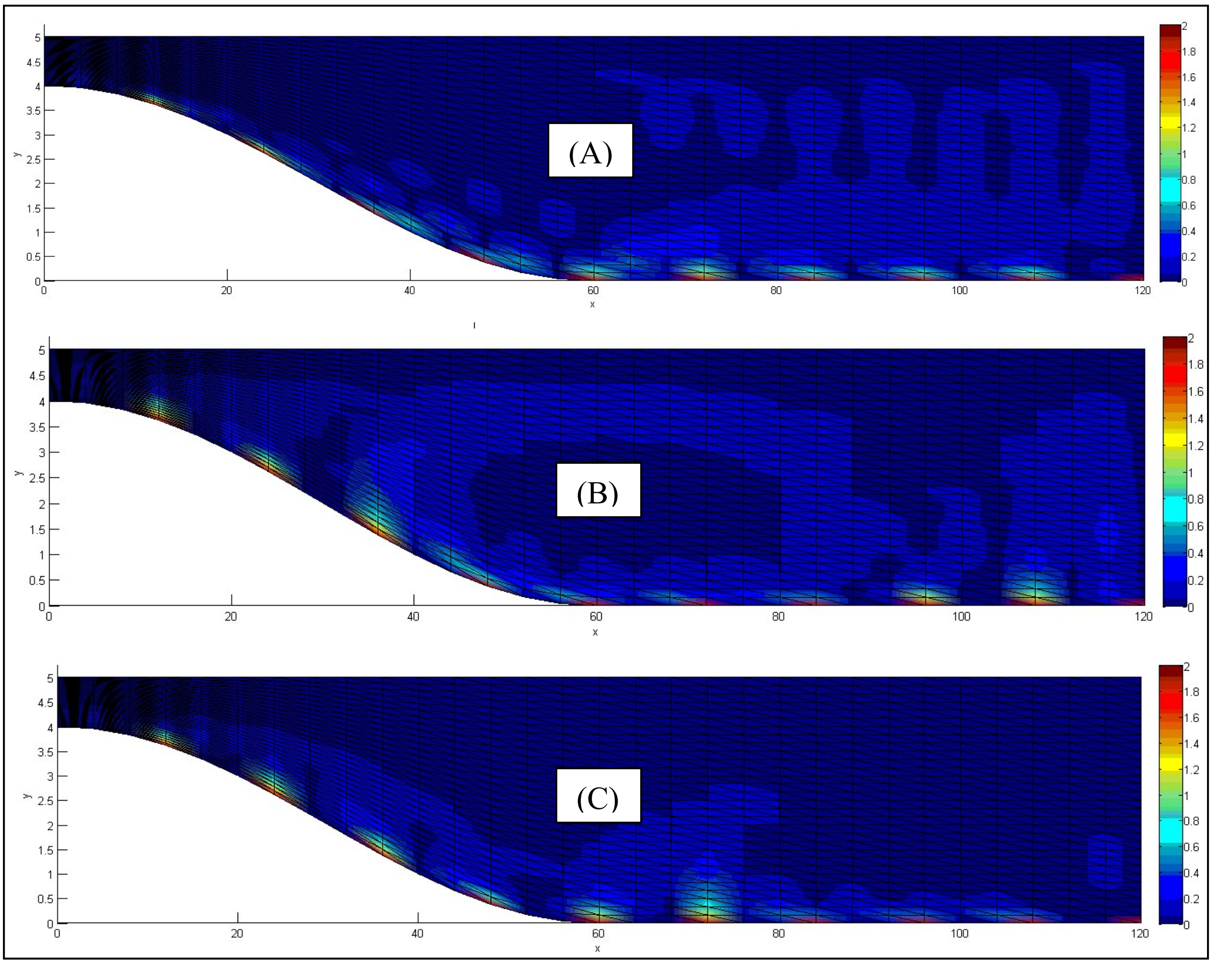


Figure 41 – Gas concentration for cyclic driven surface wind variation (Re=100).



Tags: (A) – ω_s = 1+cos2πt; (B) – ω_s = –(1+cos2πt; (C) – alternate surface vorticity.

Figures 41 A, B and C, above, show cases related to concentration profiles matching those of Figures 24 to 26 for velocity profile, that is, when the blowing wind at the surface undergoes cyclic changes of magnitude and/or direction. The flow parameters are the same as those of Figure 40.

Figure 41 A matches the case of a wind blowing in the opposite direction of the longitudinal flow with variable intensity, resulting in a concentration flattened profile but of different intensity as the one of Figure 38. Figure 41 B depicts the influence of a variable intensity blowing wind in the same direction as the flow. Alike Figure 39, the gas mixes and diffuses along the reservoir, but in different quantities due to the variable magnitude of the blowing wind. Finally, Figure 41 C is the outcome of a situation where, at first, there is no wind ($\omega_S = 0$), then a wind is set to blow in the opposite direction to the flow ($\omega_S = 1.0$) and last in the same direction as the flow ($\omega_S = -1.0$).

The situations sketched by Figures 40 and 41 imply in solving the vorticity transport equation with time varying BC, being particular cases as those already explored in Sections 1 and 2, now further explored for the simulation of the concentration distribution coupled to the flow velocity. It means also a transient variation of the surface tension, what obviously implies in different concentration profiles whose shapes are in accordance to the velocity distributions computed in the last section. The ability to capture such features, induced by environmental conditions to which the reservoirs are exposed, is another contribution of this thesis, which is provided for a future complete simulation code.

3.2 **Closure**

In Section 2, the formulation for flow velocity encompassed the particularities developed in this thesis, such as transient BCs and the use of MDBC as an outlet BC, in order to simulate features of flow in reservoirs.

As a consequence, the mathematical model tested in Section 1 was updated in order to couple the flow velocity to the concentration govern equation and computations of gas concentration profiles that occur in hydroelectric reservoirs, where gases evolve from the bottom and react in their path to the surface, were presented.

The simulations were now able to represent more faithfully concentration profiles driven by environmental conditions, such as variable inlet feed, wind blowing on the water surface and density profiles, constituting the envisaged tool that can be used to meet the requirements of a closed simulation package.

It must be observed that the outcomes presented try to capture the behavior of dynamic changing systems that is not always depicted by static figures alone. Also, it must be added that, although not explored in this section, which worked with constant diffusion and rate coefficients, the code is able to calculate local diffusion and rate coefficients once their geographical profile is known, as it can be noted in function calcSElem(e) of the code (Appendix B).

CONCLUSION

In summary, the scope of this thesis was to draw a formulation that implied in a computing method prone to be used as a tool to simulate a hypothetical hydroelectric plant reservoir. In these reservoirs, it is known that gases evolve to the atmosphere, mainly carbon dioxide and methane (WWW.KOLUMBUS.FI, 2007), as a consequence of biomass anaerobic decomposition on its bottom. Thus, it is expected that the research of a suitable method for simulation of flow velocities and gas concentration could be effectively used to counteract harmful effects of these greenhouse gases release, as well as to enable its use them as power source, as pointed out by Bambace et al. (2007).

Then, in Introduction Section, a sketch of reservoirs dynamics was made, finding basis for the study of the simulation of stratified flows as a model to represent the dynamics of these water bodies. According to practical observations collected, the evolved gases may react with dissolved oxygen in the reservoir water, reach the surface and bubble to the atmosphere or else, may be carried outside the domain by the flow, through the drains of the dam (LIMA et al., 2008). Obviously, it is a reactive flow where the main attentions must be given to the discharge flow, longitudinal, and the gas vertical flow reaching the surface, where chemical reaction occurs. As these velocity components seem to encompass the main aspects of the flow, it was decided to restrict the study to 2-D simulations, even though large reservoirs would not necessarily feature symmetry in z coordinate. Such domain is subjected to environmental conditions showing cyclic changes (CUSHMAN-ROISIN, 2014), that can be represented by time dependent and periodic functions but demand further investigation of proper BC. Having in mind that flow in reservoirs have flow at low velocities, an average hydrodynamic field was assumed and no turbulence models were introduced in the evolution equations. Density variations caused by different depth temperatures and by concentration gradients of gas were decided to be represented through the Boussinesq approximation in the vorticity transport equation, not smearing the simplicity of the model. Therefore, vorticity and stream function formulation of the Navier-Stokes equations was assumed for the system modeling. A “slice” of the reservoir was then taken supposedly aligned to inflow and outflow positioning, as illustrated by Figures 7 and 14. Numerical procedure FEM schemes were adopted, assuring the necessary flexibility to deal with problems of multidimensional reactive flows in complex geometries.

