CFD Modelling of Particle-Laden Gas Flow and Filtration Through Porous Media

Yoann Robert[1], Duygu Kocaefe[2], Yasar Kocaefe[3] and Simon Gaboury[4]
1. Postdoctoral fellow
2. Professor
3. Professor
UQAC Research Chair on Industrial Materials (CHIMI), Chicoutimi, Québec, Canada,
University Research Centre on Aluminium (CURAL), Chicoutimi, Québec, Canada,
4. Principal Advisor Environment Technologies, Aluminium Technology Solutions
Centre de recherche et de développement Arvida (CRDA), Jonquière, Québec, Canada
Corresponding author: Duygu_Kocaefe@uqac.ca

Abstract

Particle-laden flows are quite common in industry. In some cases, a reaction takes place between a component of the gas and the particles. Then, the particles are filtered through a porous media to avoid their emission to the environment. In aluminum industry, filter bags are used to retain particles. After validation, a mathematical model for such systems could be a highly useful tool to test various operational and design parameters. However, the representation of the particle deposition on a filter media is highly complex to model.

A three-dimensional transient mathematical model was developed to represent a system in which a gas flow enters, a certain concentration of small particles is injected into the gas stream, and the gas leaves through a porous media where the particles are to be filtered. The porous media with a certain thickness represents the filter bag. The conservation equations for the gas flow and solid particles are obtained using the phase equations of the Algebraic Slip Model (ASM). The turbulence model used is the standard k-ε model with the wall function treatment. The porous media settings are defined according to the Ergun equation. The model equations are solved numerically by the commercial code ANSYS-CFX19.5. A parametric study was carried out to determine the effect of some parameters such as particle injection velocity and concentration. In this paper, the model will be described, and the results are presented for some cases.

Keywords: Gas flow, CFD simulation, Porous media, Algebraic slip model.

1. Introduction

Commercial aluminum production is based on the Hall-Héroult process during which alumina is reduced to metallic aluminum in an electrolysis cell. The exhaust gas contains SO_2 coming from carbon anodes which are regularly consumed and replaced after 20–25 days. SO_2 can be removed from the exhaust gas by using dry hydrated lime. The study consists of a simulation of a laboratory scale reactor in which hydrated lime and SO_2 are brought in contact to achieve the target SO_2 removal level.

This paper describes a work in progress. The flow field within the reactor as well as the concentration distributions of various gas components - air, $Ca(OH)_2$ particles, and SO_2 - in the reactor are presented. The particle filtration and the reaction between SO_2 and hydrated lime are not yet incorporated into the model.

2. Mathematical Formulation

The model considers a simple reactor in cubic form which contains a filter bag. Figure 1 shows the geometry of the physical problem. There is one inlet for the mixture which is composed of two gas phases (air and SO_2) and one dispersed phase of solid $Ca(OH)_2$ particles, and one outlet. The filter is defined as a porous media (shown in green on Figure 1). The adopted approach in this study consists of solving the flow and the mass fraction of SO_2 and $Ca(OH)_2$ using the Algebraic Slip Model (ASM) under isothermal conditions.

