

LAGRANGIAN METHOD FOR SIMULTANEOUS PROPAGATION OF WATERBORNE SUBSTANCES IN WATER DISTRIBUTION NETWORKS

G. R. Munavalli**, **M. S. Mohan Kumar***

** Former Research scholar, Dept. of Civ. Engrg., Indian Institute of Science, Bangalore 560 012, India. Presently, Selection Grade Lecturer, Dept. of Civ. Engrg., Walchand College of Engrg., Sangli 416 416, India. Email: gurumunavalli@yahoo.co.in

*Associate Prof., Dept. of Civ. Engrg., Indian Institute of Science, Bangalore 560 012, India. Fax: (080) 3600404, Email: mismk@civil.iisc.ernet.in

ABSTRACT

The maintenance of specified residual chlorine within the distribution system is essential as a protective measure against the probable contamination. But the chlorine levels depend on the amounts of organic matter and bacterial content present in the water. Thus the concentration of these waterborne substances viz. chlorine, organic matter and bacterial content present in the water are related with each other. In the present study, simplified interrelated formulations are developed to represent the various governing processes to simulate the concentration of these substances. The resulting formulation consisting of a set of differential equations is solved using the modified Lagrangian time driven approach that was earlier used to simulate the propagation of single substance within the distribution system. The model is developed incorporating the above formulations and is able to predict the concentrations of multiple water borne substances and also the water age. The application of the model is illustrated for a real life distribution network to simulate the above-mentioned water borne substances. The chlorine concentrations are found to be dependent on the substrate content, wall reaction parameter and water age. The suitability of the model in tracking the spread of the contaminant, which has intruded into the system at any location within the distribution system, is also illustrated. For the network studied, it is observed that more the substrate the higher is the biomass growth resulting in lower chlorine concentrations. Thus the model presented in this paper is of immense help to the water supply authorities.

Key Words: Chlorine, Distribution system, Microbial quality, Substrate

1. INTRODUCTION

The microbial quality of water can be attained either by reducing the natural organic matter in the water or using the disinfectants. It is difficult to reduce the organic concentration to a value that will prevent the microbial growth. But considering the current practice of water treatment in India, the organic matter

(however small may be the concentration) is bound to be present in the treated water. Hence the latter option is practiced widely by various means to ensure microbial quality within the distribution system. The disinfection process through chlorination is more common. But being a strong oxidizing agent chlorine reacts with variety of waterborne substances and undergoes decay. Natural organic matter that are extracted from living and decaying vegetation is one these substances which interact with chlorine and thereby reducing its concentration. The compounds contributing to natural organic matter include humic and fulvic acids, polymeric carbohydrates, proteins and carboxylic acids. The possible presence of microbial content may also contribute to the reduction of chlorine concentration in water. Bacterial growth occurs at the expense of an organic or inorganic substrate. The rough surfaces encountered in metallic pipes provide the shelter for bacteria against the disinfectant action thereby enhancing their growth. Thus the concentration of these substances viz. organic, chlorine and microbial contents are interrelated with each other.

The addition of appropriate amount of chlorine is critical, as it must be kept below certain levels because of concerns about formation of carcinogenic disinfection by-products within the distribution system. Therefore the amount of disinfectant that is added into the distribution system may be inadequate to destroy microbes and prevent bacterial regrowth, particularly if much of the disinfectant is consumed by the corrosion by-products at the pipe wall. Factors which promote bacterial survival in chlorinated water supplies include attachment to surface, bacterial aggregation, age of the biofilm, encapsulation and choice of disinfectant (free chlorine or monochloramine) (LeChevallier [1]). Disinfection of drinking water does not result in complete sterilization. With large volumes of water being treated, no disinfection process can result in the complete elimination of pathogens or indicator organisms. Given the presence of nutrients, some regrowth is theoretically possible (Haas [2]). However, it is required to prevent the bacterial regrowth and supply the drinking water free from bacterial contamination to the consumers.

To get an engineering insight into the regrowth phenomenon within the distribution system, it would be useful to develop a transport model capable of predicting spatial and temporal variation of organic carbon, bacterial content and disinfectant residual within a distribution system. The developed model is intended to be useful in identifying and monitoring the potential locations of bacterial regrowth in the system. Also the spread of these components in case of contaminant intrusion through the cross connections can be simulated throughout the system by using the model developed.

