Modeling of Mixing in The Liquid Phase For Bubble Column

Dr.Ali H. Jawad*

Abstract

Hydrodynamic characteristics (mixing in the liquid phase) in a bubble column with a non-Newtonian liquid phase (aqueous solutions of carboxymethylcellulose, or CMC, at different concentrations) were measured and correlated. Experiments in a 0.2-m diameter, 2.4-m-high bubble column were carried out to determine degree of mixing in the liquid phase at various gas and liquid flow rates. The axial dispersion model was used in the two operating modes, batch and continuous, and the tanks-in-series model was used just in the case of continuous mode. The axial dispersion model with closed-closed boundary conditions fit experimental data quite well and thus was used to estimate the axial dispersion coefficient. This parameter was higher in batch mode than in continuous mode, and its trend was to increase as superficial gas velocity increased.

نموذجية للخلط في للطور السائل لعمود الفقاعي

الخلاصة

الخصائص الهيدروديناميكية (الاختلاط في المرحلة السائلة) في عمود الفقاعي للسوائل النيوتينة الغير القابلة لانضغاط (carboxymethylcellulose او CMC بتراكيز مختلفة) ، تم قياسها وحسابها رياضيا اما بالنسبة لجانب العملي أجريت في 0.2 مترا وقطره و 2.4 مترا ارتفاع العمود/ فقاعة أجريت لتحديد درجة من الاختلاط في المرحلة السائلة في معدلات تدفق مختلفة من الغاز و السائل. موديل التشتت الافقي المستخدم في تشغيل اثنين من وسائط ، دفعة(Batch) ومستمرة(Continuous) ، والخزان في سلسلة(Series) استخدم نموذج فقط في حالة طريقة مستمرة. موديل التشتت الافقي مع تظام اغلاق-اغلاق في الظروف تناسب تماما مع البيانات التجريبية ، وبالتالي كان المستخدمة لتقدير معامل التشتت محوري. هذه القيم كانت أعلى في دفعة (Batch) من طريقة في طريقة مستمرة(Continuous) ، والاتجاه إلى زيادة سطحية كما زادت سرعة الغاز.

***Material Engineering Department, University of Technology/Baghdad**

Introduction

Many models can be used to describe bubble column reactors. Some aspects to take into account when it is proposed a model are the mathematical nature of the equations and the degree of complex of their solution (Deckwer, 1992).

The liquid phase mixing has an important effect on mass transfer capabilities of bubble column. Mixing in bubble columns is due to liquid circulation caused by the rise of the bubbles through liquid phase, reducing or eliminating the concentration gradient, in the system. Because of the high ratio of length to diameter, the radial gradients are often neglected compared to axial gradients (Walter and blanch, 1983).

Several mathematical models have been proposed in the literature to describe mixing based on conservation laws or simply based on empirical relations. It is common to use an injection of a tracer at the feed and then measure tracer concentrations at the exit. These collected data are analyzed using, for example, the moment's theory or the transfer function of a mathematical model that could represent the behavior of these experimental data. The disadvantage of the moments method is that moments can be quite sensitive to measurement errors at the tail of the function $E(t)$, (Ostergaard and Michelsen, 1969). In the case of bubble columns, mixing or back mixing of each phase (degree of turbulence) is due to flow or movement of the fluids through the column.

The rising bubbles cause turbulent stochastic diffusion processes and large-scale steady circulation flows (Riquarts, 1981).

Theory

Some of the mathematical models found in literature are presented in this section.Models as perfect mixing (CSTR), partial mixing (ADM) and tubular flow (PFR) may be found in gas and liquid phases operations (Deckwer, 1992).

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1-Continuous, Stirred-Tank Reactor (CSTR)

The continuous-stirred-tank reactor is a perfectly mixed tank with steady-state inlet and exit flow streams. Therefore, the concentration in the reactor, c(t), is only function of time. The expression obtained from a mass balance for an impulse of tracer is (Froment and Bischoff, 1979):

$$c(t) = \frac{N_o}{V} \exp\left(-t/\tau\right) \quad \dots\dots (1)$$

where N_o is the mass of tracer added initially as an impulse, V is the fluid volume in the tank (considered constant), t is the time and, $c(t)$ is the exit concentration of the tracer, which is the same as the concentration inside the reactor at the any particular time, and τ is the residence time defined as the relation between reactor volume, V and volumetric flow rate of the feed, Q.

