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## BOUNDARY FIELD PROBLEMS AND COMPUTER SIMULATION
## DATORMODELĒŠANA UN ROBEŽPROBLĒMAS

# APPLICATION OF IMSL LIBRARY AND EPANET-MSX ENVIRONMENT FOR COMPARISON OF BACTERIA GROWTH SIMULATION RESULTS

# IMSL BIBLIOTĒKAS UN EPANET-MSX VIDES PIELIETOJUMS BAKTĒRIJU IZPLATĪŠANĀS SIMULACIJU REZULTĀTU SALĪDZINĀŠANAI

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## Introduction

Bacterial contamination of tap water is of no doubt an important issue that needs to be addressed. Growth of bacteria and biofilm in water distribution systems must be restrained. So, effective means are necessary that would allow monitoring and controlling bacteria growth in pipes. Development of necessary methods requires thorough research work that can be facilitated by the possibility to run simulations of bacteria development in water distribution systems using a mathematical model.

The main issue impeding successful development and application of a model is the presence of large variety of different parameters affecting bacteria growth, making it almost impossible to model. The processes (e.g. bacteria growth in water and biofilm, chlorine effect on bacteria, bacteria adsorption and desorption) which are affecting bacterial regrowth in water distribution networks are not completely understood. The bacterial regrowth is difficult to model by a heuristic approach such as multiple regression analysis of observations made at monthly basis at various sites through a distribution networks. However, there were several attempts to develop a comprehensive deterministic model that would take into account main factors and describe bacteria proliferation in water distribution systems. Examples of bacterial regrowth models now available are SANCHO [1] and PICCOBIO [2].

Zhang et al. [3] proposed a model for bacteria growth that includes factors such as convection, dispersion, deposition and detachment of bacteria as well as reproduction and mortality. Bacteria reproduction, in its turn, is affected by chlorine, substrate concentration and temperature. The model contains equations governing growth of bulk and attached bacteria as well as chlorine and substrate concentrations.

However there is lack of efforts aiming to compare models with each other and test reproducibility of the results obtained with different models. The present paper makes an attempt to compare results obtained with the model proposed by Zhang et al. [3], solved by IMSL library of Fortran and the same model with excluded dispersion term, solved by EPANET-MSX (Multi-Species eXtension) platform [4].

EPANET [5] is a well-known simulation system for water distribution networks that allows modeling of flow and pressure distribution in a drinking water network. EPANET allows finding of a hydraulic solution for ramified water distribution systems. Recently a multi-species extension to the EPANET called EPANET-MSX has been released. EPANET-MSX extension allows to model reactions and behavior of different species in water. In fact, the model developed by Zhang et al. [3] can be embedded into the EPANET-MSX and a solution for a whole network can be found.

However EPANET-MSX is not free of disadvantages. The issue that definitely needs to be addressed is the dispersion term that, unfortunately, is not included into EPANET-MSX. According to Zhang et al. neglecting of dispersion may introduce significant error into results.

The purpose of this research is to evaluate error that may arise when the dispersion term is not taken into account and to test reproducibility of results obtained by two different methods. Simulation results for two models – one with dispersion term and one without it – have been compared.

**Methods and results**

The solution for mathematical model consisting of equations proposed by Zhang et al. [3] has been obtained in two different ways. First, solution of the partial differential equations has been found by means of Fortran IMSL library, using DMOLCH routine. The routine has been already applied by Juhna et al. [6]. Then the solution of the equations excluding advection and dispersion terms has been obtained by EPANET-MSX (the advection term, however, has been taken into account in hydraulic model that is a part of EPANET-MSX platform). The results were compared and the difference in the results was evaluated.

The simulation was performed for a pipe that is 1000 m long with 100 mm diameter. The flow velocity was 0.5 m/s.

The Fortran model had the following initial and boundary conditions:

**Table 1**

Initial and boundary conditions for Fortran model

| Parameter, units | Designation | Initial value | Boundary value (left boundary) |
|---|---|---|---|
| Free (bulk) bacteria, cells/mL | Xb | 0 | 1000 |
| Attached (biofilm) bacteria, cells/cm$^2$ | Xa | 10000 | 0 |
| Substrate, mg/L | S | 0 | 0.25 |
| Chlorine, mg/L | Ch | 0 | 0 |

The EPANET-MSX model had the same boundary and initial conditions.
In addition a Neumann boundary condition was applied at the right end of the pipe for Fortran model (the derivative is kept constant). The boundary condition is required in order to find a particular solution for the partial differential equations used in the model.
Fortran model implies that the modeled region (the pipe) is divided into a certain number of nodes and concentration of every species is calculated in each node. EPANET-MSX in turn provides and average value across the pipe for every specie. In order to make the results comparable the pipe in Fortran model was divided into 120 nodes and an average of nodes 2-119 was calculated.
The results obtained for 20, 120, 420 and 720 hours of simulation are presented in Fig. 1 and Fig. 2 below.