It can be seen from the literature that the modeling of bacterial growth within a distribution system is done by two types of deterministic models. The two

categories utilize the concepts of attachment-detachment processes [SANCHO (Servais et al. [3])] and biofilm formation [PICCOBIO (Dukan et al. [4])] respectively. Lu et al. [5] presented a mathematical model that accounts for simultaneous transport of substrates, disinfectants and microorganisms to predict substantial changes in quality of distributed water. This model does not account for the substrate utilization and biomass growth in the bulk flow. But it is essential to include these in modeling the simultaneous transport of substrate, biomass and disinfectant.

The basic criteria to be adopted to develop a transport model that can predict the bacterial regrowth is to express the processes of the bacterial growth, attachment, detachment, substrate consumption and disinfectant action in bulk flow and at pipe wall through a simple mathematical expressions. The available water quality models are limited primarily to the prediction of single substance. To simulate the substrate utilization, growth or decay of biomass (bacterial content) and disinfectant (chlorine) decay spatially and temporally within the distribution system the development of a dynamic reaction transport model is necessary.

2. DYNAMIC REACTION TRANSPORT MODEL FORMULATION

The simplified expressions representing the various components need to be coupled with a robust hydraulic model. The dynamic hydraulic model, which simulates the water velocity, pressure and height of water in storage tanks within a distribution system, developed in this study, is used for the development of the multicomponent model. The flow in the pipes is considered to be advection dominated (plug flow) which is common for the normal operating conditions in a distribution system. For the water quality model, the Lagrangian Time Driven Method (TDM) (Liou and Kroon [6]) is extended to handle the multicomponent reaction transport.

2.1 Hydraulic Model

The hydraulic model, which computes the flows in the pipes of the system, is a prerequisite for the development of any water quality model. In the present work an available steady state hydraulic simulation model (Niranjana Reddy [7]) is modified to handle the extended period simulation and the modified model is applied to generate the dynamic flows in pipes. The modifications also include the modules for the simulation of water age and source trace.

2.2 Water quality model

The following equations represent the advective reactive movement of substrate, biomass and disinfectant (chlorine) along the length of a pipe i . Though

not explicitly represented, all the component concentrations used in the following equations are functions of space and time within a pipe i .

Bulk flow:

Substrate:

$$\frac{\partial S_{bi}}{\partial t} + v_i \frac{\partial S_{bi}}{\partial x} = -\mu \frac{S_{bi}}{k_s + S_{bi}} \left[X_{bi} e^{-k_{inact} C_{bi}} \right] - \frac{k_{fsbi} (S_{bi} - S_{wi})}{r_{hi}} + a [k_{mort} + k_{cl} C_{bi}] X_{bi} \quad (1)$$

Living biomass:

$$\frac{\partial X_{bi}}{\partial t} + v_i \frac{\partial X_{bi}}{\partial x} = Y\mu \frac{S_{bi}}{k_s + S_{bi}} \left[X_{bi} e^{-k_{inact} C_{bi}} \right] + k_{shear} X_{wi} - [k_{mort} + k_{cl} C_{bi}] X_{bi} - k_{fix} X_{bi} \quad (2)$$

Chlorine:

$$\frac{\partial C_{bi}}{\partial t} + v_i \frac{\partial C_{bi}}{\partial x} = -k_{b1,i} C_{bi} - \frac{k_{fci} (C_{bi} - C_{wi})}{r_{hi}} \quad (3)$$

where, $k_{b1,i}$ is given by (Kiene et al. [8])

$$k_{b1,i} = \frac{1.8 \times 10^6}{3600} \left[\frac{S_{bi}}{0.3} \right] e^{-\left(\frac{6050}{T+273} \right)} \quad (4)$$

Wall zone:

The reactions in wall zone among the components occur within an immobile layer. But the reactions such as substrate utilization and biomass growth are similar to the earlier bulk case with reduced effect of chlorine action on biomass activity. The following expressions represent the reactions occurring in the wall zone for substrate, biomass and chlorine in pipe i .

