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Study of the compartmental modelling method on the basic non-reactive tank

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Abstract: The Compartment Model allows modeling the system flow to zones visually, in which each zone is characterized by a combination of basic mixing compartments. The localization of the flow zones, as well as the calculation of the volume zones and exchange rate between zones, was done based on the velocity field determined from the numerical simulation model. This study presents the results of applying the CM method to analyze the 2D basic non-reactive tank with dimensions of 100 cm x 100 cm x 10 cm and an inlet flow of about 3 - 6 L/min. The results show that the obtained CM model has 3 main flow zones including the convection zone, circulation zone and slow flow zone. The results of comparing the tracer response curves from the CM model and experiment with the root-mean-square error below 0,11 allow confirming the established CM model.

Keywords: *compartmental model, CFD, RTD, CM.*

I. INTRODUCTION

Tanks are widely used in many industrial fields such as wastewater treatment, aquaculture, and mixing multi-phase processes. Modeling system flow to provide kinetic flow information, dead zone, and optimal mixing zone can help predict system performance. The tracer method proposed by Dankwert (1953) based on the impulse response principle is known as an approach to quantify the mixing capacity of tanks by determining the experimental residence time distribution (RTD) [1]. The RTD is calculated by measured tracer concentration distribution [2]. Levenspiel (1999) developed a method to model a system by combining basic flow blocks (plug flow, ideal mixing volume, dead volume and so on) such that the RTD of the computational model is close to the experimental RTD [3,4]. This method is simple and visual, but it is uncertain in the solution because there can be many combination solutions that have similar residence time distribution. On the other hand, the method does not identify specific flow regions in the real model.

In recent years, the Compartmental Model (CM) method allows dividing regions of the flow system according to basic flow zones combined with velocity field distribution from the computational fluid dynamics (CFD) model has been developed as an improvement of Levenspiel's method. Y Le Moullec (2010) compared three methods, including CFD simulation, CM model, and Continuous Stirred Tank Reactor (CRTR) model, to model a wastewater treatment tank [5]. Delafosse et al (2010) proposed a CM model based on the CFD simulation results of the velocity field in a biological tank. The flow compartments from the CFD simulation are created by manual or automatic zoning [6]. The research on the CM model to describe the hydrodynamic process in a

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waste stabilization tank in Cuaenda (Ecuador) was performed by Alvarado et al. (2012) [7].

In short, the setting of compartments is the key of the CM model. The CM model can be validated by comparing the residence time distribution of the model and that of the experiment. This report presents the results of building a CM model based on CFD/RTD to analyze a likely 2D, the non-chemical reactive tank having dimensions of 100 cm x 100 cm x 10 cm and establishes the relationship between the inlet flow rate and the kinetic parameters of the zones.

II. CALCULATION METHOD, RESULTS AND DISCUSSION

A. Research subjects and method

Research subjects

The research tank made from 1 cm - thickness mica has the dimensions of 100 cm x 100 cm x 10 cm corresponding to a volume of 100 L. Both inlet and outlet have an inner diameter of 4 cm, which are located at diagonal corners of the tank. The tank is illustrated in Figure 1.

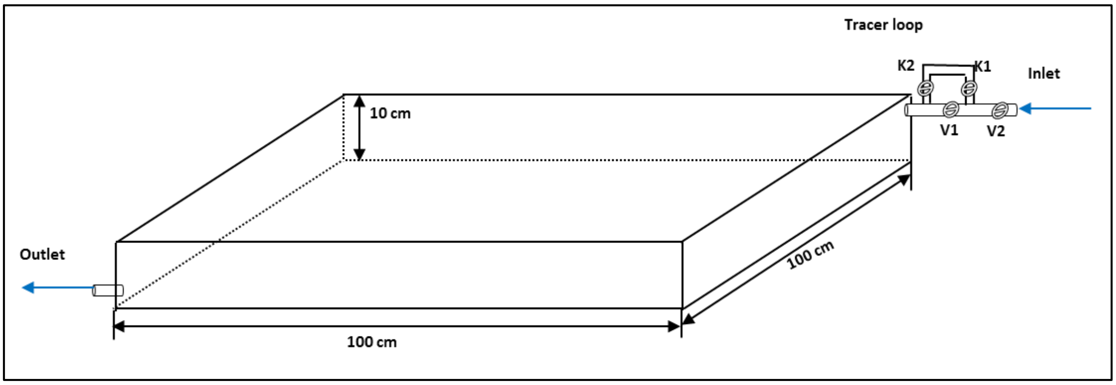

Fig. 1. Physical model diagram: V1, V2 are the flow rate control valve and K1, K2 are the tracer control valve

At the initial time, NaCl tracer solution was stored in a tracer loopwith a volume of 0.5, while both K1 and K2 valves were closed. Water was pumped into the model with a flow rate adjusted by V1 and V2 valves. When flow rate was stable, V1 was closed and K1, K2 were simultaneously opened to inject tracer to model. The NaCl tracer concentration over time was observed at the outlet by a laboratory conductivity meter.

