FINITE DIFFERENCE METHOD FOR SOLVING THE DISPERSION EQUATION IN OPEN CHANNELS

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Abstract

One dimensional advection-diffusion equation is numerically solved by using finite difference method that may be simulated to describe transport of a pollutant in open channel. A generalized Newton Raphson procedure is used to solve the system of equations. The validity of the numerical model is obtained by comparing the experimental results and numerical solution under proper initial and boundary conditions. The spatial variation of concentrations is also compared with the results of experimental measurement. The application of the model revealed good agreement and convincing between experimental and numerical results.

Keywords: Dispersion equation, open channel, finite difference, one dimensional flow, pollution.

طريقة الفروق المحدودة لحل معادلة التشتت في القنوات المفتوحة

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الخلاصة

هذا البحث يتناول حل معادلة الانتشار-التشتت عدديا باستخدام طريقة الفروق المحدودة والتي تقوم بوصف انتقال الملوث في القناة المفتوحة. استخدمت طريقة نيوتن-رفسن لحل نظام المعادلات المتكونة في المحددات. لبيان صحة تطبيق هذا الموديل الرياضي اجريت مقارنة بين النتائج المختبرية مع الحل العددي تحت شروط وقيم ابتدائية معينة وكذلك اجريت مقارنة بين تغيرات التراكيز المنتشرة مع المسافة الطولية للقناة المختبرية والحل العددي. يظهر من تطبيق الموديل الرياضي بان هناك تقارب واتفاق بين النتائج المختبرية والعددية.

List of Symbols

C : Concentration (mg/L)

u : Instantaneous velocity in the x-direction (m/s).

D_x : coefficient of turbulent diffusion (m^2/s)

q : Weighting factor.

Δt : time increment between j and j+1 (sec.).

Δx : Distance increment between I and i+1 (m).

BOD: Biochemical Oxygen Demand.

D.O : Dissolved Oxygen

Introduction

Rivers have traditionally been used for the disposal of domestic and industrial waste waters. In many cases, this has caused undesirable changes to the aquatic flora and fauna. The majority of these changes have been brought about by the discharge of Biochemical Oxygen Demand (BOD) resulting in the lowering in the concentration of the Dissolved Oxygen (DO) in the receiving water. Pollution of rivers and estuaries is also frequently caused by the discharge of toxic substances, which may break down due to chemical or bacterial action (non-conservative) or which may be resistant to break down (conservative) and other problems may arise due to the discharge of inorganic nutrients causing excessive algal growth.(Adrian, et al., 1994)

In all of these situations it is important to be able to relate the rate of discharge of the pollutant to resulting concentration pattern in the receiving water. Various methods have been devised for calculating the pattern beginning with the classic work on BOD/DO models. This laid the basis for modeling the chemical kinetics of break down. Subsequent work has concentrated on the hydrodynamic aspects- advection and diffusion along with work on stochastic and statistical models and refinement of the kinetic models (Barton, 1983).

In this paper, the mathematical model of finite difference method for solution dispersion equation is developed.

The Convective Diffusion Equation

To drive the equation of convective diffusion, consider an element volume is fixed in a fluid medium (Thongmoon, et al., 2006). The flux of material into the element across plane is cu dy dz where u is the instantaneous velocity in the x direction and c is the concentration of the tracer injected. The net change in mass of material in the element from the flux in the x direction is

$-\frac{\partial}{\partial x}(cu\,dx\,dy\,dz)$. Equating the time rate of change of mass in the element with the rate of change due to the flux in each of three coordinate directions gives:

$$\frac{\partial c}{\partial t}+\frac{\partial cu}{\partial x}+\frac{\partial cv}{\partial y}+\frac{\partial cw}{\partial z}=0 \qquad \text{……..(1)}$$

For simplicity, Eq. (1) may be written in one dimensional form as:

$$\frac{\partial c}{\partial t}+\frac{\partial cu}{\partial x}=0 \qquad \text{……..…...……(2)}$$

If a tracer slug is injected at a point in a turbulent flow it will be subjected to two distinct processes (a) it will be swept along (advected) with a velocity comparable to that of the flow, (b) it will be mixed (diffused) due to turbulence, so that the tracer becomes more dilute, but its sphere of influence expands.

