



Two Dimensional Unsteady State Mathematical Model for dispersion of Chlorine in Water in a Channel

KEYWORDS

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ABSTRACT *The two dimensional unsteady-state mass conservation equation for dispersion of chlorine in water in channel flow is solved analytically. The results obtained analytically for the model and their graphical representation is shown for various values of diffusivity, reaction rate and bulk flow velocity. The model can be used to maintain optimum chlorination in the drinking water.*

INTRODUCTION

There are a number of research papers published on chlorine concentration decay in drinking water distribution system. Clark et al. (1994) showed how chlorine residuals can vary throughout the day at different locations in the distributive systems. Clark et al. (1995) used first order kinetics and rate of chlorine decay in their model. They showed that the fluid velocity and pipe radius affect the propagation of chlorine residual levels, disinfection efficiency and the formation of disinfection by-products. Reddy et al. (1996) discussed the weighted least-square method for some parameter estimation in water distribution network, like model pressure heads, pipe flow, head loss in pipes and consumptions in flows. David and Bryan (1996) developed an advection transport model by neglecting the contribution of radials as well as axial diffusion terms. Munavali and Mohan (2005) presented a simulation-optimization model for water quality parameter estimation in the distribution system under dynamic state. Osman, and Metin (1999) solved two dimensional convection dispersive equation numerically for various boundary and initial conditions, considering the decay of chlorine in the bulk flow, but they did not consider the transfer of chlorine from bulk flow to the pipe wall. Jaipal and Bhadula (2012) presented two dimensional steady state mathematical model and unsteady state model (2013) that accounts for transport in the axial direction of diffusion and that incorporates chlorine decay within the bulk flow and transport of the chlorine from bulk flow to the pipe wall to predict the chlorine concentration in a drinking water distribution system. Eran et al (2011) studied the chlorination and ultraviolet (UV) irradiation of rotating biological contractor in treating the light-grey water. They examined the ability of chlorine and UV to inactivate indicator bacteria and specific Pathogens. Cherchi and Gu (2011) investigated the impact of the cell growth stage on chlorine disinfection efficiency and the impact of the growth stage on chlorination resistance by comparing the inactivation efficiencies of two indicator bacterial strains obtained from various growth Phases. Hoefel et al (2005) in micro trial resistant to chlorination has observed both of these in lab studies and in full scale chlorine disinfection Practice for water and Waste-water treatment. Wojcicka et al (2007) in previous studies have found that indigenous bacteria are related from different environment. Huang et al (2011) studied that the influence of chlorination on end toxin activities of secondary sewage effluent and Pure Cultured Gram-negative bacteria was instigated.

MATHEMATICAL MODELLING

The two dimensional unsteady state mass conservation equation for dispersion of chlorine in drinking water in a channel flow considering transport of chlorine flow to the wall is

$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} - U_0 \frac{\partial c}{\partial x} - V_0 \frac{\partial c}{\partial y} - k_b c - \frac{k_f(c - c_w)}{l_2} \dots\dots\dots(1)$$

Where D_x is diffusion coefficient in x direction, D_y is diffusion coefficient in y direction, U_0 and V_0 are initial velocity component along x and y axes respectively, k_b and k_f are the chlorine decay rate constant for bulk flow (s^{-1}) and mass transfer coefficient (m/s) respectively, c_w is the chlorine concentration at wall (kg / m^3) and l_2 is distance from centre to wall of the channel in direction.

Assuming that the reaction of chlorine at the pipe wall is of first order with respect to the wall concentration C_w and that it proceeds at the same rate as chlorine is transported to the wall gives the following mass balance equation for the chlorine at the wall.

$$k_f(c - c_w) = k_w c_w \dots\dots\dots (2)$$

Substituting the value of C_w from equation (2) into equation (1). We get

$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} - U_0 \frac{\partial c}{\partial x} - V_0 \frac{\partial c}{\partial y} - k_b c - \frac{k_f k_w c}{l_2(k_f + k_w)} \dots\dots\dots (3)$$

The initial boundary conditions are

$$c = 0, t = 0, x \geq 0, y \geq 0 \dots\dots\dots (4.i)$$

$$c = c_0, t > 0, x = 0, y = 0 \dots\dots\dots (4.ii)$$

Where C_0 is initial concentration

It is assumed that the change in chlorine concentration is very negligible where x approaches to length l_1 (very large distance) for $t > 0$ so.

$$\frac{\partial c}{\partial x} = 0 \text{ as } x \geq l_1 \dots\dots\dots (4.iii)$$

and wall condition is

$$\frac{\partial c}{\partial y} = 0 \text{ at } y = l_2 \dots\dots\dots (4.iv)$$

Introducing a new space variable

$$X = x + y \sqrt{\frac{D_y}{D_x}} \dots\dots\dots (5)$$

in equation (3), we get

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial X^2} - U \frac{\partial c}{\partial X} - k_b c - \frac{k_f k_w c}{l_2(k_f + k_w)} \tag{6}$$

