### COMPARISON OF SIMULATION TOOLS FOR BACTERIA REGROWTH MODELING IN WATER DISTRIBUTION SYSTEMS

# SIMULĀCIJAS METOŽU SALĪDZINĀJUMS BAKTĒRIJU PIEAUGUMA MODELĒŠANAI ŪDENS SADALES SISTĒMĀS

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Bacteria transport and proliferation in water distribution systems, no doubt, should be contained. Simulation tools are required for effective monitoring of bacteria concentration in pipelines. The issue of bacteria proliferation attracted attention of many authors. There were several attempts to develop a comprehensive model for simulation of bacteria growth in drinking water distribution networks. Factors influencing bacteria growth were also addressed. There are some difficulties hampering development of effective simulation tools. Bacteria growth is influenced by many factors, so most important are to be selected as it is virtually impossible to take them all into account.

In previous publications the model proposed by Zhang et al (2004) has been considered. It has been shown that the model can be embedded into EPANET-MSX software and the EPANET-MSX results were compared to simulation results obtained by a validated Fortran routine. Good agreement was found.

The present paper checks the validity of the model embedded into EPANET-MSX software for a small network. The results obtained by EPANT-MSX model are compared with the results obtained by Zhang et al. (2004) using split-operator method. It is shown that the results are comparable that gives hope that the Epanet-MSX model can be used as an effective simulation tool for modeling bacteria regrowth in water distribution systems.

#### Introduction

Safety and security of drinking water is of no doubt an important issue. Good bacteriological water quality must be maintained all the time. However, keeping water in distribution systems free of contaminants is not an easy challenge. There are various sources of contamination, including cross-connections, treatment plant breakthrough, installation and repair of pipes, hydrant repairs, pipe flushing events [1]. After September, 11 attacks there are rising fears of possible deliberate contamination of water distribution network of a city. Moreover, many attempts and threats to contaminate an urban drinking water supply system have already taken place [2].

So there is a need for protective means to enhance security of water distribution systems. Effective tools are necessary that would enable us to detect a contamination, to determine scale of contamination spread and finally to de-contaminate the network. The present paper focuses on efforts of developing a simulation tool allowing to model proliferation and growth of bacterial contamination of a network.

There have been many efforts to develop an accurate model for water quality [6]. However, it has never been an easy task. A comprehensive simulation tool for bacterial contamination spread in a water distribution network must include both a hydraulic model and bacteria regrowth model.

A model of bacteria concentration dynamics including convection, diffusion, deposition and detachment of bacteria as well as reproduction and mortality is proposed in [8]. Bacteria growth factor is considered to be influenced by chlorine, substrate concentration and temperature. Equations governing growth of bulk and attached bacteria as well as chlorine and substrate are included into the model.

The equations of the model [8] are:

$$\frac{\partial X_b}{\partial t} = -v \frac{\partial X_b}{\partial x} + D_d \frac{\partial^2 X_b}{\partial x^2} + \mu_b X_b + \frac{k_{det} X_a v}{R_h} - k_d X_b - k_{dep} X_b (1.1)$$

$$\frac{\partial X_a}{\partial t} = \mu_a X_a - k_{det} X_a v - k_d X_a + K_{dep} X_b R_h \tag{1.2}$$

$$\frac{\partial S}{\partial t} = -v\frac{\partial S}{\partial x} + D_d\frac{\partial^2 S}{\partial x^2} - \left(\frac{1}{Y_g\beta}\right)\left(\frac{\mu_a X_a}{R_h} + \mu_b X_b\right)$$
(1.3)

$$\frac{\partial Cl_2}{\partial t} = -v \frac{\partial Cl_2}{\partial x} + D_d \frac{\partial^2 Cl}{\partial x^2} - k_b Cl_2 - \frac{k_w}{R_h}$$
(1.4)

where  $X_b$  is bulk bacteria concentration,  $X_a$  is attached bacteria concentration, S is substrate concentration,  $Cl_2$ is chlorine concentration, v is velocity,  $D_d$  is diffusion coefficient,  $\mu_b$  and  $\mu_a$  are growth coefficients for free and attached bacteria respectively, defined by (1.5),  $k_{det}$ is detachment coefficient,  $k_d$  is bacteria mortality factor,  $R_h$  is hydraulic radius,  $Y_g$  is growth yield coefficient of bacteria,  $\beta$  is number of bacteria that are produced for each milligram of organic carbon in cell biomass,  $k_b$  is first-order kinetic constant for chlorine decay in bulk water and  $k_w$  is zero order rate constant for the wall reaction.

