Numerical Simulations of Longitudinal Advection Dispersion Contaminant Decay Model with Time-dependent Sources with COMSOL Multiphysics

Promise Mebine[1], Alabodite Meipre George[2]

[1,2]Department of Mathematics/Computer Science, Niger Delta University, Wilberforce Island, Bayelsa State, Nigeria
Email: p.mebine@yahoo.com, pw.mebine@ndu.edu.ng
[2]Department of Mathematical Sciences, Loughborough University, Leicestershire, United Kingdom
Email: A.M.George@lboro.ac.uk, georgianalgebra@gmail.com

Abstract— *A direct simulation investigations of contaminant transport has been conducted. The simulations are based on the unsteady longitudinal advection diffusion contaminant decay equation, which is discretized using finite element Galerkin's method with backward difference time formulation with the application of COMSOL Multiphysics Software Package. It was observed that the simulation results, which are illustrated pictorially via line graphs and contours, consistently represented the analytical solutions of Mebine and George (2011), thereby demonstrating interesting features of the problem effected by the variety of contaminant decay time-dependent sources.*

Keywords— Advection, COMSOL Multiphysics, Contaminant decay, Dispersion, Pollution, Time-dependent sources.

I. INTRODUCTION

Mebine and George (2011) investigated analytically the longitudinal advection-dispersion mathematical model with contaminant decay due to time-dependent sources. A variety of strategies for time-dependent sources were presented with the environmental objective to avoid intermittently high pollution levels downstream of the outfall. This was geared towards reducing environmental impact and minimising economic cost for downstream users of streams or groundwater polluted on purpose with non-conservative contaminants.

The literature is rife with several studies of modalities, methods and advocates, emphasizing the importance of time-dependent release of contaminants and their dispersion, transport, migration processes or factors in order to gain insights on how to optimally control or reduce the impacts (Dhar and Sinha, 1989; Mazumder and Dalal, 2000; Baverman et al., 1995; Kolditz et al., 1998; Sandrin et al., 2001; Sen et al., 2002; Serrano, 2001; Mebine and Smith, 2006; Mebine and Smith, 2009). Rubin and Atkinson (2001) noted particularly that the spatial and temporal distribution of contamination sources have a significant impact on contamination transport and plume distribution in the subsurface.

In recent times, the environmental, engineering and physical sciences span a broad range of issues in their disciplines such as open channel hydraulics, sediment transport, stratified flow phenomena, transport and mixing processes, water quality and atmospheric modelling, just to mention but a few. These topics are studied in various ways including theoretical analyses, physical model experiments, field studies, numerical modelling and numerical simulations. Today, the mathematical modelling and numerical solutions of some physical and engineering phenomena have been made easy due to the advent of less expensive but more powerful computers and sophisticated Commercial and Educational Software Packages with the development of user-friendly vis-à-vis easy-to-use rules and instructions yet robust modelling codes. Such packages include among others, MAPLE, MATHEMATICA, and MATLAB, which are known for their capabilities for symbolic computations and numerical simulations; CORMIX Modelling Package (http://www.cormix.info/), which is a software system for the analysis, prediction, and design of marine outfall mixing zones resulting from a continuous point discharge of effluents into open coastal waters (Doneker and Jirka, 2007), and COMSOL Multiphysics Package, which has many vital Trade Mark statements such as "COMSOL Multiphysics™ provides a powerful platform for enhancing student knowledge by first confirming the analytical solutions based upon simplifying assumptions using numerical solutions, and then extending the problem to multi-dimensions with the addition of one or more Multiphysics; COMSOL Multiphysics™ provides a robust platform to solve complicated transport phenomena problems and to generate results that lead to a better understanding of the physical significance and their real-world applications; COMSOL Multiphysics™ application can generate a broad range of results needed for a better fundamental understanding of the problem being studied" (Vasilev et al., 2015). To this end, it is the objective of this paper to use COMSOL Multiphysics for the numerical simulations of longitudinal advection dispersion contaminant decay mathematical model with time-dependent sources for the baseline comparisons of the analytical predictions in Mebine and George (2011).

The sections that follow hereafter are respectively, brief discussion of some of the applications of COMSOL Multiphysics numerical simulations; mathematical formulations of the problem and dimensionless forms of the governing equations; source types and discussion of simulation results, and general concluding remarks of the results of the previous sections.

II. COMSOL MULTIPHYSICS NUMERICAL SIMULATIONS

COMSOL Multiphysics is a Commercial Software Package that uses a finite element solver with discretization by Galerkin's Method for the purpose of stabilization to prevent spurious oscillations. The "extremely fine" settings have been used for the meshes with COMSOL backward difference formulation for the time setting. The COMSOL Multiphysics has been applied in the numerical simulations of many environmental and engineering problems including Transport phenomena (Vasilev et al., 2015); Navier-Stokes equations in supersonic flow over a double wedge airfoil (Kolluru and Gopal, 2012); Burning Candle (Gritter, 2010); Newtonian and Non-Newtonian Blood Flow (Siebert and Fodor, 2009); Topology Optimization of Heat Transfer and Fluid Flow Systems (Dede, 2009); Single Particle in Laminar Flow Regime of a Newtonian Liquid (Dinesh, 2009); Multiphase Fluid Flow Model in Porous Media (Diaz-Viera et al., 2008), and Velocity, Pressure and Temperature Distributions near a Stagnation Point in Planar Laminar Viscous Incompressible Flow (Kaufman and Gutierrez-Miravete, 2008). There is no gainsaying that these handful applications of COMSOL Multiphysics are pointers to its efficiencies, versatilities and capabilities in handling physically feasible problems.