The Eq. (1) can be expressed in terms of the age distribution function as:

$$E(t) = \frac{1}{\tau} \exp(-t/\tau) \quad \dots\dots(2)$$

For a step injection, the solution of the tracer mass balance, for a zero initial concentration in the system is:

$$c(t) = c_o \left[1 - \exp\left(-\frac{t}{\tau}\right)\right]$$

$$\dots (3)$$

Where c_o is the input concentration for t ≥ 0. When a step injection is used, the cumulative function F(t) is used instead of the distribution function E(t), and the resulting expression for a continuous stirred tank is:

$$F(t) = 1 - \exp(-t/\tau) \quad \dots\dots (4)$$

2 Plug-Flow Reactors (PFR)

In an ideal, plug-flow reactor (considered tubular), the fluid is assumed to travel through the system at uniform velocity and in straight streamlines; therefore there are no radial concentration gradients. Under these conditions, the concentration in the reactor, c(t,z), is a function of time and axial position in the reactor. A tracer mass balance on a differential element of fluid inside the reactor, taking into account as initial condition,

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c(0,z) = 0 in the case of an impulse injection, gives the final expression:

$$c(t, L) = N_o \delta(t - \tau) \quad \text{......} (5)$$

Where L is the exit point (i.e., the length of the reactor).

In case of a step injection, the exit concentration will be given by:

$$c(t, L) = c_o H(t) \quad \text{........} (6)$$

Where c_o is the maximum concentration that corresponds to feed concentration of tracer and H(t) is the Heaviside function that gives the step form of the obtained answer.

3 Tank-in-Series Model

This model is a modified CSTR model, where a mass balance of the tracer is made in a generic tank "n" of a series of identical tanks that constitute the system. When the resulting equation from the mass balance is manipulated and the initial and the boundary conditions are applied, the final expression is obtained for each form of tracer injection:

For step injection tests (Levenspiel, 1999):

$$F(t) = 1 - \exp\left(-N\frac{t}{\tau}\right) \sum_{n=1}^{N} \frac{(nt/\tau)^{n-1}}{\Gamma(n)}$$

$$\dots(7)$$

Where N is the number of tanks in the system.

For impulse injection tests (Froment and Bischoff, 1979):

$$E(t) = \frac{N^N}{\tau^N} \frac{t^{N-1} \exp(-Nt/\tau)}{\Gamma(N)}$$

$$\dots\dots (8)$$

The plots of equation (7) and (8) are presented by Levenspiel (1999) and they are shown in figures (1) and (2) respectively.

4 The dispersion model

The dispersion model is used to describe tubular non-ideal reactors. It considers that there is a Fickian dispersion of matter, i.e., described by a constitutive equation similar to the Fick's law of diffusion. The expression of the model results from a -tracer mass balance considered that is injected at the feed of the system. The model takes into account two effects: convection, which represents the bulk flow, and dispersion, which results from the molecular and turbulent

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diffusion. There are two types of contributions to dispersion: radial and axial (Riquarts, 1981). The radial effect is negligible in comparison to axial effect when the aspect ratio L/D is greater than 4. The model is then called axial-dispersion model. In this case, the concentration c(t,z) is a function of time and axial position in the reactor, and it is described by the following expression:

$$\frac{\partial c}{\partial t} = D_z \frac{D^2}{\partial z^2} - u \frac{\partial c}{\partial z} \quad …..(9)$$

Where c is the concentration of the trace, u the fluid velocity, D_z the axial coordinate, and t the time. This equation can be written in dimensionless from:

$$\frac{\delta c^*}{\delta \theta} = \frac{1}{Bo_z} \frac{\delta^2 c^*}{\delta z^{*2}} - \frac{\delta c^*}{\delta z^*} \quad …..(10)$$

Where the new variables are defined as:

$$c^* = \frac{c}{c_o} \qquad ……..(11)$$

$$\theta = \frac{t\,u}{L} \qquad ……..(12)$$

$$z^* = \frac{z}{L} \qquad ……..(13)$$

$$Bo_z = \frac{u\,L}{D_z} \qquad ……..(14)$$

Where L is the characteristic length (in this case, the length of the reactor) and Bo_z is the bodenstein number in the axial direction. For simplicity, the Bodenstein number will be expressed as Bo instead Bo_z.

The Bodenstein number is the ratio of transport rate by convection to the transport rate by dispersion. The inverse of the Bodenstein number is called dispersion number.

The solution to the differential equation on the boundary conditions are needed, one at z=o the injection point, and one at z=l the point at which the response is measured each condition depends on whether there is dispersion before the injection (z=0) and after the response point (z=L) If there is dispersion on both sides of any these points, it is an open boundary; otherwise it is called a closed boundary. Combinations are possible for a reactor open-open, open –closed, closed –open and closed –closed boundaries result in a mathematical

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discontinuity in concentration by a discontinuity in dispersion.