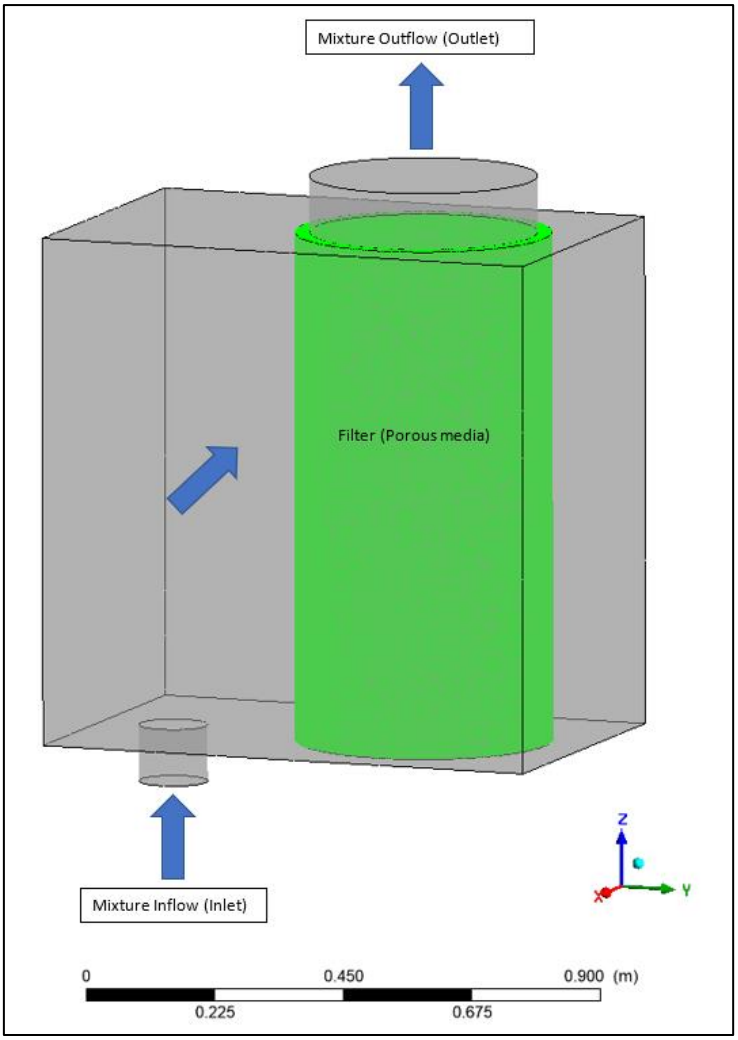

Figure 1. Schematic representation of the physical model.

It was assumed that:

- The flow field is turbulent, and
- The gravity effects are negligible.

The ASM formulation of a multi-phase model for n-interpenetrated phases of a multi-fluid model was first introduced by Ishii [1]. In this model, a system is represented with a mass and a momentum balance for the whole mixture and a mass conservation equation for the n-1 phases. Manninen and Taivassalo [2] presented the complete derivation of the model.

2.1 Phase Equations

Considering an individual phase α, the continuity equation is given for this phase as:

$$\frac{\partial}{\partial t}(r_\alpha \rho_\alpha) + \frac{\partial}{\partial x^i}(r_\alpha \rho_\alpha u_\alpha^i) = 0 \tag{1}$$

and the momentum equation of the phase α is:

$$\frac{\partial}{\partial t}(r_\alpha \rho_\alpha u_\alpha^i) + \frac{\partial}{\partial x^j}(r_\alpha \rho_\alpha u_\alpha^i u_\alpha^j) = -r_\alpha \frac{\partial p}{\partial x^i} + \frac{\partial}{\partial x^j}(r_\alpha \tau_\alpha^{ji}) + r_\alpha \rho_\alpha g^i + M_\alpha^i \tag{2}$$

where:

i, j	Orthogonal directions
$\frac{\partial}{\partial x^i}, \frac{\partial}{\partial x^j}$	Spatial partial derivatives with respect to directions *i* and *j*, respectively, m^{-1}
$\frac{\partial}{\partial t}$	Time partial derivative, s^{-1}
r_α	Volume fraction of the phase α, unitless
ρ_α	Phase density, kg/m^3
p	Pressure, Pa
g^i	Gravitational acceleration, m/s^2
τ_α^{ji}	Stress tensor, N/m^2
u_α^i and u_α^j	Phase velocity for components *i* and *j*, respectively, m/s
M_α^i	Momentum transfer with other phases, $N/m^3 \cdot s$.

2.2 Mixture Equations

The governing equations for the mixture are as follows. The continuity equation for the mixture is:

$$\frac{\partial}{\partial t}(\rho_m) + \frac{\partial}{\partial x^i}(\rho_m u_m^i) = 0 \tag{3}$$

The momentum equation is obtained by the summation of Equation (2) over all phases:

$$\frac{\partial}{\partial t}(\rho_m u_m^i) + \frac{\partial}{\partial x^j}(\rho_m u_m^i u_m^j) = -\frac{\partial p}{\partial x^i} + \frac{\partial}{\partial x^j}(\tau_m^{ji} + \tau_D^{ji}) + \rho_m g^i \tag{4}$$

where:

u_m^i and u_m^j	Mixture velocity for component *i* and *j*, respectively, m/s
ρ_m	Mixture density, kg/m^3
τ_m^{ji} and τ_D^{ji}	Mixture stress, and the diffusion stress, respectively, N/m^2.

