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Model based investigation of transport phenomena in water distribution networks for contamination scenarios

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Abstract

Water distribution networks (WDNs) are critical infrastructures that are exposed to deliberate or accidental contaminations. The project SmaRT-Online^{WDN} aims to develop an online security management and reliability toolkit for water distribution networks. One task focuses on the contaminant transport modeling. This paper deals with modeling transport processes at T- and cross-junctions. The mixing model depends on the flow conditions, the pipe condition and the crossing geometry. Preliminary results will be presented using computer fluid dynamic (CFD) for 2D and 3D modeling of transport processes for different flow conditions. These results are evaluated in comparison to existing mixing and propagation models.

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Keywords: Water Distribution Networks; CFD; transport model; T-junction mixing; cross-junction mixing; axial propagation model

1. Introduction

Water distribution networks (WDNs) are critical infrastructures that are exposed to deliberate or accidental contaminations. In the immediate future water suppliers will install water quantity and water quality sensors throughout their networks that will provide a continuous and huge stream of data. This allows for the first time to develop a system that is able to monitor and protect WDNs in real-time. Obviously, in case of a toxic contamination, the WDN operators have to react very fast as humans have to be protected against toxic drinking

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water. Hence, the operators are highly interested in getting an answer to these questions very quickly: Where is the contamination source? What impact will the contamination have on the water distribution network? Which actions are necessary (e.g. which main pipes have to be shut)? The SMaRT-Online^{W_{DN}} management toolkit (SMaRT-Online^{W_{DN}} (2013)) aims to give a high quality decision support regarding these questions. The objective of the project SMaRT-Online^{W_{DN}} is the development of an online security management and reliability toolkit for water distribution networks. It combines modules for classification of contamination events, real-time water quantity and water quality, source identification, contaminant plume identification and sensor placement.

The online security management toolkit is based on sensor measurements (hydraulic and water quality sensors) and online hydraulic and transport models and will allow (i) an estimation of the localization of the contamination source and (ii) the simulation of short-time future scenarios in order to estimate the impact of a contamination source. For both tasks the transport model is one of the central modules as the accuracy of predictions (or re-simulations) for the distribution of solute substances throughout the WDN depends on the accuracy of the transport model. Hence, a main objective of research is to enhance the transport model for the use in online simulation. While the general phenomena of transport modeling are well understood (mathematically described by a partial differential equation which models spatio-temporal behavior of diffusion, advection, reactions and sources resp. sinks). However, all actually available software packages for the simulation of hydraulics and water quality in WDN (e.g. EPANET (2013)) are based on a one-dimensional (1D) formulation. Due to that restriction in many cases where the 3D geometry of the WDN has an impact to spreading of substances (e.g. at junctions and crossings of pipes) the 1D description may not be accurate enough.

Hence, in recent years some research has been done in order to improve the performance of 1D transport models. So far axial propagation for the most part is modeled by plug flow. Though this is a good approximation for turbulent flow it does not hold up for laminar and transitional flow. E.g. in Romero-Gomez (2010), Romero Gomes et al. (2008, 2011) a more realistic model of the axial dispersion in 1D-models has been introduced. Furthermore, improvements of the modeling of the mixing behavior in 1D models has been achieved. Classical mixing models used in most simulation software tools (e.g. EPANET) are based on the assumption of complete mixing of the substances. Experimental investigations have shown that for certain flow conditions at cross-junctions and double-T-junctions ideal mixing is not fulfilled (Choi et al. (2008)). Hence some more enhanced approaches have been investigated in order to find a more realistic model to describe an incomplete mixing of substances in 1D transport and flow models (e.g. estimations based on experimental results in AZRED (Choi et al. (2008)), bulk-mixing model implemented in EPANET 2 BAM (Ho (2009))). But in practice it is often difficult to apply these models as they contain one or more parameters, which have to be determined by several experiments for each individual junction. This is not applicable for real world networks which contain hundreds or thousands of junctions. Furthermore, AZRED model does not cover the laminar flow regime.

The objective of the work presented in this paper is to develop a 1D mixing model for laminar mixing of transient contamination pulses in water distribution networks, based on 2D CFD simulations. Future work will extend the investigations to turbulent flow and 3D CFD simulations as basis for the derived 1D mixing models.

