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Modeling the Transport of Textile Dye Contaminants on Aquatic Environments in Laminar Flow: MATLAB and COMSOL Multiphysics Approaches

Mina Abbasipour[a*]

[a]*Montreal, Quebec, Canada*

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Abstract

In this study, COMSOL Multiphysics is employed to model the transport of textile dye contaminants in a riverine system, with a focus on their dispersion along laminar flow. The objective is to understand the impact of these pollutants on aquatic ecosystems. Initially, the flow in the river is assumed to be in a steady state, facilitating the development of a comprehensive numerical model for contaminant dispersion. Numerical solutions for momentum and mass transfer in the river are derived through MATLAB simulations and compared with simulations obtained through COMSOL Multiphysics to assess the accuracy and reliability of the computational model in replicating real-world scenarios. The parameters used in the COMSOL simulation include geometry and materials, defining the river's structure and properties, as well as physics modules governing momentum and mass transfer. Sensitivity analyses are conducted by varying parameters such as the length and depth of the river to understand their impact on velocity and concentration profiles. Additionally, the modeling of mass transfer for textile dye contaminants reacting with water is investigated, considering carbon dioxide and iron (II) oxide as models of contaminants that react with water. This multifaceted approach aims to provide a thorough understanding of how textile dyes spread and interact in riverine environments, contributing valuable insights for environmental protection and remediation efforts.

Keywords: Textile dye contaminate, Riverine system simulation, Laminar flow dispersion, COMSOL Multiphysics, MATLAB

[1]* Corresponding author. Mina Abbasipour, Montreal, Quebec, Canada
E-mail address: mina.abbasipour@gmail.com

1. Introduction

Textile dye contaminants present a significant environmental challenge due to their widespread use in the textile industry and their potential to adversely affect aquatic ecosystems [1]. The textile industry is one of the largest industrial polluters globally, primarily due to the immense volumes of water and chemicals involved in the dyeing and finishing processes [2]. These processes result in the discharge of various pollutants, including textile dyes, into water bodies such as rivers and lakes [3]. Once released into aquatic environments, textile dye contaminants can persist for extended periods, posing threats to aquatic life and human health [4, 5].

The environmental impact of textile dye contaminants stems from their chemical composition, which often includes hazardous substances such as heavy metals, aromatic compounds, and synthetic organic compounds [6]. Many of these compounds are known to be toxic, carcinogenic, or mutagenic, raising concerns about their potential ecological and human health risks [2, 7]. Additionally, textile dye contaminants can disrupt aquatic ecosystems by altering water quality parameters such as pH, dissolved oxygen levels, and light penetration, thereby affecting the health and biodiversity of aquatic organisms [8].

Understanding the behavior and fate of these contaminants in aquatic environments is crucial for effective environmental management and sustainable textile production practices [9]. In recent years, computational modeling has emerged as a powerful tool for studying contaminant transport dynamics, offering insights into dispersion mechanisms and aiding in the development of mitigation strategies [10].

This study aims to utilize COMSOL Multiphysics to model the transport of textile dye contaminants in aquatic environments, focusing on riverine systems as a primary case study. Textile manufacturing processes are known for their extensive water usage and chemical discharge, which significantly contribute to water pollution. By focusing on modeling contaminant transport using COMSOL Multiphysics, this study aims to explore the complex dynamics of textile dye pollutants in riverine systems.

2. COMSOL Parameters

2.1. Geometry

As shown in Figure 1., a rectangular geometry was utilized to model a river. The length and width of the river were chosen from 1 to 5 m (in steps of 1) and 0.1 to 0.5 m (in steps of 0.1), respectively.

