

A transient 2-D water quality model for pipeline systems

Un modèle 2-D transitoire de qualité de l'eau pour des systèmes de canalisation

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ABSTRACT

This study develops a water quality model in a pipeline during transient conditions using a two-dimensional (2-D) approach including advection, diffusion, and reaction terms. More specifically, using a modified Vardy-Hwang hydraulic model, a 2-D transient model for flow is coupled with a 2-D advection-diffusion-reaction model for chemical constituent concentration. A five-region turbulence model is used to compute turbulent shear stresses. Using a fixed grid method of characteristics, the hydraulic equations are integrated numerically to determine the velocity and pressure head. Then, an explicit/implicit finite difference method is used to integrate the advection-diffusion-reaction equation (ADRE). A reservoir-pipe-valve-reservoir system illustrates the 2-D behaviour of transient flow due to a sudden valve opening and results are compared with a one-dimensional (1-D) counterpart. Although the system response using the two models is not dramatically different, the 2-D results do show some discernable increases in realism and insight over the 1-D model. Interestingly, the study also reveals that the Taylor model produces insufficient dispersion in a large-diameter pipe carrying a fully turbulent flow with large Reynolds number.

RÉSUMÉ

Cette étude développe un modèle de qualité de l'eau dans une canalisation pendant des états transitoires en utilisant une approche bidimensionnelle (2-D) comprenant la convection, la diffusion, et les termes de réaction. Plus spécifiquement, en utilisant un modèle hydraulique modifié de Vardy-Hwang, un modèle 2-D transitoire pour l'écoulement a été couplé à un modèle 2-D de convection-diffusion-réaction pour la concentration chimique des constituants. Un modèle de turbulence en cinq zones est employé pour calculer les efforts de cisaillement turbulents. En utilisant une méthode des caractéristiques en grille fixe, les équations hydrauliques sont intégrées numériquement pour déterminer la vitesse et la charge. Puis, une méthode de différences finies explicite/implicite est employée pour intégrer l'équation de convection-diffusion-réaction (ADRE). Un système de réservoir-conduite-vanne illustre le comportement 2-D de l'écoulement transitoire suite à une ouverture soudaine de vanne et les résultats sont comparés à une approche unidimensionnelle (1-D). Bien que les réponses des deux modèles ne soient pas nettement différentes, les résultats 2-D montrent un peu plus de réalisme et de discernement par rapport au modèle 1-D. D'une manière intéressante, l'étude montre également que le modèle de Taylor produit une dispersion insuffisante dans une conduite de large diamètre avec un écoulement pleinement turbulent et un grand nombre de Reynolds.

Keywords: Chemical constituent decay, finite difference method, method of characteristic, transient flow, turbulence model, two-dimensional model water quality

1 Introduction

Transient flow is an important phenomenon that must be considered in the design of all significant pipeline systems. Transient pressures may be large enough to damage pipelines, pumps and other system elements, and the rapidly oscillating flows can re-suspend sediments or draw external contaminants into the pipe, leading to the water quality problems and posing a threat to safe drinking water. In fact, a water distribution system (WDS) is a complicated dynamic system in which different physical, chemical, and microbiological events may occur simultaneously resulting in changes to the quality of water. Besides the hydraulic issues, factors such as pipe corrosion and various chemical and biological reactions between disinfectants and organic and inorganic compounds can all contribute to water quality changes. Transient velocities may potentially accelerate these chemical

and biological reactions, and therefore, significantly alter the odour, taste, colour, and in general the quality of water in the system. Such considerations motivate the current search for a better understanding of the hydraulic-related deterioration of the water quality during the transient water hammer conditions.

Assuming steady hydraulics and transport conditions, various authors have studied the fate of chlorine as the system approaches the equilibrium state (Boulos *et al.*, 1993; Clark *et al.*, 1988; Taylor, 1953). Unsteady chlorine concentrations under steady hydraulic conditions were considered by others (Boulos *et al.*, 1995; Grayman *et al.*, 1988; Liou and Kroon, 1987; Rossman, 1993; Rossman and Boulos, 1996). Such approaches, while ignoring inertia and compressibility effects, form the core of the most commonly used water quality software.

Using unsteady conditions for both chlorine and flow, Fernandes and Karney (2004) proposed a one-dimensional (1-D)

water quality model considering advection, diffusion, and reaction terms. The approach combined a finite difference method (FDM, to numerically integrate the ADRE) and method of characteristics (MOC, to numerically integrate hydraulic equations for transient flow). However, a steady state formula (Darcy-Weisbach equation) and Taylor's model were applied to calculate the turbulent shear stresses and the diffusion coefficient. The 1-D unsteady model considered realistic conditions for flow and chlorine concentration such as the changes in flow velocity, compressibility and inertia effects. However, the model is based on a uniform concentration along the cross section of the pipe; whereas in a real WDS, the difference between the concentration of a constituent at the pipe wall and that at the pipe centerline can be quite considerable. For example, the difference between the pH of water at the pipe wall and that at the pipe centerline may be three to even four pH units (AWWARF, 1996). This remarkable difference highlights the need for a better representation of velocity profile effects. Considering the chlorine decay within the biofilm and using a finite difference approach, Ozdemir and Ger (1998, 1999) proposed a quasi two-dimensional (2-D) model for water quality including advection (in the longitudinal direction), diffusion and reaction. In their model, they allowed unsteady conditions for water quality but only steady conditions for flow. They observed a penetration for the transient chlorine micro-profile within the biofilm with a rate depending on the chlorine bulk concentration. By using an exponential variation for decay coefficient with the chlorine concentration within the biofilm, they were able to achieve a close agreement between the experimental and model results.

The current research develops a 2-D water quality model by coupling a mass transport equation (including advection, diffusion, and reaction) for a chemical constituent (e.g., chlorine) with a comprehensive hydraulic model. This is accomplished by coupling two numerical schemes, one for mass transport and the other for system hydraulics. The numerical results of the model are compared with the results of an available 1-D model. Interestingly, Taylor's model has been traditionally used in 1-D models to determine the dispersion along a pipe. Originally developed for a short and small-diameter but extremely rough pipe for a relatively low-Reynolds-number turbulent flow (Taylor, 1953, 1954), the capability of the Taylor model to produce sufficient dispersion in a large-diameter pipe carrying a fully turbulent flow (with large Reynolds number) is also investigated in this study.