Where $D = D_x \left(1 + \frac{D_y^2}{D_x^2} \right), U = U_0 + V_0 \sqrt{\frac{D_y}{D_x}}$

The initial and boundary condition become

$$c = 0, t = 0, X \geq 0 \tag{7.i}$$

$$c = c_0, t > 0, X = 0 \tag{7.ii}$$

$$\frac{\partial c}{\partial x} = 0, t \geq 0, X \rightarrow \infty \tag{7.iii}$$

Again introducing the following transformation

$$c(X, t) = P(X, t) \exp \left[\frac{UX}{2D} - \left(\frac{U^2}{4D} + K \right) t \right] \tag{8}$$

Where $K = k_b + \frac{k_w k_f}{l_2(k_w + k_f)}$

Equation (3) reduced into

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial X^2} \tag{9}$$

The initial and boundary condition (7.i) to (7.iii) become

$$P(X, t) = 0, X \geq 0, t = 0$$

$$P(X, t) = c_0 \exp \left[\left(\frac{U^2}{4D} + K \right) t \right], X = 0, t = 0$$

$$\frac{dP}{dX} = 0, t \geq 0, X \rightarrow \infty \tag{10.iii}$$

Solving equation (9) together with initial boundary conditions (10.i) to (10.iii) by Laplace transformations technique and then putting the value of $P(X, t)$ in equation (8), we get

$$c = \frac{c_0}{2} \left[\exp \left\{ \left(\frac{U}{2D} X \right) - X \left(\frac{U^2 + 4KD}{2D} \right)^{1/2} \right\} \operatorname{erfc} \left(\frac{X - (U^2 + 4KD)^{1/2} t}{2\sqrt{Dt}} \right) + \exp \left\{ \left(\frac{U}{2D} X \right) + X \left(\frac{U^2 + 4KD}{2D} \right)^{1/2} \right\} \operatorname{erfc} \left(\frac{X + (U^2 + 4KD)^{1/2} t}{2\sqrt{Dt}} \right) \right] \tag{11}$$

RESULTS AND DISCUSSION

The numerical values of chlorine concentration given by

equation (11) are obtained using MATLAB for different values of parameters such as fluid velocity, diffusivity and chlorine consumption rate and fluid velocity etc are shown in figure 1 to figure 4, table 1 and table 2.

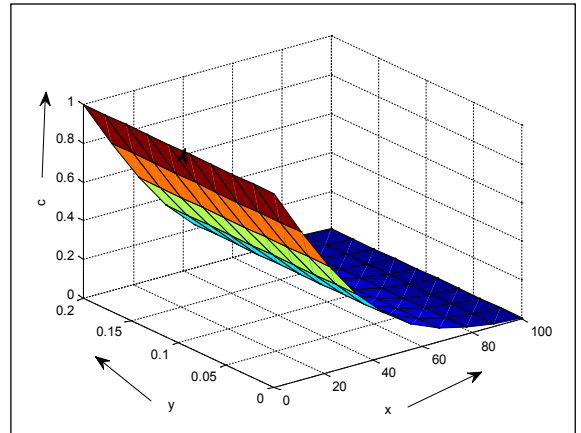


Fig.1 Variation of chlorine concentration with X and y (at $D_x = 0.00003, D_y = 0.00006, U_0 = 0.40, V_0 = 0.002, c_0 = 1.0, K = 0.035, T = 10.0$).

It is clear from fig.1 that chlorine concentration decreases very fast from $X = 0$ to $X = 65$ while from $X = 65$ to $X = 90$ chlorine concentration decreases slowly and after that chlorine concentration becomes almost constant and negligible. So we have to inject chlorine again after $X = 90$. It appear that there is no variation of C with y . It is because of that the change of chlorine concentration with y is very small and so it cannot be observed from the figure. To clarify this we can see table 1 which shows that at $y = 0, C = 0.78568012996958$ while at $y = 0, C = 0.78272107133604$ at same distance $X = 10$.

Table 1

y	c at $K = 0.035$	c at $K = 0.07$
0.0	0.78568012996958	0.78568029051031
0.1	0.78272107133604	0.78272123500595
0.2	0.77976515659284	0.77976532241207

For $D_x = 0.00003, D_y = 0.00006, U_0 = 0.40, V_0 = 0.002, c_0 = 1.0, T = 10.0$ at $x=10.0$

It clears that chlorine concentration decreases (however small) with y . To see the effect of reaction rate K (that also includes transport of chlorine from bulk flow to the wall) on chlorine concentration we compare fig.1 (for $K = 0.035$) and fig.2 (for $K = 0.07$) both the figure look similar and the effect of K on C cannot be observed from these figures.