Following, Section 1 dealt with the research of a computing method for simulation of chemical species concentration in a two-dimensional reactive flow subjected to time dependent inputs. Preparatory work was carried out in order to fulfill gaps still existing in the scope of this work, like the development of multidimensional analytic solutions of the species conservation equation applied to cyclic loads (Annex A) and the development of proper downstream BCs for the same class of environmental conditions (Annex B). These works were reported in the Proceedings of the Brazilian Society of Computational and Applied Mathematics (OLIVEIRA FILHO; MANGIAVACCHI, 2017) and the Brazilian Journal of Chemical Engineering (OLIVEIRA FILHO et al., 2017), respectively. They comprise analytical developments reaching a new formulation by employing a BC that extend the physics of the problem to the domain boundaries, in an effort to capture variations in the domain limits due to time dependent inputs. This kind of BC was already suggested by the literature, as it may be found in Bristeau et al. (1987), but it does not seem to be ever implemented. Here, it was termed Material Derivative Boundary Condition (MDBC), due to its mathematical layout and is one of the main contributions of this thesis.

A MATLAB code prototype using a simple GFEM formulation was developed to test computations using the MDBC. Aware that this simple numerical scheme could experience instabilities and oscillations, appropriate criteria were used for time step and element size, as described in Section 1. In these experiments, velocity and concentration profiles were uncoupled in order to achieve verification through comparison with published and developed analytical solutions for concentration profiles. Analysis of the obtained solutions showed that MDBC could better capture the effect of periodic input at the boundaries than traditionally used BCs (Table 1).

Section 2, by its turn, coupled the flow velocity profile to species concentration problem, by taking into account density variations due to dissolved gas with the use of Boussinesq hypothesis. In this section, the MDBC was used in a novel formulation for vorticity transport (Equation 82), another main contribution of this work, making it possible to adopt similar treatment for the governing equations for species transport. The computational implementation was done by expansion and completion of the previous code prototype and then, two-dimensional flow velocity profiles were able to be simulated, taking into account several situations driven by environmental conditions. A major difficulty, faced in this phase of the research, was the proper handling of vorticity at the solid boundaries, due to the lack of correspondent BCs. This difficulty was overcame by the equation system uncoupling, as suggested by the literature. So, first, the stream function was solved, then wall vorticity was computed, both from Equation 62. Then, field vorticity was calculated from Equation 82.

The finite elements scheme used here also relied simply in GFEM for space discretization, without using any upwinding technique. The use of a fully implicit time discretization scheme together with proper mesh refining made possible to approach solutions for Reynolds Numbers up to 1000, without exploiting the effects of the numerical viscosity. Although running in limited hardware capability, simulations with meshes up to 2025 elements were performed in practical computational times with acceptable oscillations smoothing. Thus, it was possible to cover the span of simulations of flows more likely to happen in reservoirs, in other words, those driven mainly by surface winds and buoyancy forces, with large retention times. The accuracy of the solutions was demonstrated by the application of the core of the algorithm to the well-known problem of lid-driven cavity flow. This benchmark was adopted for verification because the reservoir model is, itself, close to cavity flow. Outcomes verify the code (Figure 32 and Table 5) which may be assumed to represent the schematic behavior of the flow characteristics.

Section 3 brought together the techniques developed in previous ones and shows 2-D outcomes for gas concentration profiles obtained by the computation of the governing equations system comprised by Equations 2, 3 and 4 but with a coupled velocity profile for the species transport equation (Equation 105). For the same span of Reynolds Numbers and mesh refining as before, gas concentration profiles were simulated and aspects of different situations were discussed. It was found that gas distributions changed in accordance with flow Reynolds Numbers, diffusion coefficients and decay ratio and also are influenced by environmental effects, reinforcing the verification achieved by the model in Sections 1 and 2.

Thus, it may be finally concluded that the envisaged tool was attained and that the features listed in the Closure of Introduction Section were also provided.

This thesis occupies itself much more of the development and verification of a new mathematical model rather than a closed simulation code. Looking this way, it does not exhaust the object. Nevertheless, multiple paths were open to pursuing new research that might hit other outstanding goals.

In the field of applied mathematics, for instance, the supposition of inclined outlet flow, as suggested by Equation 73, could generalize the MDBC solution for vorticity transport, although more difficult to implement. The introduction of a two fluid or two-phase model, rather than the homogeneous flow model used here may also lead to novel and very contributing formulations and make it possible more precise simulations. Considerations for introducing the Energy Equation in the system of governing equations, coupling the temperature field, could also be made. But this coupling must be carefully weighted because of environmental weather conditions that strongly influence and often force the temperature field. Although implying in a very large computational effort, it looks promising that a three-dimensional model be developed with the use of the vector potential (AZIZ; HELLUMS, 1967) in order to keep on applying stream function and vorticity concepts. This model would provide, undoubtedly, means of achieving a complete simulation in such a large basin as a reservoir, extending the periodicity of outlet conditions, so well represented by MDBC, to the z coordinate. Turbulence models could also be applied in the construction of a new model. However, this must be subjected to analysis, maybe based on experimental data, in order to evaluate in what types of basin, in which situations and when it would be rewarding to adopt them.

In the field of computational programming and simulation, it is to note that, although written in MATLAB, a high level programming language, an effort was made in order to make feasible an easy translation of the algorithm into a low level language, like C++ or FORTRAN. As it can be verified in Appendices B and C, the codes were programmed in several functions that practically constitute subroutines. In these functions, logic, meshes and matrices are mostly built by hand, not necessarily using MATLAB resources, and integrations are solved numerically through the use of GQ, also specifically programmed. Thus, a following step might as well be to translate these codes in some of those closer-to-hardware languages. This might enhance the possibilities of the simulation, just as refining further the mesh and obtaining more accurate solutions within practical computational times, without exceeding the capacity of the hardware usually available in our universities and research institutes. For three-dimensional models simulations, for instance, it seems crucial. An easier task could be to make more prominent the nonlinear feature of the code in respect to concentration profile computation. Although not explored within this thesis, the code is able to calculate local diffusion and rate coefficients once their geographical profile is known, as it can be noted in function calcSElem(e) of the code (Appendix B). Also not explored, due to time limitations, is the generation of a moving mesh, in order to simulate seiches that imply in varying surface levels that often takes place in large reservoirs (PACHECO, 2009). A raw programming for this feature was made, but the computational cost was very high and, for now, it was left aside.

Finally, if a simulation package is intended to be of practical use, it obviously needs to make use of experimental data collected in laboratory and on field. Thus, future works in the experimental field are envisaged. For instance, development of methods and appliances, as well as selection of dams and of parameters to be measured comprise a huge, expensive and complex task that is bound to be pursued as soon as possible.

REFERENCES

ARAL, M. M.; LIAO, B. Analytical solution for two-dimensional transport equation with time-dependent dispersion coefficients. *J. Hydrol. Engrg*., vol. 1, nº. 1, pp. 20-32, 1996.

AREGBESOLA, Y. A. S.; BURLEY, D. M. The vector and scalar potential method for the numerical solution of two and three-dimensional Navier-Stokes equations. *J. Comp. Phys*, nº. 24, pp. 398-415, 1977.

AZIZ, K.; HELLUMS, J. D. Numerical solutions of the three-dimensional equations of motion for laminar natural convection. *The Physics of Fluids*, vol. 10, nº. 2, pp. 314-324, Feb. 1967.

BAMBACE, L.A.W.; RAMOS, F. M.; LIMA, I. B. T.; ROSA, R. R. Mitigation and recovery of methane emissions from tropical hydroelectric dams. *Energy*, vol. 32, pp. 1038-1046, 2007.

BASTVIKEN, D.; EJLERTSSON, J.; TRANVIK, L. Measurement of methane oxidation in lakes: a comparison of methods. *Environ. Sci. Technol.,* vol.36, nº. 15, pp. 3351-3361, 2002.

BOEGMAN, L. Currents in stratified water bodies 2: internal waves. In: LINKENS, G. E. (Editor). *Encyclopedia of Inland Waters.* Oxford: Elsevier, 2009, v.1, pp. 539-558.

BRISTEAU, M. O.; GLOWINSKI, R.; PERIAUX, J. Numerical methods for the Navier-Stokes equations; applications to the simulation of compressible and incompressible viscous flows. *Comp. Phys. Rep.*, vol. 6, pp. 73-187, Feb. 1987.

CAMPION-RENSON, A.; CROCHET, M. J. On the stream function-vorticity finite element solutions of Navier-Stokes equations. *Int. j. numer. methods eng.,* vol. 12, pp. 1809-1818, 1978.

CHAPMAN, B. M. Dispersion of soluble pollutants in non-uniform rivers – I. theory, *J. Hydrol.*, nº. 40, pp. 139-152, 1979.

CHAPRA, S.C.; CANALE, R. P. *Numerical methods for engineers, 6^{th} ed*. New York: Mc Graw-Hill, 2010. 968 p.

CHEN, J. S.; LIU, C. W. Generalized analytical solutions for advection-dispersion equation in finite spatial domain with arbitrary time-dependent inlet boundary condition. *Hydrol. Earth Syst. Sci*., nº. 15,pp. 2471-2479, 2011.

COMINI, G.; MANZAN, M.; NONINO, C. Finite element solution of the streamfunction-vorticity equations for incompressible two-dimensional flows. *Int. J. Numer. Meth. Fluids*, vol. 19, pp. 513-525, 1994.