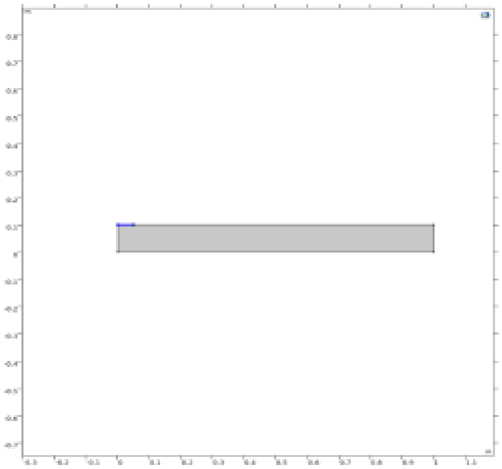

Figure 1. A rectangular geometry to model a river

2.2. Material

Water was selected as the material for modeling fluid flow, while the concentration of contaminants ranged from 100 to 150 mol/m3 (in steps of 10). The diffusion coefficient of contaminants was assumed to vary from 0.01 to 0.001 m^2/s.

2.3. Physics

Laminar flow and transport of diluted species modules were chosen as physics.

2.4. Momentum transfer

Momentum transfer is modeled in COMSOL using laminar and incompressible flow, and Newtonian fluid assumptions. The bottom of the rectangle was considered as no slip condition since the top was set as open boundary. The upper side of the rectangle is set as open boundary because it was supposed as surface of river. Also, the top side of rectangles is defined as a moving wall with a velocity of 0.1-0.5 m/s (step 0.1).

2.5. Mass transfer

Mass transfer in COMSOL was modeled by setting the inlet of contaminants with concentrations ranging from 100 to 150 mol/m3 in the left rectangle. The source of contaminants was assumed to be along the line from point (0, 0) to (0.05, 0) on the top side of the rectangle (Figure 1). The right rectangle was set as the outlet. The upper edge of the right rectangle was defined as an open boundary, while the bottom of the river and the source boundary were set to have no flux.

Table 1. presents the parameters considered for modeling in COMSOL.

Table 1. COMSOL parameters

Parameter	**Range**	**Step**
Length (L)	1-5 m	1
Width (W)	0.1-0.5 m	0.1
Velocity (V)	0.1-0.5 m/s	0.1
Concentration (C)	100-150 mol/m^3	10
Diffusion coefficient (D)	0.01-0.001 m^2/s	0.01, 0.009, ..., 0.001

3. Numerical calculation

Mass and momentum transfer were performed to calculate the velocity profile and mass diffusion through water using MATLAB. To perform numerical calculation, steady state conditions ($\partial/\partial t=0$), laminar flow, constant temperature (T), and incompressible flow (ρ=constant) were assumed. The fluid was considered Newtonian (μ=constant) and $V_z=V_z(x)$. In addition, the system was considered cartesian coordinate.

4. Numerical calculation VS. COMSOL momentum balance

As Table 2. shows, COMSOL results for average velocity differed from the numerical solution due to neglect of the transition region and convection effects.

Table 2. Numerical calculation vs COMSOL momentum balance

Property	Numerical calculation	COMSOL result
$V_{average}$ (m/s)	0.45	0.4988

5. Velocity

The velocity profile obtained from COMSOL is illustrated in Figure 2. In Region 1, situated at the top boundary, the velocity remains constant at 0.5 m/s due to the absence of external forces. Consequently, velocity variations within this region are minimal. In Region 2, located at the bottom, the velocity is constrained to zero owing to the no-slip boundary condition (Figure 2a).
The cut line No. 1, (point (0.1, 0) - (0.1, 0.5)) was selected to plot velocity changes with respect to x-axis. The COMSOL result shows that the Vmax ~ 0.5 m/s which is equal to numerical result. The graph obtained from numerical calculation and COMSOL is shown in Figure 2b. Figure 6. shows that the velocity graph obtained from numerical calculation is different from COMSOL, because in the numerical calculation the convection effects did not account.