A turbulent flow may be conceived as consisting of two constituents, namely a time- averaged velocity, $u_{av,}$ and a fluctuating velocity u_f so that

$$v = u_{av} + u_f \qquad \text{……...(3)}$$

The concentration of the tracer in turbulent flow may be split into the two component (time average c_{av} and fluctuating c_f so that

$$c = c_{av} + c_f \qquad \text{……..(4)}$$

The equations (3) and (4) can be substituted into equation (2) and each term averaged to give:

$$\frac{\partial}{\partial t}(c_{av}+c_f)+\frac{\partial}{\partial x}(c_{av}+c_f).(u_{av}+u_f)_{av}=0 \qquad \text{……(5)}$$

The differentials of products may be expanded giving

$$\frac{\partial c_{av}}{\partial t}+u_{av}\frac{\partial c_{av}}{\partial x}+c_{av}\frac{\partial u_{av}}{\partial x}+\frac{\partial}{\partial x}(u_f c_f)_{av}=0 \qquad \text{……(6)}$$

The form of $\frac{\partial u_{av}}{\partial x} = 0$ in equation (6) is the continuity equation.

Equation (6) simplifies to

$$\frac{\partial c_{av}}{\partial t} + u_{av}\frac{\partial c_{av}}{\partial x} + \frac{\partial}{\partial x}(u_f c_f)_{av} = 0 \qquad \text{…….(7)}$$

The cross product terms such as $u_f\, c_f$ represent the net convection of mass due to the turbulent fluctuations and with Fick's Law of molecular diffution they can be represented by an equivalent diffusive mass transport system in which the mass flux is proportional to the mean concentration gradient and the flux is in the direction of the mean concentration gradient. Hence

$$(u_f c_f) = -D_x \frac{\partial c_{av}}{\partial x} \qquad \text{……(8)}$$

Where D_x is coefficient of turbulent diffusion. Equation (7) can be rewriting omitting the time average subscripts as

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} - \frac{\partial}{\partial x}(D_x \frac{\partial c}{\partial x}) = 0 \qquad \text{…….(9)}$$

Equation (9) is the one dimensional convective diffusion equation. Values for the turbulent diffusion coefficient must be obtained from tracer measurements or by curve fitting exercise.

Numerical Solution of Advection diffusion Equation

A typical implicit approximation method (Preissmann Scheme) approximates derivatives in the Equation (9), leading to the following finite difference at node I:

$$\frac{1}{2\Delta t}(c_{i+1}^{j+1} + c_i^{j+1} - c_{i+1}^{j} - c_i^{j}) + u\left[\frac{q}{\Delta x}(c_{i+1}^{j+1} - c_i^{j+1}) + \frac{1-q}{\Delta x}(c_{i+1}^{j} - c_i^{j})\right] - \frac{D_x}{2\Delta x^2}\left[c_{i+1}^{j+1} - 2c_i^{j+1} + c_{i-1}^{j+1} + c_{i+1}^{j} - 2c_i^{j} + c_{i-1}^{j}\right] = 0 \qquad \text{……. (10)}$$

Where q is weighting factor , Δt =time increment between j and j+1 and Δx = distance increment between i and i+1 (Young,and Wallis.,1993, and Valentine and Word, 1979)

Equation (10) is nonlinear with respect to the three unknown concentrations , c, at time j+1. However, one unknown is common for any two neighboring rectangular grid. Consequently, the (N-1) pairs of equations, in which N is the number of computational nodes in the channel, contains 2N unknown. two additional supplied by the boundary condition make this system of equations mathematically determinable. One boundary condition is specified at each end of the channel. A concentration is assumed at the inlet and outlet

$$c_1^{j+1} = c_0 \qquad \text{…….. (11)}$$

$$c_N^{j+1} = c_L \qquad \text{……..(12)}$$

Equations (10) , (11) and (12) are solved by using generalized Newton Raphson iteration method. Computer program in quick basic is developed for numerical solution.A schematic of algorithm program for the model is presented in **Figure 2**.(Gubashi, 2000).