CUSHMAN-ROISIN, B. *Environmental transport and fate, chapter 5 – lake dynamics*. Thayer School of Engineering, Darthmouth College, Hanover, USA, 2012. Available at: < https: // engineering. dartmouth. Edu /~ d30345d /courses/ engs43/ Chapter5. pdf>. Retrieved: 26 Aug 2016.

______. *Environmental fluid mechanics – lake and reservoir dynamics*. Thayer School of Engineering, Darthmouth College, Hanover, USA, 2014. Available at: <https://engineering.dartmouth.edu/~d30345d/courses/engs151/EFM-Lakes.pdf>. Retrieved: 26 Aug 2016.

CZERNUSZENKO, W. Dispersion of pollutants in rivers, *Hydr. Sci. J.*, vol. 32, nº. 1, pp. 59-67, 1987.

DHATT, G.; FOMO, B. K.; BOURQUE, C. A *ψ-ω* finite element method for the Navier-Stokes equations. *Int. J. Num. Meth. Engnrg.*, vol. 17, pp. 199-212, 1981.

ENVIRONMENTAL NEWS SERVICE (ENS). *Methane from dams: greenhouse gas to power source*, 2007. Available at: < http://www.ens-newswire.com/ens/may2007/ 2007-05-09-04.asp >. Retrieved 28 Oct 2013.

ERTURK, E. et al. Numerical solutions of 2-d steady incompressible driven cavity flow at high Reynolds numbers. *Int. J. Numer. Meth. Fluids*, vol. 48, pp. 747-774, 2005.

FEARNSIDE, P. M. Greenhouse gas emissions from a hydroelectric reservoir (Brazil's Tucuruí dam) and the energy policy implications. *Water Air Soil Pollut*, nº. 133, pp. 69-96, 2002.

FINLAYSON, B. A. *The method of weighted residuals and variational principles, with application in fluid mechanics, heat and mass transfer*. New York: Academic Press Inc., 1972, 412 p.

______. Nonlinear analysis in chemical engineering. New York: Mc Graw-Hill, 1980, 366 p.

GALEÃO, A. C.; ALMEIDA, R. C.; MALTA, S. M. C; LOULA A. F. D. Finite element analysis of convection dominated reaction-diffusion problems. *Appl. Num. Math.*, nº. 48, pp. 205-222, 2004.

GHADI, F.; RUAS, V.; WAKRIM, M. Numerical solution of the time-dependent incompressible Navier-Stokes equations by piecewise linear finite elements. *J. Comp. Appl. Math.*, nº. 215, pp. 429-437, 2008.

______. Finite element solution of a stream function-vorticity system and its application to the Navier-Stokes equations. *Appl. Math.*, vol. 4, pp. 257-262, 2013.

GHIA, U.; GHIA, K. N.; SHIN, C. T. High-re solutions for incompressible flow using the Navier-Stokes equations and a multigrid method. *J. Comp. Phys.*, nº. 48, pp. 387-411, 1982.

GLAISNER, F.; TEZDUYAR, T. E. Finite element techniques for the navier-stokes equations in the primitive variable formulation and the vorticity stream-function formulation. Houston: Department of Mechanical Engineering, University of Houston, 1987. 61p. NASA Interim Report.

GLOWINSKI, R.; PIRONNEAU, O. Numerical methods for the first biharmonic equation and for the two-dimensional Stokes problem. Stanford: Computer Science Department, Stanford University, 1977. 81p. Report STAN-CS-77-615.

GOLZ, W. J.; DORROH, J. R. The convection-diffusion equation for a finite domain with time varying boundaries. *Appl. Math. Lett.,* vol. 14, pp. 983-988, 2001.

GUÉRIN, F.; ABRIL, G.; RICHARD, S.; BURBAN, B.; REYNOUARD, C.; SEYLER, P.; DELMAS, R. Methane and carbon dioxide emissions from tropical reservoirs: significance of downstream rivers. *Geoph. Res, Lett.*, vol. 33, L21407, Nov 2016.

HIRASAKI, G. J. *A general formulation of the boundary conditions on the vector potential in three-dimensional hydrodynamics*. 1967. 49p. Dissertation - Rice University, Ann Arbor, 1967.

HOFFMAN, K. A.; CHANG, S. T. *Computational fluid dynamics -vol. I, 4th. ed*. Wichita: Engineering Education System, 2000. 486 p.

ITAIPU BINACIONAL. *A maior geradora de energia limpa e renovável do planeta,* 2016. Available at:<https://www.itaipu.gov.br/sala-de-imprensa/fotos>. Retrieved: 10 Jan 2017.

JIAN-GUO, L.; WEINAN, E. Simple finite element method in vorticity formulation for incompressible flows. *Math. of Comp*., vol. 70, nº. 234, pp. 579-593, 2000.

JOHN, V.; SCHMEYER, E. Finite element methods for time-dependent convection-diffusion-reaction equations with small diffusion. *Comp. Meth. Appl. Mech. Engrg*, nº. 198, pp. 475-494, 2008.

KASCHIASHVILI, K.; GORDEZIANI, D.; LAZAROV, R.; MELIKDZHANIAN, D. Modelling and simulation of pollutants transport in rivers. *Appl. Math. Mod*., nº. 31, pp. 1371-1396, 2007.

KAWALA, A. M.; ODDA, S. N. Numerical investigation of unsteady free convection on a vertical cylinder with variable heat and mass flux in the presence of chemically reactive species. *Adv. P. Math*, nº. 3, pp. 183-189, 2013.

KONZEN, P. H.; De BORTOLI, A. M.; THOMPSON, M. Finite element method applied to the solution of a convective-diffusive-reactive flow, In: XXX CONGRESSO NACIONAL DE MATEMÁTICA APLICADA E COMPUTACIONAL – XXX CNMAC (Annals), Florianópolis (2007). Available at: http://www.sbmac.org. br /eventos/ cnmac/ xxx_cnmac /PDF/294.pdf. Retrieved: 08 Sept 2015.

LAUNAY, M.; Le COZ, J.; CAMENEM, B.; WALTER, C.; ANGOT, H.; DRAMAIS, G.; FAURE, J.-B.; COQUERY, M. Calibrating pollutant dispersion in 1-d hydraulic models of river networks. *J. Hydro-env. Res*., nº. 9, pp. 120-132, 2015.

LEE, M. E.; SEO, I. W. Analysis of pollutant transport in the Han river with tidal current using a 2D finite element model. *J. Hydro-env. Res*., vol. 1, nº.1, pp. 30-42, 2007.

______. 2D finite element pollutant transport model for accidental mass release in rivers. *KSCE J. Civ. Eng*., vol. 14, nº.1, pp. 77-86, 2010.

LEWIS, R. W.; NITHIARASU, P.; SEETHARAMU, K. N. *Fundamentals of the finite element method for heat and fluid flow*. Chichester: John Wiley & Sons, 2005. 341 p.

LIMA, I. B. T.; RAMOS, F. M.; BAMBACE, L.A.W.; ROSA, R. R.. Methane emissions from large dams as renewable energy sources: a developing nation perspective. *Mitig. Adapt. Strat. Glob. Change*, nº. 13, pp. 193-206, 2008.

LOGAN, J. D. Solute transport in porous media with scale-dependent dispersion and periodic boundary conditions. *J. Hydr*., vol. 184, nº. 3, pp. 261-276, 1996.

______. *A first course in the finite element method - 4th edition*. Ontario: Thomson, 2007, 808p.

LOGAN, J. D.; ZLOTNIK, V. The convection-diffusion equation with periodic boundary conditions. *Appl. Math. Lett*.,vol. 8, nº. 3, pp. 55-61, 1995.

MARCHI, C. H.; SUERO, R.; ARAKI, L. K. The lid-driven square cavity flow: numerical solution with a 1024 x 1024 grid. *J. of the Braz. Soc. Of Mech. Sci & Eng*, vol. XXXI, nº. 3, pp. 186-198, Jul.-Sept. 2009.

NARVENKAR, G.; NAQVI, S. W. A.; KURIAN, S.; SHENOY, D. M; PRATIHARY, A. K.; NAIK, H.; PATI, S.; SARKAR, A.; GAUNS, M. Dissolved methane in Indian freshwater reservoirs. *Environ. Monit. Assess*., nº. 185, pp. 6989-6999, Feb. 2013.

OLIVEIRA FILHO, A. G. de; MANGIAVACCHI, N.; PONTES, J. Simulation of species concentration distribution in reactive flows with unsteady boundary conditions. *Braz. J. Chem Eng*, vol. 34, nº. 04, 2017 (to appear).

OLIVEIRA FILHO, A. G. de; MANGIAVACCHI, N. Multidimensional unsteady solutions to the convection-diffusion-reaction equation with a time dependent boundary condition. In: CONGRESSO NACIONAL DE MATEMÁTICA APLICADA E COMPUTACIONAL, 36, 2016, Gramado. *Proc. Braz. Soc. Comp. Appl. Math*, vol. 5, nº. 1, 2017. Available at: < https://proceedings.sbmac.org.br/sbmac/article/view/1675 /1684>. Retrieved: 03 Jul 2017.