The paper is structured as follows. In section 1 some of the most popular mixing models are presented, namely the Complete Mixing Model, the Bulk Advective Mixing Model (BAM) and AZRED. Furthermore, an exemplary statistics on the junctions of the water distribution network (WDN) in Strasbourg is presented. Section 2 introduces the CFD-based method for the derivation of enhanced 1D mixing Models. Simulation Results of Mixing at T- and N-Junctions are presented in section 3. A conclusion and an overview of future work is provided in section 4.

1.1. Mixing Models

In the sequel the most popular mixing models are presented, namely the Complete Mixing Model, the Bulk Advective Mixing Model (BAM) and AZRED.

The *Complete Mixing Model* assumes that mixing in pipe junctions is instant and complete. This means that the concentration of fluid leaving the junction is identical at each outlet pipe. This simple model can be formulated in a single equation for the mass balance of the solute species in the junction as follows:

$$c_{complete} = c_{out,i} = \frac{\sum_{j=1}^n Q_j c_j}{\sum_{j=1}^n Q_j} \quad (1)$$

The concentration of solute leaving each outlet pipe i is given by $c_{out,i} [mol/m^3]$. $c_j [mol/m^3]$ is the concentration of the flow entering the junction with the flow rate $Q_j [m^3/s]$ at inlet pipe $j = 1 \dots n$. Since the fluid is assumed to be incompressible the sum of flows entering the junction equals the sum of flows leaving it. Due to its easy implementation the Complete Mixing Model is often used to determine the spreading of contaminations in water distribution networks, as for example the implementation in EPANET.

Modeling solute mixing in this way however, does not represent the physical process of solute mixing in pipe junctions adequately. That has been established in experiments as well as CFD simulations presented in Ho (2009). It has been shown that for X-junctions in a state of flow as shown in Fig. 1, with adjacent inlet and outlet pipes the results differ significantly from the Complete Mixing Model. These findings lead to the development of the *Bulk Advective Mixing (BAM)* model which is intended to extend the Complete Mixing Model in cases where it lacks precision. The BAM model describes the mixing in X-junctions with adjacent inlet and outlet pipe and equal diameters and is presented in Ho (2009). It is based on the observation that for unequal momentum of the flow in the adjacent pipes a part of the bulk flow crosses over the junction. In respect to this fact the BAM Model assumes that mixing is solely effected by the bulk flow in the junction. Influences like diffusion or turbulent mixing at the flow interfaces are neglected. In effect, where the Complete Mixing Model can be seen as maximum bound for mixing at X-junctions, the BAM Model represents a minimal bound. The state of flow for the BAM Model is defined by the ratio of the inflow rates Q_1/Q_2 and the ratio of the outflow rates Q_3/Q_4 .

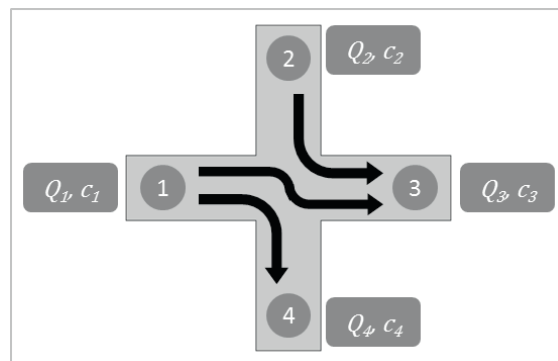


Fig. 1: Definition of state of flow, pipe nomenclature and flow variables for BAM Model.

To calculate the concentration of the fluid at the outlet pipes (c_3 and c_4) we need the known flow rates Q_i at the inlet pipes ($i = 1,2$) and outlet pipes ($i = 3,4$) as well as the concentrations at the inlet c_1 and c_2 . In the first step the flow rate that crosses over the junction has to be determined. To do this the sum of the flow rates of the opposing pipes is defined. The direction with the higher sum is the one that crosses over. For equal pipe diameters the crossing bulk flow can be determined by the difference of the flow in the adjacent inlet and outlet pipes pairs $|Q_1 - Q_4|$ or $|Q_2 - Q_3|$. With these values the concentration of the outlet pipe that is not concerned with the crossing bulk flow is that of the adjacent inlet pipe ($c_4 = c_1$), cf. the flow state depicted in Fig. 1.