The tracer experiments

The tracer experiments were conducted on the physical model with the inlet flows of 3.0 L/min, 4.5 L/min and 6.0 L/min, respectively, to determine the experimental residence time distribution curve.

At $0 \leq t \leq 5$ s, 0.5 L of NaCl tracer solution with12.14 g/L concentration (D = 1000 kg/m3) was injected into model at the inlet. At the outlet, salt concentration C(t) was measuredby the conductivity sensor HANNA HI98197 (Romania).

By definition, RTD is calculated by the following formula [2]:

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)dt} \qquad (1)$$

The computational dynamics fluid (CFD)

The spatial velocity distribution and the RTD of the tank with different flow rates were calculated on the numerical model corresponding to the experimental parameters using FLUENT software (ANSYS ACADEMIC 2020 R2, USA). The software can simulate tracer transport in the tank in three approaches: (1) Eulerian-Lagrangian involving the application of the Eulerian method to the continuous phase and the Lagrangian method to the dispersed phase; (2) Eulerian-Eulerian applying the Eulerian method to phases regardless of the phase contact surface; (3) Volume of Fluid (VOF) applying the Eulerian method to phases where the phase contact surface is calculated based on volume. In this study, VOF is interested. The equation shows the transport of each phase (water – continuous phase, tracer – dispersed phase) [8]:

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho v) = \sum S_k \quad (2)$$

$$\frac{\partial (\rho v)}{\partial t} + \nabla.(\rho v v) = -\nabla \pi + \rho g + F \quad (3)$$

Where ρ is the phase density, v is the velocity of phase, Sk is the mass transfer, g is the gravity acceleration, F is the momentum exchange between phases. The above equations are solved using the properties of the fluid mixture because it has more than one fluid in a unit volume:

$$\rho = \sum \alpha_k \rho_k \quad (4)$$

Where α_k is the volume fraction of phase k in a unit volume defined by the following equation:

$$\frac{\partial \alpha_k}{\partial t} + (v_k.\nabla)\alpha_k = S_k \quad (5)$$

The CM method

In the CM method, the flow system is characterized by multiple compartments with the zoning criterion based on the velocity field of the system obtained from CFD. The procedure of building CM method includes 5 steps:

- ***Step 1.*** *Calculatingspatial velocity distribution using FLUENT*

This study used FLUENT software to calculate fluid dynamics and define spatial velocity distribution in the model corresponding to experimental conditions. The finite element method was used to solve continuous and momentum conservation equations. The model had a total of 12500 grid cells with each grid cell witha dimension of 2 cm x 2 cm x 2 cm and the standard turbulence model k – ε was used to calculate three velocity components, turbulent kinetic energy and the rate of dissipation of turbulent kinetic energy in each grid cell with the necessary convergence.

- ***Step 2***. *Zoning based on the velocity field of the system obtained from CFD*

The zoning program is built on MATLAB 2014b software based on the velocity field of the system obtained from CFD. The zoning algorithm is as follows [9, 10]:

- Initialization: Selecting the tolerance value Δv. The smaller the tolerance value Δv was, the larger the number of zones generated. At the beginning, all grid cells are free.

- Zoning creation: Selecting a free grid cell is the seed cell of the new zone. The seed cell has the maximum velocity (v_{seed}).

- Zoning development: If other free cells have velocity satisfied the condition of $|v - v_{seed}| \le \Delta v$, those cells are in the new created zone.

- Closing: If there are still existing free cells, , please return to the initialization step. Otherwise, the zoning step ends.