Solution of Finite Difference Equation

To illustrate the procedures that estimated to find a new unknown concentration at time j+1, it be assumed initial values of variables c are introduced into equations 10, 11, and 12, the right hand sides become the residuals. Let the residuals be denoted by R_i^K , and the system of equations may be represented in a genral way by

$$\begin{aligned} &f_1(c_1, c_o) = R_1^K \\ &f_2(c_1, c_2) = R_2^K \\ &f_3(c_2, c_3) = R_3^K \\ &\cdots\cdots\cdots\cdots \\ &\cdots\cdots\cdots\cdots \\ &f_N(c_N, c_{N-1}) = R_N^K \end{aligned} \qquad \text{……. (13)}$$

In which f_1 is the specified concentration at the inlet given by equation (11), f_2 is the diffusion equation (10) at i , f_3 is the equation (10) at cell i+1 and f_N is the boundary condition at outlet.

Improved estimates are obtained by using Newton- Raphson recurrence formula for each time which results in the following set of equations:

$$\begin{aligned} &\frac{\partial f_1}{\partial c_1} dc_1 = -R_1^K \\ &\frac{\partial f_2}{\partial c_1} dc_1 + \frac{\partial f_2}{\partial c_2} dc_2 = -R_2^K \\ &\frac{\partial f_3}{\partial c_2} dc_2 + \frac{\partial f_3}{\partial c_3} dc_3 = -R_3^K \\ &\cdots\cdots\cdots\cdots\cdots\cdots \\ &\cdots\cdots\cdots\cdots\cdots\cdots \\ &\frac{\partial f_N}{\partial fc_N} dc_N = -R_N^K \end{aligned} \qquad \text{…… (14)}$$

In which dc_i is the concentration correction for cell i for k_{th} iteration cycle. Equation (14) can be written as

$$\mathbf{A\ X\ dA = -B} \qquad \text{…….. (15)}$$

In which **A** is a matrix of coefficients**, dA** a column vector of corrections and **B** is a column vector of residuals from equations 10 to 12. The matrix **A** is banded about the center diagonal as shown in the following form:

$$\begin{bmatrix} \frac{\partial f_1}{\partial c_1} & & & & \\ \frac{\partial f_2}{\partial c_1} & \frac{\partial f_2}{\partial c_2} & & & \\ & \frac{\partial f_3}{\partial c_2} & \frac{\partial f_3}{\partial c_3} & & \\ & & \cdots\cdots\cdots & & \\ & & & \cdots\cdots\cdots & \\ & & & & \frac{\partial f_N}{\partial c_N} \end{bmatrix} \quad \ldots\ldots\ldots \quad (16)$$

Band solvers Gaussian elimination method can be employed to provide the values of dc_i. Then, the values of the variables of iteration cycle k+1 are obtained by the following form:

$$c_i^{k+1} = c_i^k + dc_i \qquad \ldots\ldots\ldots\ldots \quad (17)$$

The computations can be terminated whenever the difference between the values of variable c in two consecutive iteration cycles falls below tolerance value.

Experimental Studies

Laboratory experiments were carried out in a rectangular flume with dimensions, 20 m long, 0.9 m wide, and it constructed of steel structure with Perspex panels walls of (1.2 cm), and the effective wide is 0.85m. Water is pumped by an electrically driven centrifugal provide a maximum flow of ($13\,L/s$) to the flume from the laboratory sump tank ($3.5m^3$) and four small pumps with ($0.5L/s$). The discharge is regulated by a 4 inch gate-valve. The entrance to the flume is filled with filter material (multi short lengths of mesh wire 12mm) which served to break up any large eddies in the flow, water from the main sump under the laboratory flume is pumped at a fixed rate up to the header tank and entered large tanks at the end of the flume .