The concentration in the outlet pipe with bulk mixing is calculated as the mean value of the adjacent inlet and the crossing bulk flow. In the case of Fig. 1 this results in

$$c_3 = c_{BAM} = \frac{Q_2 c_2 + (Q_1 - Q_4) c_1}{Q_3} \quad (2)$$

As stated before the Complete Mixing Model and the BAM model can be seen as an upper and lower bound. In Ho (2009) it is suggested that a combination of both models could be used to approximate the real mixing process through a weighting factor s . This leads to a final outlet concentration at the mixed outlet pipe of

$$c_{combined} = c_{BAM} + s(c_{complete} - c_{BAM}). \tag{3}$$

The weighted approach implies that the influence of diffusion and turbulent instabilities is constant for all inlet and outlet flow ratios.

The third model called *AZRED* has been developed at the University of Arizona (Choi et al. (2008)). In contrast to the theoretical approach of the BAM Model, this model is based on experimental results and is not bound to cross-junctions. The state of flow is defined by the Reynolds number $Re = U_i D / \nu$ for the inlet and outlet pipes. Here U_i is the average velocity in pipe i , D is the diameter of the pipe and ν is the dynamic viscosity. To be able to describe all flow scenarios at the junction the ratios of Reynolds numbers for the inlets and outlets are introduced.

$$Re_{inlet} = \frac{Re_1}{Re_2}, \quad Re_{exit} = \frac{Re_3}{Re_4} \tag{4}$$

Due to the fact that the *AZRED* model concentrates on junctions with equal pipe diameters this presentation concurs with the relative inlet and outlet flow rates given in Ho (2009). The experiments presented in Choi et al. (2008) show, that in the turbulent flow regime the ratios of the Reynolds numbers and the type of junction are the predominant variables influencing the mixing process. Since the model is based on experimental results the extreme values of the flow rates cannot be determined. This means that in these cases the model is extrapolated.

The objective of our work is to develop a model based on CFD simulations that can give a better description of the mixing process especially for the extreme ratios of the flow rates with a special focus on the laminar mixing process.

1.2. Exemplary Statistics on Junctions of a Water Distribution Network

To get an idea of the relevant junction types exemplary statistics on the junctions of the WDN of Strasbourg have been done. These statistics are based on a 24 hour simulation of the hydraulic model of Strasbourg and its surroundings implemented in PORTEAU (Porteau (2013)). The hydraulic model is represented by a reduced network with 12,730 pipes, 10,460 junctions and a complete length of 964 km is used. A more detailed model with over 52,000 pipes is in preparation to give a more complete picture. The values of interest for the CFD model are the dominant junction types and the relevant flow conditions.

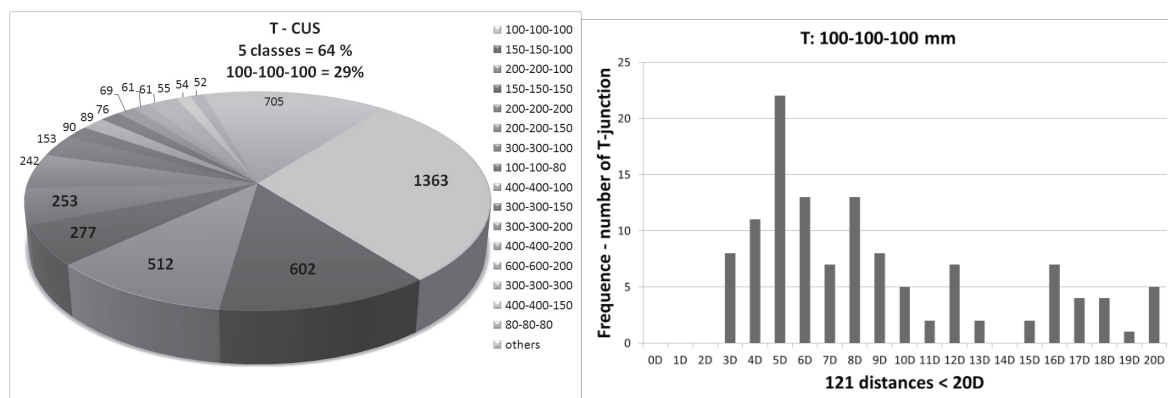


Fig. 2: (a) classes of T-junctions by diameters of branches in Strasbourg network model; (b) number of distance between two junctions in diameter proportion.