III. MATHEMATICAL FORMULATIONS

The rate of contaminant transport in groundwater or river flow is governed by many factors including advection, dispersion, diffusion, dilution or mixing, retardation, and decay. These factors are usually incorporated into transport equations which describe transport phenomena such as heat transfer, mass transfer, fluid, waves, momentum transfer and many others. A generic transport equation that describes transport phenomena as in Siddig (2016) is stated as

$$\frac{\partial \phi}{\partial t} + \nabla \cdot f\left(t, \bar{x}, \phi, \nabla \phi\right) = g\left(t, \bar{x}, \phi\right), \tag{1}$$

where ϕ, f, t, g and $\bar{x}$ are respectively the quantity to be transferred, flux, time, source and the Cartesian coordinates (x, y, z) and $\nabla \equiv i\frac{\partial}{\partial x} + j\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}$, and where $i, j, \hat{k}$ are unit vectors. Equation (1) is indicative that all transfer processes constitute certain conservation principles, flux expressions, constitutive equations, initial conditions, and boundary conditions to a particular environmental and engineering system geometry for all dependent variables in relation to the independent variables involved. This implies that the specific application of equation (1) depends on the issue of interest under investigation.

The factors that characterize the transport of species are known for their specific roles such that the generic transport equation (1) could be simplified accordingly bearing in mind the necessary and sufficient transport physics. To this end, as in Mebine and George (2011), for consideration of one-dimensional domain contaminant transport or migration undergoing advection, dispersion, sorption isotherms and first-order contaminant decay, the governing equation is written as

$$\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} - \lambda c, \tag{2}$$

where $V = \frac{U}{R}, D = \frac{\kappa}{R}, R = 1 + \frac{\rho_b k_d}{\theta}$. The appropriate initial and boundary conditions (Israel-Cookey et al., 2002; Williams and Tomasko, 2008) are written as

$$t \le 0 : c(x,t) = 0,$$
$$t > 0 : \begin{cases} c(0,t) = c_0 g(t), \\ c(\infty, t) \to 0. \end{cases} \tag{3}$$

Here $c(x,t)$ represents contaminant concentration; x, longitudinal or downstream coordinate; t, time; U, advective velocity; κ, dispersion coefficient; λ, first-order contaminant decay, degradation, or kinetic reaction parameter which accounts for the overall water-bed exchange of the contaminant; R, accounts for contaminant retardation (equilibrium absorption) due to sorption and other physical processes; its values are generally less than 10; ρ_b, bulk density; k_d, contaminant distribution coefficient. The distribution coefficient is a physically meaningful parameter as it is a simple ratio of the amount sorbed to the amount dissolved in phase at equilibrium, and θ, effective porosity. It is important to note that the cross-sectional averaged contaminant concentration $c(x,t)$is released at a rate $c_0 g(t)$from the point source at $x = 0$ for all t; c_0 is the solute concentration after mixing over the cross-section of the stream; $g(t)$ is time-dependent function, which accounts for the time-dependent source.

It is in order to render the equations (2, 3) dimensionless through the variables and parameters

$$X = \frac{x}{L}, \tau = \frac{Vt}{L}, C = \frac{c}{c_0}, Pe = \frac{VL}{D}, \Lambda = \frac{L\lambda}{V} \tag{4}$$

Such that the equations (2, 3) are written as

$$\frac{\partial C}{\partial \tau} + \frac{\partial C}{\partial X} = \frac{1}{Pe}\frac{\partial^2 C}{\partial X^2} - \Lambda C, \tag{5}$$

$$\begin{aligned} &\tau \le 0 : C(X,\tau) = 0, \\ &\tau > 0 : \begin{cases} C(0,\tau) = g(\tau), \\ C(\infty,\tau) \to 0, \end{cases} \end{aligned} \tag{6}$$

where L is a characteristic length of interest; X, the reduced or dimensionless downstream distance; Λ, strength of contaminant decay, and Pe, the column Peclet number (van Genuchten and Alves, 1982). Physically, the Peclet number measures the characteristic time of the diffusion process $\left(L^2/D\right)$ relative to the convection process (L/V). Therefore, while large Pe values represent less mixing at the advective/convective front causing a sharper front, smaller Pe values represent more mixing causing a broader front.

The equations (5, 6) are physically appropriate for investigating the effect of influent boundary, which varies over time due to variable discharge rate when considering the contaminant release and discharge problem in coastal industrial sites. This situation is realistic in the sense that generally industries or waste sites release pollution in a finite time period, either because industrial firms have a finite life or the pollution problem is controlled after a certain time with the awareness of the contamination or government regulation. Mebine and George (2011) utilized equations (5, 6) in proffering various analytical solutions, which could serve as toolkits for the testing of numerical experimentations and simulations. This is the definite objective of this paper with the application of COMSOL Multiphysics.

To be at par with the results of Mebine and George (2011), the parametric values used for the simulations are $\tau = 0.25, 0.50, 0.75, 1.00; Pe = 1000; \Lambda = 0.25, 0.50, 1.00,$ but for the longitudinal distance, X, it ranges as indicated on the line graphs.

IV. CONTAMINAT SOURCE TYPES AND SIMULATION RESULTS

The following time-dependent contaminant source types are considered for the numerical simulations: (i) accelerated source, (ii) continuous source, and (iii) exponential decay source.