A bed of plastic covered with 12mm broken gravel with a slope of 1:1416 is laid in the flume, the slope was chosen as representative of a natural open channel flow with the aspect ratios that could be obtained in the flume, as shown in **Plate(1) and Figure 1**. This flume is at hydraulic laboratory of the Engineering College at AL-Mustansiriyah University (Gubashi, et al., 2007).

In these experiments Pure KCl salt has been used as a tracer in water. Twenty five runs are performed with different flow rate that varied between 0.5 and 12.5 L/s. Results of concentration-time profiles of KCL is shown in**Figure 3**.

Results and Discussion

Results of proposed numerical model are compared with that of laboratory experiments to calibrate and validate the proposed mathematical model. **Figure 4** shows experimental and numerical concentration-time profiles. The temporal and spatial of concentration in present model and experimental are plotted in **Figures 5 and 6**. As shown in the figures the agreement between measured and numerical concentration profiles. The statistical correlation coefficient is presented in all figures and shows greater than 90%.

Conclusions

A numerical model solution is used for determining the temporal and spatial variation of pollution concentration in open channel. The developed model is applied to a hypothetical flume conditions. The validity of the present model is shown by comparing with the results of the experimental solution under certain boundary and initial assumed conditions. The comparison presented good agreement between them and coefficients of square correlation, R^2 are greater than ninety percent as shown in figures.

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Plate (1) General view of the flume.