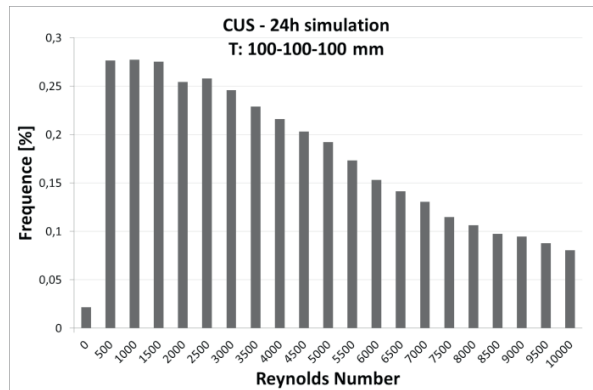


Fig. 3: Reynolds algebraic values around T 100-100-100 mm for one-day simulation.

Fig. 2 (a) shows the frequency of pipe diameters for all T-junctions in the network. We can see that the diameter of $d = 100 \text{ mm}$ is dominant. 29 % of the T-junctions have equal pipe diameters of $d = 100 \text{ mm}$, further junctions with identical pipe diameters account for 44 % of all T-junctions. Fig. 2 (b) shows a statistic on the relevant distance between two T-junctions. From literature we know that a contamination can be considered completely mixed after a pipe length of around $l < 20d$. In the diagram we see that the most common distance between two T-junctions is about $l < 5d$. In Fig. 3 the frequency Reynolds numbers at all T-junctions is depicted over a simulated period of 24 hours. It is evident that the laminar flow regime is relevant in wide areas of the network. The statistics support the approach to simulate the laminar mixing process in different configurations of T-junctions.

2. CFD-based Method for the derivation of enhanced 1D mixing Models

The objective of our work is to set up a one-dimensional transport model for water distribution networks based on CFD simulations. In the following section we describe the basic models, model parameters and the method for evaluation of the CFD simulation.

2.1. CFD Model for T- and N-Junctions with Contamination Source

The governing equations for the flow in the two and three-dimensional domain are described by the Navier-Stokes equations. In the case of solute mixing in pipe junctions we can apply certain simplifications to their general formulation. The fluid observed in the studies is incompressible and body forces are neglected (same elevation at the junction scale). Due to the fact that we simulate time dependent mixing in a steady state flow, time derivatives can be disregarded. Under these conditions the Navier-Stokes equations can be stated by the conservation equation and the momentum equation as follows:

$$\rho \nabla \cdot \mathbf{u} = 0 \quad (5)$$

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)]. \quad (6)$$

The constant density is given by ρ , the pressure by p and the velocity field by \mathbf{u} .

The transport equation for modeling the distribution of a conservative contaminant (i.e. no biological degradation, no chemical reactions) is given by the convection and diffusion equation for single-phase transport.

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c) + \mathbf{u} \cdot \nabla c = 0 \quad (7)$$

Here c gives the concentration of the contamination. The diffusivity of the contaminant is given by the diffusion coefficient D . The velocity field for the convective transport is determined by the Navier-Stokes equations. Since we do not consider any sources inside the domain the right hand side is equal to zero. The inlet of a contamination source is considered by a time dependent boundary condition, which is described in the sequel.

The geometric domain for the T-junction is depicted in Fig. 4 (a). For further proceedings a nomenclature for naming the pipes is defined here. For the 3-way junction the main inlet pipe is referred to by ①, the main outlet pipe is referred to by ③ and the secondary pipe is referred to by ②. Fig. 4 (b) shows the domain for the N-junction. The following nomenclature can also be applied for the U-junction with equilateral secondary pipes. In a 4-way junction the main inlet ① and the main outlet ③ are defined the same way as at the T-junction. Additionally, the secondary inlet pipe is referred to by ② and the secondary outlet pipe is referred to by ④. Based on the investigations of CUS the pipe diameter is defined as $d = 100 \text{ mm}$.