$$\rho_m = \sum_{\alpha=1}^{n} r_\alpha \rho_\alpha \tag{5}$$

$$\rho_m u_m^i = \sum_{\alpha=1}^{n} r_\alpha \rho_\alpha u_\alpha^i \tag{6}$$

$$\tau_m^{ji} = \sum_{\alpha=1}^{n} r_\alpha \tau_\alpha^{ji} \tag{7}$$

$$\tau_D^{ji} = -\sum_{\alpha=1}^{n} r_\alpha \rho_\alpha (u_\alpha^i - u_m^i) u_\alpha^j \tag{8}$$

where:

n Total number of phases, unitless.

2.3 Drift and Slip Relations

From the previous equations, the slip velocity is determined as the phase velocity relative to the continuous phase by the following relation:

$$u_{S\alpha}^i = u_\alpha^i - u_c^i \tag{9}$$

and the drift velocity is given as:

$$u_{D\alpha}^i = u_\alpha^i - u_m^i \tag{10}$$

where:

$u_{S\alpha}^i$ Slip velocity of the phase α, m/s
u_c^i Velocity of the continuous phase, m/s
$u_{D\alpha}^i$ Drift velocity of the phase α, m/s.

2.4 Drag Force

The motion of particles (dispersed phase) in the continuous gas phase leads to a drag force acting on the particles. The drag force expression is given by Ishii and Mishima [3],

$$F_{\alpha d} = -\frac{3}{4} C_D \frac{r_\alpha \rho_c}{d_{\alpha d}} |u_{S\alpha}| u_{S\alpha}^i \tag{11}$$

where:

$F_{\alpha d}$ Drag force, N/m^3
ρ_c Density of the continuous phase, kg/m^3
$d_{\alpha d}$ Particle diameter of the dispersed phase, m
C_D Drag coefficient, unitless.

2.5 Porous Media

The filter bag is represented as a porous media where the volume porosity is the ratio of the volume *V'* available to flow in an infinitesimal control cell surrounding the point, and the physical volume *V* of the cell.

$$V' = \varepsilon V \tag{12}$$

where:

V'	Volume available to flow in an infinitesimal control cell, m^3
V	Physical volume of the cell, m^3
ε	Volume porosity, unitless.

The volume porosity is calculated from the Ergun equation [4] using the expression:

$$\Delta p = \frac{150\mu L}{D_p^2}\frac{(1-\varepsilon)^2}{\varepsilon^3}v_s + \frac{1.75L\rho}{D_p}\frac{(1-\varepsilon)^2}{\varepsilon^3}v_s|v_s| \tag{13}$$

where:

Δp	Pressure drop, Pa
L	Length of the bed, m
D_p	Equivalent spherical diameter of the packing, m
P	Density of the fluid, kg/m^3
μ	Dynamic viscosity of the fluid, Pa·s
v_s	Superficial velocity, m/s.

2.6 Initial and Boundary Conditions

As initial conditions, the system is taken as isothermal and the relative pressure at the outlet of the system is set to 0 Pa.

The boundary conditions for the flow field are given as follows:

$$Inflow = \begin{cases} u = 0, v = 0, w = U_f \\ T = T_f \\ r_{SO_2} = r_{SO_2}^{initial} \\ r_{Ca(OH)_2} = r_{Ca(OH)_2}^{initial} \\ d = d_{Ca(OH)_2} \end{cases} \quad Outflow = \begin{cases} p = 0 \\ u = 0, v = 0, w = 0 \\ T = T_f \\ r_{SO_2} = 0 \\ r_{Ca(OH)_2} = 0 \end{cases} \tag{14}$$

where:

u, v, w	Orthogonal velocity components, m/s
T	Temperature, °C
r_{SO_2}	Mass fraction of SO_2
$r_{Ca(OH)_2}$	Mass fraction of $Ca(OH)_2$
d	Particle diameter, m.