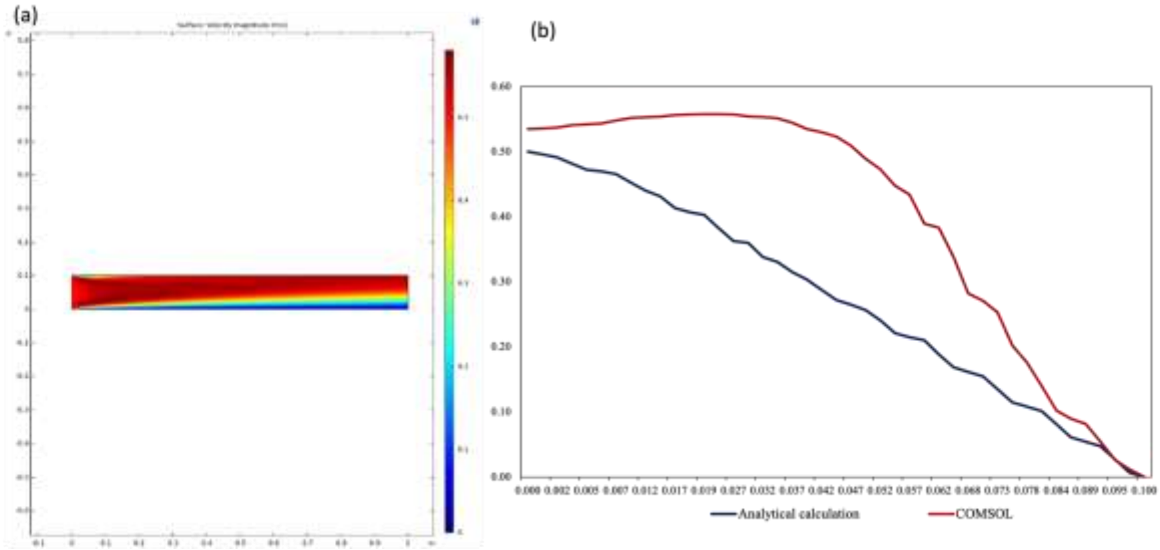

Figure 2. (a) Velocity profile obtained from COMSOL, (b) comparison of velocity graphs from cut line 1 obtained from MATLAB and COMSOL.

6. Concentration

The concentration profile obtained from COMSOL is shown in Figure 3. In despite of the source boundary, the rest region shows uniform concentration. At the right edge, the concentration is equal to zero, because the right edge was assumed as inflow boundary.
The result obtained from MATLAB is shown in Figure 3c. In numerical calculation, concentration tends to zero because of different boundary conditions (at x=0, CA=CA0). In addition, the convection term in x direction and diffusion term in z direction were neglected. However, the concentration profile obtained from COMSOL showed uniform

distribution, except near the source boundary where the concentration was highest. The numerical solution predicted a concentration tending towards zero, but COMSOL showed a concentration of 41 mol/m^3 (Figure 3b).