When open –open boundary conditions are used, they can be written as:

$$c^*(-\infty, 0) = finite$$

$$c^*(\infty, 0) = finite$$

The corresponding analytical solution of equation (10) at z^*=1 is (Froment and Bischoff, 1979):

$$c^* = \frac{c}{c_0} = \frac{1}{2}\sqrt{\frac{-Bo}{\pi\theta}} exp\left(\frac{-Bo(1-\theta)^2}{4\theta}\right)$$

$$\dots\dots(15)$$

And the response curves for an impulse injection is shown in figure (3)

On the other hand, the following closed-closed boundary conditions, normally called Danckwerts boundary conditions, may be used

$$z^* = 0, -\frac{1}{B_0}\frac{\partial c^*}{\partial z^*}\bigg|_{0+} + C^*\big|_{0+} = 1$$

$$z^* = 1, \frac{\partial c^*}{\partial z^*}\bigg|_{1+} = 0$$

and the corresponding analytical solution at $z^* = 1$ is (Froment and Bischoff, 1979):

$$C^* = \frac{C}{C_0} = 4\varepsilon_{n=0}^{\infty}\frac{\delta_n(B_0 \sin\delta_n + 2\delta_n \cos\delta_n)}{B_0^2 + 4B_0 + 4\delta_n}\ exp\left[\frac{B_0}{2} - \frac{(B_0^2 + 4\delta_n^2)}{4B_0}\theta\right]$$

$$\dots\dots(16)$$

Where the Eigen values δn of this series solution are the roots of the following equation:

$$\cot\delta_n = \frac{1}{2}\left(\frac{2\delta_n}{B_0} - \frac{B_0}{2\delta_n}\right).. (17)$$

Figure (4) shows the response curves for impulse injection of tracer in these boundary conditions.

On the other hand, when there are at least two phases in the system, the equation (9) needs to be modified as follows:

$$\frac{\delta c}{\delta t} = -\frac{u_l}{1-\varepsilon_G}\frac{\delta c}{\delta z} + D_Z\ \frac{\delta_c^2}{\delta_Z^2}$$

$$\dots\dots(18)$$

Where c is the tracer concentration in the Liquid phase.

When figures 2 through 4 are compared, the trends of figures 2 and 4 are similar because both models consider that the mixing is inside the system and in enter and exit zones there are not mixing.

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Many researchers have studied the back mixing in bubble columns showing the dependence on the column diameter, gas distributor, and gas velocity, but the influence of the velocity and properties of the liquid phase on the mixing of the same phase, especially when the liquid phase is non-Newtonian is not known. Some experimental and mathematical works are described below.

Ohki and Inoue (1970) determined longitudinal dispersion coefficient in batch bubble column with 0.04, 0.08 and 0.16 m diameters. They stated that the one - dimensional diffusion model is valid when the distance between injection tracer and measuring points are sufficiently long. They use the one-dimensional diffusion model resulting from Eq. (9) when the convective term is neglected:

$$\frac{\delta_c}{\delta_t} = D_z \frac{\delta_c^2}{\delta_z^2} \qquad ...... (19)$$

The boundary conditions used by authors are:

$$\frac{\delta_c}{\delta_z} = 0 \ at \ z = 0 \ and \ z = L$$

While the initial condition is:

$$c(z, 0) = \begin{cases} c_o \ for \ 0 \leq z \leq \beta \\ 0 \ for \ z \geq \beta \end{cases}$$

Where p is a height filled with tracer. The solution to the differential equation is:

$$\frac{c(t,z)}{c_E} = 1 + \frac{2L}{\pi\beta} \sum_{N=1}^{\infty} \left\{ \frac{1}{n} sin\left(\frac{n\pi}{L}\beta\right) cos\left(\frac{n\pi}{L}z\right) exp\left[-\left(\frac{n\pi}{L}\right)^2 D_z t\right] \right\}$$

$$....(20)$$

Where C_E is related through the expression:

$$C_E L = C_o \beta \qquad ...... (21)$$

The researchers determined the dispersion coefficient from the expression:

$$D_Z = \left(\frac{L}{\pi}\right)^2 \frac{\Delta\theta}{\Delta t} \qquad .... (22)$$

D_Z is obtained from the fitting of Eq. (20) to experimental data, where the authors plotted c/ c_E as a function of $\pi D_Z \ t/L$ and took $\Delta\theta$ as the distance in the abscise marked when the value of c/ c_E = 0.7 and c/ c_E = 0.3 intercept the curve obtained from the model for a z/ L. The authors correlated the data and proposed two

1998

expressions that depend on prevailing flow regime:

Homogeneous regime:

$$D = 0.3\, d_c^2\, u_G^{12} + 170 d_o$$

……. (23)

Slug flow regime:

$$D = \frac{14 d_c}{(1 - \varepsilon_G)^2}$$

…. (24)

They got agreement of the proposed expression with experimental data.

Experimental

The experimental setup is shown in Figure (5).

The main components are: a column made up by two cylindrical sections of Plexiglas of 0.20 m of inner diameter and an entrance

cone, a self-metering pump, two plastic feed tanks, filter devices, a rotameter to measure the gas flow rate, and a pressure transducer connected to a data acquisition system.