O'LOUGHLIN, E. M.; BOWMER, K. H. Dilution and decay of aquatic herbicides in flowing channels. *J. Hydrol.*, nº. 26, pp. 217-235, 1975.

PACHECO, F. S. *Study of water masses movements through lagrangian drifters and implications for the understanding of ecological processes* (In Portuguese). 2009. 88f. Dissertation (Master in Applied Ecology) – Ecology Program, Universidade Federal de Juiz de Fora, Juiz de Fora, 2009.

PEETERS, M. F.; HABASHI, W. G.; DUECK, E. G. Finite element stream function-vorticity solutions of the incompressible Navier-Stokes equations. *Int. J. Num. Meth. Fluids*, vol. 7, pp 17-27, 1987.

PEETERS, F.; KIPFER, R. Currents in stratified water bodies 1: density-driven flows. In: LINKENS, G. E. (Editor). *Encyclopedia of Inland Waters.* Oxford: Elsevier, 2009, vol.1, pp. 530-538.

PÉREZ GUERRERO, J. S.; PONTEDERO, F. M.; VAN GENUCHTEN, M. Th.; SKAGGS, T. H. Analytical solutions of the one-dimensional advection-dispersion solute transport equation subject to time-dependent boundary conditions. *Chem. Eng. J.*, nº. 221, pp. 487-491, 2013.

PIASECKI, M.; KATOPODES, N. D. Control of contaminant releases in rivers I: adjoint sensitivity analysis, *J. Hydraul. Eng.*, vol. 123, nº. 6, pp. 486-492, 1997.

REHM, R. G.; BAUM, H. R. The equations of motion for thermally driven buoyant flows. *J. Res. Nat. Bureau St.*, vol.83, nº. 3, pp. 297-308, May-June 1978.

REHM. R. G.; BAUM, H. R.; BARNETT, P. D. Buoyant convection computed in vorticity, stream-function formulation. *J. Res. Nat. Bureau St.*, vol.87, nº. 2, pp. 165-185, March-April 1982.

SERT, C. *Lecture Notes for ME 582 finite element analysis in thermofluids*. Department of Mechanical Engineering, Middle East Technical University, Ankara, Turkey, 2015. Available at: <http://users.metu.edu.tr/csert/teaching_notes.htm>. Retrieved: 15 Sept 2016.

St LOUIS, V. L.; KELLY, C. A.; DUCHEMIN, E.; RUDD, J. W. M.; ROSENBERG, D. M. Reservoir surfaces as sources of greenhouse gases to the atmosphere: a global estimate. *Bioscience*, nº. 50, pp. 766-775, 2000.

TAYLOR, C.; HOOD, P.; A numerical solution of the Navier-Stokes equations using the finite element technique. *Computer and Fluids*, vol.1, pp. 73-100, 1973.

TEZDUYAR, T. E.; GLOWINSKI, R.; LIOU, J. Petrov-Galerkin methods on multiply connected domains for the vorticity-stream function formulation of the incompressible Navier-Stokes equations. *Int. J. Num..Meth. Fluids*, vol. 8, pp. 1269-1290, 1988..

TEZDUYAR, T. E.; LIOU, J.; GANJOO, D. K.; BEHR, M. Solution techniques for the vorticity-stream function formulation of two-dimensional unsteady incompressible flows. *Int. J. for Num. Meth. in Fluids*, vol. 11, pp. 515-539, 1990.

TEZDUYAR, T. E.; LIOU, J. On the downstream boundary conditions for the vorticity-stream function formulation of two-dimensional incompressible flows. *Comp. Meth. Appl. Mech. Engnrg*., nº. 85, pp. 207-217, 1991.

TUTTY, O. R. On vector potential-vorticity methods for incompressible flow problems. *J. Comp. Phys*, nº. 64, pp. 368-379, 1986.

VAN GENUCHTEN, M. TH.; ALVES, W. J. *Analytical solutions of the one-dimensional convective-dispersive solute transport equation*. Washington: US Department of Agriculture, 1982. 149 p. Agric. Res. Service Tech. Bulletin nº. 1661.

VILHENA, M.T.; LEAL, C. A. Dispersion of non-degradable pollutants in rivers. *Int. J. Appl. Radiat. Isot.*, vol. 32, pp. 443-446, 1981.

VILHENA, M.T.; SEFIDVASH, F. Two-dimensional treatment of dispersion of pollutants in rivers. *Int. J. Appl. Radiat. Isot.*, vol. 36, nº. 7, pp. 569-572, 1985.

WONG, A. K.; REIZES, J. A. An effective vorticity-vector potential formulation for the numerical solution of three-dimensional duct flow problems. *J. Comp. Phys*, nº. 55, pp. 98-114, 1984.

WRIGHT, N. G.; GASKELL, P. H. An efficient multigrid approach to solving highly recirculating flows. *Computers & Fluids,* vol. 24, nº. 1, pp. 63-79, 1995.

Www.kolumbus.fi. *Basic information on biogas*. In: https://web.archive.org/ web/ 20100106022729/http://www.kolumbus.fi/suomen.biokaasukeskus/ en/ enperus.html. 2007. Retrieved: 10 Jan 2017.

YU, F. X.; SINGH, V. P. Improved finite element method for solute transport. *J. Hydraul. Eng*., vol. 121, nº. 2, pp. 145-158, 1995.

YU, T. S.; LI, C. W., Instantaneous Discharge of Buoyant Fluid in Cross-flow, *J. Hydraul. Eng*., vol. 124, nº. 1, pp. 1161-1176, 1998.

ZIENKIEWICZ, O. C.; TAYLOR, R. L. *The finite element method, vol 1: the basis, 5th ed*. Oxford: Butterworth-Heinemann, 2000. 689 p.

ZISKIND, G.; SHMUELI, H.; GITIS, V. An analytical solution of the convection-dispersion-reaction equation for a finite region with a pulse boundary condition. *Chem. Eng. J*., nº. 167, pp. 403-408, 2011.

APPENDIX A – STREAM FUNCTION, VORTICITY AND VELOCITY TEST COMPUTATIONS WITHOUT BOUYANT TERM

This appendix collects tests carried on within the Reynolds Numbers span expected as covering most usual flow patterns that occur in hydroelectric reservoirs basins. These tests were carried in order to secure conditions where the code would perform stable and also to experiment some of its features. It can be noted that the outcomes have different mesh sizes and shapes and that integration is performed with GQ of different numbers of points.

The corrugated surface that is observed in the discretized domains was tested, but not implemented in the text, because it requires a more elaborate programming that is left for a future work. It was also found that the computational time for its implementation could imply in deviation of the core of this work

All results presented correspond to the case where there is no wind blowing on the water surface, what means imposing a surface boundary condition for vorticity such that ω_s =0.0.

A.1 Longitudinal velocity computation tests

Figure 42 – Stream function, vorticity and longitudinal velocity (Re = 10; outlet NBC; 1800 triangular elements mesh; GQ of seven points).

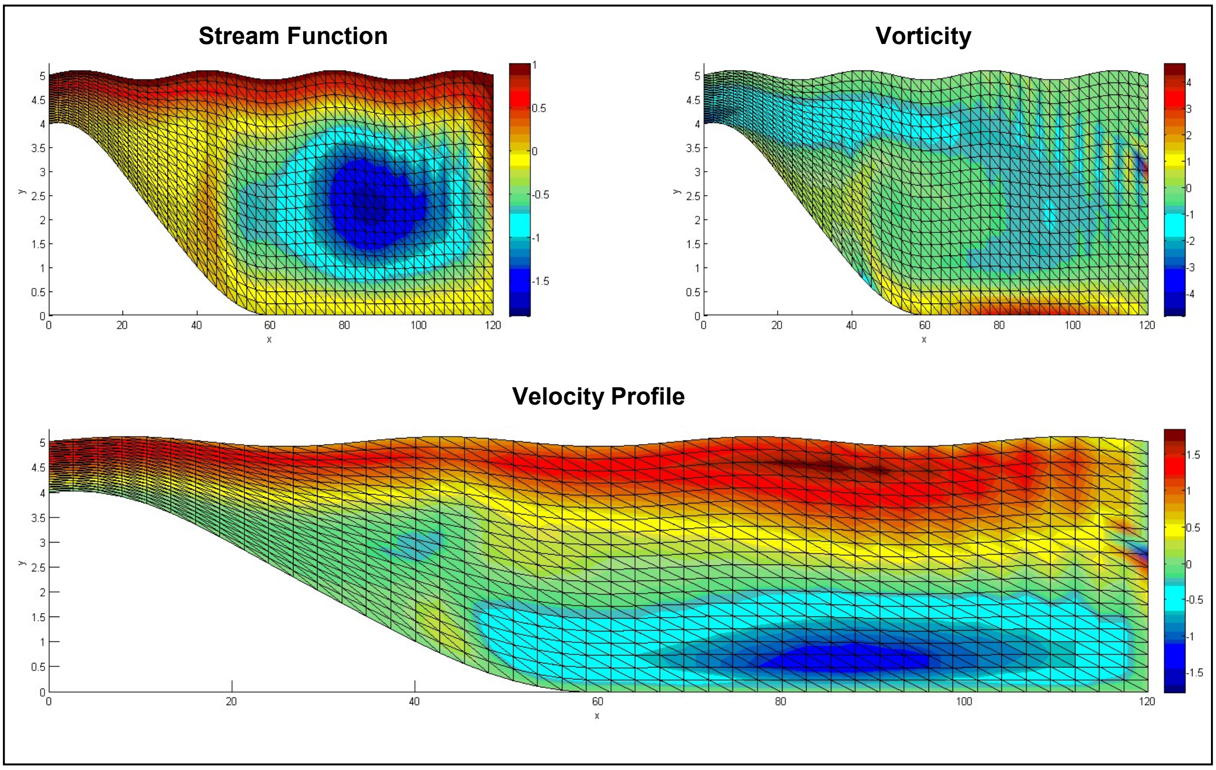


Figure 43 – Stream function, vorticity and longitudinal velocity (Re = 10; outlet MDBC; 1800 triangular elements mesh; GQ of seven points).