- ***Step 3.*** *Calculatingvolume and exchange rate between zones*

The exchange rate between zones need calculating after zoning. The exchange rate between two adjacent zones is the sum of the convective flux Q_v^{conv} and the turbulent flux Q_v^{turb}:

The convective flux Q_v^{conv} is calculated as the following equation:

$$Q_v^{conv} = \sum_{i=1}^{N} q_{iv}^{conv} = \sum_{i=1}^{N} S_i . v_i^{conv} \qquad (6)$$

Where Q_v^{conv} is the convective flux between two adjacent zones, q_{iv}^{conv} is the convective flux, S_i is the area of the interface, v_i^{conv} is the flow velocity on the surfaces constituting the interface between two adjacent cells.

The turbulent flux Q_v^{turb} is calculated as follows

$$Q_v^{turb} = \sum_{i=1}^{N} \left(\frac{\sqrt{A_i^2 + 8A_i}}{4A_i} - \frac{1}{4} \right) . q_{iv}^{conv} \qquad (7)$$

$$A_i = \frac{q_{iv}^{conv} . \Delta x_i . Sc_t . \in_i}{2 . S_i . C_\mu . k_i^2} \qquad (8)$$

In the above equations, Q_v^{turb} is the turbulent flux between two adjacent zones, C_μ is a constant of the k – ε turbulent model, k_i and ε_i are the turbulent kinetic energy and the turbulent dissipation rate of each cell, respectively, Sc_t is the turbulent Schmidt number, S_i is the area of the interface between two adjacent cells, Δx_i is the distance between the cell centers of two adjacent cells.

- ***Step 4.*** *Building CM model*

The CM model having the compartments corresponding to the basic flow zones is established using Progepi RTD 4.2.1.0 software. It is a useful tool to determine CM based on fluid dynamics characteristic of system developed by the Laboratory of Chemical Engineering (France) [2,11].

- ***Step 5.*** *Confirming the established CM model based on the tracer experiment and CFD simulation*

The established CM model was confirmed by comparing the RTD curve from the CM model to experiment in the physical model and CFD simulation.

B. Results

The simulation results of spatial velocity distribution in the model with three inlet flow rates of 3.0 L/min, 4.5 L/min and 6.0 L/min are presented in Figure 2. Visually, the model has three main velocity zones: high-velocity zone from the inlet to the outlet, medium-velocity zone and slow-velocity zone at the center of the model.

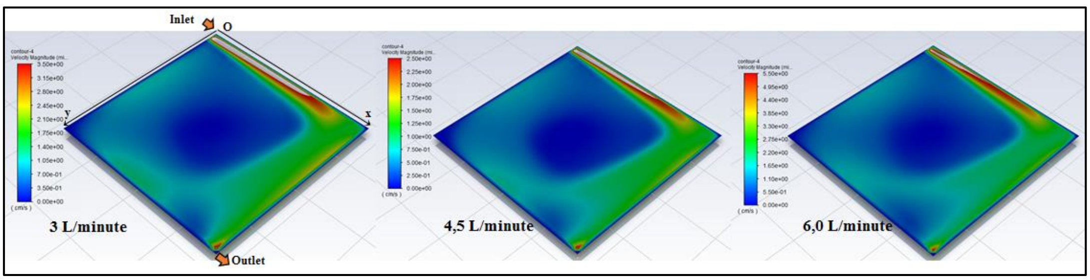

Fig. 2. Spatial velocity distribution corresponding to three inlet flow rates

Based on spatial velocity distribution results, the model was partitioned, the volume and exchange flow rate between zones were calculated by MATLAB 2014b software classified 3 main flow zones in the tank including convection flow zone – zone 1 (green), cyclic flow zone – zone 2 (yellow) and slow exchange zone – zone 3 (red) with volume and exchange flow rate between zones were presented as Figure 3 and Table I.