Two types of experiments were carried out: continuous (the gas and liquid phases are fed continuously in the column in the bottom of the column, flowing in this case in ascendant and

cocurrent mode) and semicontinuos modes (the gas phase flow in ascendant mode while the liquid phase was charged to the column at the beginning of the operation). First the CMC solution was prepared in one of the feed tanks. Runs were carried out at various gas and liquid superficial velocities and at various concentrations of CMC.

Aqueous solutions of carboxymethylcellulose (provided by Noviant) at different concentrations, which are known to exhibit non-Newtonian behavior, were used in the experiments.

exit concentrations of tracer in the residence time distribution experiments were analyzed through the axial dispersion model and tank-in-series model using the moment theory and direct fit of the experimental data to the model. As a result of this procedure, the number of tanks in series, Bodenstein number and axial dispersion coefficient in the liquid phase were found, taking into account the multiphase system used in this case

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(gas and liquid phases involved in the experiments). Axial dispersion coefficient data were correlated for each flow regime as a function of superficial velocities of gas and liquid phases, and rheological parameters of the power-law model.

Results and discussion

This section. Additionally, the fit of experimental data by a proposed correlation through the minimization of the sum of squares of errors using a Mathcad @ subroutine is presented, together with the best estimate of the parameter and the moments calculated from the parameter. Figure (6) shows there is not a significant difference in the exit-tracer concentration between the two radial positions; therefore, it is reasonable to consider only the effect of axial position in the dispersion model.

The mixing in the liquid phase was studied considering the operation mode. In each case (batch and continuous mode), experimental data and the equation of the model considered could fit these data were

plotted. The parameter of the proposed model was adjusted to find its best value that permitted the best fit. This procedure was developed through Mathcad® software and its minimization technique.

In the case of batch mode, the programmed expression was Eq. (20) and the results of this model shows that it fitted quite well experimental data as it is observed in Figure (7) for tap water. Similar plots are shown in Figures (8) and (9) for 0.20 and 0.40% CMC solutions.

In continuous mode, Eq. (8) for the tanks-in-series model and Eq. (15) for the axial dispersion model with boundary conditions open-open were programmed in Mathcad®.

Figure (10) shows the experimental data and the models tested for tap water. It is observed that the axial dispersion model (ADM) with open-open boundary conditions does not fit the experimental data. Figures (11) and (12) show results for 0.20 and 0.40% CMC solutions that were similar to those obtained with tap

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water. These results were similar at the other gas and liquid superficial velocities considered

Conclusions

In the bubble column, no changes in the concentration curves at the same operating conditions were found at different radial positions.

The dispersion model for semi continuous mode fit quite well experimental data and tanks-in-series model fit well experimental data for continuous mode. The calculations of the axial dispersion coefficient from the model with closed-closed boundary conditions showed consistency in the expressions of the three moments derived for this model. The axial dispersion model with open-open boundary conditions did not fit experimental data.

Axial dispersion coefficient exhibited higher values in the batch mode than in continuous mode.

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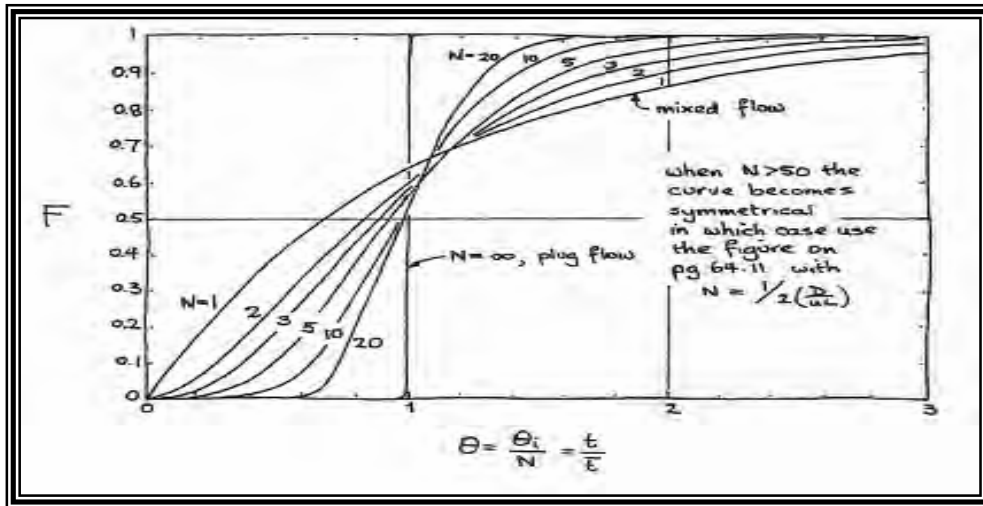
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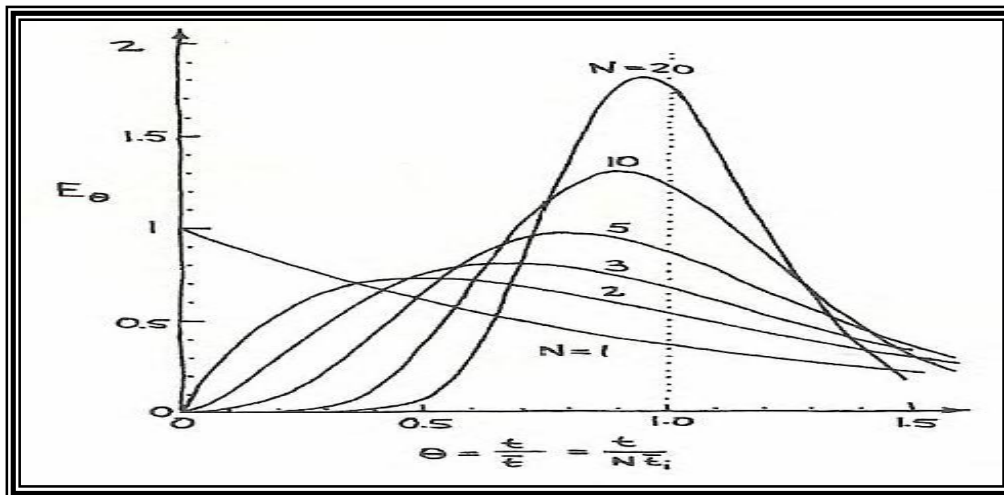Modeling of Mixing in The Liquid