2 Flow equations

The governing equations for 2-D unsteady turbulent conduit flow (continuity and momentum equations) can be expressed as follows (Zhao and Ghidaoui, 2003):

$$\frac{g}{a^2} \frac{\partial H}{\partial t} + \frac{\partial U}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r}(rV) = 0 \quad (1)$$

$$\frac{\partial U}{\partial t} + g \frac{\partial H}{\partial x} = \frac{1}{r\rho} \frac{\partial}{\partial r}(r\tau) \quad (2)$$

in which, H is piezometric head; U and V are longitudinal and radial velocity components; τ is the total shear stress, ρ is the density of water; r and x are coordinates in cylindrical system; and t is time. Adopting the Boussinesq's assumptions, the turbulent shear stress is expressed as:

$$\tau = -\overline{\rho u'v'} + \nu_m \frac{\partial U}{\partial r} = (\nu_t + \nu_m) \frac{\partial U}{\partial r} \quad (3)$$

in which ν_t and ν_m are the turbulent and molecular kinematic viscosity coefficients; u and v are the velocity fluctuations in longitudinal (x) and radial (r) directions, respectively. The bar-sign over the quantities indicates a temporal average.

3 Water quality model

Following the work of several researchers (e.g., Biswas *et al.*, 1993; Fernandes and Karney, 2004; Ozdemir and Ger, 1998; Rossman *et al.*, 1994), a first-order decay model is assumed. The following 2nd-order parabolic PDE in cylindrical coordinate system represents the unsteady ADRE for the chemical constituent concentration:

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} + V \frac{\partial C}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r}(rJ_r) + \frac{\partial J_x}{\partial x} - K_b C \quad (4)$$

in which C is the concentration at point (x, r) and time t ; K_b is the bulk decay coefficient; J_x and J_r are the mass fluxes in the longitudinal and radial directions, respectively. The first two terms on the right side account for diffusion of the chemical constituent toward the pipe-wall (radial direction) and along the pipe (longitudinal direction). As Rodi (1993) argued, it is assumed that the turbulent mass transport is related to the gradient of the transported quantity in direct analogy to the turbulent momentum transport. Hence

$$J_x = -\overline{uc} + D_m \frac{\partial C}{\partial x} = (\Gamma + D_m) \frac{\partial C}{\partial x} \quad (5a)$$

$$J_r = -\overline{vc} + D_m \frac{\partial C}{\partial r} = (\Gamma + D_m) \frac{\partial C}{\partial r} \quad (5b)$$

in which c is the fluctuations of concentration of the chemical constituent and Γ and D_m are the turbulent and molecular diffusivity coefficients, respectively. The details of the 1-D model are given in (Fernandes and Karney, 2004).

Powell *et al.* (2000) studied the performance of six different kinetic models for the bulk decay of chlorine through a comparison with field data. Their models included 1st-order, 2nd-order with respect to chlorine, 2nd-order with respect to chlorine and another reactant, nth-order, limited 1st-order, and parallel 1st-order models. They showed that, besides its simplicity, the 1st-order kinetic model predicted the chlorine decay reasonably well. However, the studies by Zhang *et al.* (1992) and Jadas-Hecart *et al.* (1992) revealed a major limitation for the first order model in reproducing the steep decay observed immediately following chlorination. For this case, the 2nd-order model better represents the results. However, difficulty in defining the value of the decay parameters currently restricts its use for network modeling purposes (Powell *et al.*, 2000). As a result, the 1st order kinetics is used in this study to model the bulk decay of chlorine.

3.1 Turbulence model

The Reynolds shear stress terms in the hydraulic model and the turbulent diffusivity of each constituent within the flow can readily be calculated using the eddy-viscosity and diffusivity concepts. In principle, the current simulation model could be used with any prescribed turbulence model based on the eddy viscosity concept. However, to overcome the complexity in the determination of the turbulent shear stresses and to reduce the computational burden, the standard five-region turbulence model (Kita *et al.*, 1975) was used to model velocity fluctuations. This approach, which is an equilibrium turbulence model originally developed for steady flows, uses different mechanisms to damp turbulence: molecular viscosity is dominant in the region near to the pipe wall (i.e., in the viscous sublayer) while eddy viscosity is the main damping-mechanism in the core region (near the pipe centerline). The full description of the hydraulics of this model is given in Kita *et al.* (1975).

According to Rodi (1993), using the Reynolds analogy between the mass transport and the momentum transport, the turbulent diffusivity coefficient is closely related to the eddy-diffusivity concept and the dimensionless turbulent Schmidt number. The Schmidt number—which shows the ratio of turbulent kinematic viscosity to turbulent diffusion—has been found to have only small variations across flows or from flow to flow Rodi (1993). Thus, following a common convention, the turbulent Schmidt number is considered constant in this study. A more detailed study of this effect is found in Naser (2006).

4 Numerical solution

Using the MOC, the hyperbolic PDEs of flow, (1) and (2), are converted into a pair of ordinary differential equations (ODEs) along the positive and negative characteristic lines and then integrated numerically. The longitudinal and radial discretizations of the pipe flow domain are shown in Fig. 1 where N_x and N_r are number of reaches and cylinders in longitudinal and radial directions (further details in Naser *et al.*, 2004).

A finite difference-based scheme, namely the Alternating Direction Implicit (ADI) approach, is used to numerically integrate (4). ADI scheme provides an efficient 2nd-order numerical solution to the parabolic PDEs through inverting only tridiagonal matrices (Ferziger, 1981). Knowing the concentrations at the previous time level (n) and using the ADI scheme in both the radial and longitudinal directions, the discretization of (4) for the next time level ($n + 1$) is executed into two half steps.