The turbulence intensity is set to medium level (*i.e.*, 5 %). The transport and physical properties are summarized in Table 1.

Table 1. Parameters used in the simulation.

Property	Value
U_f (m/s)	5, 7, 10
Tf (°C)	25
$r_{SO_2}^{initial}$ (%)	0.03
$r_{Ca(OH)_2}^{initial}$ (%)	10, 15
$d_{Ca(OH)_2}$ (μm)	45

3. Numerical Solution

The multiphase flow is solved in a fluid domain which also includes a porous media by using a commercial software ANSYS-CFX19. A mesh consisting of 2 500 917 elements in the fluid and solid domain (filter) with an adaptative time step between 0.125 and 1.000 second was used for all the cases. The CPU time for the simulation of 15 seconds of the process is 1 h on Intel®Xeon® E5 v4 2.20GHz computer.

4. Results and Discussion

The following sections present the velocity field for three inlet velocities and the mass fractions of each phase in the system.

Since the filtration of particles (retention of particles on the filter surface) is not simulated, they penetrate through the porous media and leave the system. Also, the reaction for SO_2 removal is not included. Consequently, all SO_2 that enters, leaves the system. These features are being currently incorporated into the model and are, therefore, considered to be beyond the scope of the present work:

- When the particle retention on the filter surface is functional, there would be no particles inside the filter and at the outlet of the system:
    - The particle layer thickness would grow as a function of time and would need to be removed regularly
- When the chemical reaction between SO_2 and $Ca(OH)_2$ is represented in the model, the SO_2 concentration would decrease due to the contact with the particles:
    - Its concentration at the outlet would indicate the removal efficiency as a function of different parameters.

In its current form, the model shows the level of particle-SO_2 interaction, which is important for an efficient SO_2 removal. Without the particle retention by the filter and the chemical reaction for SO_2 capture, the results presented in this article correspond to those of the steady-state simulation.

4.1 Velocity Field

In Figure 2, the computed velocity field for three different inlet velocities, *i.e.*, 5, 7, and 10 m/s is shown. For each case, the gas mixture flow enters the system through the inlet, expands in the tank and around the filter. Then, it goes through the filter and exits by the outlet. The gas velocity decreases quickly in the system before its exit. Table 2 summarizes the values predicted in the system for the three cases.