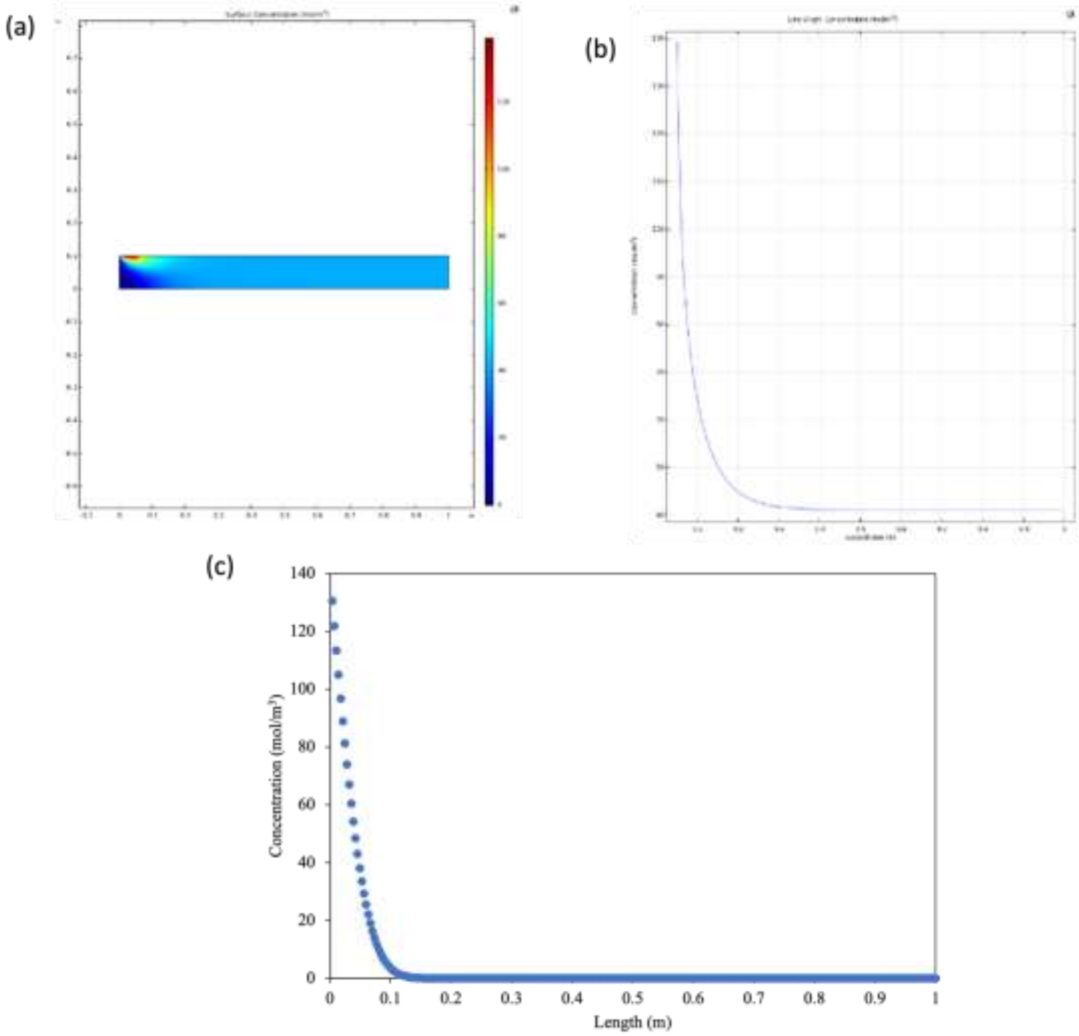

Figure 3. (a) Concentration profile at primary concentration of 139.19 mol/m3 and diffusion coefficient of 0.01 m^2/s, (b) the concentering diffusion obtained from COMSOL (c) the concentering diffusion obtained from numerical calculation

The mass transfer equation obtained from the numerical method was plotted using MATLAB (CA0=1339.19 mol/m^3, D=0.01 m^2/s). The results obtained from MATLAB showed good agreement with COMSOL. In MATLAB, it was assumed at the final stage that the contaminants never reach the bottom of the river ($x \to \infty$, C_A=0). This assumption influenced the results.