The bulk bacteria growth coefficient  $\mu_a$  has the form:

$$\mu_{a} = \begin{cases} \mu_{max,a} \left(\frac{S}{S+k_{s}}\right) \exp\left[-\frac{Cl_{2}-Cl_{2,ta}}{Cl_{2,c}}\right] \exp\left[-\left(\frac{T_{opt}-T}{T_{o}pt-T_{i}}\right)^{2}\right] & \text{for } Cl_{2} > Cl_{2,ta}, \\ \mu_{max,a} \left(\frac{S}{S+k_{s}}\right) \exp\left[-\frac{Cl_{2}-Cl_{2,ta}}{Cl_{2,c}}\right] & \text{for } Cl_{2} \le Cl_{2,ta}. \end{cases}$$
(1.5)

The attached bacteria growth coefficient  $\mu_b$  is expressed in similar way.

More detailed description of the model can be found in [8].

Table 1. Parameters of the pipe

Parameter	Value	Units
Length of the pipe Diameter of the pipe Flow	120 150 7.7 - 27.3	${ m meters} \ { m millimeters} \ { m m}^3/{ m h}$

The model (1.2)-(1.4) was embedded into a Fortran routine and experimentally validated in [3]. However there are difficulties in applying the model for a complex water distribution network due to lack of means of combining a hydraulic model with the regrowth model. Recent release of the multi-species extension for the Epanet software (Epanet-MSX) provides a basis for combining a hydraulic model and a regrowth model. The software allows to use data of the hydraulic simulation for a network as the input data for a mathematical model of bacteria regrowth.

The objective of the current study is to adapt the model proposed in [8] to the Epanet-MSX software and test it. The testing procedure includes comparing results obtained with the Epanet-MSX model for a pipe to the results obtained with the validated Fortran routine mentioned in [3] and then comparing Epanet-MSX model results for a small network to the results obtained for the same network in [8] using the alternating split-operator method.

#### Methods

Simulations have been performed both for a straight pipe segment and for a small network. Totally, results of the Epanet-MSX model were compared with the results of two other simulation tools: the data obtained by the validated Fortran model [3] and the data provided in [8], obtained with the help of the alternating split-operator method. All the tools are based on the model [8]. A remark should be made of the Epanet-MSX model. The equations proposed in the model [8] are partial as convection and diffusion are involved. Unfortunately, the Epanet-MSX software deals with ordinary differential equations only. Therefore, diffusion term must be neglected. Convection term, in its turn, is not necessary as the hydraulic model is calculated by Epanet software and the results are used for the transport model. The Epanet-MSX model has been tested against other simulation tools in two steps. First, simulations have been performed for a 120m long pipe. The parameters of the pipe are presented in Table 1. Two cases are considered. A normal operation of the pipe containing substrate, chlorine and bacteria (assumed to be non-dangerous) is modelled in the first case. An intrusion with high bacteria inflow into a clean pipe is modelled in the second case. The parameters of the model in both cases are shown in Table 2 and Table 3.

Table 2. Conditions for the normal operation

Parameter	Boundary value	Initial value	Units
Free Bacteria	$10^{8}$	$10^8$	cell/m <sup>3</sup>
Biofilm	$10^{7}$	$10^7$	cell/cm <sup>2</sup>
Substrate	0.4	0.4	mg/l
Chlorine	1.0	1.0	mg/l

Table 3. Conditions for the intrusion

Parameter	Boundary value	Initial value	Units
Free Bacteria	$10^9$	0.0	cell/m <sup>3</sup>
Biofilm	0.0	0.0	cell/cm <sup>2</sup>
Substrate	0.4	0.0	mg/l
Chlorine	1.0	0.0	mg/l