The boundary conditions for the fluid flow in the T-junction are given by the flow rate at the inlet pipe ① and the main outlet pipe ③. At the secondary outlet pipe ② a free pressure outlet boundary condition is set. Since this model is set in laminar flow conditions an entrance length of $L_{entr} = 6,2m$. For the concentration only for the main inlet pipe a contamination impulse is set. To simulate a contamination injected into the concentration has a Gaussian distribution focused at the pipe center. For the temporal distribution of the pulse a Gaussian distribution is chosen as well. The boundary conditions for the 4-way junction are chosen similarly. The only difference is that the flow rate secondary inlet pipe is defined.

2.2. Model Parameters

The parameters for the physical models and the parameter studies are presented in this section. For the physical model the material properties of water are defined by the density $\rho = 998.21[\text{kg}/\text{m}^3]$ and the dynamic viscosity $\mu = 1,002[\text{Pa} \cdot \text{s}]$, for room temperature of 20°C . The contamination is defined by sodium chloride. The density is defined as constant and equal to that of water, the diffusivity is set to $D_{NaCl} = 1,5 \cdot 10^{-9}[\text{m}^2/\text{s}]$.

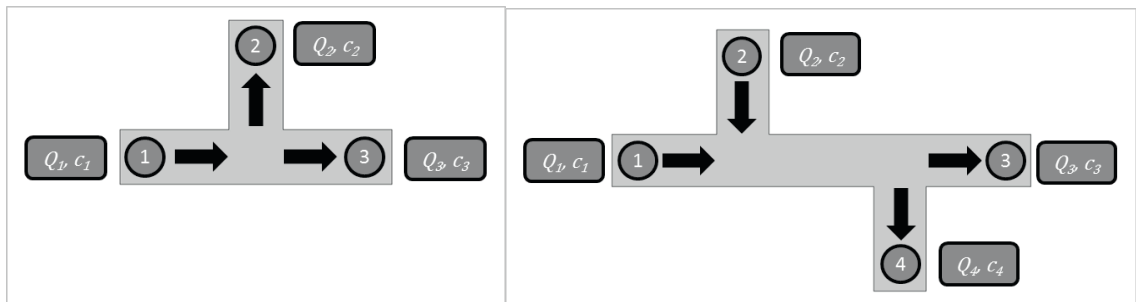


Fig. 4: (a) Nomenclature for pipes, definition variables and state of flow for T-junction.; (b) Nomenclature for pipes, definition variables and state of flow for N-junction

In the mixing models described in the introduction two ways are defined to describing the state of flow in a 4-way junction. In the BAM model it is defined by the ratio of inlet flow rates Q_1/Q_2 and the ratio of the outlet flow rates Q_3/Q_4 . In AZRED the flow state is defined by the ratios of the Reynolds numbers. Since both models are intended for junctions with equal pipe diameters these ratios are basically the ratios of flow velocities at the inlet and the outlet. In respect to the fact that the approach to modeling mixing in junctions presented in this paper may be extended for junctions with unequal pipe sizes we define the relative inlet and outlet flow rate ratios

$$Q_{in,rel} = \frac{Q_1}{Q_{total}}, Q_{out,rel} = \frac{Q_3}{Q_{total}} \quad (8)$$

with

$$Q_{total} = Q_1 + Q_2 = Q_3 + Q_4. \quad (9)$$

For the T-junction only the relative outlet flow rate is defined. The ratios are each defined at one of the inlets and one of the outlets and divided by the total flow rate. This way a linear scale can be introduced to describe the flow state in a junction. Further it is possible to describe the extreme ratios of the flow rates where one pipe has no bulk flow either as 0 or 1.

For N-junctions a third factor of interest is introduced. It is defined by the dimensionless distance L between two T-junctions, $L = l/d$. Here l stands for the distance between the two T-junctions. It is set in relation to the pipe diameter d . The statistics from CUS presented before give a good measure for the range of interest of the dimensionless distance of $3 < L < 20$.

2.3. Method for the Evaluation of the transient mixing Behavior

Our model simulates the time dependent mixing in stationary flow conditions. This is due to the fact that we simulate contamination pulses, which seems close to reality. The time dependent concentration at the inlet pipe is defined as Gaussian pulse as shown in Fig. 5 (solid line). The resulting time dependent concentrations at the outlet pipes for a T-junction are also shown in Fig. 5 (for $Q_{out,rel} = 0.75$). Due to this time dependent scenario, which is much closer to reality than stationary conditions, the mixing process is evaluated by means of the inflowing/outflowing mass cumulated over time.