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Figure (1) Response for a step injection of tracer in

the tanks-in-series model (Levenspiel, 1999)

Figure (2) Response for an impulse injection of tracer in
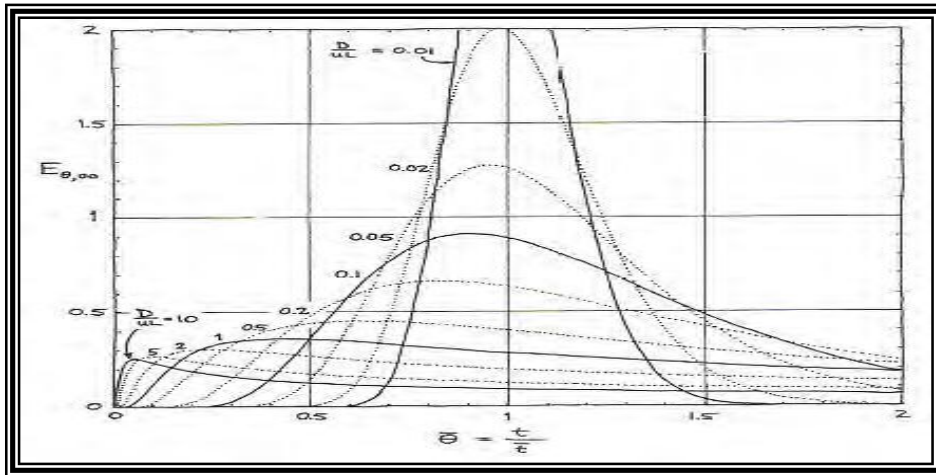
the tanks-in-series model (Levenspiel, 1999)