For the first half step, the technique is implicit in the radial direction but explicit in the longitudinal direction, providing the following set of tri-diagonal equations for the unknown chemical constituent concentrations at each node at the intermediate time level $n + 1/2$:

$$A_1 C_{i,j+1}^{n+1/2} + B_1 C_{i,j}^{n+1/2} + E_1 C_{i,j-1}^{n+1/2} = F_1 \tag{6}$$

The subscript i denotes the position of the node in longitudinal direction with $i = 1$ and $i = N_x + 1$ corresponding to the inlet and outlet sections; the subscript j denotes the position of the node in

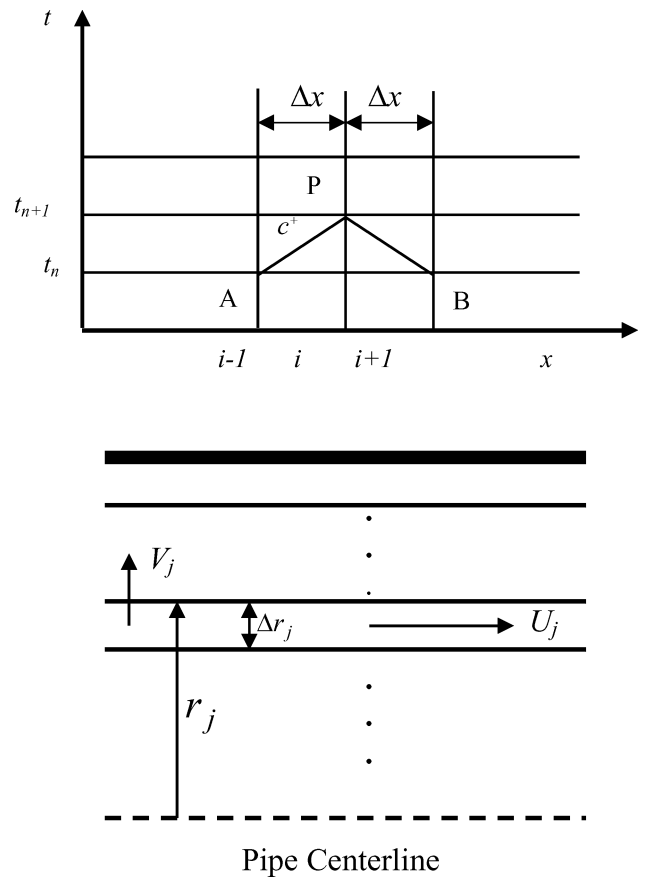


Figure 1 Longitudinal and radial discretization of pipe

the radial direction with $j = 1$ and $j = N_r$ corresponding to the first cylinder (at pipe’s centerline) and the last cylinder (at pipe wall), respectively.

For the second half step, the scheme is explicit in the radial direction but implicit in the longitudinal direction, providing another set of tridiagonal matrices for the unknown chemical constituent concentrations at each node at the time level $n + 1$:

$$A_2 C_{i+1,j}^{n+1} + B_2 C_{i,j}^{n+1} + E_2 C_{i-1,j}^{n+1} = F_2 \tag{7}$$

This pair repeats over the whole simulation period. Overall, the solution of these two sets of equations provides the unknown concentrations at each node for the corresponding time level. Expressions for the coefficients in Eqs (6) and (7) are given in the Appendix.

To solve Eqs (1), (2), and (4), boundary conditions that consider the chemical constituent concentration at the upstream, downstream, pipe wall, and pipe centerline boundaries, and the initial conditions, must be specified. For the current study, a no-flux condition is applied at the pipe wall, at the centerline, and at the downstream end of the system. The upstream end is considered as a fixed concentration node and the water in the pipe is assumed free from the considered chemical constituent initially.

5 Case study: Flow initialization from valve opening

The results of the 2-D simulation model for a hypothetical reservoir-pipe-valve-reservoir case fully described in Fernandes



Figure 2 Schematic of the pipe system for the case study

and Karney (2004) are now compared with the corresponding 1-D simulation results of Fernandes and Karney (2004). For clarity, Fig. 2 depicts the pipeline system with its two terminal constant-head reservoirs. The pipeline is 1000 m long, 1128.4 mm in diameter, and has a wave speed of 1000 m/s. A steady state Darcy-Weisbach factor of 0.05 was assumed for the pipe's friction factor during every stage of flow (Fernandes and Karney, 2004). Certainly, the constant friction factor assumption is quite approximate during the initial stage of the flow but becomes progressively more accurate as the new steady state is approached.

The water is at an elevation of 200 and -100 meters for the upstream and downstream reservoirs, respectively. The final steady-state flow rate (with the valve fully open) is 2000 l/s. The coefficient of head-loss of the downstream valve is assumed as $0.117 \text{ m}^2\text{-s}^5$. Initially, there is no flow in the system (the valve is fully closed), but then the valve is suddenly opened to introduce a transient state during which 0.5 mg/l of chlorine is continuously supplied at the upstream end. The bulk-flow decay coefficient is 0.0006 s^{-1} and there is no chlorine consumption at the pipe wall.

To facilitate comparison of results between the 1-D and 2-D models, the local concentration of the 2-D simulation is averaged over the pipe's cross section. For the purpose of numerical simulation, the pipe is divided into 400 reaches in longitudinal direction (for both 1-D and 2-D models) and 600 cylinders in the radial direction (for the 2-D model). These numbers were selected through a preliminary numerical investigation seeking to achieve good numerical convergence within a reasonable computational time. Numerical convergence is discussed in more detail later.

Within a numerical cell the pressure wave propagates both with a speed related to the wall material (water hammer velocity) and with the speed of advection of a scalar quantity (the average flow velocity). These two speeds produce an inconsistency between the time scale of water quality and that of the transient flow simulations. This difficulty is often solved by interpolating the velocity field. However, an accumulative-approach is used here to achieve a better agreement between the advective and hydraulic propagation. In essence, the mass flux is added over a number steps by using water quality time-step (Δt_{wq}) that is an integer multiplier of the hydraulic time-step (Δt_{lf}). Using a trial and error approach the ratio of the time-step for water quality to the corresponding term for transient flow for the current case study was selected as 24 and 50 for the 2-D and 1-D simulation models, respectively. The smaller time-ratio needed for the 2-D model likely arises from the larger velocity variation in the 2-D model.

6 Model application for a system start-up

The transient event in this system is created by a sudden valve opening, which initially depressurizes the water near the valve. This depressurization creates traveling pressure and velocity waves that move through the system, interacting as they do with the pipe wall and the upstream boundary condition. Interestingly, the unsteady friction literature has been preoccupied with closure events and few detailed considerations have been given to such an opening event (Bergant *et al.*, 2002; Vitkovsky *et al.*, 2006).

The resulting system responses for the maximum and minimum pressure head along the pipeline are given in Fig. 3 for both 1-D and 2-D model. The created pressure and velocity waves propagate through the system until they decay to a new steady state. It is the compressibility and inertia associated with the valve opening that creates the temporary fluctuations in both pressure head and flow discharge. The figure clearly shows that the five-region turbulence model produces higher energy dissipation than the Darcy-Weisbach formula in the 1-D model. Interestingly, although there is almost no significant difference in minimum pressure head between 1-D and 2-D results, the difference in maximum pressure heads is quite noticeable. The reason for this becomes clear from a consideration of velocity.