A useful description for the time dependent mixing can be given by the mass fractions. This method evaluates the mass of the contaminant leaving each outlet pipe in relation to the total mass of the contaminant entering the junction. This approach makes it possible to evaluate the results from the existing mixing models, since the mass fraction is calculated through the integral over time of the concentration distribution.

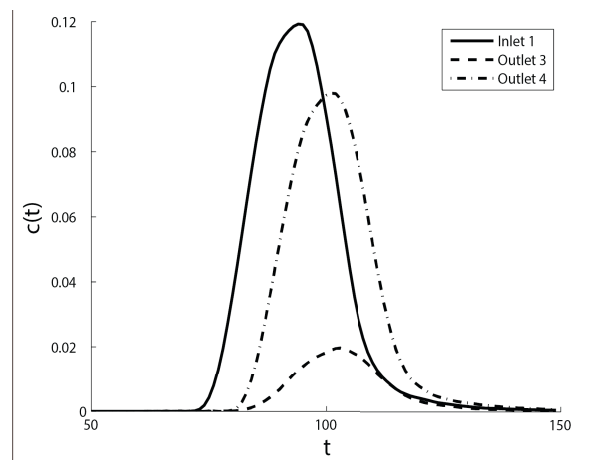


Fig. 5: Time dependent concentrations at a T-junction for inlet (solid line) and outlets ($Q_{out,rel} = 0.75$).

For the given values of the concentrations of the contaminant $c_{cont,i}$ and the flow rates Q_i at each pipe, the mass fraction w for the stationary models can be calculated by

$$\dot{m}_{cont,i} = Q_i c_{cont,i} \tag{10}$$

$$w_{stationary,i} = \frac{\dot{m}_{cont,i}}{\dot{m}_{cont,total}} \tag{11}$$

with $i = 3,4$. Here $\dot{m}_{cont,total}$ stands for the total rate of contaminant entering the junction. Since the concentrations and flow rates are constant over time the mass fraction can be calculated by the bulk flow. For the CFD model the bulk flow is given through a time dependent distribution similar to that in. The mass fraction can there for be calculated by

$$w_{transient,i} = \frac{\int \dot{m}_{cont,i}(t)dt}{\int \dot{m}_{cont,total}(t)dt} \tag{12}$$

3. Simulation Results of Mixing at T- and N-Junctions

Fig. 6 shows the results of the simulations for a T-junction. It shows the mass fraction w for the main and secondary outlet pipe in percent over the relative flow rate for the outlet $Q_{out,rel}$. The diagram contains the results for the two dimensional CFD simulation and the results for ideal mixing obtained by the Complete Mixing Model.

In the Complete Mixing Model the mass fractions directly follow the flow rates at the outlet pipes. As a result we can see that the mass fractions at the outlets are linked proportional to the relative outlet flow rates. For the CFD model the results match those of the Complete Mixing Model in the extreme values of the relative outflow rate and the central point of $Q_{out,rel} = 0,5$. Due to the shape of the concentration pulse modeled in our simulation we have higher mass fraction for the outlet with the higher flow rate. The difference in the mass fraction between the CFD model and the ideal mixing is shown in the second diagram of Fig. 6. This difference reaches a maximum of about 10% at the relative flow rates of $Q_{out,rel} = 0,25$ and $Q_{out,rel} = 0,75$.

The results of our CFD simulations for the X-junction and a N-junction with a dimensionless distance between the T-junctions of $L = 5$ are presented in Fig. 7 (a) and (b). For the state of flow across the junction, defined by the relative inflow $Q_{in,rel}$ and outflow $Q_{out,rel}$, the mass fraction leaving the junction through the primary outlet pipe w_3 is depicted. In the same way the results attained by the BAM Model and AZRED are shown in Fig. 8 (a) and (b). The diagram for the BAM Model was created from the model described in the introduction. The diagram for AZRED is based on data from the implementation in EPANET.