1.1 Accelerated Source

The accelerated source has application in MHD free-convection and mass transfer flow on a porous medium in a rotating fluid by enhancing radiative heat transfer (Israel-Cookey et al., 2002). This is represented by $g(\tau) = \tau.$

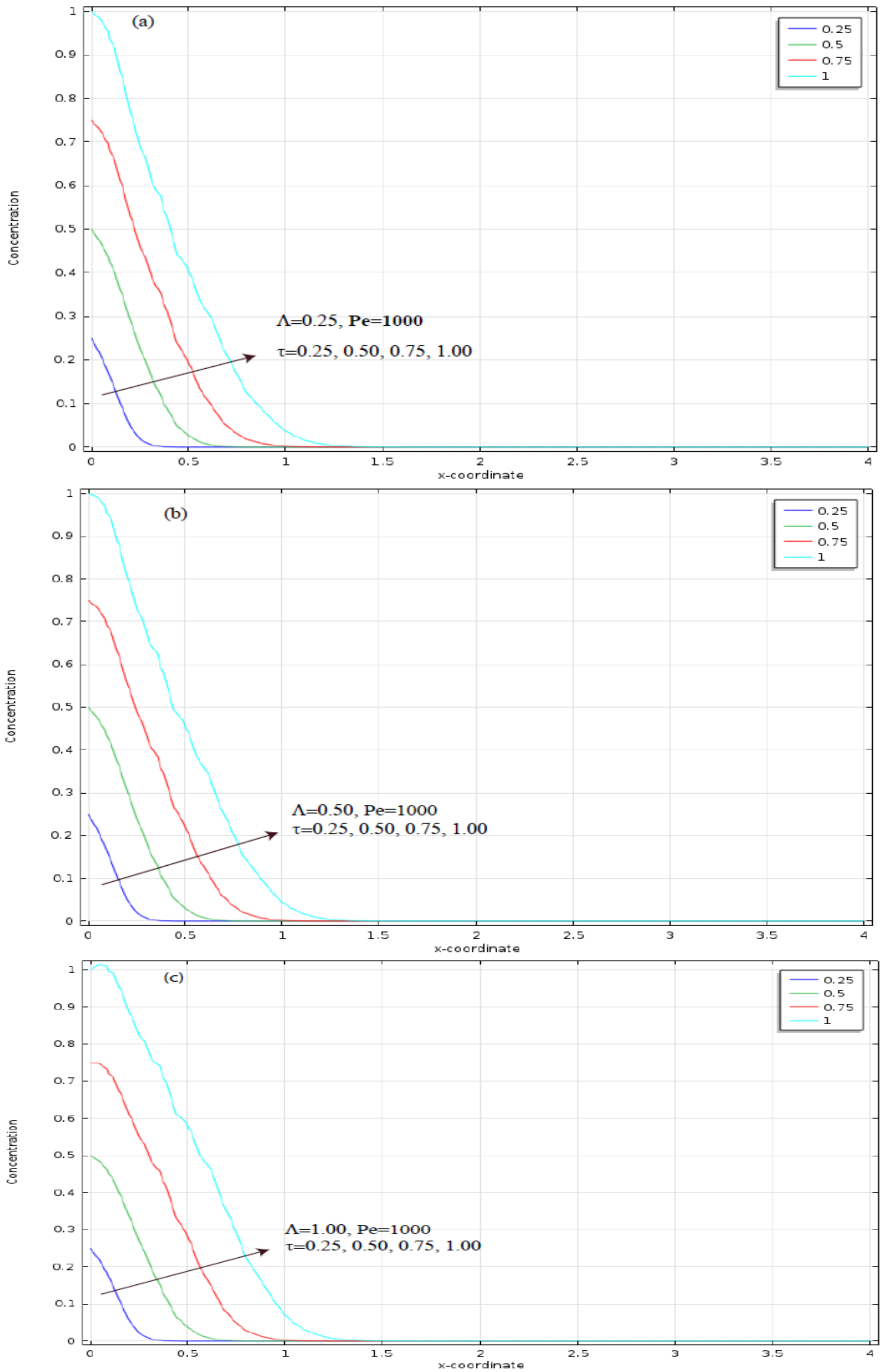

FIGURE 1: ACCELERATED SOURCE LINE GRAPHS FOR CONCENTRATION VS. LONGITUDINAL DISTANCE

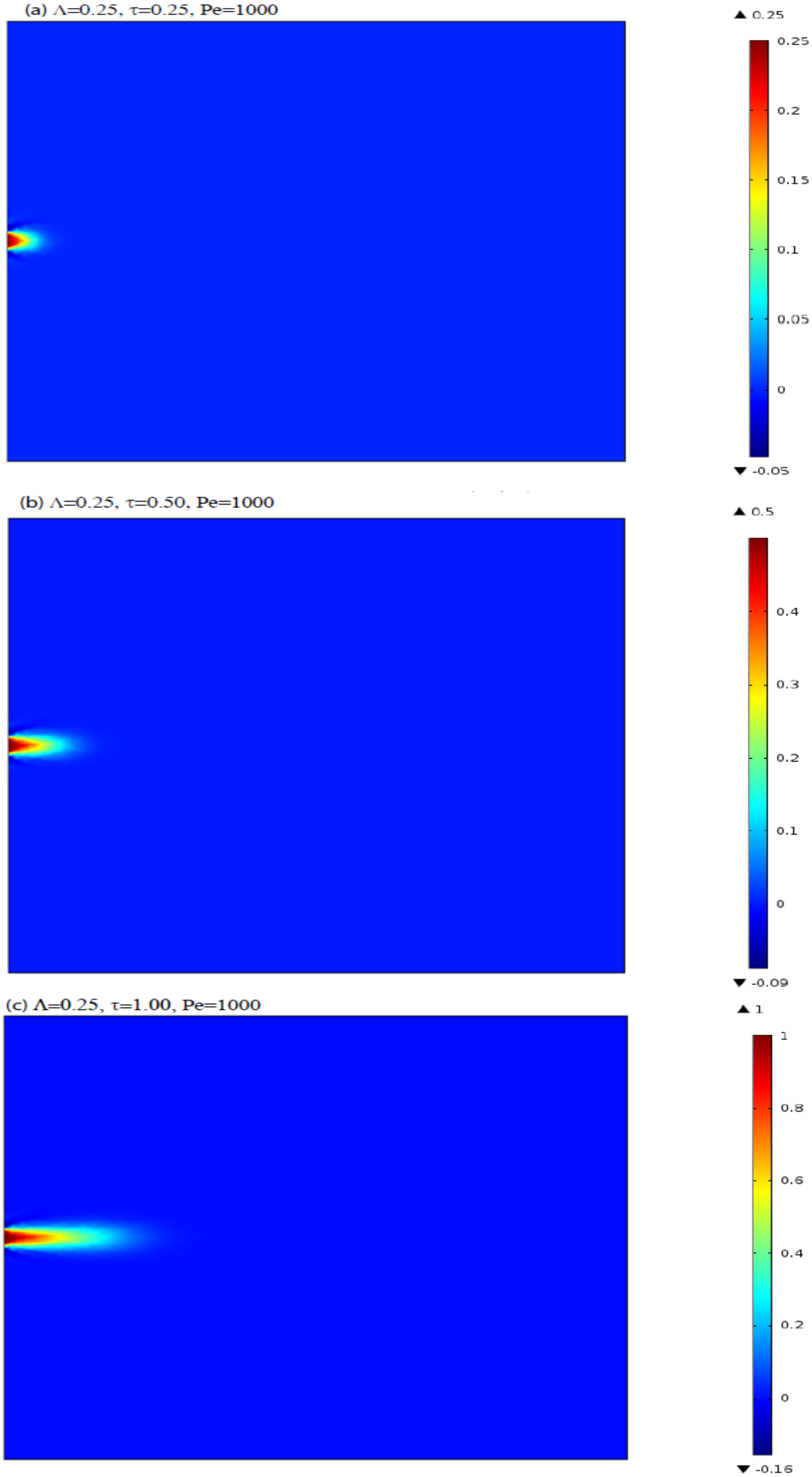

FIGURE 2: ACCELERATED SOURCE SURFACE CONCENTRATIONS

1.2 Continuous (Impulsive) Source

The continuous source depicts a known or constant injection concentration, where $g(\tau)=1$. In Laser heat source applications, Al-Khairy and Al-Ofey (2009) regarded the continuous source as a model of long duration of laser pulse when short times (of the order of few or tens of relaxation time) are considered.