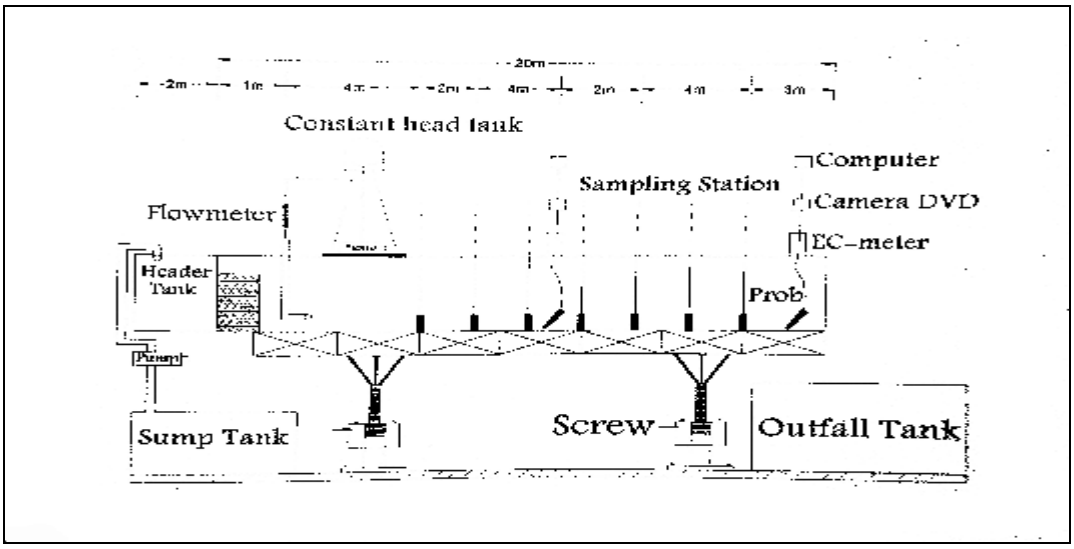

Figure 1 Layout diagram of laboratory flume

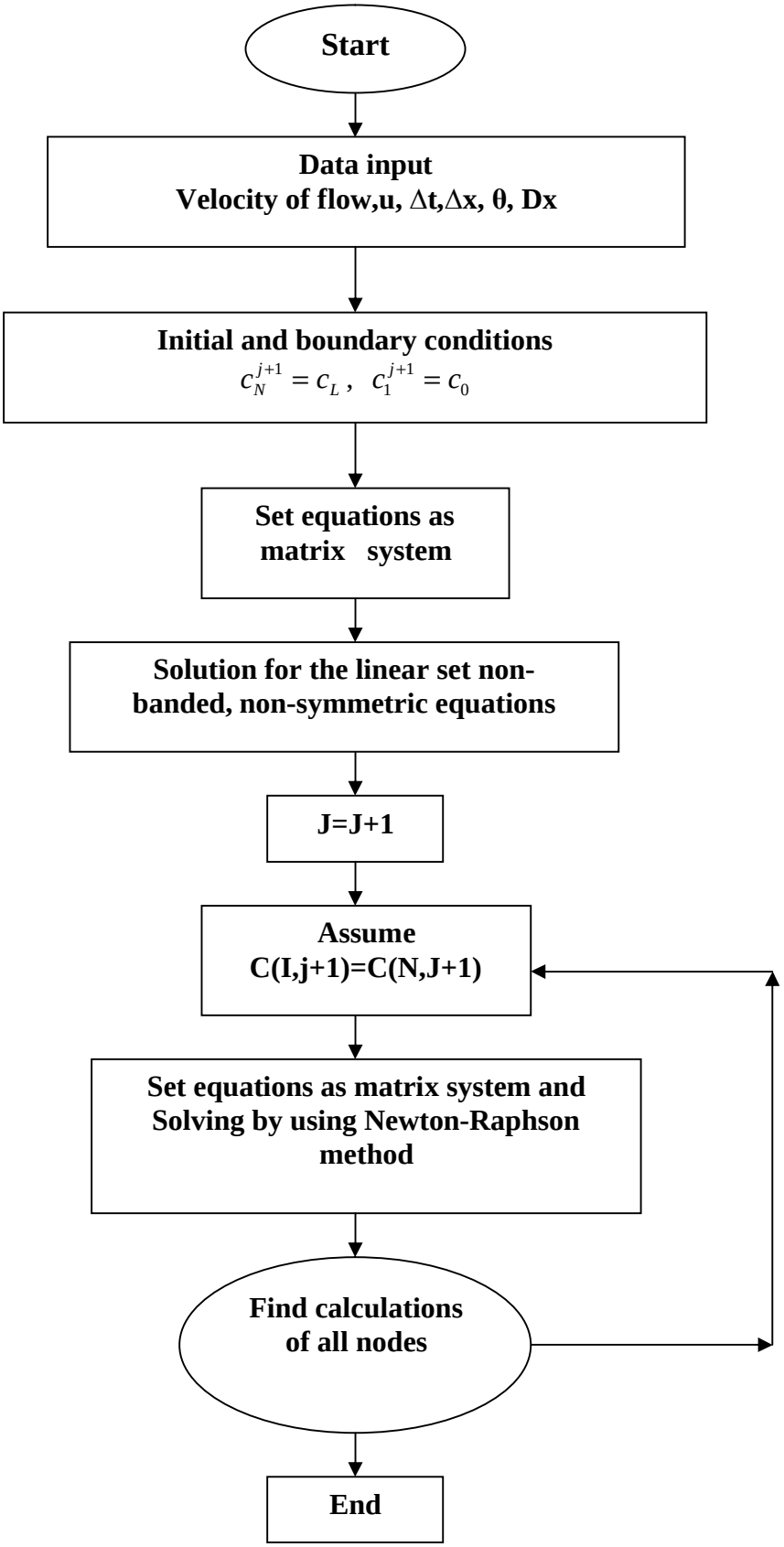

Figure 2 Layout of algorithm program

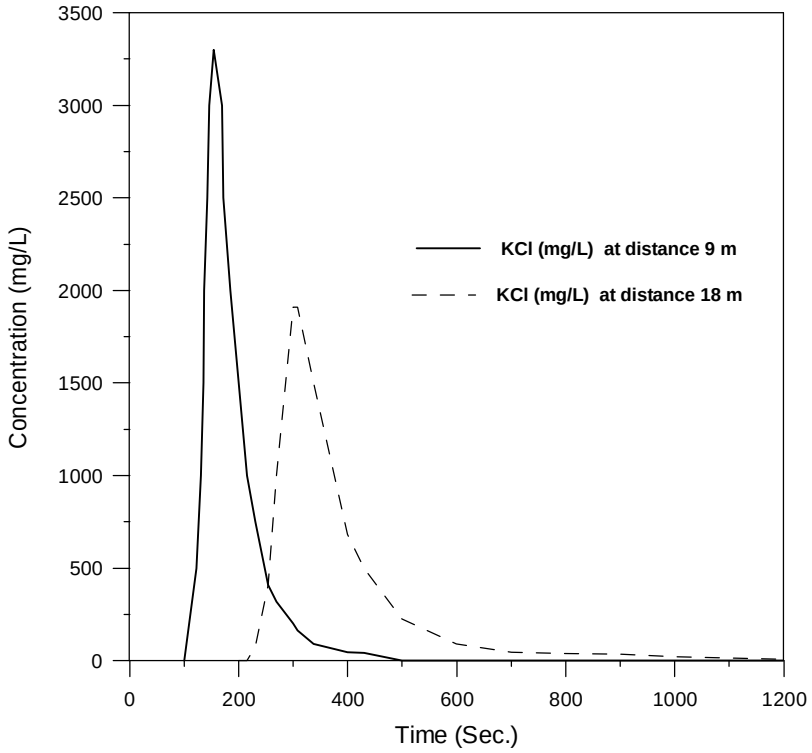