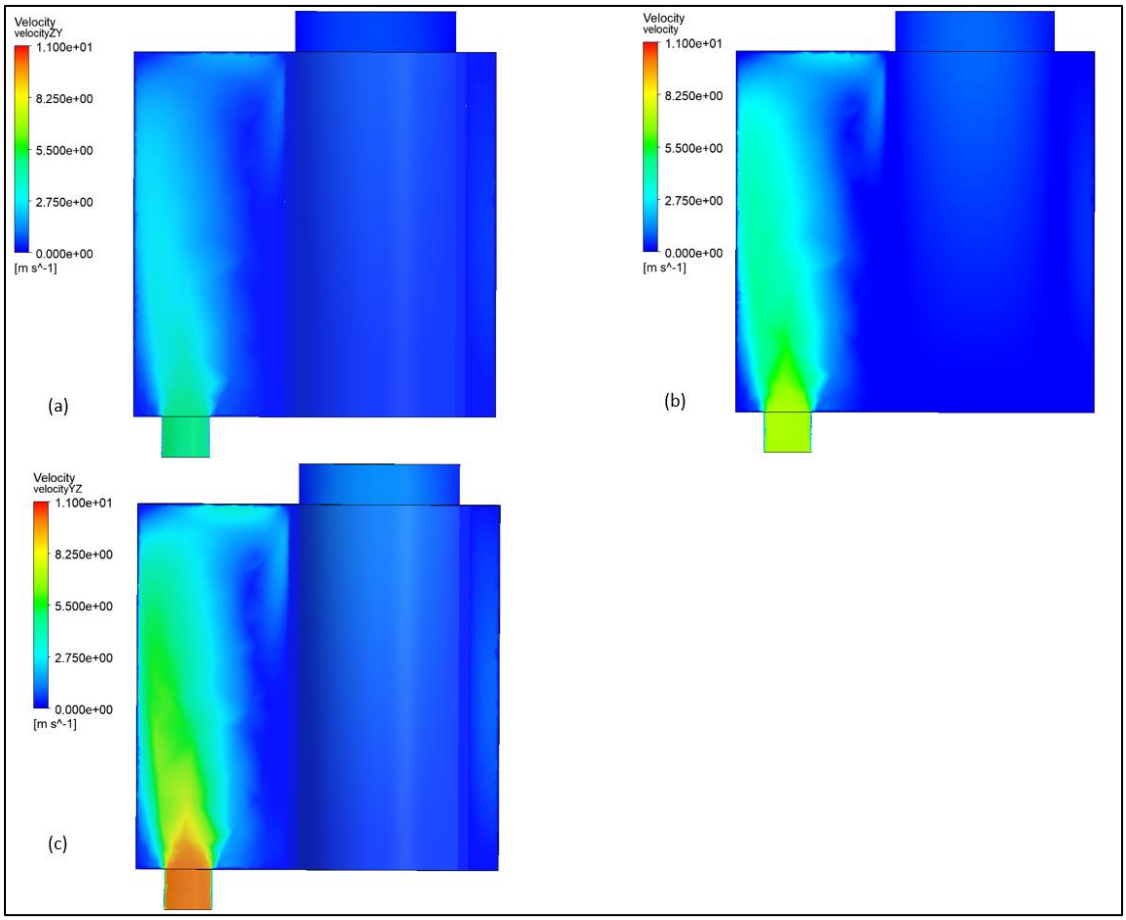

Figure 2. Gas velocity field for different inlet velocities. (a) 5 m/s, (b) 7 m/s, and (c) 10

Table 2. Mixture velocities in the system.

Inlet velocity (m/s)	**5**	**7**	**10**
Inlet mass flow (kg/s)	0.05	0.07	0.10
Outlet mass flow (kg/s)	-0.05	-0.07	-0.10
Outlet velocity (m/s)	0.45	0.63	0.90
Mean velocity (m/s)	1.02	1.16	1.98
Max. velocity (m/s)	5.32	7.18	10.57
Min. velocity (m/s)	0.011	0.006	0.014

When the inlet velocity is 5 m/s, the mean velocity in the system is 1.02 m/s; for an inlet velocity of 10 m/s, it is 1.98 m/s. The reaction between SO_2 and $Ca(OH)_2$, and consequently the SO_2 removal, would be expected to increase with an increase in inlet velocity. Once the experimental system is in place, the model (after the incorporation of particle filtration and chemical reaction) will be validated.

4.2 Phase Mass Fractions

Figure 3 shows the mass fraction of three phases (air, $Ca(OH)_2$, and SO_2) for the inlet velocities of 5, 7, and 10 m/s. Air (continuous phase) occupies a large part of the system with a mass fraction

between 70 and 95 % except in small regions (corners) where the particles are accumulated due to low velocities. Considering other phases, a major part of the gas phase of SO_2 and the dispersed phase of $Ca(OH)_2$ are observed around the filter. Thus, the reactor geometry favors a good contact between these two reactants. The $Ca(OH)_2$ and SO_2 mass flowrates increase with an increase in inlet velocity. As it can be seen in the figure, the presence of these components increases as the inlet velocity is increased.