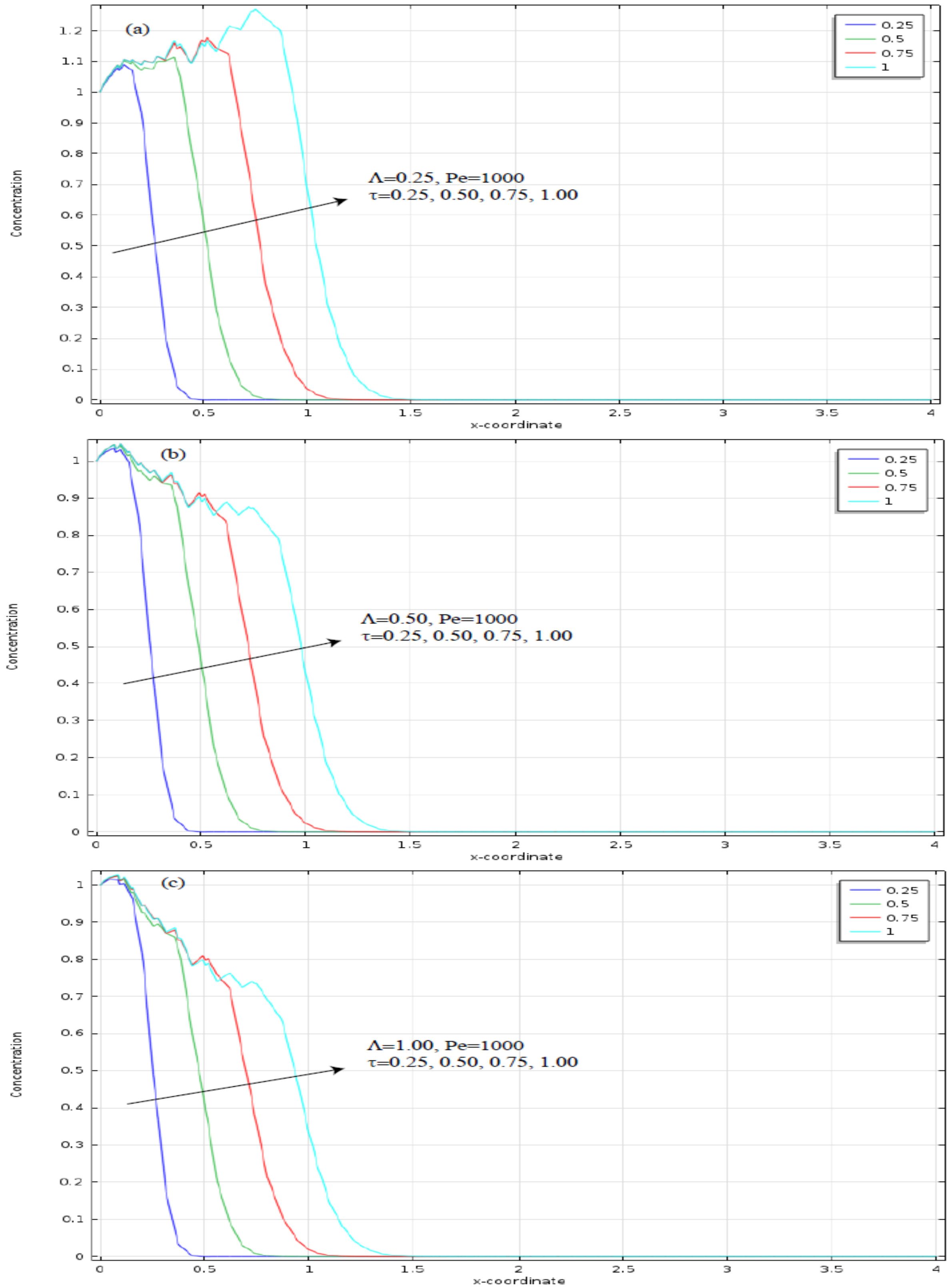

FIGURE 3: CONTINUOUS SOURCE LINE GRAPHS FOR CONCENTRATION VS. LONGITUDINAL DISTANCE

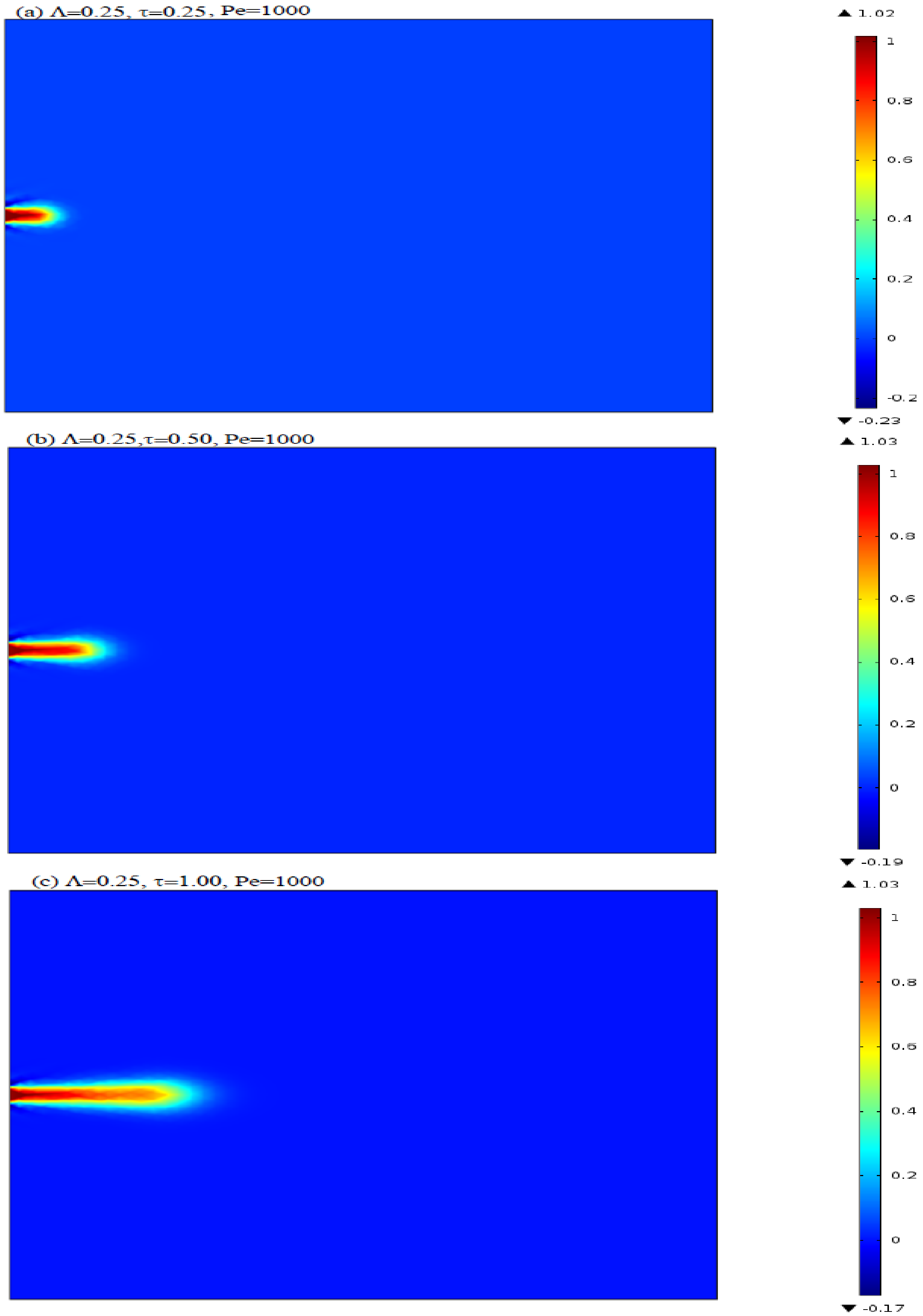

FIGURE 4: CONTINUOUS SOURCE SURFACE CONCENTRATIONS

1.3 Exponential Decay Source

For exponentially decaying source, $g(\tau)=\exp(-\beta\tau)$, where β is the source term decay constant which is different from the contaminant decay constant. Applications of exponentially decaying source are found in models of degradation of chlorinated compounds (Aziz et al., 2000). For radioactive waste disposal field and long-term behaviour of recalcitrant non-aqueous phase liquid (NAPL) spills, Williams and Tomasko (2008) reported that model physical processes are best conceptualized with exponentially decaying source. Another very important application of the exponentially decaying source is in the field of pharmaco-kinetics (Joshua, 2008) for the examination of drug absorption in the gastrointestinal track.