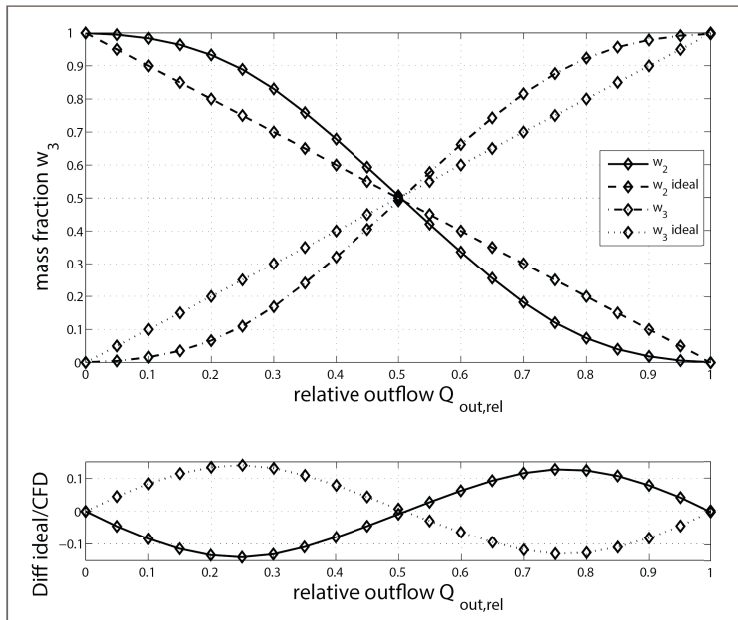


Fig. 6. Simulated and Ideal mass fractions at a T-junction for $Q_{out,rel} = 0 \dots 1$.

For the extreme values of $Q_{in,rel}$ and $Q_{out,rel}$ all models show similar behavior. For the relative inflow rate $Q_{in,rel} = 0$ the mass fraction is $w_3 = 0$ since no contaminant is injected into the junction. In the case of the relative inflow rate $Q_{in,rel} = 1$ we can see that the behavior of the T-junction is reproduced. This means the T-junction could be interpreted as a special case of a 4-way junction. For the relative outflow rate $Q_{out,rel} = 0$ the mass fraction is $w_3 = 0$ here this can be explained by the fact that we have no flow rate at the main outlet pipe. Contrary to that the mass fraction is $w_3 = 1$ for the relative outflow rate $Q_{out,rel} = 1$ due to the fact that the flow exits the junction at a single pipe. For the point at $Q_{in,rel} = 0, Q_{out,rel} = 1$ the value cannot be defined properly. In our model we set the mass fraction to zero.

If we compare Fig. 7 (a) and (b) we can identify the influence of the distance between the two T-junctions. While the X-junction has a relative sharp separation between mixing and no mixing, this area is smoothed for the N-junction. This can be explained by the mixing that occurs in the pipe between the two junctions. Simulations show that longer distance between the junctions result in better mixing. For longer distances L the model approaches the Complete Mixing Model.

When we compare the two diagrams for the X-junction Fig. 7(a), Fig. 8 (a) and Fig. 8 (b) we can confirm what we have expected. The three models generally show good accordance. In the area around $Q_{in,rel} + Q_{out,rel} = 1$ we can see better mixing for the CFD model than in the BAM Model since BAM neglects some mixing effects. In the comparison between the CFD model and AZRED we can see even stronger mixing for AZRED. This can be explained by the fact that AZRED is a model for turbulent mixing.