Figure 4 displays the results of both 1-D and 2-D models for discharge variations at the section at the pipe's midpoint during the first 25 s of the event. The 1-D simulation indicates that it takes approximately 20 s for the system to reach the steady state flow of 2000 l/s; the corresponding time for the 2-D approach is around 15 s. The figure clearly shows a sequence of deceleration and acceleration events, which ultimately bring the system to essentially the same discharge but through a sequence of slightly different average velocities. Interestingly, during the acceleration phase the average velocity is slightly higher for the 1-D model than that for the 2-D simulation particularly for the first two cycles (2.8 and 2.7 m/s in the first cycle) due to lower dissipation effects in the 1-D model. However, there is little difference between the average velocities in both models during the deceleration phase. In essence, the greater decay or dissipation of energy in the 2-D case brings the flow more quickly and closely to the final

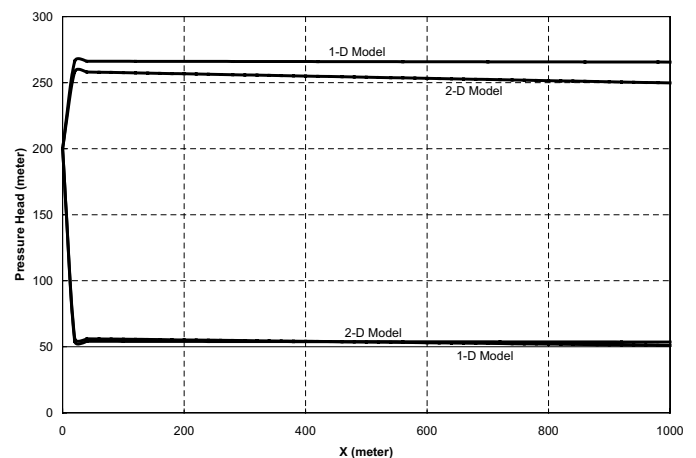


Figure 3 Maximum and minimum pressure head caused by sudden opening

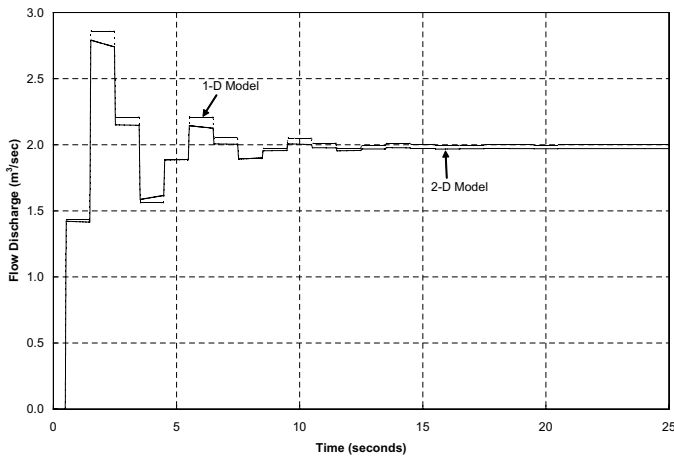


Figure 4 Comparison between 1-D and 2-D models for flow discharge at midpoint of pipe

steady state velocity. Thus, the small difference in the minimum pressure heads in Fig. 3 is explained as is the larger difference in maximum head values. These differences have implications for several aspects of the system response including the propagation of chemical constituent.

Compared to the longitudinal velocity component (2.0 m/s), the radial velocity component is relatively small in magnitude and indeed no consideration is given to these velocities in 1-D transient models. However, they can potentially contribute not only to the momentum exchange between layers of flow (hence preserving the assumption of uniformity of the piezometric head at a cross section) but also to the transport of chemical constituent or other constituents in the radial direction. As the transient wave dies out, so does the radial velocity.

Figure 5(a,b) represent the results of the 2-D approach for temporal and spatial variations of velocity profile along the pipe. Thus, these figures reflect the boundary layer growth. As it is obvious in Fig. 5(a), the velocity profile is initially very flat over the pipe cross section (at $t = 5.0$ s). However, as the boundary layer grows the profile spreads out. Moreover, splitting the pipe cross section into a wall-region and a core-region, the fluid of