Figure 3 KCl Concentration-time profiles at distances 9 m and 18 m in flume

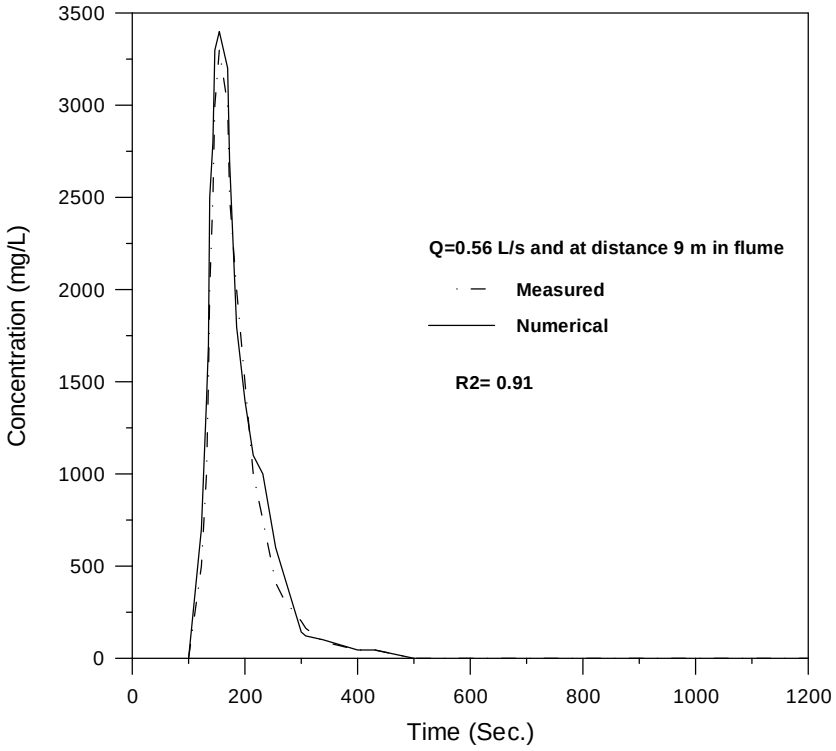

Figure 4 Comparison between numerical and experimental concentration-time profiles