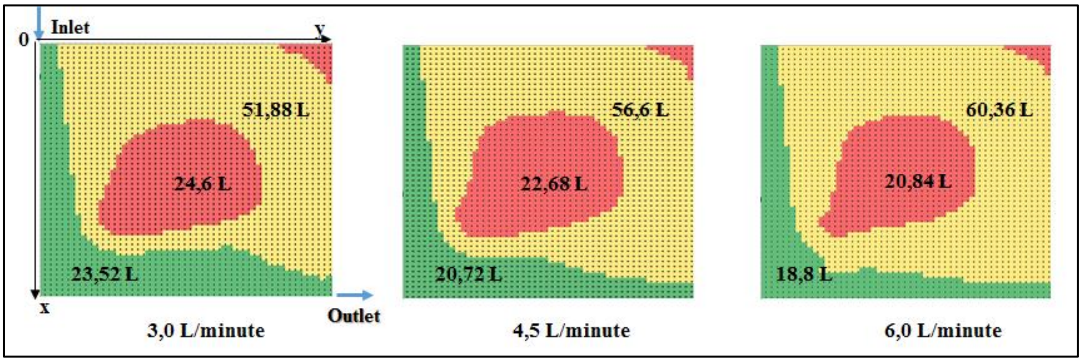

Fig. 3. Zoning is based on velocity distribution and volume of each zone

Table I. The volume and exchange flow rate between zones

Parameters	Inlet flow rate		
	3.0 L/min	**4.5 L/min**	**6.0 L/min**
Volume of zone 1 – green (L)	23.52	20.72	18.80
Volume of zone 2 – yellow (L)	51.88	56.60	60.36
Volume of zone 3 – red (L)	24.60	22.68	20.84
Exchange rate between zone 1 – 2 (L/min)	7.20	11.40	15.00
Exchange rate between zone 1 – 3 (L/min)	0.00	0.00	0.00
Exchange rate between zone 2 – 3 (L/min)	3.60	4.92	6.00

Figure 3 shows that the model exists as a circulation flow. The connection between zones is illustrated in Figure 4. Zone 1 has high-velocity, connects with zone 2 and extends from the inlet to the outlet in the direction of flow. Zone 2 has medium-velocity, interacts with zone 1 and 3 and tends to be cyclic in the system. Region 3 is a low-velocity zone that only interacts with zone 2 but not with zone 1.

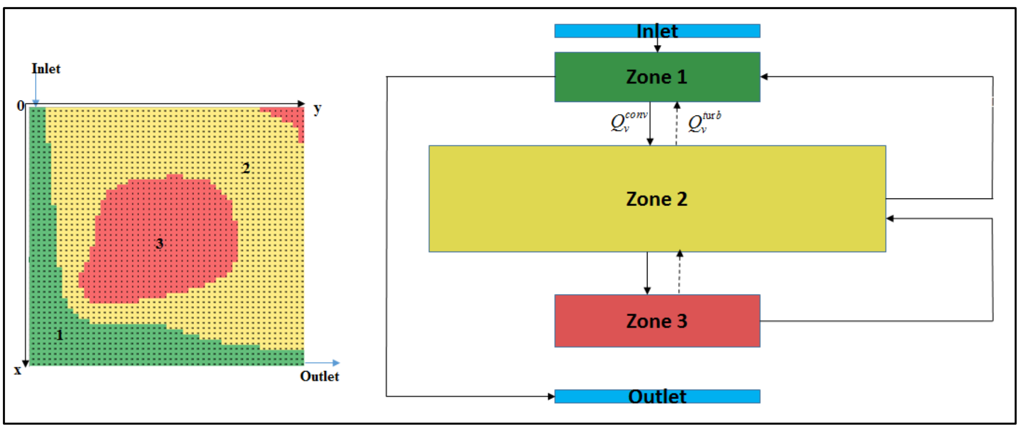

Fig. 4. The illustration of the connection between zones in the model with a flow rate of 4.5 L/min

After the information about the volume and the connection between zones was collected, the Compartmental Model was built by Progepi RTD 4.2.1.0 software. The volume and the exchange flow rate between zones were adjusted corresponding inlet flow rate.

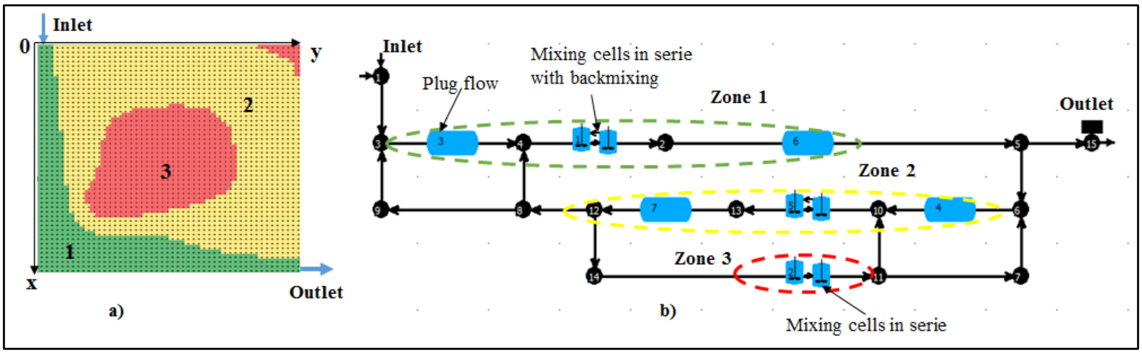

Fig. 5. Zoning system (a) and Compartmental model (b) with a flow rate of 4.5 L/min

The tracer normalized residence time distribution obtained from CM, CFD simulation and tracer experiment were compared. The result with the root-mean-square error of less than 0.11 which allows confirming the established CM model, is shown in Figure 6 and Table II.