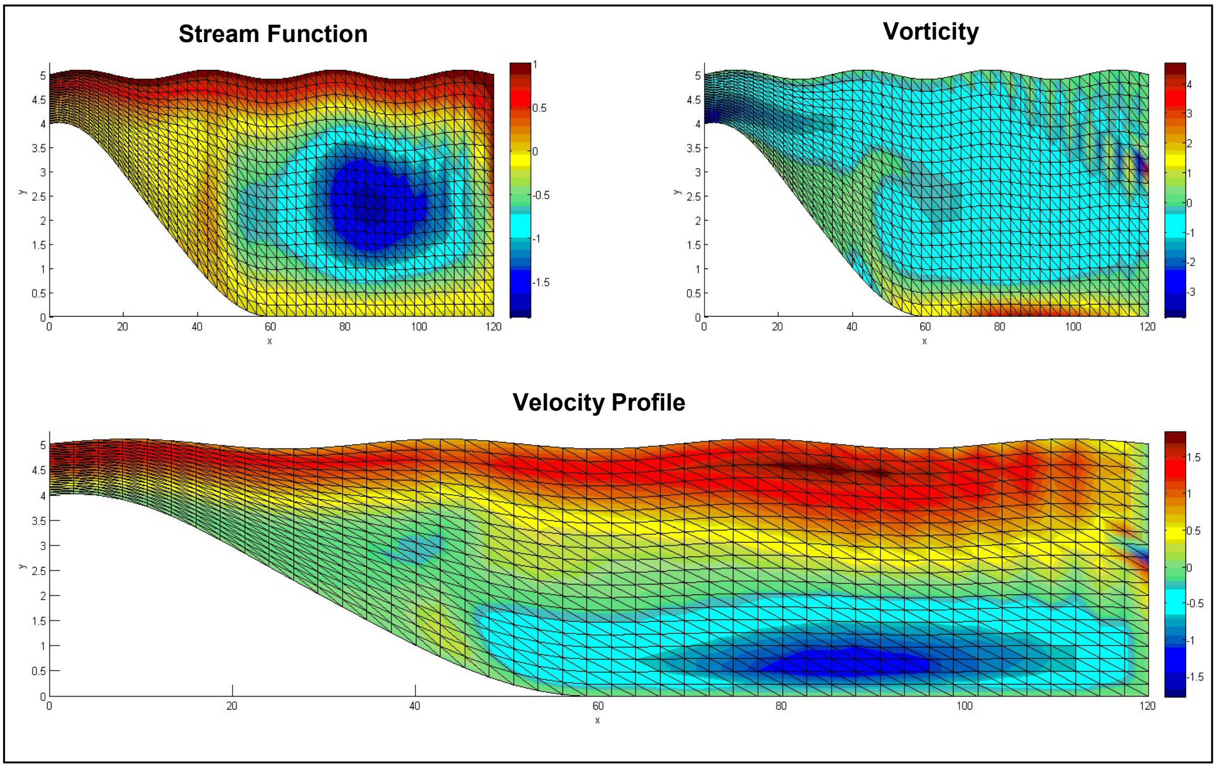


Figure 44 – Stream function, vorticity and longitudinal velocity (Re = 50; outlet EBC; 900 quadrangular elements mesh; GQ of nine points).

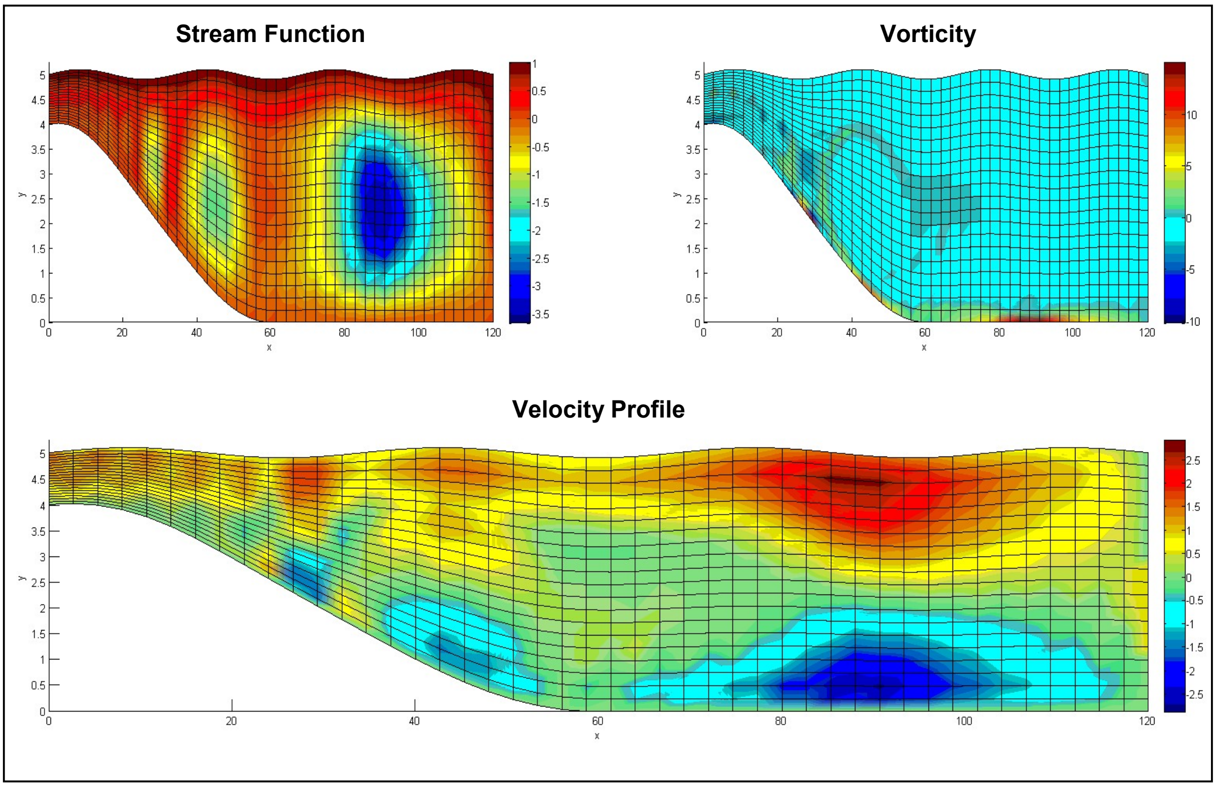


Figure 45 – Stream function, vorticity and longitudinal velocity (Re = 100; outlet MDBC; 900 quadrangular elements mesh; GQ of nine points).