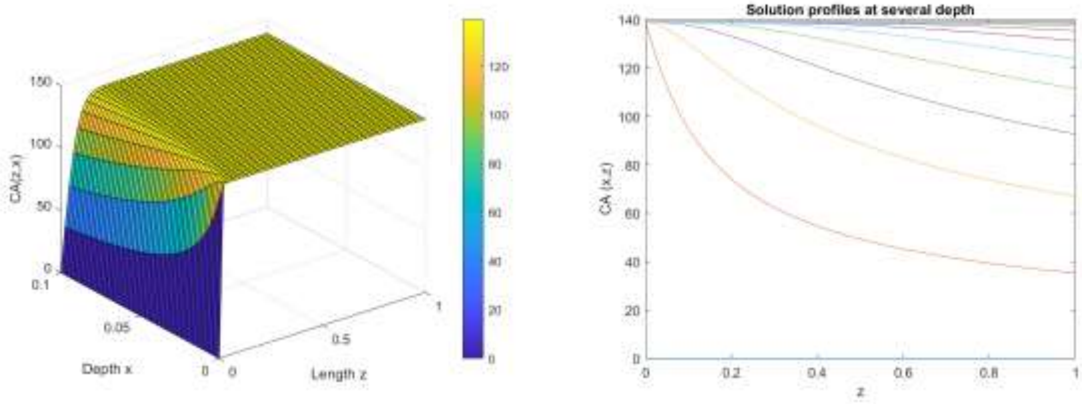

Figure 4. Changes of concentration along the length of river in different depth using MATLAB

The Effect of length and depth of river on velocity profile and concentration profile were investigated.

Length of the river had no effect on the velocity and concentration profiles (Figure 5a and 5b), but Vmax decreased with increasing length (Figure 5b).

Figure 5c shows the velocity profile and concentration profile with respect to the depth of river. As figure 5c shows, the velocity profile is independent of depth of river. However, by increasing depth of river, the concentration changes significantly. For example, in the width of 0.2, the distribution in concentration is more than other widths (Figure 5d).

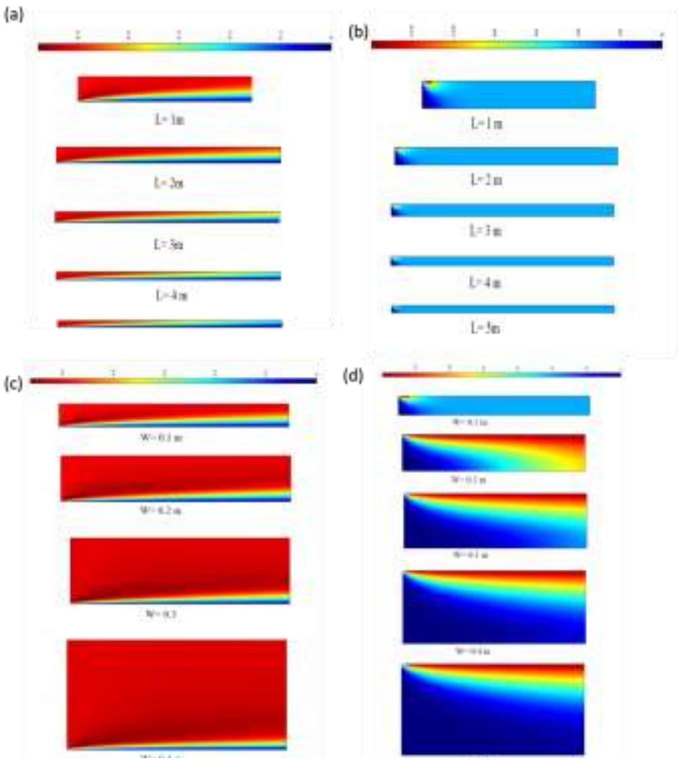

Figure 5. (a) Velocity and (b) concentration profiles with respect to different length; (c) velocity and (c) concentration profiles with respect to different depth

7. Modeling of mass transfer of contaminants reacted with water

7.1. Carbon dioxide (CO_2)

In the textile industry, some dyeing or finishing processes involve chemicals such as bicarbonates, carbonates and organic acids that react with water and release carbon dioxide (CO_2). These materials are typically used for specific purposes such as neutralizing or removing certain substances [11].

CO_2 gas was considered as a contaminant, and its reaction with water was modeled using laminar flow, transport of diluted species, and chemistry modules. Parameters for the simulation were selected as described in Table 3.

$$CO_2 + H_2O \rightarrow H_2CO_3$$

Table 3. Used parameters for COMSOL simulation [1].