Table II. The root-mean-square error of the tracer which normalized residence time distribution was obtained from CM, CFD simulation and tracer experiment.

RMSE	Inlet flow rate		
	3.0 L/min	**4.5 L/min**	**6.0 L/min**
CM – CFD	0.04	0.04	0.05
CM – Experiment	0.1	0.08	0.11

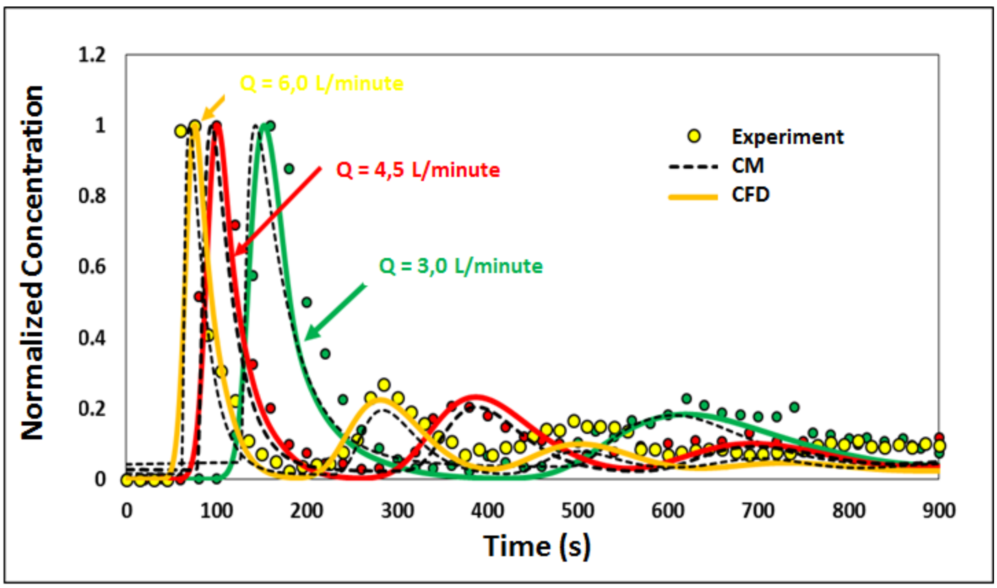

Fig. 6. The results of comparing the tracer response curves from the CM model, CFD simulation and experiment with an inlet flow rates of 3.0 L/min, 4.5 L/min and 6.0 L/min

C. Discussion

The results of CM zoning and RTD analysis show that when the tracer is injected at the inlet, the tracer moves convectively in Zone 1, partly moves to the outlet, the rest of the tracer moves to Zone 2, simultaneously diffuses into Zone 3, and then back to Zone 1. This process repeats to create circulation in the system. As a result, the tracer residence time distribution in different flow rates is multi-peak. Obviously, the first peak is influenced by tracer convection in Zone 1, while the other peak is a result of the circulation flow through Zone 2 and Zone 3.

This study investigates the correlation between flow rate and volume of zones, exchange flow rate between zones. The results show that there is a linear correlation as Figure 7. The circulation volume (Zone 2), the exchange flow rate between Zone 2-3 and Zone 2-1 increases with the increment of the inlet flow rate. Therefore, it is necessary to determine the optimal flowrate when designing the actual tank , in which the circulation zone has the largest volume and the slow exchange zone volume is as small as possible .