Substrate:

$$\frac{\partial S_{wi}}{\partial t} = -\mu \frac{S_{wi}}{k_s + S_{wi}} \left[X_{wi} e^{-k_{inact} C_{wi}} \right] + \frac{k_{fsbi} (S_{bi} - S_{wi})}{r_{hi}} + a k_{lysis} \left[k_{mort} + \frac{k_{cl} C_{bi}}{k_{r1}} \right] X_{wi} \quad (5)$$

Living Biomass:

$$\frac{\partial X_{wi}}{\partial t} = Y\mu \frac{S_{wi}}{k_s + S_{wi}} \left[X_{wi} e^{-\frac{k_{inact} C_{wi}}{k_{r2}}} \right] + k_{fix} X_{bi} - \left[k_{mort} + \frac{k_{cl} C_{wi}}{k_{r1}} \right] X_{wi} - k_{shear} X_{wi} \quad (6)$$

Chlorine:

$$\frac{\partial C_{wi}}{\partial t} = -\frac{k_{w1,i} C_{wi}}{r_{hi}} + \frac{k_{fci} (C_{bi} - C_{wi})}{r_{hi}} \quad (7)$$

(For notations please refer nomenclature)

At the nodes where two or more pipes meet, the mixing of fluid is considered to be complete and instantaneous. The water parcels leaving such nodes will carry the

constituent concentration that is the flow-weighted average of concentrations coming from the incoming pipes.

2.2 Lagrangian Solution Methodology

TDM is a Lagrangian time-based approach, which tracks the fate of discrete parcels of water as they move along the pipes and mix together at junctions between fixed-length time steps. These water quality time steps are typically much shorter than the hydraulic time step to accommodate the short times of travel that can occur within pipes. This method breaks the system into segments, and tracks the concentration and size of a series of non overlapping segments of water that fill each link of the network. TDM approach is extended herein for the simulation of multiple water borne substances. The following steps occur in this method:

- 1) Initially each pipe in the network is divided into a mobile (bulk) and an immobile (wall) segment. The quality of mobile segment equals the initial quality assigned to the downstream node.
- 2) For each water quality time step:
 - a) The reacted concentrations of all the substances in a mobile segment have to be determined considering the substances from the immobile segment in the wall zone associated with this mobile bulk flow segment.
 - b) At each node, a cumulative account is kept for the total mass of each substance and flow volume entering from the most downstream mobile segment of inflow pipes. The volume contributed from each pipe equals the product of its flow rate and the water quality time step. If this volume exceeds that of the most downstream segment then that segment is destroyed and the next one in line behind it begins to contribute its volume. The contributions from outside sources are added to the quality values at the nodes. Then the water from incoming pipes is blended together to compute new values of water quality at each node using the flow-weighted equation. The quality in the storage tanks is updated using a complete mixing model.
 - c) New mobile segments are created in pipes with flow out of each node, reservoir, and tank. The mobile segment volume equals the product of the pipe flow and the water quality time step. The water quality of these new segments is equal to the new quality value computed for the upstream node. Excessive generation of mobile segments is controlled by the creating new segments only when the new node quality differs in concentration of any substance by a specified tolerance from that of existing most upstream segment in the outflow pipe. If difference in quality is below the tolerance then the size of the current most upstream segment in the outflow pipe is simply increased by the volume flowing into the pipe over the time step.

- Next, it is required to rearrange the immobile segments in the wall zone corresponding to the bulk segment volumes of water. In other words the number of immobile wall segments should be made equal to the number of mobile bulk segments. In doing so, it is essential to redistribute the mass/concentration of components between old and new immobile wall segments so that the mass balance is achieved between the two segments. The process of redistribution is shown in Fig. 1, which illustrates the state of the segments before and after creation of new bulk segments and redistribution of mass/concentration. An efficient algorithm is developed to redistribute the mass/concentration between old and new wall segments.
- d) The above process is repeated for the next water quality time step until the next hydraulic change is encountered.
 - 3) At the start of the next hydraulic time step the order of segments in any pipes that experience a flow reversal is switched. Otherwise no other adjustment is necessary.
 - 4) The process is terminated when the total simulation time is reached.