Figures 1, 3 and 5 represents respectively the accelerated, continuous and exponential decay source line graphs of the simulated concentration distribution versus longitudinal distance at different pore volumes (time) τ with Peclet number, $Pe = 1000$ and decay strength, $\Lambda = 0.25, 0.50$ and 1.00, respectively. The results excellently agree with those of the analytical results thereby replicating the characteristics of the accelerated, continuous and exponential decay sources, which were extensively discussed in Mebine and George (2011). However, it is observed that the line graphs of the continuous and exponential decay sources experienced some spurious or turbulent effects at the concentration peaks. This may be, physically, due to the cross dispersion coefficients that were used in the simulations. Equally, overshoots are visibly seen in the line graphs, which are reduced as the decay strength increases. From the Figures it is seen that the source term concentration is lower than the concentration behind the advective fronts. The introduction of the decay strength reduces the contaminant concentration behind the advective fronts with increasing longitudinal distance from the source. This is so because the contaminant at the advective front has undergone more degradation during transport.

On the other hand, Figures 2, 4 and 6 indicates the accelerated, continuous and exponential decay sources surface concentration distributions for the decay strength, $\Lambda = 0.25$ for various pore volumes, $\tau = 0.25, 0.50$ and 1.00, respectively. It is observed that increasing pore volumes causes the contaminant concentrations to decrease everywhere in the flow (the red colour), thereby increasing the green colour (the safe zone). In effect, the downstream experienced minimum environmental impact of the non-conservative contaminant.

V. CONCLUDING REMARKS

The concentration distribution behaviour of non-conservative contaminants is depicted by the results of the simulations of the advection-diffusion-reaction mathematical model with time-dependent sources. The simulations have clearly shown that the choice of time-dependent contaminant release can have a persistent and marked effect upon the concentrations experienced far downstream, thereby making visible the characteristics and objectives of the problem. In addition, the simulations showed cross dispersions in terms of spurious or turbulent effects, which were not observed in the analytical solutions. Physically, the spurious or turbulent effects account for mixing. The overall testament of the investigation is that the simulations have, indeed, confirmed the fact that the analytical results of Mebine and George (2011) are usable for preliminary predictive tools for simulating contaminant migration in streams due to time-dependent contaminant releases, and they can attest to the effectiveness of COMSOL Multiphysics.