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Figure (3) Response curves for an impulse injection of tracer in the ADM model with Open-open boundary conditions (Levenspiel, 1999)
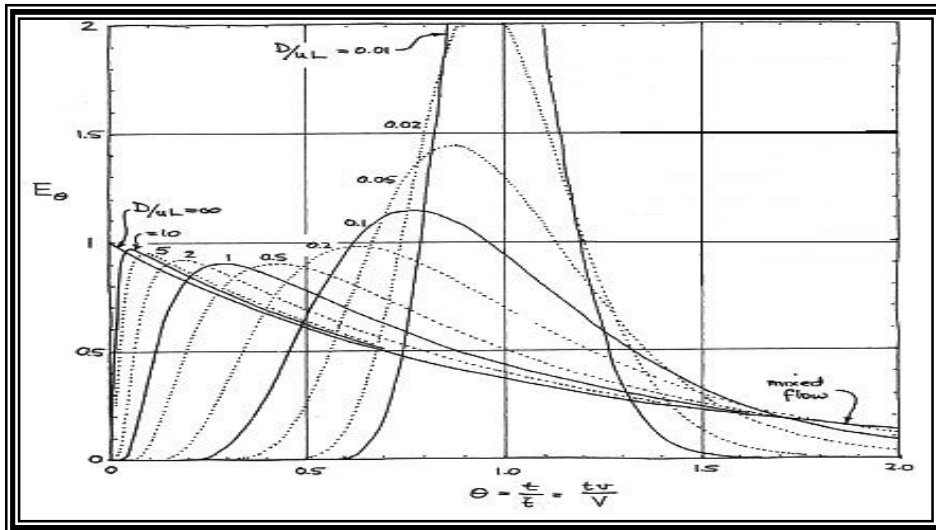
Figure (4) Response curves for an impulse injection of tracer in the ADM model with closed - closed boundary conditions (Levenspiel, 1999)
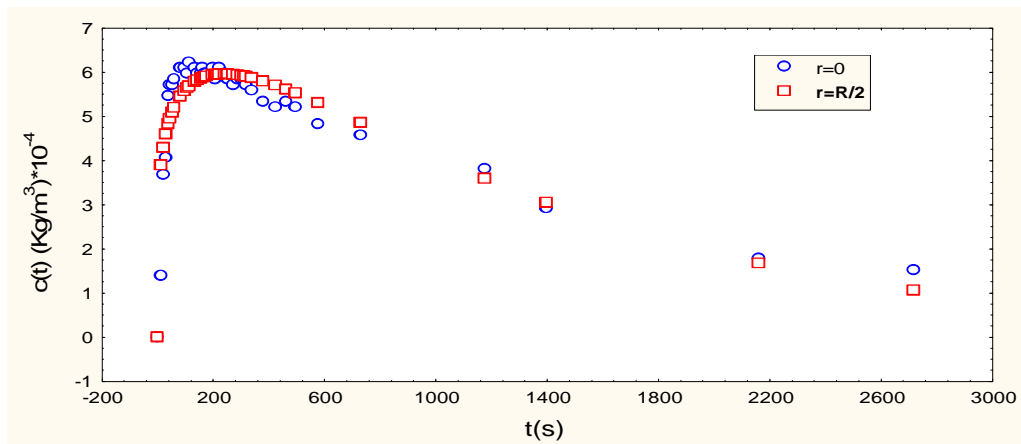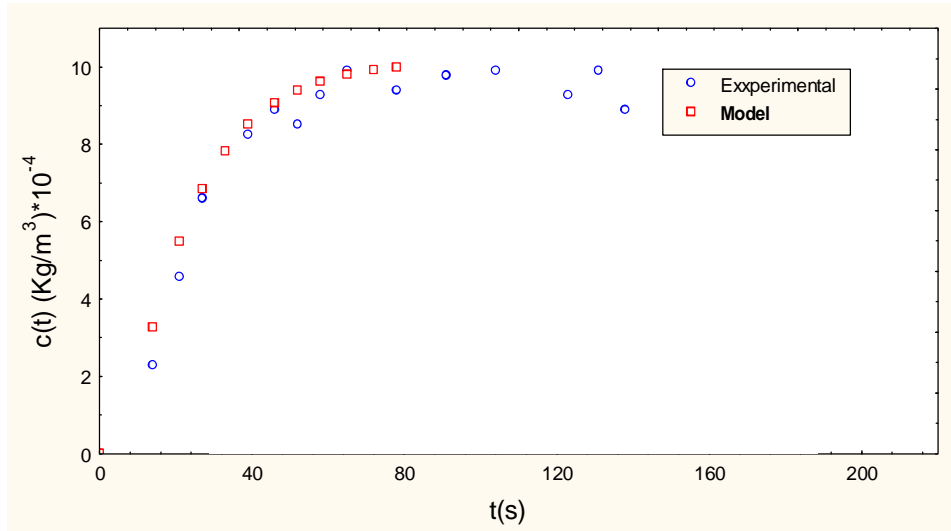
2003