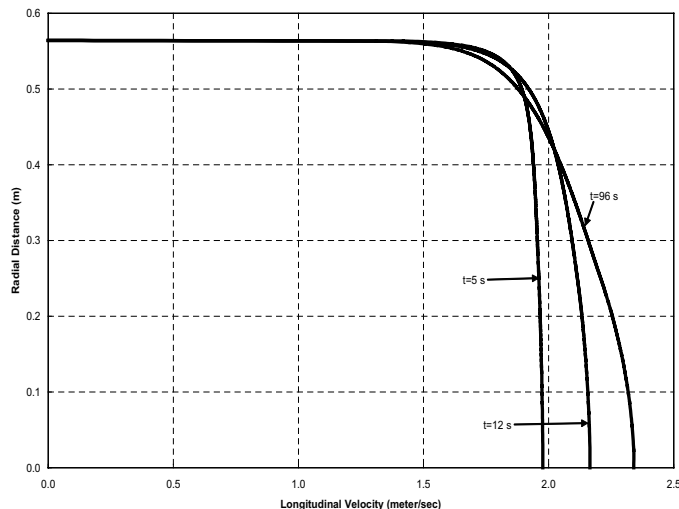


Figure 5(a) Velocity profile at midpoint of pipe

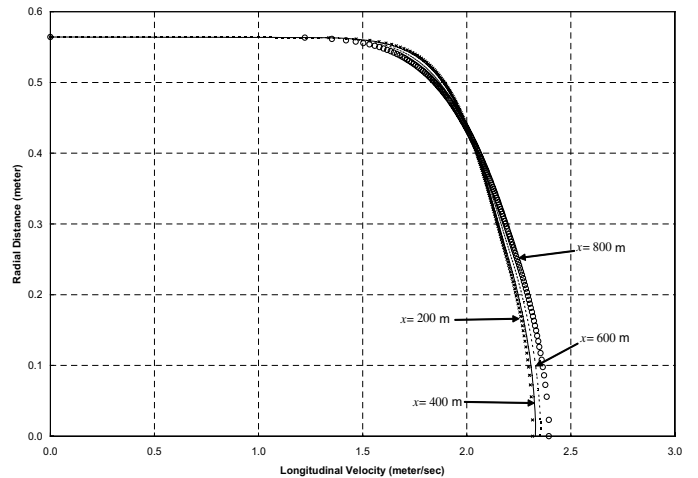


Figure 5(b) Steady velocity profile at various sections

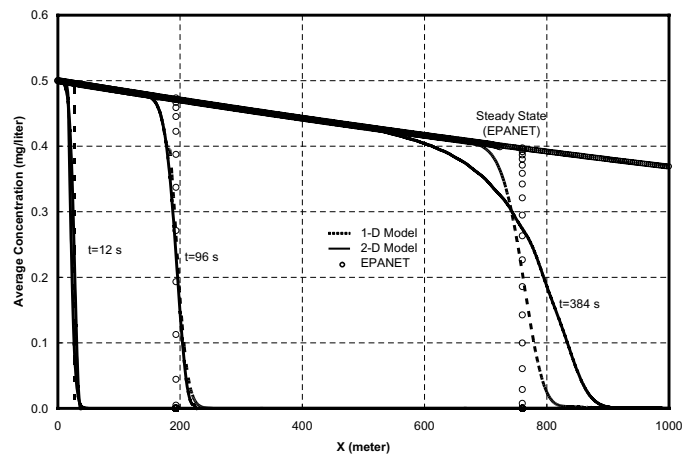


Figure 6 Chemical constituent front evolution

each region moves with the same average velocity in the 1-D model (2.0 m/s), unlike in the 2-D model. Although the system reaches steady state after about 20 s, as Fig. 5(b) indicates, the velocity profile is still developing along the pipe. The figure also shows a slight increase in the boundary layer thickness along the pipe length even after the system hydraulically approaches the new steady state.

The influence of flow hydraulics on the chemical constituent transport can be recognized in Fig. 6, which depicts the wave front evolution for the average concentration through the pipeline during the transient event based on the results of both the 1-D and 2-D models. Using the software EPANET (Rossman, 1993), steady-state analysis was also performed and the corresponding results indicated. The figure clearly shows a symmetric dispersion around the mean front for the 1-D result, whereas some asymmetry is evident in the 2-D counterpart. This symmetric property in 1-D results can be interpreted as a consequence of the uniform velocity along a pipe cross section unlike the 2-D velocity profile. The nonuniformity in velocity profile in 2-D model causes a different rate for chemical constituent decay and movement at core region than that of the wall region (higher rate at core region), which consequently creates an asymmetric chemical constituent front in the 2-D model. Thus, the chemical

front is slightly steeper for the 1-D results. This variation arises for two reasons: first the difference in energy dissipation mechanisms and therefore in average velocity between 1-D and 2-D models during the acceleration and deceleration cycles (overall the difference in the history of flow), and through the effects of a developing velocity profile along the pipe. As it is obvious EPANET chemical constituent front is entirely vertical; by contrast, a dispersion is obvious in both 1-D and 2-D results. This is because EPANET considers advection as the only mass transport mechanism in a WDS, while both 1-D and 2-D models take into account the effects of dispersion.

Interestingly, however, the new study clearly shows that although the difference between 1-D and 2-D results at the beginning of the transient event is negligible, it becomes more significant as the time progresses. In other words, the figure clearly shows less dispersion for the 1-D approach. Taylor's model used in the 1-D approach in this study is summarized as:

$$\Gamma = 20.2DU\sqrt{f/8} \quad (8)$$

It is useful to note that Taylor developed his studies (Taylor, 1953, 1954) for a very short (2.473 m length), small-diameter (9.525 mm) but extremely rough (1/6 relative roughness) pipe for a relatively low-Reynolds-number turbulent flow (with an average velocity of 1.46 m/s). Thus, the noticeable difference between the 1-D and 2-D models may reflect an inability in the Taylor's model to produce sufficient dispersion for a large-diameter and less-rough pipe carrying, as it does here, a fully turbulent flow of large Reynolds number. In order to investigate this, a sensitivity study was performed for a small 100.0 m pipe with 1.0 cm diameter, a Darcy-Weisbach friction factor of 0.022, and with 0.095/s discharge. The 2-D and 1-D results are plotted in Fig. 7. Although Taylor found more satisfactory results for the case in his study, the figure clearly highlights a higher dispersion for the 2-D approach. In fact, the good agreement between the model's results and experimental data in Taylor's study can be largely attributed to the high roughness of the pipe. Given the system characteristics in Taylor study, the Darcy-Weisbach friction factor was of the order of 0.14, which consequently provides enough dispersion in

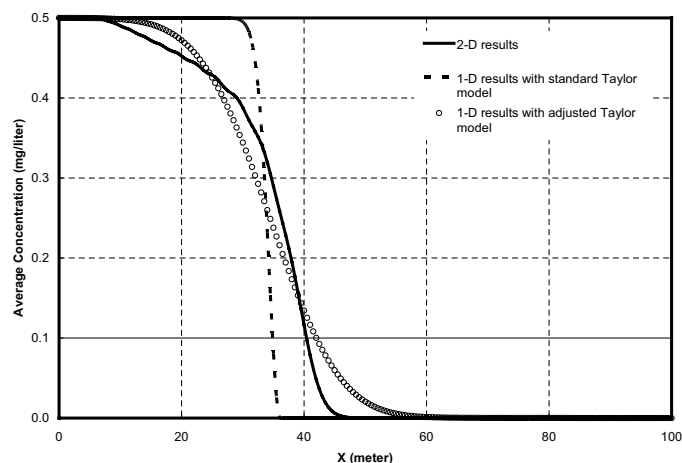


Figure 7 1-D and 2-D chemical front evolution (at $t = 30$ s) for the capillary-tube case

the flow via (8). The 1-D results for the case in this study were adjusted by increasing the dispersion term in the Taylor model by a factor of 500. The results of this simulation (Fig. 7) show greater consistency with the 2-D results.