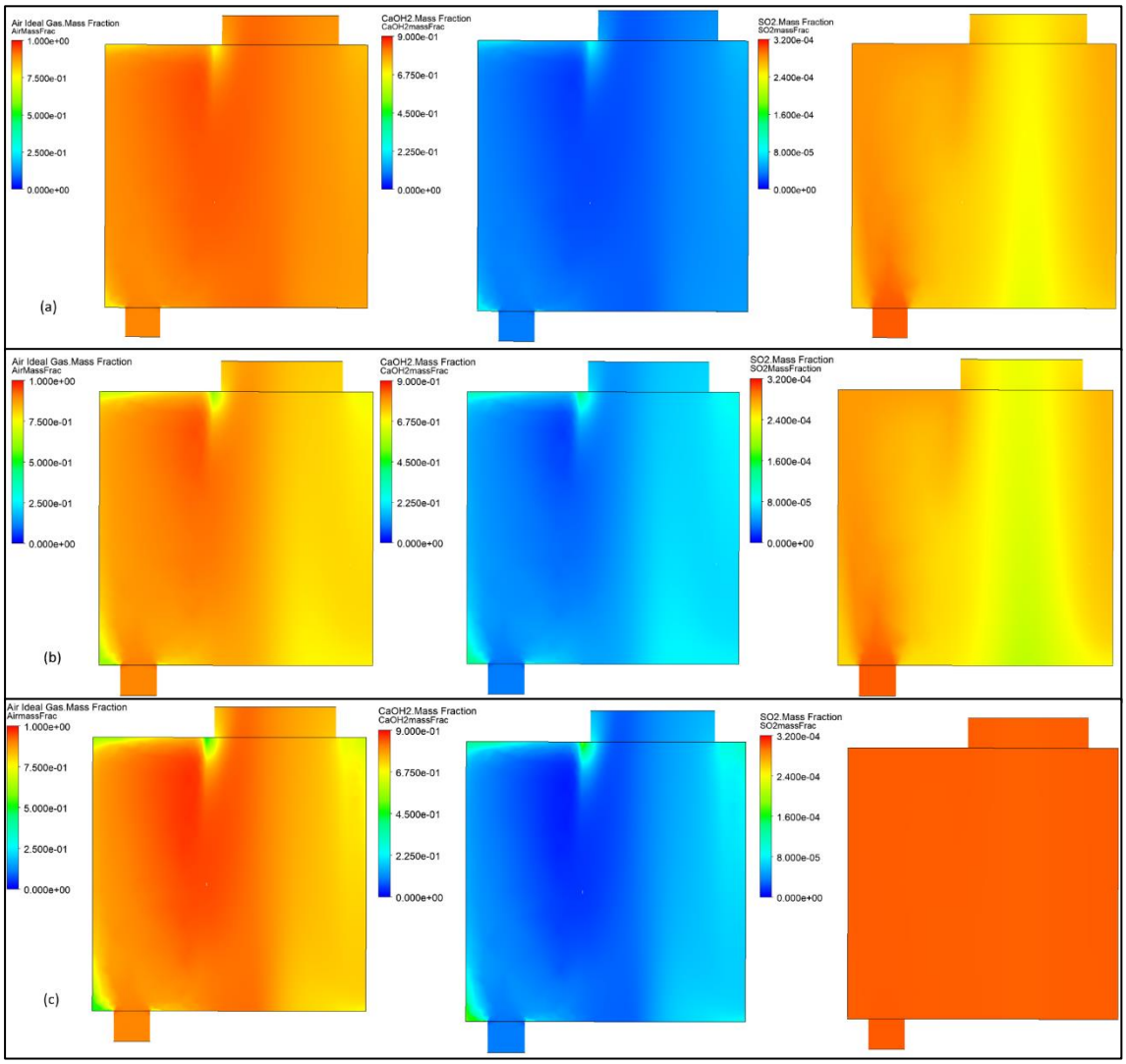

Figure3. Mass fractions of air, $Ca(OH)_2$, and SO_2 for different inlet velocities, considering a Ca(OH)2 inlet mass fraction of 10 %. (a) 5 m/s, (b) 7 m/s, and (c) 10 m/s.

Figure 4 presents the $Ca(OH)_2$ concentration distributions for 7 m/s and 10 m/s inlet velocities and $Ca(OH)_2$ mass fractions of 10 and 15 % at the inlet. It can be seen that the impact is much less pronounced for 7 m/s case compared to 10 m/s one. The higher the velocity and the inlet mass fraction are, the higher the quantity of SO_2 and $Ca(OH)_2$ injected into the system. At 10 m/s and 15 % inlet mass fraction, more particle accumulation is observed around the corners.

The model will help determine the conditions under which the sulfur capture is more favorable.