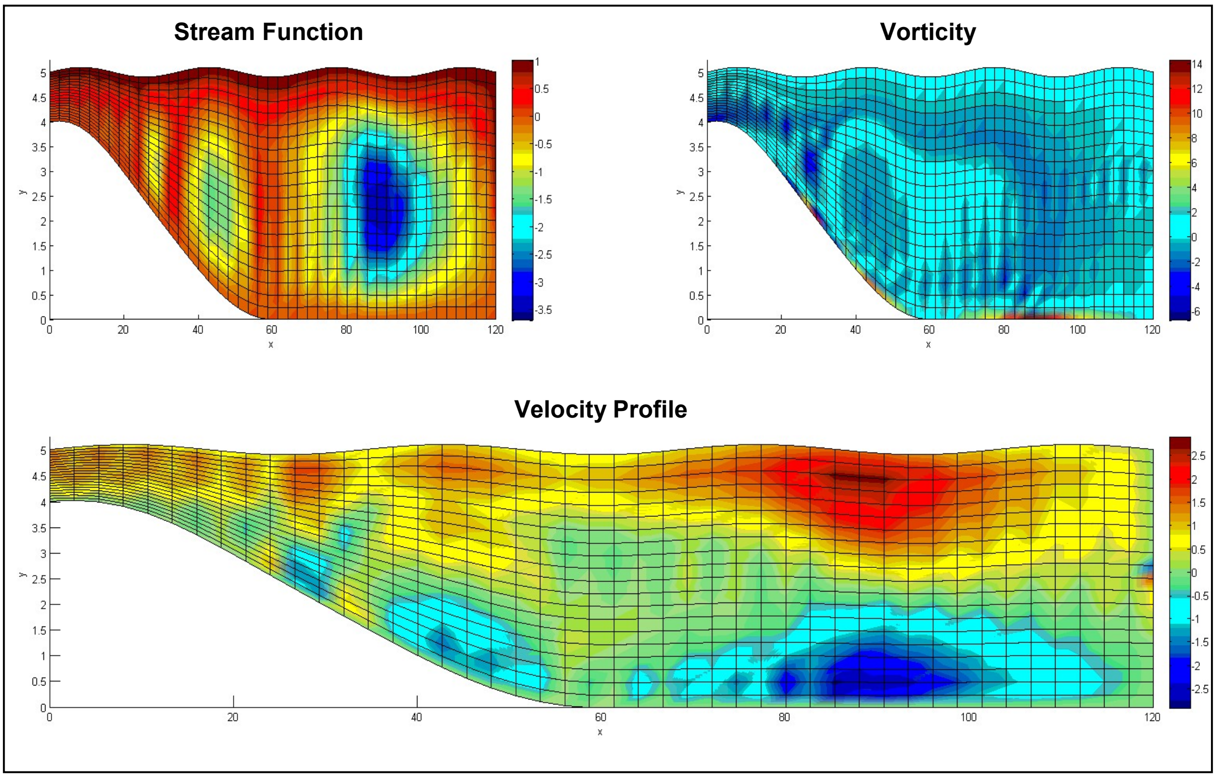


Figure 46 – Stream function, vorticity and longitudinal velocity (Re = 100; outlet EBC; 1800 triangular elements mesh; GQ of seven points).

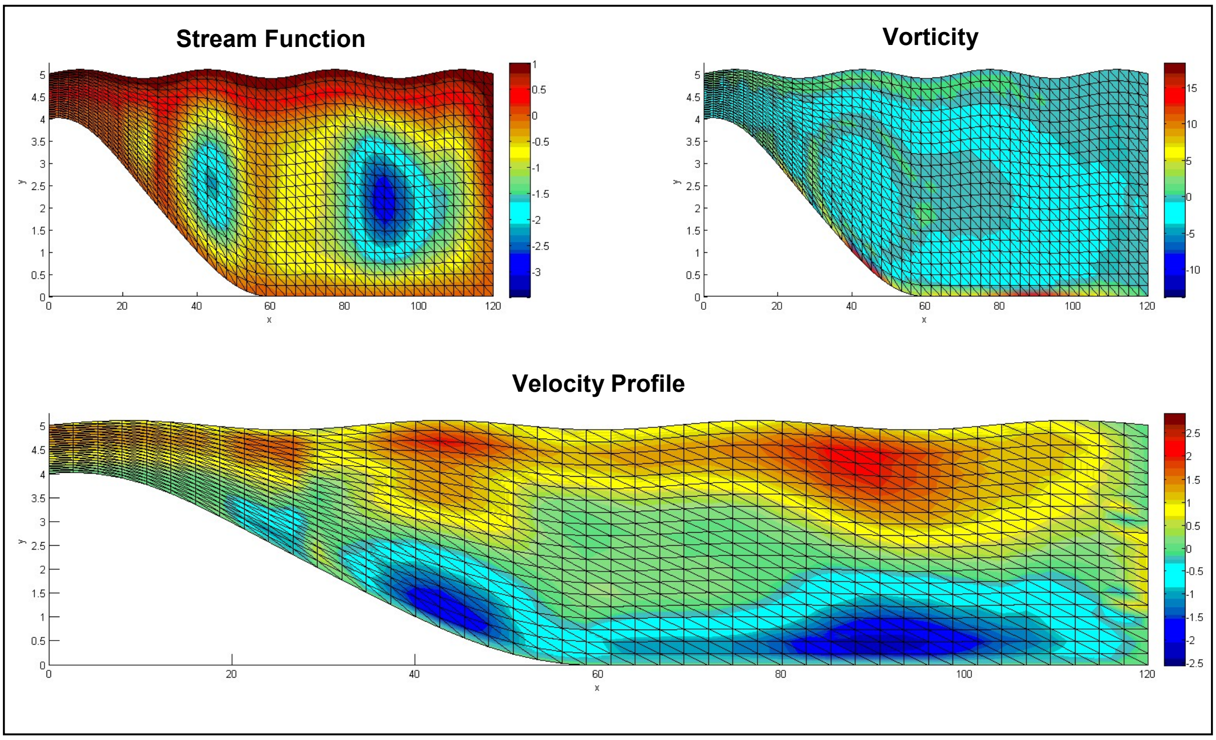


Figure 47 – Stream function, vorticity and longitudinal velocity (Re = 100; outlet NBC; 1800 triangular elements mesh; GQ of seven points).

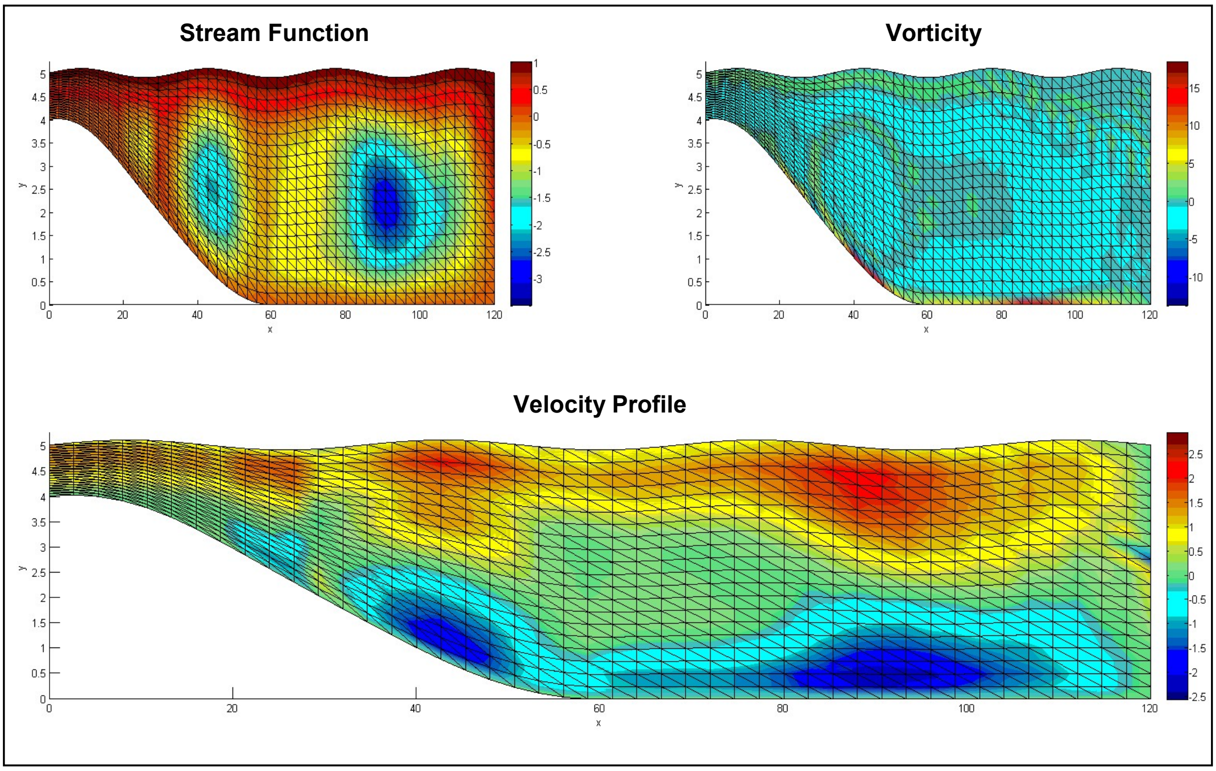


Figure 48 – Stream function, vorticity and longitudinal velocity (Re = 500; outlet EBC; 1800 triangular elements mesh; GQ of seven points).