For the case on normal operation, typical values of free and attached bacteria, substrate, chlorine concentration for water distribution networks are selected. Bulk bacteria concentration in several water networks of Europe and North America was found to be in the range of  $10^7 - 10^9$  cell/m<sup>3</sup> [7]. Concentration of cell/m<sup>3</sup> is used for simulations. Biofilm  $10^{8}$ concentration is assumed to be  $10^7$  cell/cm<sup>2</sup> in compliance with data of [4, 5]. Concentration of BDOC (substrate) in water distribution systems of the USA is reported to be up to 1 mg/litre [7]. The value of 0.4 mg/litre is chosen for the simulation of normal network operation. Chlorine concentration is set to 1 mg/litre. The BDOC and chlorine concentration also complies with [8]. The initial conditions for the case of normal operation are the same as boundary conditions.

For the case of intrusion it is assumed that water with bacteria concentration ten times higher than the normal concentration enters the pipe. Initial conditions for the pipe are all zeroes. That corresponds to the case when the pipe is clean from bacteria, substrate and chlorine. Simulation for the both cases are performed for a pipe. Two solution tools are used: the Fortran routine [3] and the Epanet-MSX model. The obtained results are compared to check how close are the results of the Epanet-MSX model to the results of the validated Fortran model and whether the Epanet-MSX model may be suitable for simulation of bacteria regrowth in a pipe.

Simulation of bacteria behavior and dynamics in a small water network is performed as well. A small hypothetical network used in [8] is used for simulation (Figure 1). The network model has been created in the Epanet-MSX software environment and simulations were performed. The obtained results were compared to the results provided in [8]. The model is solved in [8] with the alternating split-operator algorithm. Solving the model under the same conditions by the Epanet-MSX method allows to compare the two methods and verify if Epanet-MSX environment is suitable for bacteria growth simulation in a network.



Figure 1. Small hypothetical network used for simulation.

3

4  $\mathbf{5}$  1200

1000

2000



Figure 2. Chlorine concentration in nodes.

0.063

0.009

0.036

Table 4. Hypothetical network					
Link	Length (m)	Diameter (mm)	Flowrate (m3/h)	Velocity (m/	
1	1000	200	15.3	0.135	
2	800	150	4.0	0.063	

200

150

150

7.1

0.6

2.3



Figure 3. Bulk bacteria concentration in nodes.

The parameters of the network are shown in Table 4. The simulation for a small network was performed under the same initial and boundary conditions as in [8], that is free bacteria concentration at the entrance is  $10^4$  cell/litre, substrate concentration is 0.4 mg/litre, chlorine con centration is 1.0 mg/litre. The initial conditions for all other pipes and nodes are zeroes.

Duration or simulation for the pipe was 120 hours, for the network – 60 days. Simulation for the pipe was performed for three various velocity values.

# SCIENTIFIC JOURNAL OF RIGA TECHNICAL UNIVERSITY Series - Computer Science - Boundary Field Problems and Computer Simulation - 51<sup>st</sup> thematic issue 2009 Results and discussion the obtained results give basis for consideration

Bacteria concentration values for the pipe obtained from the Epanet-MSX model agree well with the values obtained from the Fortran model. Good agreement between the results is seen for three flow velocities and for both normal operation and intrusion cases. As the Fortran model has been validated experimentally [3], the obtained results give basis for consideration that the Epanet-MSX model might be suitable for predicting growth and proliferation of bacteria in a pipe. The results are presented in Figure 4. The charts show bacteria concentration in the pipe after 120 hours of operation. The concentration is averaged over the pipe length.



Figure 4. Results of bacteria regrowth obtained with EPANET and Fortran models for various cases: a) normal operation of a pipe, biofilm concentration; b) normal operation of a pipe, bulk bacteria concentration; c) intrusion into a pipe, biofilm concentration; d) intrusion into a pipe, bulk bacteria concentration. Concentration units are cell/m<sup>3</sup> for bulk bacteria and cell/cm<sup>2</sup> for biofilm.