In order to briefly investigate the effect of flow history on chemical constituent propagation the simulation was rerun but for a steady flow scenario. The system is exactly the same as before except that chemical constituent is injected at the upstream reservoir 10 min after the valve has opened and thus after the flow has achieved a steady condition. No significant differences were observed for the 1-D and 2-D results at the beginning of the evolution, but the differences gradually become more obvious. In fact, even under a steady hydraulic condition, the velocity profile is flat at the upstream end but becomes more nonuniform toward the downstream end (Fig. 5b). These velocity differences again create a longer tail for the chemical front in the 2-D approach. The fact that the effects of boundary layer growth and velocity profile are included in the 2-D approaches could be a significant advantage. Thus, in the current study, 2-D effects are more important than the transient effects, but in fairness it should be stated that the 1-D model actually performs quite well.

The dimensionless turbulent Schmidt number is the ratio of the eddy viscosity to the diffusivity of the scalar constituent. Using the Reynolds analogy, it can be argued that the turbulent Schmidt number is around unity (Rubin and Atkinson, 2001). A sensitivity analysis was conducted by varying the Schmidt number from 0.5 to 1.5 where smaller numbers are associated with greater diffusion. Interestingly, however, the numerical results show little change in predicted concentrations. This small role highlights the fact that the dominant mass transport mechanism in this case study is advection.

7 Effect of pipe diameter

In order to investigate the effect of pipe diameter on chemical constituent decay, two simulations were performed with different diameters of 1100 and 200 mm. The water level was lowered to 100 m for the downstream reservoir, while it unchanged at the upstream end. To achieve an average longitudinal velocity of 2 m/s, the valve coefficients for the smaller- and larger-diameter pipes were set at 0.2 and 0.009 $m^{2.5}/s$, respectively. For both simulations 500 reaches were used in longitudinal direction and 300 cylinders in radial direction (for the 2-D model). A difference in average velocities was noted between the two systems during the acceleration and deceleration phases. Not surprising, the analysis reveals a higher transient velocity for the system with a larger pipe diameter: a peak velocity 3.2 m/s for larger pipe compared to 3 m/s for the smaller. Both systems reached the 2 m/s steady velocity after about 20 s. The implications of this for chemical constituent propagation are shown in Fig. 8 at 383 s after valve opening. The figure displays a noticeable difference in chemical front for systems with different diameter. It should be also noted that this difference can partly be due to radial velocity effects, which is much greater for larger diameters, thus highlighting the importance of 2-D effects. Moreover, the assumptions of

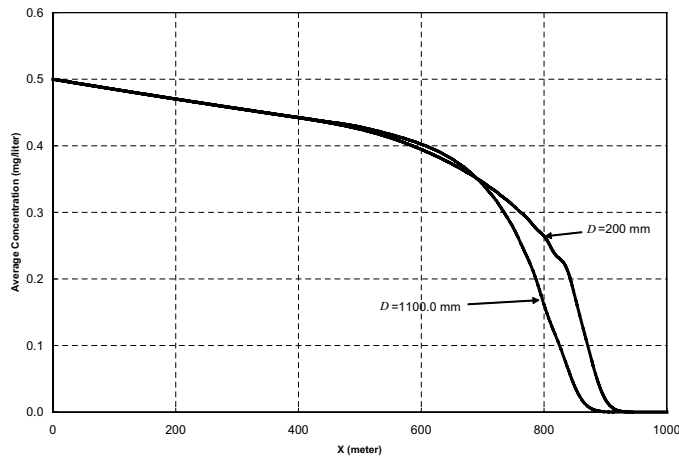


Figure 8 Pipe diameter effect: 2-D results for chemical front 383 s after valve opening

a constant velocity field and wall friction factor mean that the Taylor model (8) in 1-D approach produces slightly different diffusion for systems with different diameter (200 and 1100 mm). However, considering the fact that at least for the current case study advection is the main mass transport mechanism, the 1-D water quality model would produce similar results for chemical propagation.

8 Stability and convergence of the numerical model

As many have confirmed (e.g., Karney and Ghidaoui, 1997), the Courant condition ($C_r = a \times \Delta t / \Delta x \leq 1.0$) is indeed necessary to assure a stable numerical solution for the hyperbolic equations of continuity and momentum. This certainly affects the water quality model through the numerical-cell advective numbers ($\Delta t / \Delta x$ and $\Delta t / \Delta r$), Peclet numbers ($U \Delta t / \Delta x$ and $V \Delta t / \Delta r$), and diffusion numbers ($v_l \Delta t / \Delta x^2$ and $v_l \Delta t / \Delta r^2$) appearing in Eqs (6) and (7). It has been provisionally verified in the literature (Ferziger, 1981) that, although each individual differenced equation from one time level (n) to the next ($n + 1$); namely (6) and (7), is conditionally stable, the two-step ADI algorithm is a stable technique when it applies to the parabolic PDEs with constant coefficients, whereas in the case of transient-flow problems the coefficients change in both time and space. Therefore, the stability criterion clearly depends on the nature of the transient flow. A careful study is required to further refine and clarify the criterion. However, several preliminary runs were conducted to investigate the mesh size effects (in both radial and longitudinal directions) on the numerical convergence. Due to page limitation, not all the results were given here. However, two typical results for radial discretization effect are given in Figs 9 and 10 showing average chemical constituent concentration (by 2-D model) along the pipe 96 s after valve opening. The figures clearly show the proposed 2-D model becomes progressively more accurate as a finer numerical mesh is chosen. However, simulation times naturally increase.

A preliminary study was conducted to investigate the mesh size effect on computational time. For this purpose, the

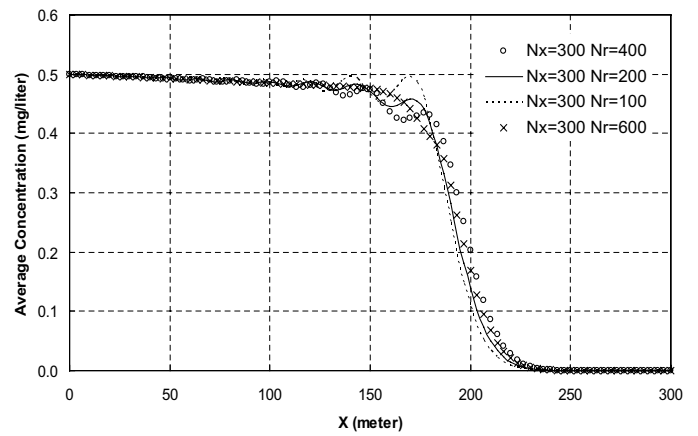


Figure 9 Convergence analysis of 2-D model: results with finer mesh size in radial direction 96 s after valve opening