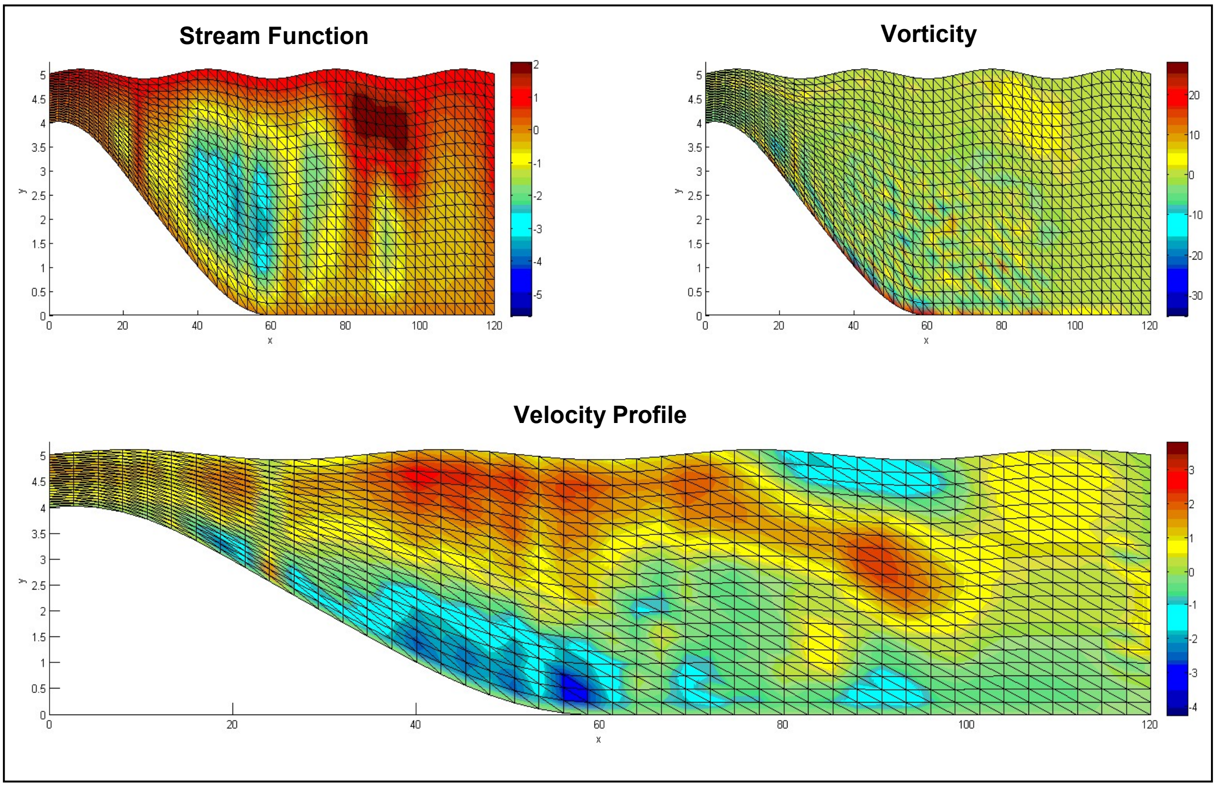


Figure 49 – Stream function, vorticity and longitudinal velocity (Re = 500; outlet NBC; 1800 triangular elements mesh; GQ of seven points).

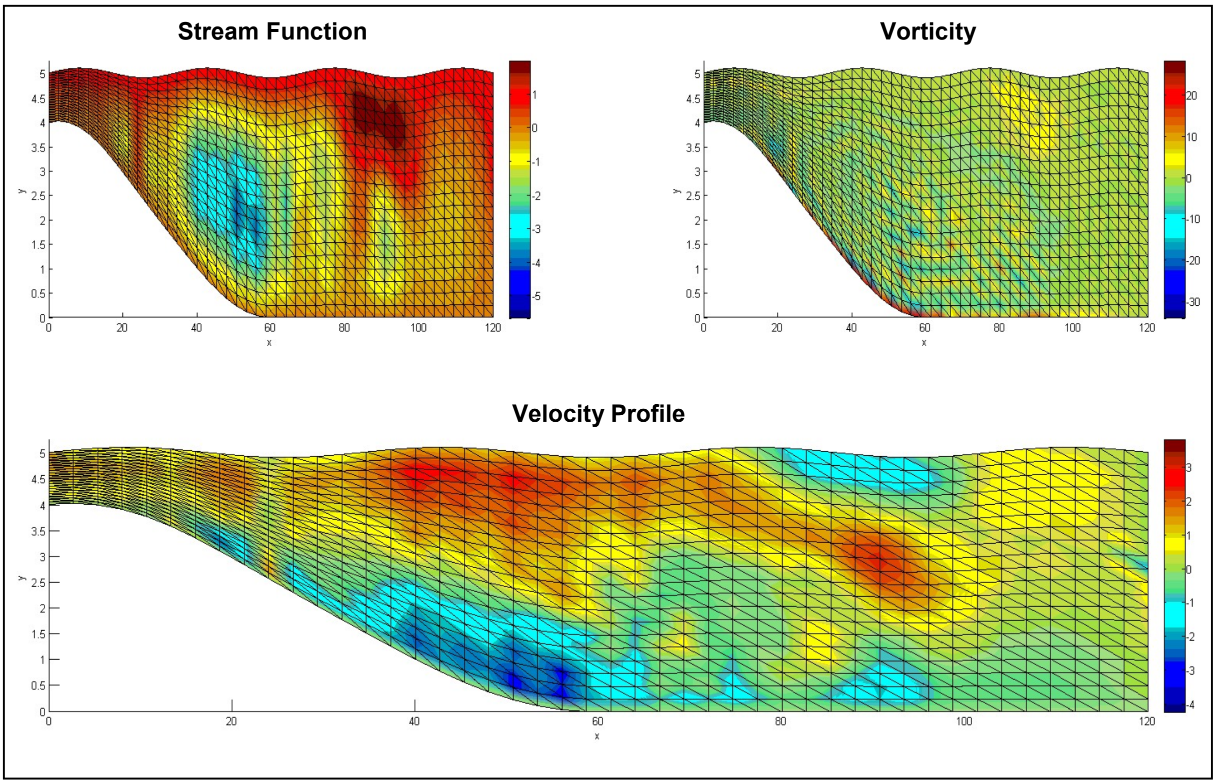


Figure 50 – Stream function, vorticity and longitudinal velocity (Re = 1000; outlet EBC; 1800 triangular elements mesh; GQ of seven points).