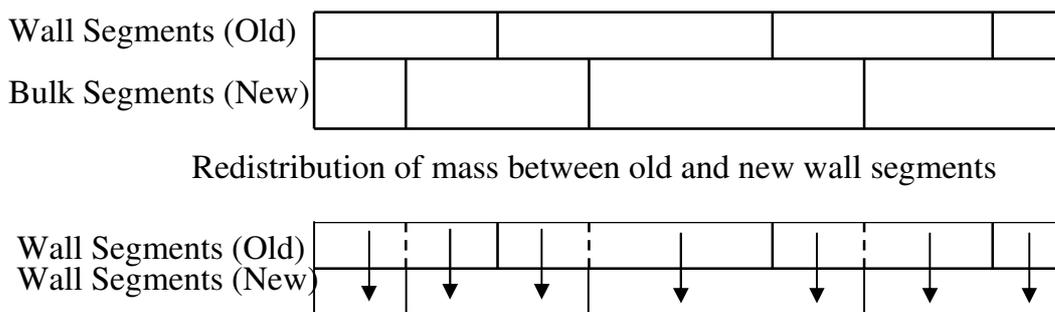


Figure 1. Redistribution of mass between old and new wall segments

3. MODEL APPLICATION: RESULTS AND DISCUSSION

The application of the model discussed above is illustrated using a real life network configuration and hypothetically assumed dynamic operating conditions. Also, the application of the model to track the contaminant being spread due to its intrusion at any node in the system. The network is analyzed for two different cases. In the first case, it is assumed that the water leaving the treatment plant is free from biomass. And the components such as substrate and chlorine are simulated. The simulation is carried out till such a period at which the repetitive pattern of these components emerges. In the second case, a contaminant intrusion through a cross connection at some node in the system is assumed in the established conditions of the first case and the various components are simulated. The node at which the contaminant enters the system is modeled as a flow paced water quality source node. The contaminant entering the system is assigned with the assumed values of substrate and biomass concentrations. The spread of the

contaminant within the distribution system can be studied by using the results of the model.

Example Network

The application of the model is illustrated using the water transmission main network of Bangalore city in India. The details of the system are given in the reference Munavalli and Mohan Kumar [9]. To summarize briefly, the whole system is grouped based on the age of the pipes in to three zones and the network is shown in the Figure 2. The pipes 1 to 36, 37 to 71 and 72 to 94 with Hazen-Williams Coefficient (HWC) of 106.90, 127.50 and 103.60 (Datta and Sridharan [10]) form the three groups respectively.