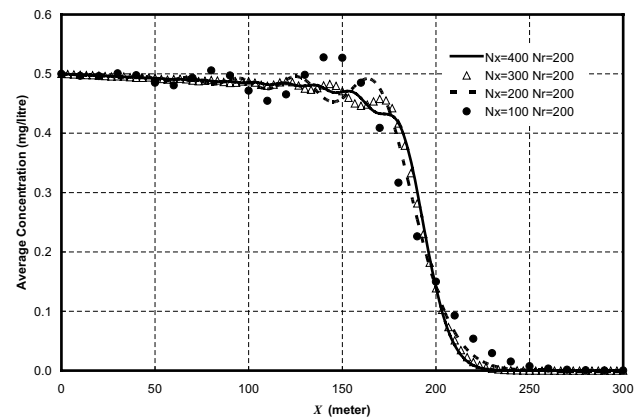


Figure 10 Convergence analysis of 2-D model: results with finer mesh size in longitudinal direction 96 s after valve opening

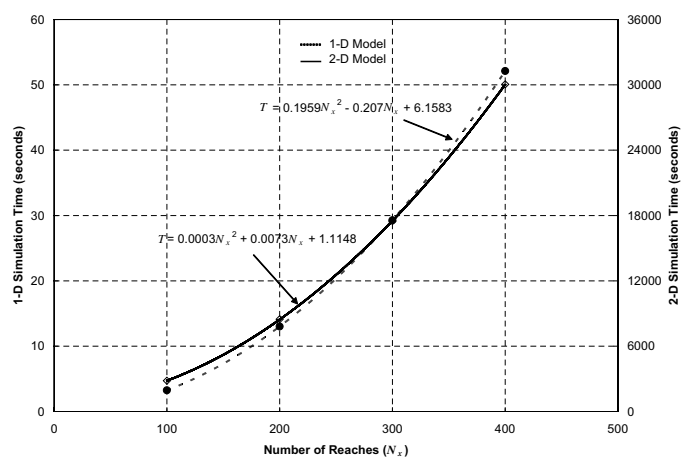


Figure 11 Simulation time for 1-D and 2-D model: effect of mesh size in longitudinal direction (with 350 cylinders in radial direction for 2-D model)

computational times for the reservoir-pipe-valve-reservoir example were recorded for various mesh sizes. The simulations were performed on a DELL INSPIRON-8200 Pentium 4 laptop (1.8 GHz). Figure 11 indicates the influence of number of reaches in longitudinal direction (N_x) on total CPU time required to run both the 2-D (when pipe cross section was divided into 350

cylinders in radial direction) and 1-D models. Clearly decreasing the mesh size increases the simulation time enormously. As expected, although the figure clearly indicates a quadratic increase in CPU time for an increase in number of reaches for both models, the 1-D approach is more efficient regarding computational time. The quadratic relationship is expected and arises through the dual effect of time step (determined using a Courant condition) and the number of reaches.

A similar study was also conducted to determine the dependency of total CPU time on the number of cylinders (N_r) in 2-D model. These results show a linear increase in simulation time by an increase in the number of cylinders ($T = 88.9N_r - 160.0$). However, the number of cylinders is important factor not only in stability of the numerical approach but also for an accurate implementation of the five-region turbulence. Since the five-region turbulence model uses molecular viscosity as the main mechanism for energy dissipation in the viscous sublayer zone, there must be at least one cylinder in this zone.

9 Conclusions

In the context of a WDS design and analysis, water quality problems during transient events have been traditionally modeled using a 1-D representation not only for hydraulic parameters, but also for the time evolving concentrations along the pipeline. 1-D models clearly ignore the variations in both velocity and concentration profiles during unsteady conditions.

Using the five-region turbulence model, a 2-D hydraulic model for transient flow was created and then coupled with a 2-D ADRE for the concentration of chemical constituent. Overall, the study reveals that although in some cases there is qualitatively excellent agreement between the 1-D and 2-D models in average sense, the 2-D model represents a more realistic variation for chemical constituent concentration along the pipe section. The proposed 2-D study showed a strong influence of velocity profile and boundary layer growth on the chemical constituent front evolution; such an influence cannot be directly investigated by a 1-D approach. Since the difference between the concentration of the constituent at the pipe wall and that at the pipe centerline can be considerable in a real WDS, there is a potentially significant advantage to 2-D simulation as opposed to 1-D. In particular, the difference for the pH of water at the pipe wall and that at the pipe centerline may be three or four pH units (AWWARF, 1996). It is planned to explore further implications of these findings on transient water quality in the next stages of this modeling effort.

The current study also shows that although the difference between 1-D and 2-D results at the beginning of the transient event is negligible, it becomes more significant as the time progress highlighting less dispersion for the Taylor's model in the 1-D approach, which was originally developed for a very short and small-diameter but extremely rough pipe for a relatively low-Reynolds-number turbulent flow. Thus, the noticeable difference between the 1-D and 2-D models may reflect an inability in the Taylor's model to produce sufficient dispersion for a

large-diameter and less-rough pipe carrying a fully turbulent flow with large Reynolds number (the case in this study).

A sensitivity analysis on pipe diameter effect showed a faster transient propagation in large diameter systems even though the systems approach the same steady state hydraulic condition. This again highlights the effect of velocity profile, which is not captured in a 1-D approach.

The study reveals a deficiency in the five-region turbulence model to determine energy dissipation in relatively rough pipes. Although it is possible to hydraulically calibrate the model using an equivalent pipe concept, this may cause serious distortions in other parameters. A more sophisticated turbulence modeling is likely needed for the rough pipe cases.

Although the results of the current study exhibited few significant differences between the 1-D and 2-D models for the cross sectional average concentration, there could be some important advantages inherent in a 2-D model over its 1-D counterpart for certain situations such as corrosion and biofilm effects in which the chemical reactions happen mostly at pipe wall.

Unfortunately, the relatively larger execution time for the 2-D simulation model may render its adoption questionable especially when it is used for the analysis of a real and complex WDS with many pipes and devices. Since collectively the pipes in a real WDS are relatively long, a finite difference approach with an explicit scheme for the longitudinal direction, and implicit scheme for the radial direction, converts the ADRE into a tri-diagonal system which, not only can be easily solved for the desired unknowns, but also considerably reduces the computational time. More research is needed to explore the costs and benefits of the 2-D model.