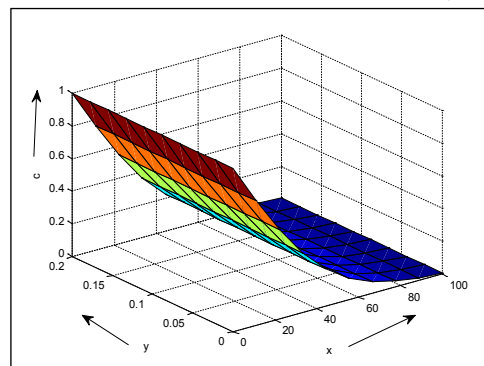


Fig.2 Variation of chlorine concentration with X and y

(at $D_x = 0.00003$, $D_y = 0.00006$, $U_0 = 0.40$, $V_0 = 0.002$, $C_0 = 1.0$, $K = 0.07$. $T = 10.0$).

Again we see table 1, and observe that when the reaction rate K changes from 0.035 to 0.07(keeping other parameters same), then chlorine concentration increases towards y for example at $y = 0.2$, $C = 0.77976515659284$ (at $K = 0.035$) while $C = 0.77976532241207$ (at $K = 0.07$). Since the reaction rate K in our work, includes the term of transport of the chlorine from bulk flow to the wall. Therefore increasing of C with increasing value of K at the same location of y is justified.

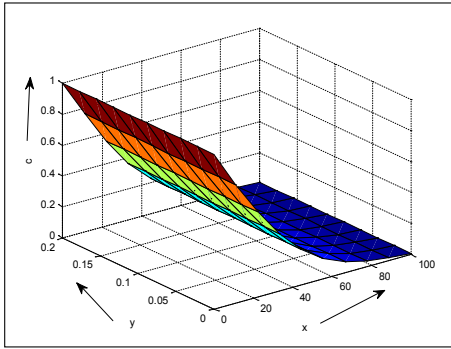


Fig.3 Variation of chlorine concentration with X and y (at $D_x = 0.00003$, $D_y = 0.00006$, $U_0 = 0.60$, $V_0 = 0.002$, $C_0 = 1.0$, $K = 0.035$. $T = 10.0$).

To see the effect of diffusivity we compare fig.3 (for $D_y = 0.00006$) and fig.4 (for $D_y = 0.00012$). It is observed from these figures that when diffusivity increases in y direction then more mixing takes place and so chlorine concentration become constant at some earlier distance for example when $D_y = 0.00006$ (fig.3) then chlorine concentration decreases very fast at $X = 0$ to $X = 65$ (approximately) then from $X = 65$ to $X = 90$ variation is slow and $X = 90$ onwards it becomes constant.

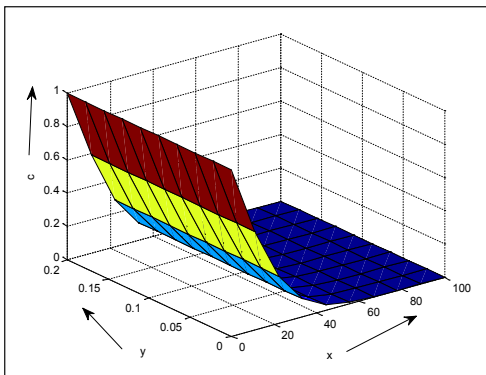


Fig.4 Variation of chlorine concentration with X and y

(at $D_x = 0.00003$, $D_y = 0.00012$, $U_0 = 0.60$, $V_0 = 0.002$, $C_0 = 1.0$, $K = 0.035$. $T = 10.0$).

When $D_y = 0.00012$ (fig.4) then chlorine concentration decreases very fast from $X = 0$ to $X = 45$ then from $X = 45$ to $X = 55$ variation is slow and after $X = 60$ chlorine concentration becomes constant. Thus chlorine concentration become constant after $X = 90$ when $D_y = 0.00006$ while chlorine concentration becomes constant after $X = 60$ for $D_y = 0.00012$ due to more mixing.

Table 2

y	C at $U_0 = 0.40$	C at $U_0 = 0.60$
0.0	0.17371465183261	0.17700254390629
0.10	0.17249972996704	0.17577915873285
0.16	0.17177383413740	0.17504816087294
0.20	0.17129117538641	0.17456209083238

For $D_x = 0.00003$, $D_y = 0.00006$, $C_0 = 1.0$, $K = 0.035$, $T = 10.0$ at $X = 50.0$

The effect of fluid velocity in X direction on chlorine concentration can be observed from table 2 in which we have observed the chlorine concentration for fluid velocity $U_0 = 0.40$ and $U_0 = 0.60$ at same location $X = 50$ keeping other parameters same we observed that at $y = 0$, $X = 50.0$ chlorine concentration $C = 0.1737$ for $U_0 = 0.40$ while $C = 0.1770$ for $U_0 = 0.60$ at the distance in X direction. Thus at same distance X , chlorine concentration C increases with increasing value of fluid velocity in X direction which is due to advection effect.

CONCLUSION

The analytical solution of two dimensional unsteady-state mathematical model presented in the paper predicts good dispersion of chlorine in water. The model can be use effectively to optimize the chlorination for safe drinking water.

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