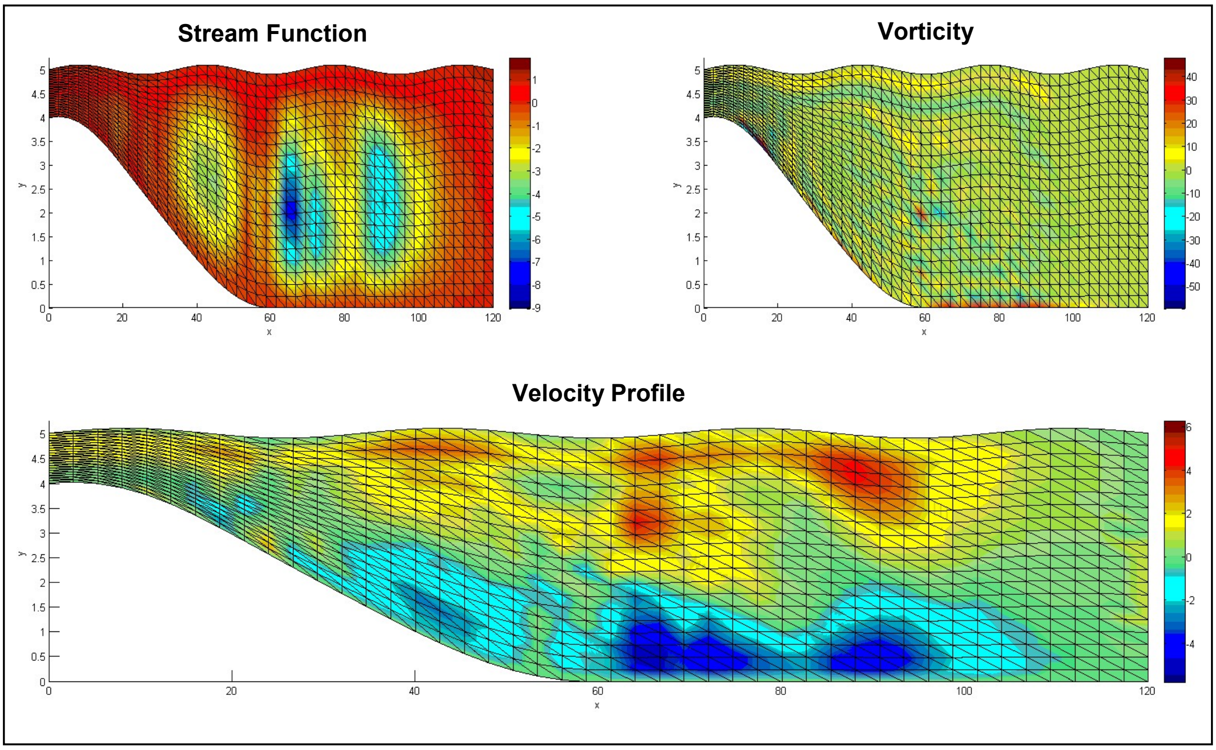
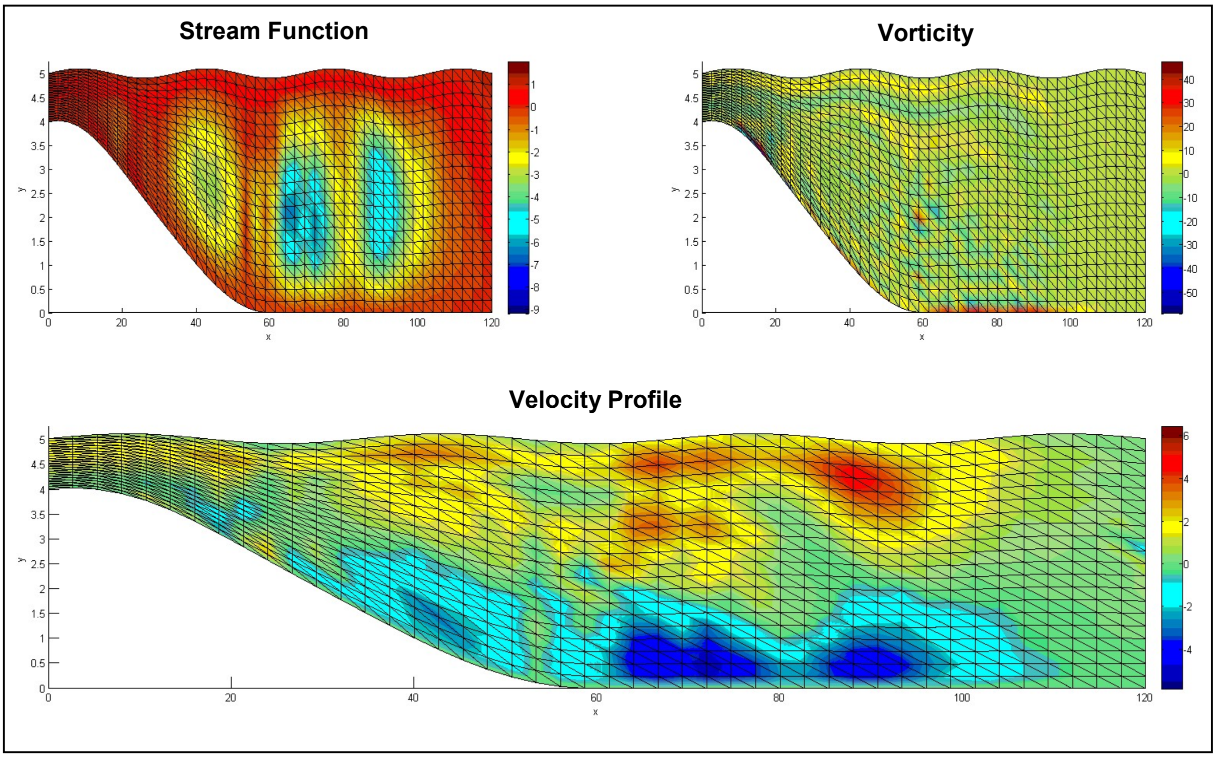
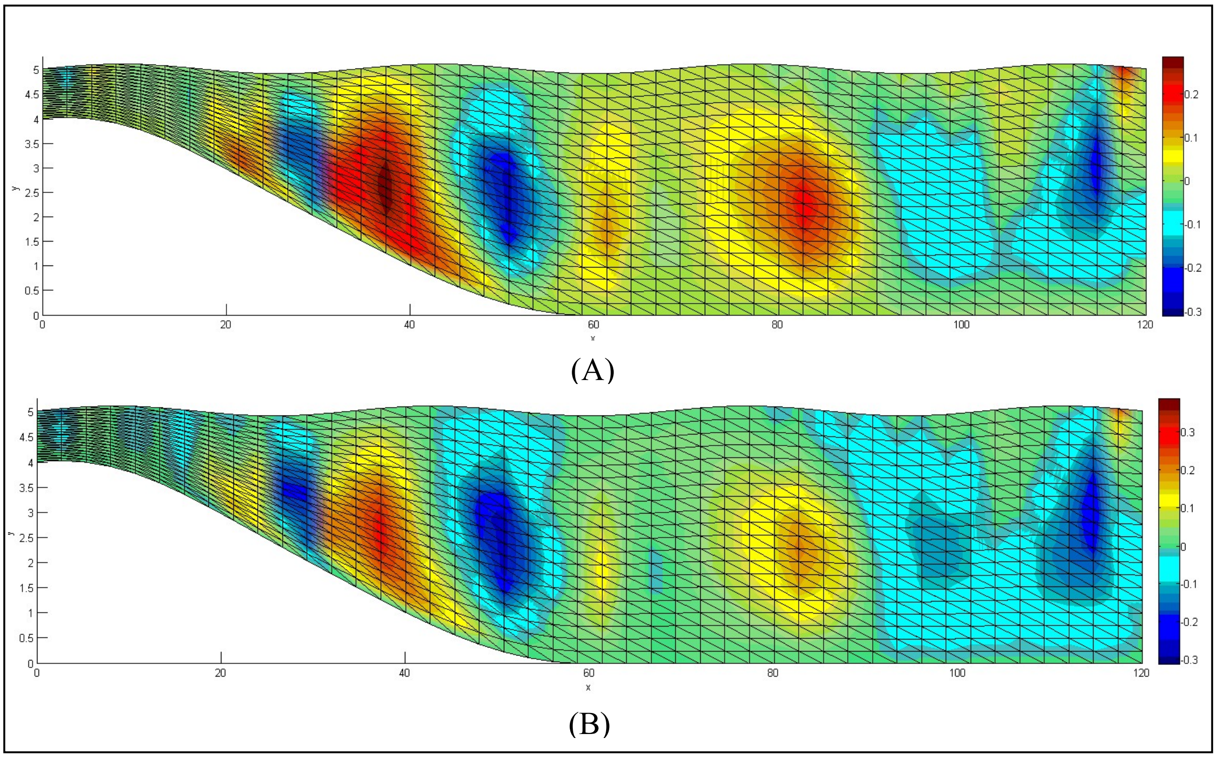


Figure 51 – Stream function, vorticity and longitudinal velocity (Re = 1000; outlet MDBC; 1800 triangular elements mesh; GQ of seven points).



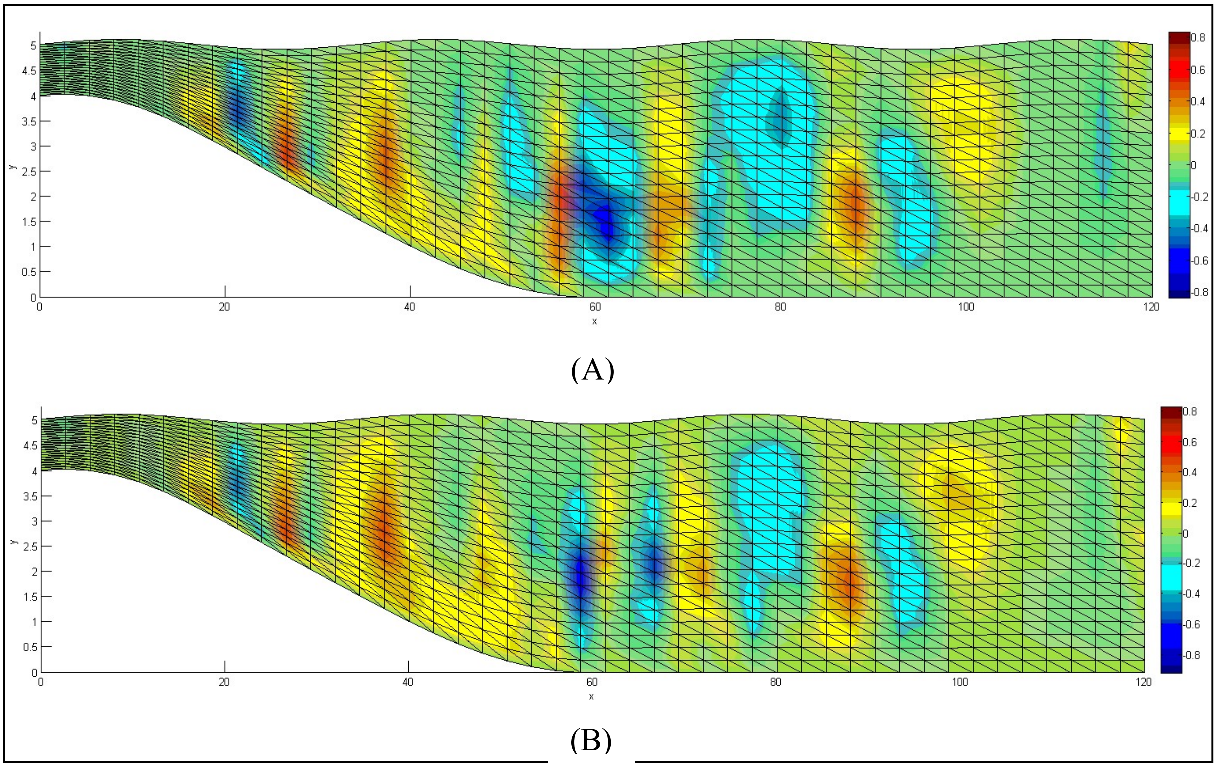
A.2 Vertical velocity computation tests

Fig 52 – Vertical velocity computation (Re = 100; 1800 triangular elements mesh; GQ of seven points)



Tags: (A) – outlet NBC; (B) – outlet MDBC.

Fig 53 – Vertical velocity computation (Re = 500; 1800 triangular elements mesh; GQ of seven points)



Tags: (A) – outlet NBC; (B) – outlet MDBC.