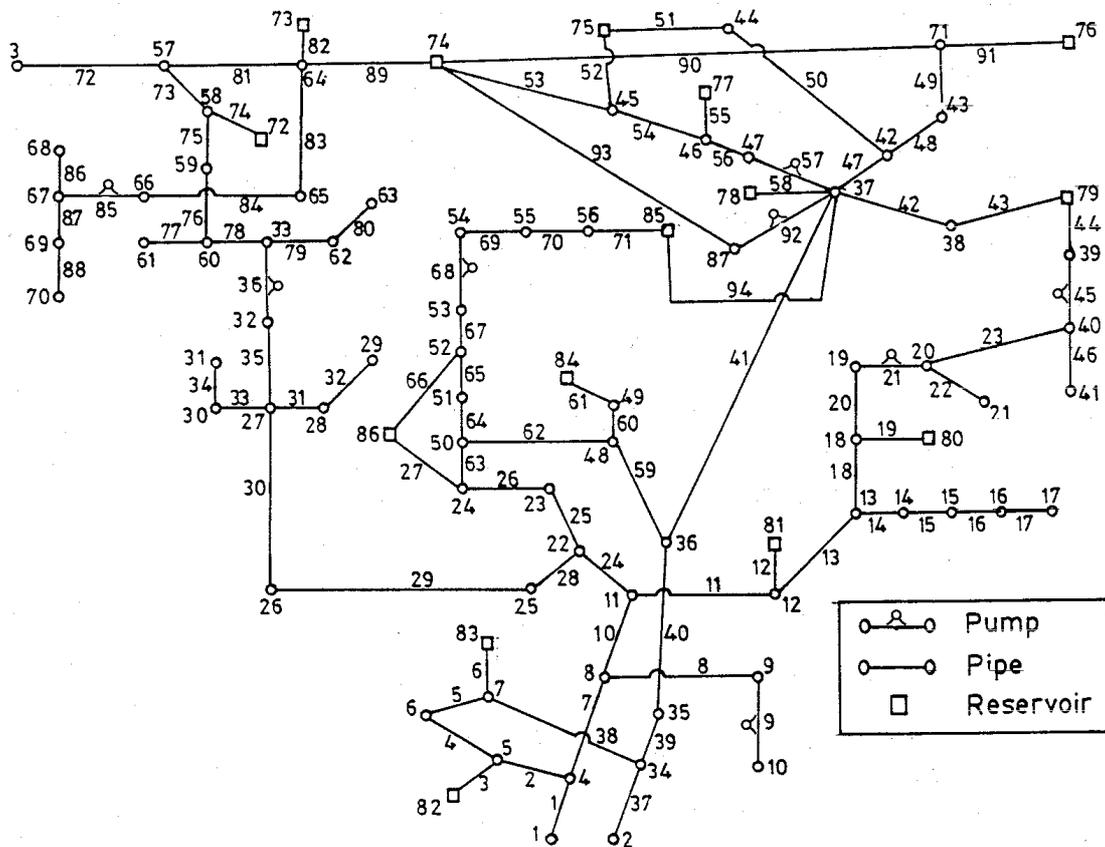


Figure 2. Schematic of Bangalore Water Transmission Main Network

The first-order wall reaction parameters assigned are 0.75 m/d, 0.50 m/d and 1.0 m/d for the three groups of pipes respectively. A constant chlorine concentration of 0.75 mg/L is assumed to be injected from all the three sources of supply, whereas the total organic carbon in the three supplies is assumed to be 2 mg/L, 2 mg/L and 1 mg/L respectively.

Table 1: Demand Patterns for Example Network

Period	Hourly Demand Flow Patterns (m ³ /s)				
	Pattern 4	Pattern 5	Pattern 6	Pattern 7	Pattern 8
1	0	0	0	0	0
2	0	0	0	0	0
3	0	0	0	0	0
4	0	0	0	0	0
5	0	0	0	0	0
6	0	0	0	0	0
7	0.053	0.042	0.189	0.179	0.2
8	0.053	0.042	0.189	0.179	0.2
9	0.053	0.042	0.189	0.179	0.2
10	0.053	0.042	0.189	0.179	0.2
11	0.053	0.042	0.189	0.179	0.2
12	0.053	0.042	0.189	0.179	0.2
13	0	0	0	0	0
14	0	0	0	0	0
15	0	0	0	0	0
16	0	0	0	0	0
17	0	0	0	0	0
18	0	0	0	0	0
19	0.053	0.042	0.189	0.179	0.2
20	0.053	0.042	0.189	0.179	0.2
21	0.053	0.042	0.189	0.179	0.2
22	0.053	0.042	0.189	0.179	0.2
23	0.053	0.042	0.189	0.179	0.2

Table 2: Nodes with Demand Patterns (Example Network)

Pattern	Node
1	10, 17, 21, 29, 41, 61, 63
2	68, 70
3	31
4	30, 6
5	14, 16
6	28
7	33
8	44
9	54
10	55, 69
11	60
12	62

The system is made to behave dynamically by applying the varying demand flow patterns at various nodes in the network. The demand patterns 1, 2, and 3 have constant hourly demands of 0.0631 m³/s, 0.021 m³/s and 0.0315 m³/s throughout the simulation period of 24 hour. Table 1 shows the other demand patterns applied and Table 2 represents the nodes with their corresponding patterns. The nodes 72 to 86 have unknown consumptions and are determined by the forward simulation hydraulic analysis.

Case (i)

The reaction transport model is run for a simulation period of 3 days during which the repetitive pattern of concentrations is established. A quality time step of 3 min and a zero concentration tolerance for all the three substances are used. The comparative results of chlorine and substrate concentrations simulated by the model at nodes 27, 63, 70, and 85 are shown in Figs. 3 (a) and 3 (b) respectively. The results shown in these figures represent the concentrations in the last cycle time (48 h to 72 h) of the simulation period. It can be seen from these figures that the nodes (27, 63, 85) having higher substrate concentrations are contributed more by the sources 1 and 2, whereas node 70 being contributed by source 3 has lesser substrate concentration.