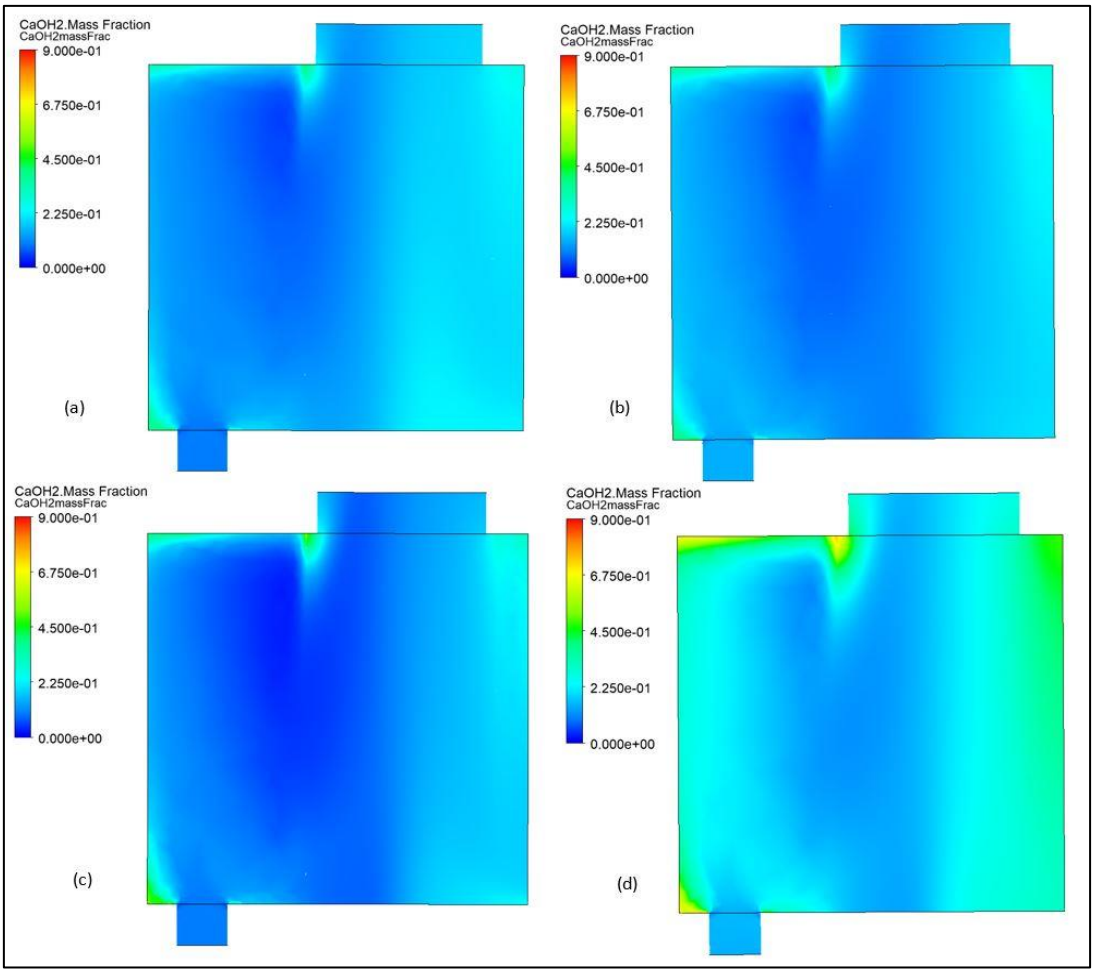

Figure 4. $Ca(OH)_2$ mass fractions for different inlet velocities and $Ca(OH)_2$ inlet mass fractions, respectively. (a) 7 m/s and 10 %, (b) 7 m/s and 15 %, (c) 10 m/s and 10 %, and (d) 10 m/s and 15 %.

5. Conclusions

A numerical simulation of a fluid flow through a filter (porous media) has been carried out by solving the algebraic slip model equations for a mixture of a gas phase (air) containing SO_2 and a dispersed phase for $Ca(OH)_2$. The computational fluid dynamic software, ANSYS CFX19 is employed to solve the system of continuity and momentum equations for the mixture and each phase. The results show expected trends. Work is continuing to incorporate the particle filtration and the chemical reaction for sulfur removal.

6. References

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