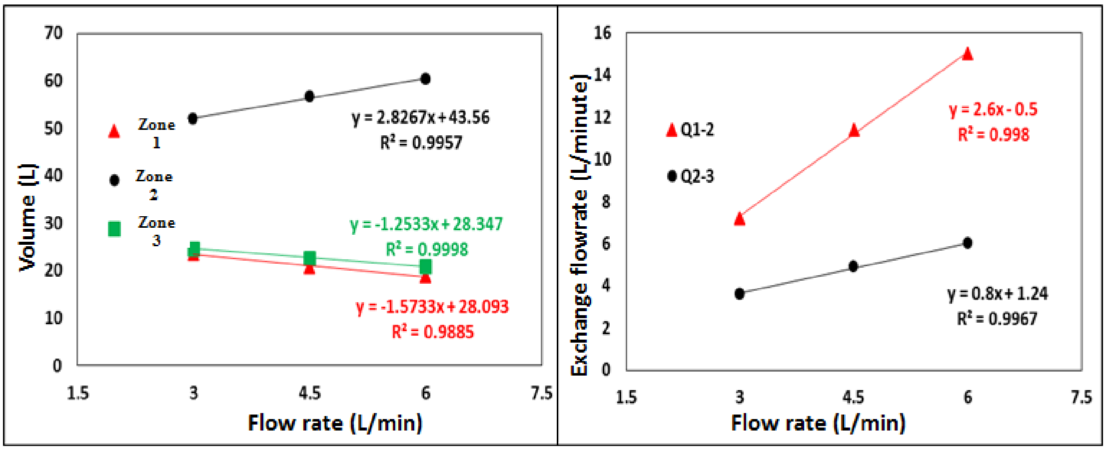

Fig. 7. The correlation between inlet flow rate and volume, exchange flow rate between regions

The research shows that the kinetic parameters of the CM are strongly dependent on the inlet flow rate in a specified tank. Therefore, the CM method can be effectively applied in non-reactive system optimization and design.

III. CONCLUSIONS

This paper presents the results of applying the CM method to analyze some basic parameters of the flow in the 2D basic non-reactive tank with the dimensions of 100 cm x 100 cm x 10 cm at different inlet flow rates (3 - 6 L/min). The results show that the obtained CM model has 3 main flow zones including the convection zone, circulation zone and slow-exchange flow zone. The results of comparing the tracer response curves from the CM model and experiment with the root-mean-square error of less than 0.11 allow confirming the established CM model.

The research results show that the volume and the exchange rate of the circulation zone are proportional to the inlet flow rate. This has important implications for optimizing the system's performance.

The obtained results in this study are the premise for further studies on the application of the CM method in stirring systems with chemical reactions. The improvement of the partitioning algorithm and the calculation of fluid dynamics needs to be optimal in the future.

REFERENCES

[1]. P.V. Danckwerts, "Continuous flow system. Distribution of Residence Times", *Chemical Engineering Sciences*, 2, 1-13, 1953.

[2]. International Atomic Energy Agency, *Radiotracer Residence Time Distribution Method for Industrial and Environmental Applications*, IAEA, Vienna, 2008.

[3]. Octave Levenspiel, *Chemical Reaction Engineering, 3rd Edition*, John Wiley & Sons, 1999.

[4]. Jérémie Haag, et al., "Modelling of Chemical Reactors: From Symtemic approach to Compartmental modelling", *International Journal of Chemical Reactors Engineering*, Vol 16, Issue 8, 1-22, 2018.

[5]. Le Moullec, et al., "Comparision of Systemic, compartmental and CFD modelling approaches: Application to the simulation of the biological reactor of wastewater treatment", *Chemical Engineering Sciences*, 65, 343-350, 2010.

[6]. Delafosse, et al., "Development of a compartmental model based on CFD simulations for description of mixing in bioreactors", *Biotechnology, Agronomi, Society and Environment*, 14, 517 - 522, 2010.

[7]. Alvarado, et al., "A compartmental model to describe hydraulics in a full scale waste stabilization pond", *Water Research*, 46, 521-530, 2012.

[8]. Carl-Fredrik Mandenius, "Bioreactors: Design, Operation and Novel Applications", *Wiley-VCH Verlag GmbH & Co. KgaA*, 2016.

[9]. Sharma, et al., "Review of CFD applications in biotechnology process", *Biotechnology Progress*, 27(6), 1497-1510, 2011.

[10]. Bezzo, et al., "A General Methodology for Hybrid multizonal/CFD Models: Part II" *Automatic Zoning Computation Chemical Engineering*, 28, 513–525, 2004.

[11]. International Atomic Energy Agency, *Radiotracer technology as applied to industry*, IAEA-TECDOC-1262, IAEA, Vienna, 2001.