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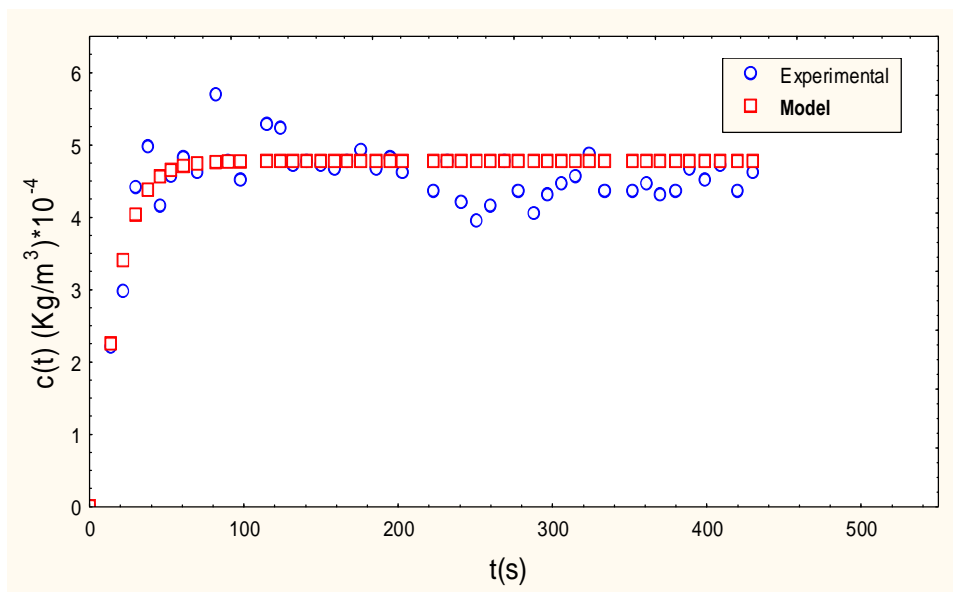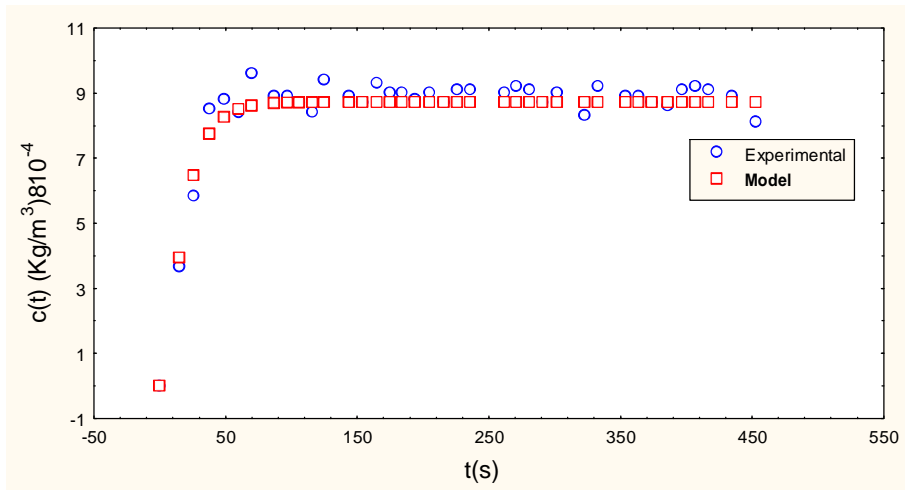
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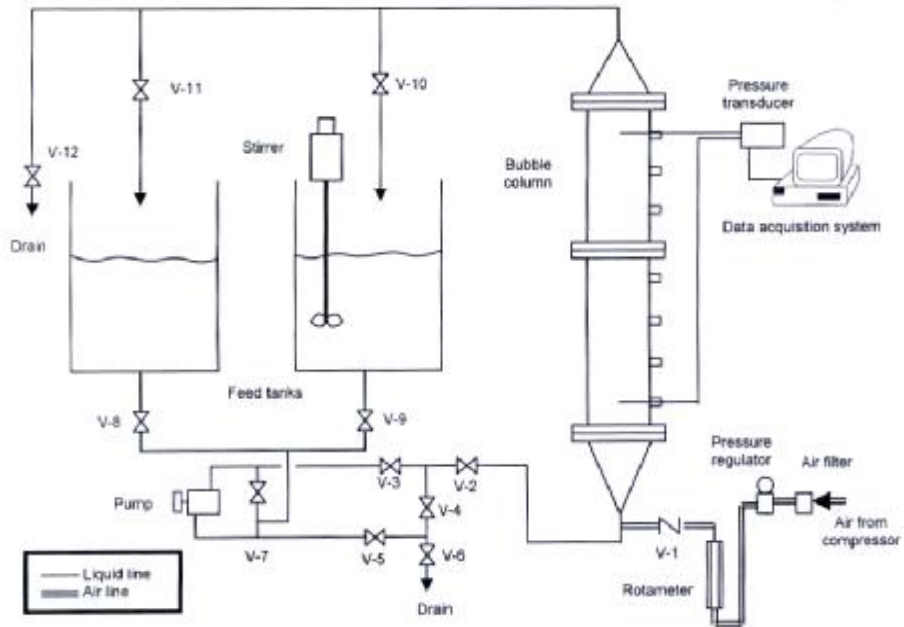
Figure (5) Experimental setup

Figure (6) Exit-tracer concentration for tap water in continuous mode
(u_G=0.0112 m/s and u_L=0.0017 m/s) at two radial positions