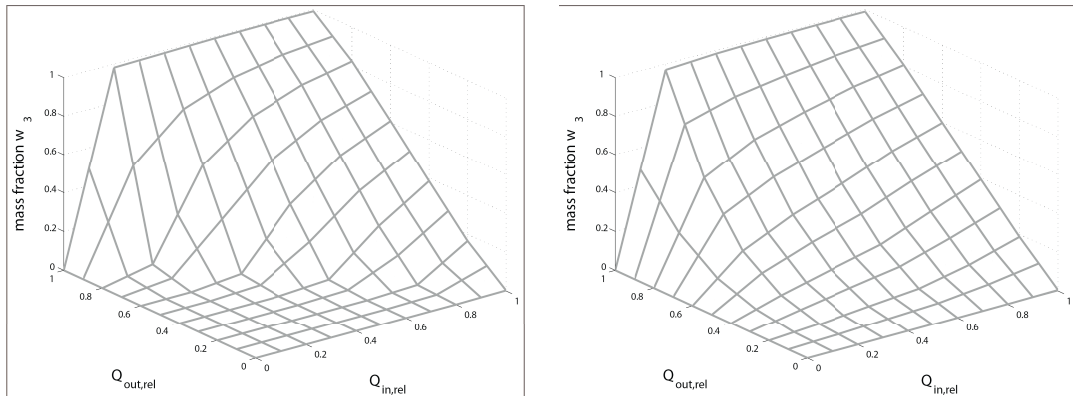


Fig. 7: mass fraction w_3 at main outlet pipe for $Q_{in,rel} = 0 \dots 1$ and $Q_{out,rel} = 0 \dots 1$. (a) CFD ($L=0$); (b) CFD ($L=5$)

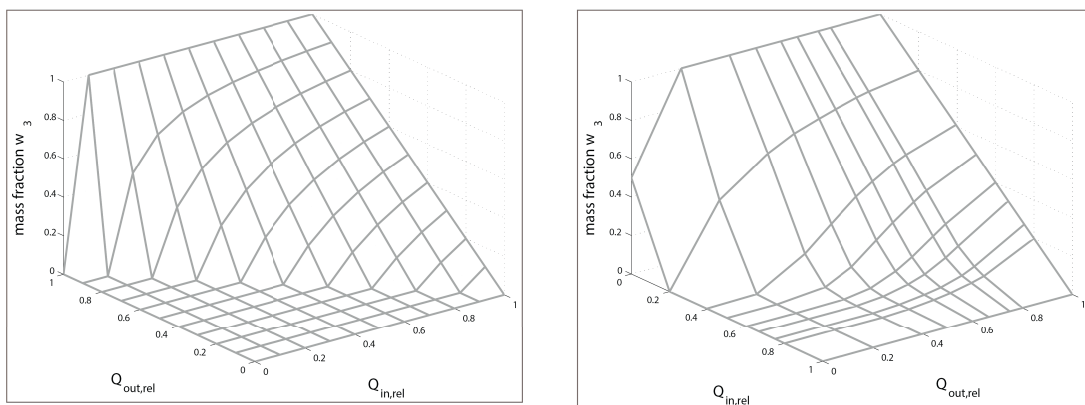


Fig. 8: mass fraction w_3 at main outlet pipe for $Q_{in,rel} = 0 \dots 1$ and $Q_{out,rel} = 0 \dots 1$. (a) BAM ($L=0$); (b) AZRED ($L=0$)

During our investigations we have seen that the mass fractions do not give a comprehensive description of the solute transport. Fig. 6 shows the course of the concentration at each pipe of the junction. Through the laminar transport along the pipe the profile degraded from the perfect Gaussian shape defined in the boundary conditions. This effect is also known as axial dispersion and can be modeled as an axial dispersion reactor Hart et al. (2013), Sun et al. (2009). The influence of axial dispersion is not modeled in our approach yet.

4. Conclusion and future work

In this work we have investigated the mixing behavior of several types of junctions (T, X and N junctions) based on a 2D CFD model in the laminar flow regime. A close to reality transient contamination scenario has been assumed (pulse-like inflow of contamination). We have seen that for the X-junction the CFD based approach is comparable to the BAM Model and AZRED. With the CFD based approach slight improvements compared to BAM models are achieved due to consideration of diffusion. Regarding N-junctions (which are not covered by BAM), the CFD based approach in the laminar regime is more accurate than AZRED, as in AZRED these values are extrapolated from turbulent regime. Regarding T-junctions, for certain flow conditions the CFD based approach has a deviation of more than 10 % compared to the simple ideal mixing mode. The T-junctions are not considered in AZRED model, hence a comparison with AZRED is not possible.

A general advantage of our approach is that even extreme values of the relative inflow and outflow are considered. This is a weakness of AZRED which extrapolates results for such extreme inflow / outflow conditions.

The work on the mixing model will be continued in various directions. First, the investigations will be extended to transitional and turbulent flow regime. Second, a 3D CFD model will be used as basis for the derivation of the 1D mixing model. Furthermore, more complex junctions will be investigated (e.g. junctions with different pipe diameters). Non-constant boundary conditions, a slow varying flow rate, will also be tested. During the ongoing SMaRT-Online^{WDN} project the resulting 1D model will be implemented in a hydraulic solver and will be validated in experiments at a medium sized test network.

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