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Appendix

Using the central finite difference discretization scheme, the coefficients in Eqs (6) and (7) were derived as following (the subscripts i and j denote the position of the node in longitudinal and radial directions, respectively and the superscript n denotes the time level):

Intermediate Time Level $n + 1/2$: The scheme is implicit in radial direction but explicit in longitudinal direction, hence:

$$A_1 = \frac{1}{\bar{r}_{j+1} - \bar{r}_{j-1}} \times V_{i,j}^{n+1/2} - \alpha_1 \quad (A1)$$

$$B_1 = \frac{2}{\Delta t} - \beta_1 + K_b \quad (A2)$$

$$E_1 = \frac{-1}{\bar{r}_{j+1} - \bar{r}_{j-1}} \times V_{i,j}^{n+1/2} - \gamma_1 \quad (A3)$$

$$F_1 = \left[\frac{-U_{i,j}^n}{\Delta x} + \alpha_2 \right] \times C_{i+1,j}^n + \left[\frac{2}{\Delta t} + \beta_2 \right] \times C_{i,j}^n + \left[\frac{U_{i,j}^n}{\Delta x} + \gamma_2 \right] \times C_{i-1,j}^n \quad (A4)$$

$$\alpha_1 = \frac{1}{\bar{r}_j (\bar{r}_{j+1} - \bar{r}_j)} \times \left[\frac{\bar{r}_{j+1}}{\bar{r}_{j+1} - \bar{r}_j} \times \Gamma_{i,j+1/2}^{n+1/2} \right] \quad (A5)$$

$$\gamma_1 = \frac{1}{\bar{r}_j (\bar{r}_{j+1} - \bar{r}_j)} \times \left[\frac{\bar{r}_j}{\bar{r}_j - \bar{r}_{j-1}} \times \Gamma_{i,j-1/2}^{n+1/2} \right] \quad (A6)$$

$$\beta_1 = -(\alpha_1 + \gamma_1) \quad (A7)$$

$$\alpha_2 = \frac{1}{\Delta x^2} \times \Gamma_{i+1/2,j}^n \quad (A8)$$

$$\gamma_2 = \frac{1}{\Delta x^2} \times \Gamma_{i-1/2,j}^n \quad (A9)$$

$$\beta_2 = -(\alpha_2 + \gamma_2) \quad (A10)$$

Advanced Time Level $n+1$: The scheme is explicit in radial direction but implicit in longitudinal direction, hence

$$A_2 = \frac{U_{i,j}^{n+1}}{\Delta x} - \alpha_4 \quad (A11)$$

$$B_2 = \frac{2}{\Delta t} - \beta_4 + K_b \quad (A12)$$

$$E_2 = \frac{-U_{i,j}^{n+1}}{\Delta x} - \gamma_4 \quad (A13)$$

$$F_2 = \left[\frac{-V_{i,j}^{n+1/2}}{\bar{r}_{j+1} - \bar{r}_{j-1}} + \alpha_3 \right] \times C_{i,j+1}^{n+1/2} + \left[\frac{2}{\Delta t} + \beta_3 \right] \times C_{i,j}^{n+1/2} + \left[\frac{V_{i,j}^{n+1/2}}{\bar{r}_{j+1} - \bar{r}_{j-1}} + \gamma_3 \right] \times C_{i,j-1}^{n+1/2} \quad (A14)$$

$$\alpha_3 = \frac{1}{\bar{r}_j (\bar{r}_{j+1} - \bar{r}_j)} \times \left[\frac{\bar{r}_{j+1}}{\bar{r}_{j+1} - \bar{r}_j} \times \Gamma_{i,j+1/2}^{n+1/2} \right] \quad (A15)$$

$$\gamma_3 = \frac{1}{\bar{r}_j (\bar{r}_{j+1} - \bar{r}_j)} \times \left[\frac{\bar{r}_j}{\bar{r}_j - \bar{r}_{j-1}} \times \Gamma_{i,j-1/2}^{n+1/2} \right] \quad (A16)$$

$$\beta_3 = -(\alpha_3 + \gamma_3) \quad (A17)$$

$$\alpha_4 = \frac{1}{\Delta x^2} \times \Gamma_{i+1/2,j}^{n+1} \quad (A18)$$

$$\gamma_4 = \frac{1}{\Delta x^2} \times \Gamma_{i-1/2,j}^{n+1} \quad (A19)$$

$$\beta_4 = -(\alpha_4 + \gamma_4) \quad (A20)$$

in which Δt , Δx are the time step and the length of each reach in longitudinal direction. The term \bar{r} is defined as following:

$$\bar{r}_j = (r_j + r_{j-1})/2 \quad (A21)$$

Notation

- a = Acoustic wave speed of pipe wall material (LT⁻¹)
 C = Concentration of a chemical (ML⁻³)
 c = Turbulent fluctuation of a chemical's concentration (ML⁻³)
 C_r = Courant number
 D = Pipe diameter (L)
 D_m = Molecular diffusivity coefficient (L²T⁻¹)
 D_{eq} = Equivalent pipe diameter (L)
 f = Darcy-Weisbach friction factor
 g = Acceleration due to gravity (LT⁻²)
 H = Piezometric head (L)
 i, j = Nodal subscripts in longitudinal and radial directions
 J_x, J_r = Mass flux in longitudinal and radial directions (ML⁻²T⁻¹)
 K_b = Bulk decay/growth coefficient (T⁻¹)
 n = Superscript denotes the time level
 N_x = Number of reaches in longitudinal direction
 N_r = Number of cylinders in radial direction
 x, r = Longitudinal and radial coordinate axis (L)
 t = Time (T)
 T_{tf} = Transient flow time scale (T)
 T_{wq} = Water quality time scale (T)
 U = Longitudinal component of time-averaged velocity (LT⁻¹)
 u = Velocity fluctuations in the longitudinal direction (LT⁻¹)
 V = Radial component of the time-averaged velocity (LT⁻¹)
 v = Velocity fluctuations in the radial direction (LT⁻¹)
 Γ = Turbulent diffusion coefficient (L²T⁻¹)
 ν_t, ν_m = Turbulent and molecular kinematic viscosity coefficients (L²T⁻¹)
 $\Delta t_{tf}, \Delta t_{wq}$ = Time step for transient flow and water quality analysis (T)
 Δx = Mesh sizes in longitudinal direction (L)
 Δr = Mesh sizes in radial direction (L)

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