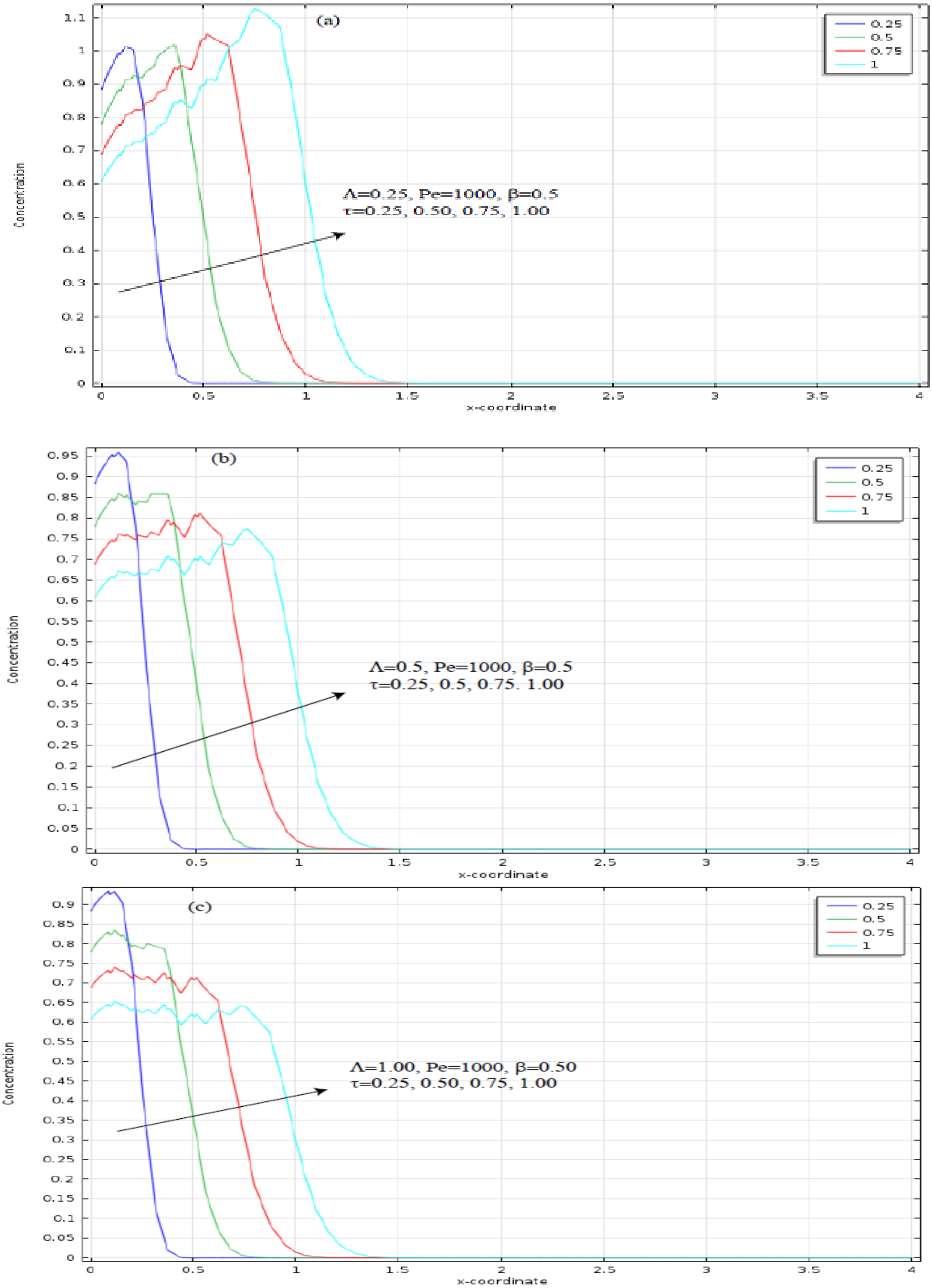

FIGURE 5: EXPONENTIAL SOURCE LINE GRAPHS FOR CONCENTRATION VS. LONGITUDINAL DISTANCE

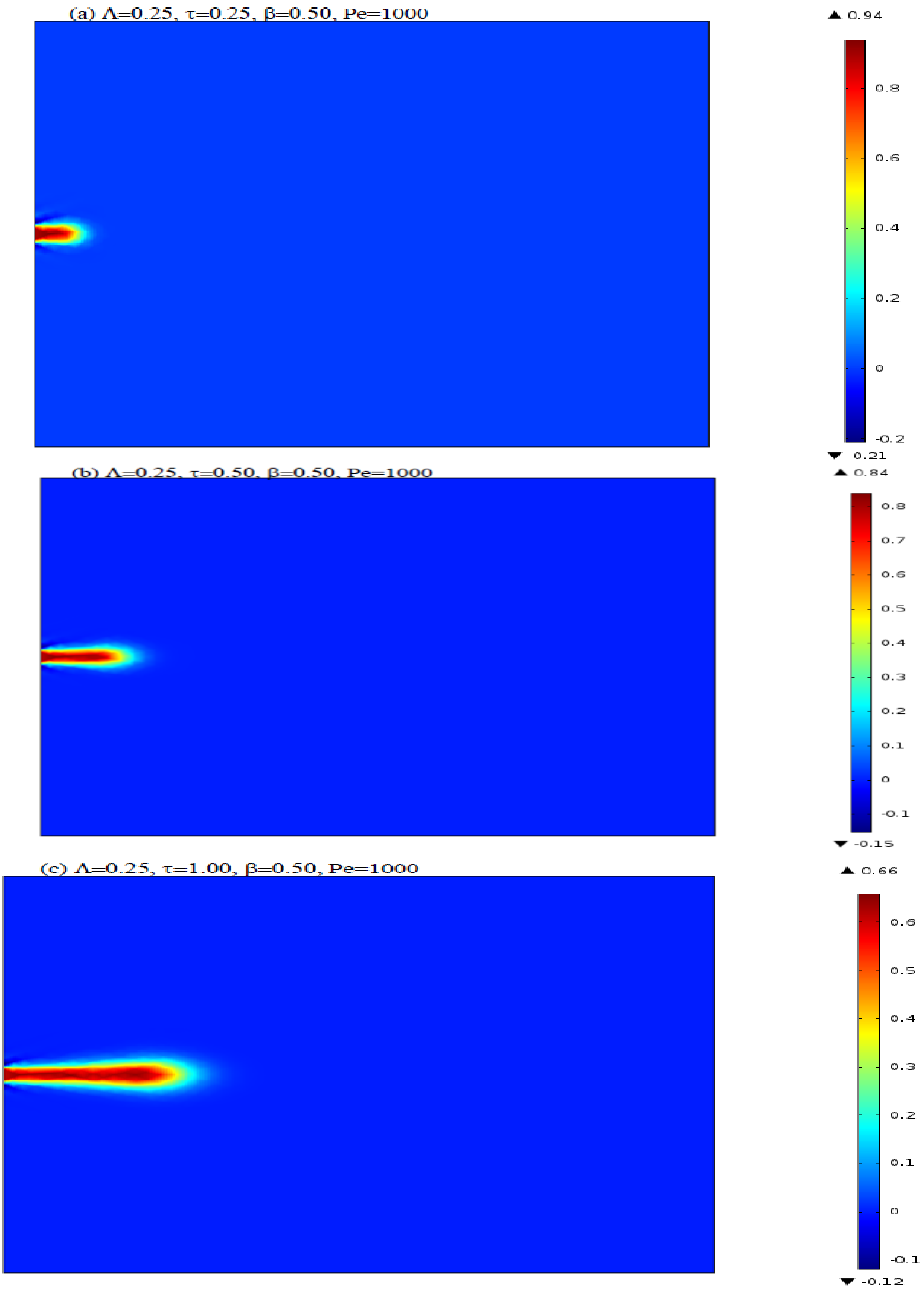

FIGURE 6: EXPONENTIAL SOURCE SURFACE CONCENTRATIONS

REFERENCES

[1] P. Mebine and A. M. George, “Contaminant Decay Effected Longitudinal Advection Dispersion Models with Time-dependent Sources,” Int. J. of Appl. Math. and Mech. 7(16): 42-55, 2011.

[2] P. K. Dhar and D. K. Sinha, “Time-dependent optimal Control of gaseous pollutants from a point source,” Applied Mathematical Modelling 13(1), pp. 27 – 31, 1989.