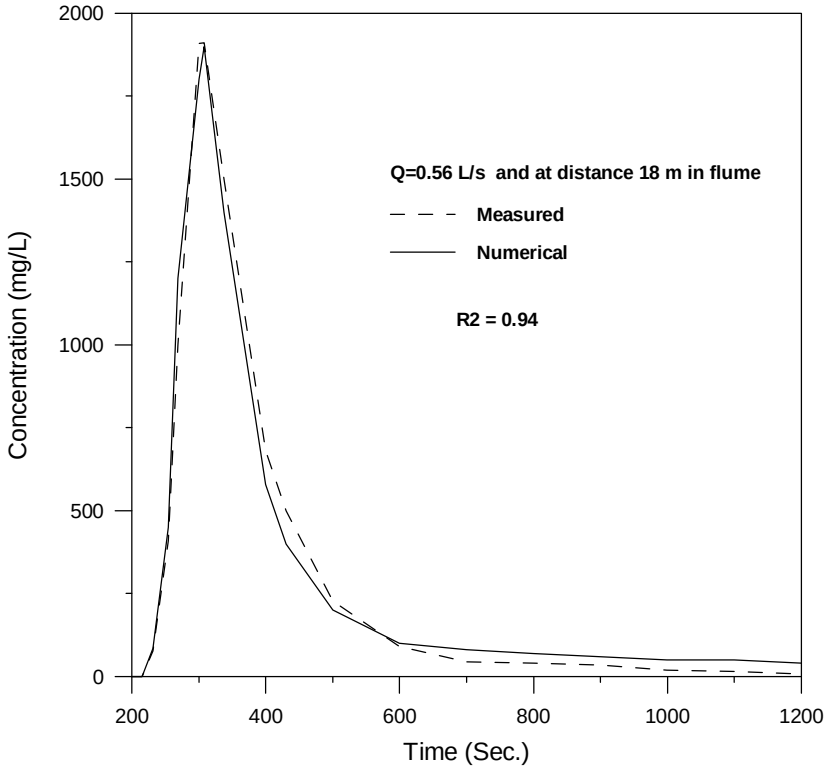

Figure 5 Comparison between numerical and experimental concentration-time profiles

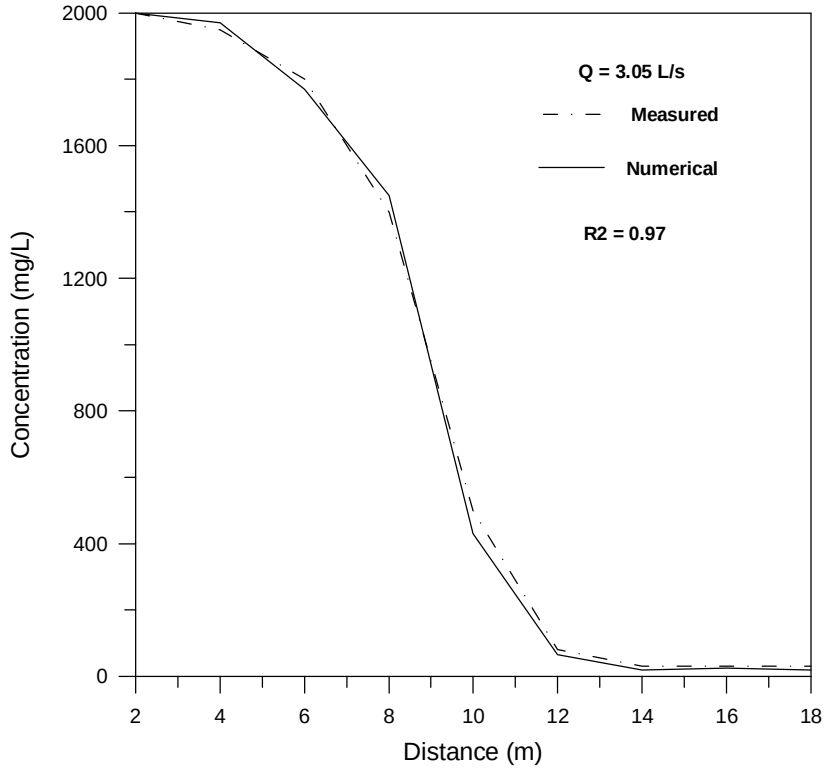

Figure 6 Comparison between numerical and experimental spatial variation of concentration