The results for the network obtained with the Epanet-MSX model are shown in Figure 2 for chlorine and in Figure 3 for bulk bacteria. The results agree well with the results provided in [8], given the first-order kinetic constant for chlorine decay by wall demand value is taken in reasonable range (in this study the value 0.0048 is used instead of 2.6, as originally proposed, as such a high value leads to instant decay of chlorine). Good agreement of the results obtained by different tools is in favor for consideration that both tools are suitable for simulation.

So, the Epanet-MSX model might be enough accurate to be used for simulation of bacteria regrowth in water networks.

However, the ultimate challenge is to compare the results obtained with the Epanet-MSX model to experimental results. As experiments with urban water distribution networks entail technical difficulties, a pilot device is needed simulating a part of a water distribution network. Bacteria concentration data obtained by measurements at the pilot device ought to be compared with the results from the model.

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#### Juhna T., Nazarovs S., Rubulis J. Simulācijas metožu salīdzinājums baktēriju pieauguma modelēšanai ūdens sadales sistēmās

Baktēriju transports un izplatīšanās ūdens padeves sistēmās ir jākontrolē. Simulācijas rīki ir nepieciešami, lai varētu veikt efektīvu baktēriju koncentrācijas monitoringu. Daudzi autori pētīja baktēriju augšanu ūdensvados. Tika mēģināts izstrādāt modeli baktēriju augšanas simulācijai ūdensvados. Tika pievērsta uzmanība arī faktoriem, kas ietekmē baktēriju augšanu. Diemžēl, ir dažādas problēmas, kas apgrūtina modeļa izveidošanu. Piemēram, baktēriju augšanu ietekmē daudzi faktori, tātad jāizvēlas svarīgākie, jo pilnīgi visus faktorus ņemt vērā nav iespējams.

Iepriekšējos pētījumos tika izskatīts modelis, ko piedāvāja Zhang et al (2004). Tika paradīts, ka modeli var iekļaut Epanet-MSX programmatūrā un rezultāti, kas bija iegūti ar EPANET-MSX programmatūras palīdzību tika salīdzināti ar rezultātiem no validētas Fortran programmas. Salīdzinājums parādīja, ka rezultāti ir stipri līdzīgi.

Šī pētījuma ietvaros tika pārbaudīta EPANET-MSX modeļa pielietojamība nelielam ūdensvadu tīklam. Rezultāti, kas tika iegūti ar EPANET-MSX programmas palīdzību tika salīdzināti ar rezultātiem, ko ieguva Zhang et al (2004). Tika parādīts, ka rezultāti ir salīdzināmi, tātad var cerēt, ka EPANET-MSX modeli varēs izmantot baktēriju izplatīšanās modelēšanai arī ūdensvadu tīklos.

# Юхна Т., Назаров С., Рубулис Я. Сравнение методов симуляции роста бактерий в водопроводных системах

Распространение бактерий в водопроводных системах, без сомнения, должно быть ограничено. Для эффективного мониторинга и моделирования концентрации бактерий в трубах необходимы инструменты, позволяющие симулировать рост бактерий. Задача о создании таких инструментов рассматривалась многими авторами. Было несколько попыток разработать модель для симуляции роста бактерий в системах подачи питьевой воды. Также изучались факторы, влияющие на рост бактерий. Однако существуют некоторые трудности, препятствующие разработке эффективных методов симуляции. На рост бактерий влияют многие факторы. Все их включить в модель практически невозможно, поэтому важно выбрать те из них, которые оказывают наибольшее влияние.

В предыдущих публикациях рассматривалась модель, предложенная в публикации Zhang et al (2004). Было показано, что модель можно включить в программу EPANET-MSX и результаты были сравнены с результатами, полученными с помощью экспериментально проверенной модели, реализованной на языке Fortran. Было обнаружено хорошее соответствие результатов.

Настоящая работа имеет своей целью проверку применимости модели, включенной в программу EPANET-MSX, для небольшой водопроводной сети. Результаты, полученные с помощью модели, были сопоставлены с результатами, полученными в публикации Zhang et al (2004). Показано, что результаты сравнимы. Это дает надежду, что модель, включенная в программу EPANET-MSX, может быть использована как эффективный инструмент симуляции роста и распространения бактерий в системах подачи питьевой воды.