Parameter	Value	Description
M_A	0.04401 [kg/mol]	Molar weight, carbon dioxide
rho_A	1.98 [kg/m^3]	Density, carbon dioxide
cA0 (rho_A/M_A)	44.99 [mol/m^3]	carbon dioxide concentration, inlet
M_B	0.018 kg/mol	Molar weight, water
rho_B	1000 kg/m^3	1000 kg/m^3
cB0 (rho_B/M_B)	55556 mol/m^3	Water concentration, inlet
M_C	0.06203 kg/mol	Molar weight, carbonic acid
rho_C	1670 kg/m^3	density, carbonic acid
A	0.03 1/s	Frequency factor
E	15900 J/mol	activation energy
dH	59810 J/mol	heat of reaction
ke	0.559 W/(m·K)	Thermal conductivity
myref_B	0.001 Pa·s	Reference dynamic viscosity, water
Tref_my	293 K	Reference temperature viscosity

Concentration and velocity profiles of species were shown in Figure 6. As shown in Figure 6a, the concentration of CO_2 is uniform, indicating an instantaneous reaction where all CO_2 is converted to carbonic acid. Figure 6b presents the concentration profile of carbonic acid, illustrating areas with varying concentrations due to the reaction. Notably, the velocity profile in Figure 6c shows significant changes compared to the scenario without any reaction.

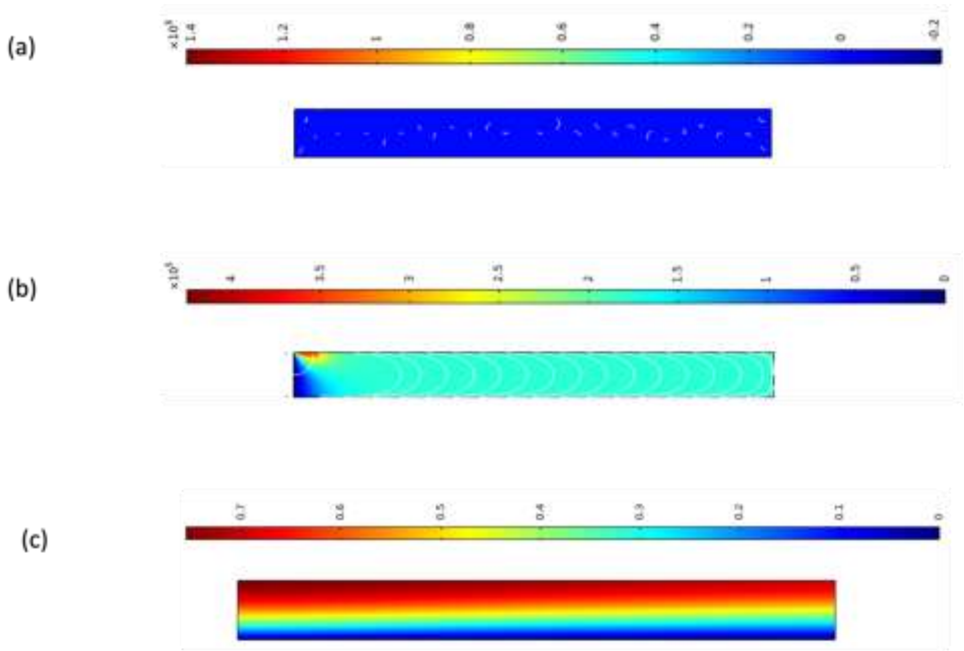

Figure 6. Concentration profile of (a) CO_2, (b) carbonic acid and (c) velocity profile

7.2. Iron (Fe)

Iron contaminants in the textile industry wastewater primarily originate from dyes, water supplies, and corrosion of metal equipment. Elevated iron levels can cause discoloration, sludge formation, and environmental toxicity, adversely affecting aquatic life and water quality [12]. The reaction of FeO with water was modeled to investigate the effect of reaction rate on concentration and velocity profiles. Table 4 shows the parameter used to simulate Fe reaction with water.

Table 4. Used papameters for Fe reaction with water [13].