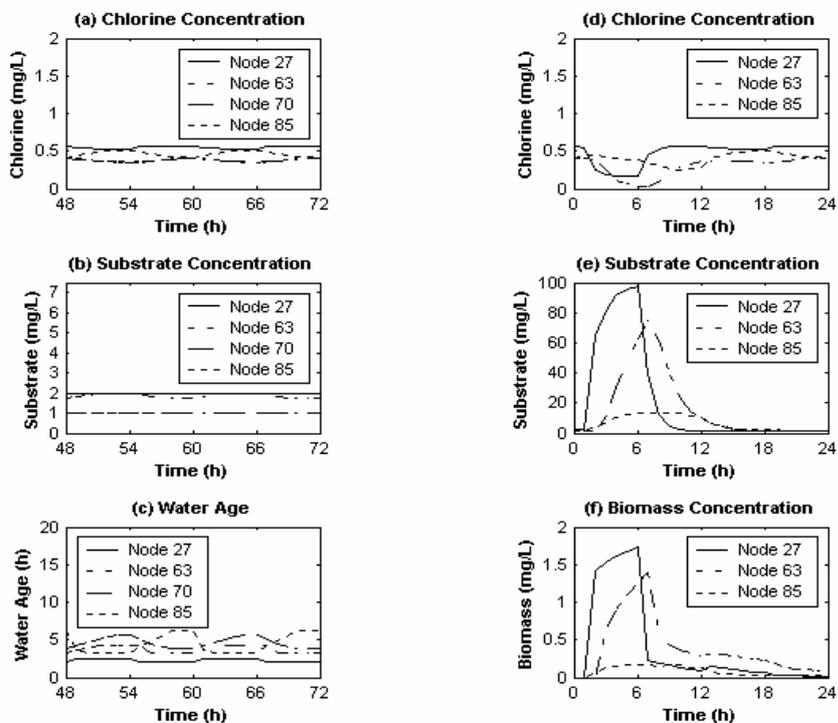


Figure 3: Results of Case (i) and Case (ii)

The chlorine concentrations are comparatively higher for the nodes 27 and 85 even though the substrate levels are higher at these nodes. This is due to the lower wall reaction parameters associated with the sources 1 and 2. The node 70 has lower chlorine concentrations due to its association with higher wall reaction rate pipes. Further, the effect of water age on chlorine levels can be seen in the Fig. 3 (c) the nodes 63, 70 and 85. Thus it can be summarized that the chlorine concentrations depend on the substrate content, wall parameter and water age.

Case (ii)

In this case the disturbances caused by the contaminant intrusion in the established steady substance concentrations generated in Case (i) are studied. The disturbances are represented in the form of changes in substrate concentrations with respect to Case (i). The contaminant having 100 mg/L of substrate and 2 mg/L of biomass is assumed to be entering the system at the node 22 for duration of first six hours in a period of 24 h. And spreading of the contaminant is studied for a typical 24 h simulation period. The results at the nodes 27, 63, and 85 are represented in Figs. 10 (d) and 10 (e) (for chlorine and biomass concentrations) and 10 (f) (for substrate concentrations). It can be seen from these figures that the above nodes, which are on the downstream side of the intrusion point, are affected to varying degree of influence. A general observation for all the nodes presented in figures is that more the substrate the higher is the biomass growth resulting in lower chlorine concentrations.

4. CONCLUSIONS

An integrated hydraulic and water quality forward simulation model is developed for the simulation of water borne substances. The model formulated is solved using Lagrangian time driven approach that divides the pipe into mobile (bulk) and immobile (wall) zones. The mass redistribution process is introduced at every quality time step so that mobile segments are in reference to the corresponding immobile segments. The model is flexible enough to represent the bulk chlorine decay as a function of organic carbon. The applicability of the model is illustrated using a real life distribution network. It is found that the model can properly simulate the substrate, chlorine and biomass concentrations. The capability of the model to represent the spread of contaminant intrusion is also illustrated. Thus the model is useful to water supply agencies for simulating multiquality of water within their distribution system.

NOMENCLATURE

a = fraction of dead biomass converted to substrate after analysis

C_{bi} = chlorine concentration in bulk in pipe i
 C_{wi} = chlorine concentration at wall zone in pipe i
 $k_{b,li}$ = first order bulk reaction parameter for pipe i
 k_{cl} = chlorine induced mortality coefficient
 k_{fci} = mass transfer coefficient of chlorine in pipe i
 k_{fix} = attachment coefficient
 k_{fsbi} = mass transfer coefficient of substrate in pipe i
 k_{inact} = inactivation constant of living biomass (bulk) by chlorine
 k_{mort} = natural mortality coefficient
 k_{r1} = resistance factor of attached bacteria versus free bacteria to chlorine induced mortality
 k_{r2} = resistance factor of attached bacteria versus free bacteria to chlorine induced inactivation
 k_s = half saturation constant
 k_{shear} = detachment coefficient
 $k_{w,li}$ = first order wall reaction parameter for pipe i
 r_{hi} = hydraulic radius of pipe i
 S_{bi} = substrate concentration in bulk in pipe i
 T = temperature
 v_i = velocity of flow in pipe i
 X_{bi} = living biomass concentration in bulk in pipe i
 X_{wi} = living biomass concentration at wall zone in pipe i
 Y = growth yield of bacteria
 μ = maximum substrate utilization rate

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