2004

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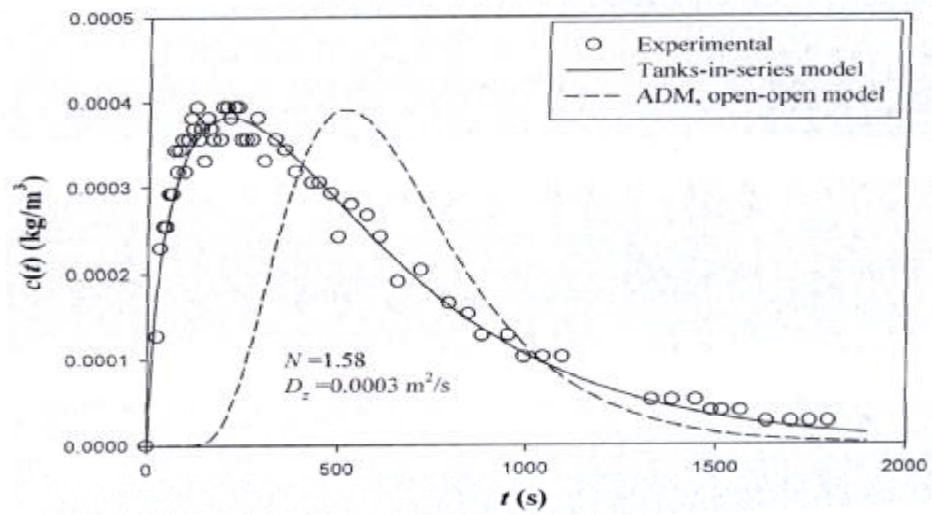
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Figure (7). Exit-tracer concentration for tap water in batch

mode (u_G=0.0083m/s and u_L=0 m/s)

Figure (8) Exit-tracer concentration for 0.20% CMC

solution in batch mode (u_G=0.0308m/s and u_L=0 m/s)

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Figure (9). Exit-tracer concentration for 0.40% CMC

solution in batch mode (u_G=0.462m/s and u_L=0 m/s)

Figure (10). Exit concentration of an impulse of tracer for tap

water at continuous mode (u_G=0.0010 m/s and u_L=0.0025 m/s)

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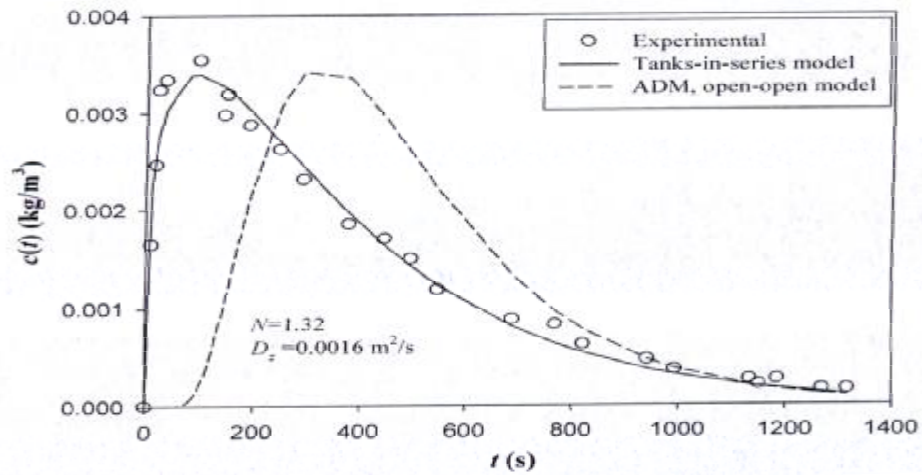
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Figure (11). Exit concentration of an impulse of tracer for 0.20% of CMC

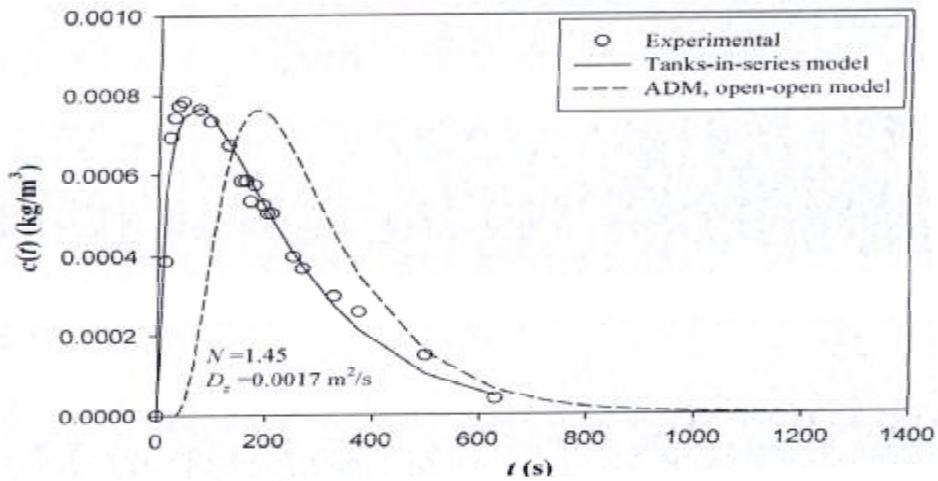**solution at continuous mode (u_G=0.0462m/s and u_L=0.0045 m/s)**

Figure (12). Exit concentration of an impulse of tracer for 0.40% of CMC solution at

continuous mode (u_G=0.0462m/s and u_L=0.0045 m/s)

2007