Parameter	Value	Description
M_A	0.055845 [kg/mol]	Molar weight, Iron
rho_A	7874 [kg/m^3]	Density, Iron
cA0 rho_A/M_A	1.41e5 [mol/m^3]	Iron concentration, inlet
M_B	0.018 kg/mol	Molar weight, water
rho_B	1000 kg/m^3	1000 kg/m^3
cB0 (rho_B/M_B)	55556 mol/m^3	Water concentration, inlet
M_C	0.071844 kg/mol	Molar weight, carbonic acid
rho_C	5740 kg/m^3	density, FeO
A	3e11 1/s	Frequency factor
E	2.4e5 J/mol	activation energy
dH	59810 J/mol	heat of reaction
ke	-266.5 W/(m·K)	Thermal conductivity
myref_B	0.001 Pa·s	Reference dynamic viscosity, water
Tref_my	293 K	Reference temperature viscosity

As shown in Figure 7a, the concentration profile of Fe is highest on the left side, representing the entry of Fe contaminants into the river. The concentration decreases as the Fe disperses and dilutes downstream. Figure 7b illustrates the concentration profile of FeO, showing an increase as Fe is oxidized to FeO away from the entry point. Notably, the velocity profile in Figure 7c shows significant changes due to the introduction and reaction of Fe contaminants, reflecting alterations in flow dynamics.

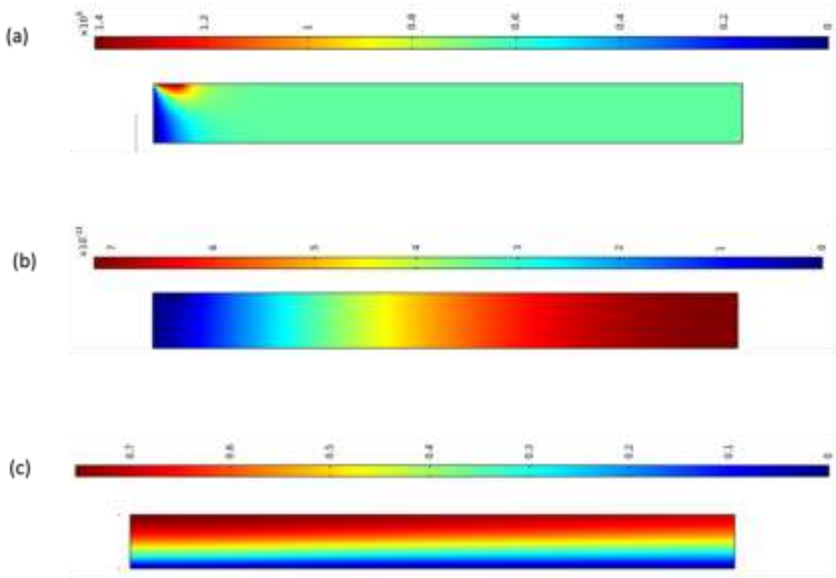

Figure 7. Concentration profile of (a) Fe, (b) FeO and (c) velocity profile

8. Conclusion

This paper aims to simulate the mass transfer of contaminants in a river. The obtained results from COMSOL modeling and numerical calculations are compared. In the numerical calculation, the concentration tends to zero due to different boundary conditions (at x=0, C_A=C_{A0}). Additionally, the convection term in the x direction and the diffusion term in the z direction were neglected. However, the COMSOL result shows that the concentration tends to 41 mol/m^3. The mass transfer equation obtained from the numerical method was plotted using MATLAB (C_{A0}=1339.19 mol/m^3, D=0.01 m^2/s). The results obtained from MATLAB showed good agreement with the COMSOL results because in the hand calculation, it is assumed that the contaminants never reach the bottom of the river ($x \to \infty$, C_A=0). Therefore, this assumption affected the results. Some parameters, such as the length and width of the river were changed to study their effect on the concentration and velocity profiles. It was found that the length of the river does not affect the velocity and concentration profiles, but Vmax decreases with an increase in the length of the river. The velocity profile is independent of the width of the river, but the concentration shows considerable changes with increasing width.

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