[3] B. S. Mazumder and D. C. Dalal, “Contaminant dispersion from an elevated time-dependent Source,” Applied Mathematics 126(1 - 2), pp. 185 – 205, 2000.

[4] C. Baverman, L. Moreno and I. Neretnieks, “A fast coupled geochemical and transport program and applications to waste leaching and contaminant transport,” International Journal of Rock Mechanics and Mining Science & Geomechanics Abstracts 32(7), pp. 317A - 318A, 1995.

[5] O. Kolditz, R. Ratke, H.G. Diersch and W. Zielke, “Coupled groundwater flow and transport: 1. Verification of variable density flow and transport models,” Advances in Water Resources 21(1), pp. 27 – 46, 1998.

[6] S. K. Sandrin, F. L. Jordan, R. M. Maier and M. L. Brusseau, “Biodegradation during contaminant transport in porous media: 4. Impact of microbial lag and bacterial cell growth,” Journal of Contaminant Hydrology 50(3 - 4), pp. 225 – 242, 2001.

[7] T. K. Sen, N. Nalwaya and K. C. Khilar, “Colloid-associated contaminant transport in porous media: 2. Mathematical modelling,” AIChE Journal 48(10), pp. 2375 – 2385, 2002.

[8] S. E. Serrano, “Contaminant transport under non-linear sorption and decay,” Water Research 35(6), pp. 1525 – 1533, 2001.

[9] P. Mebine and R. Smith, “Effects of contaminant decay on the diffusion centre of a river” Environmental Fluid Mechanics 6, pp. 101 – 114, 2006.

[10] P. Mebine and R. Smith, “Effect of pollutant decay on steady-state concentration distributions in variable depth flow,” Environmental Fluid Mechanics 9(6), pp. 573 – 586, 2009.

[11] H. Rubin and J. Atkinson, Environmental Fluid Mechanics. Marcel Dekker, New York, NY, USA, 2001.

[12] R. L. Doneker and G. H. Jirka, CORMIX User Manual: A Hydrodynamic Mixing Zone Model and Decision Support System for Pollutant Discharges Into SurfaceWaters,MixZon, Portland, Ore, USA, 2007, http://www.cormix.info.

[13] M. Vasilev, P. Sharma and P. L. Mills, “Application of COMSOL Multiphysics in Transport Phenomena Educational Processes,” Excerpt from the Proceedings of the COMSOL Conference in Boston, 2015.

[14] R. Kolluru and V. Gopal, “Numerical Study of Navier-Stokes Equations in Supersonic Flow over a Double Wedge Airfoil using Adaptive Grids,” Excerpt from the Proceedings of COMSOL Conference in Banglore, 2012.

[15] L.T. Gritter, J.S. Crompton, S.Y. Yushanov and K.C Koppenhoefer, “Analysis of Burning Candle,” Excerpt from the Proceedings of COMSOL Conference in Banglore, 2010.

[16] M. W. Siebert and P. S. Fodor, “Newtonian and Non-Newtonian Blood Flow over a Backward-Facing Step – A Case Study,” Excerpt from the Proceedings of COMSOL Conference in Boston, 2009.

[17] E. M. Dede, “Multiphysics Topology Optimization of Heat Transfer and Fluid Flow Systems,” Excerpt from the Proceedings of COMSOL Conference in Boston, 2009.

[18] J. Dinesh, “Modelling and Simulation of a Single Particle in Laminar Flow Regime of a Newtonian Liquid,” Excerpt from the Proceedings of COMSOL Conference in Bangalore, 2009.

[19] M. A. Diaz-Viera, D. A. Lopez-Falcon, A. Moctezuma-Berthier and A. Ortiz-Tapia, “COMSOL Implementation of a Multiphase Fluid Flow Model in Porous Media,” Excerpt from the Proceedings of COMSOL Conference in Boston, 2008.

[20] E. Kaufman and E. Gutierrez-Miravete, “Computation of Velocity, Pressure and Temperature Distributions near a Stagnation Point in Planar Laminar Viscous Incompressible Flow,” Excerpt from the Proceedings of COMSOL Conference in Boston, 2008.

[21] N. H. B. Siddig, “Mathematical modeling of solutes transportation in arterial blood flow,” Journal of Scientific and Engineering Research, 3(3), pp. 319 – 324, 2016.

[22] C. Israel-Cookey, P. Mebine and A. Ogulu, “MHD Free-Convection and Mass Transfer Flow on a Porous Medium in a Rotating Fluid due to Radiative Heat Transfer,” Modelling, Measurement & Control, AMSE 71(1), pp. 1 – 7, 2002.

[23] R. T. Al-Khairy and Z. M. AL-Ofey, “Analytical Solution of the Hyperbolic Heat Conduction Equation for Moving Semi-Infinite Medium under the Effect of Time-Dependent Laser Heat Source,” Journal of Applied Mathematics Volume 2009, Article ID 604695, 18 pages, doi:10.1155/2009/604695

[24] C. E. Aziz, C. J. Newell, J. R. Gonzales, P. Haas, T. P. Clement and Y-W. Sun, BIOCHLOR Version 1.0 User Manual, EPA /6000/R-00/008, EPA, Washington, D. C, 2000.

[25] G. P. Williams and D. Tomasko, “Analytical solution to the advective-dispersive equation with a decaying source and contaminant,” Journal of Hydrologic Engineering 13(12), pp. 1193 – 1196, 2008.

[26] E. E. Joshua, “Drug absorption in the gastrointestinal tract: a mathematical model,” J. Nigerian Mathematical Society 27, pp. 109 – 122, 2008.