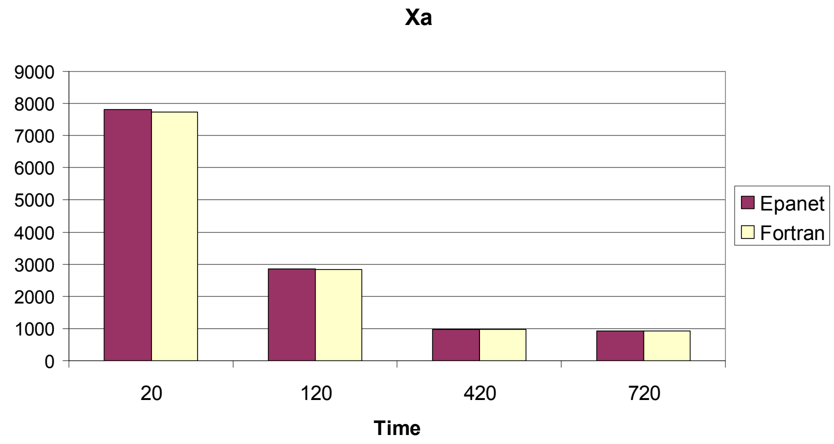


**Fig. 1.** Attached bacteria concentration (Xa, cells/cm$^2$) calculated with EPANET-MSX and Fortran

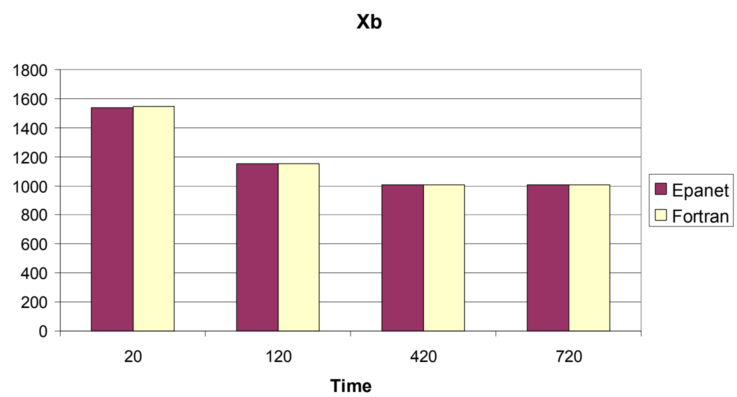


**Fig. 2.** Bulk bacteria concentration (Xb, cells/mL) calculated with EPANET-MSX and Fortran

As it can be seen from the results, the difference between Fortran and EPANET results is less than one per cent. This allows drawing two important conclusions.
First of all, as EPANET-MSX and Fortran use two different numerical methods for integration of the differential equations and still the results are similar, then, probably, integration errors in both methods are kept minimal. Moreover, it should be stressed that EPANET MSX neglects dispersion terms and nevertheless allows getting the same results as Fortran that does include dispersion. Therefore, dispersion might not be a significant factor for flows at velocities typical for distribution networks.
More thorough research also indicated that bacteria concentration follows logical trends in both cases (e. g. bacteria concentration growth is suppressed if substrate is low and vice versa).

## Conclusion

The two methods of finding solution for the equations, a bacterial regrowth model is based on, have been compared with each other. The two methods are: application of EPANET-MSX platform and IMSL library of Fortran. The results demonstrate a good reproducibility for the two methods. As the EPANET-MSX method does not take dispersion into account, and still the results obtained with this method well agree with Fortran results, one can conclude that dispersion term might not be significant, in some cases.

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**Juhna T., Kolyshkin A., Nazarovs S., Rubulis J. IMSL bibliotēkas un Epanet-MSX vides pielietojums baktēriju izplatīšanās simulāciju rezultātu salīdzināšanai**

*Risinājums baktēriju izplatīšanās problēmai ūdensvados tika meklēts vairākos pētījumos. Dažādi autori mēģināja izveidot modeļus, kas dotu iespēju simulēt baktēriju augšanu dzeramā ūdensvada tīklos un noteikt kādi faktori ietekmē baktēriju attīstību. Baktēriju augšanu ietekmē daudzi faktori, kas apgrūtina aprēķinu un ietvert tos visus modelī nav iespējams.*
*Tomēr eksistē modeļi, kas no vienas puses ņem vērā vissvarīgākos faktorus, no kuriem ir atkarīga baktēriju izplatīšanās, un no otrās puses ir pietiekoši kompakti, lai viņus varētu pielietot vidēja līmeņa datoriem, kas ir pieejami laboratorijās. Tomēr jāveic pētījumi ar mērķi salīdzināt dažādus modeļus un pārbaudīt rezultātu atkārtojamību gadījumā, ja rezultāti tiek iegūti ar dažādām modelēšanas programmām. Šajā pētījumā tika salīdzināti rezultāti, kas iegūti ar Fortran IMSL bibliotēku un Epanet-MSX programmas paketi.*
*Zhang et al (2004) piedāvāja matemātisko modeli, kas apraksta baktēriju augšanu ūdensvados. Šajā pētījumā modeļa vienādojumi tika atrisināti taisnas caurules gadījumam, izmantojot Fortran IMSL bibliotēku. Tie paši vienādojumi, izņemot dispersijas locekli tika ievadīti Epanet-MSX vidē. Rezultāti tika salīdzināti savā starpā.*

*Tika atrasts, ka rezultāti, kas bija iegūti ar Fortran IMSL palīdzību, labi sakrīt ar rezultātiem no Epanet-MSX programmas. Var secināt, ka dispersijas loceklis vienādojumos var būt ne īpaši nozīmīgs atsevišķos gadījumos.*

**Juhna T., Kolyshkin A., Nazarovs S., Rubulis J. Application of IMSL library and Epanet-MSX environment for comparison of bacteria growth simulation results**

*The issue of bacteria proliferation in water distribution networks has been addressed by several authors. Attempts have been made to develop a comprehensive model that would allow simulating growth of bacteria in drinking water distribution networks and determining how different factors are influencing bacteria growth. There are some difficulties, however, that one developing a bacteria growth model has to overcome. Bacteria development is influenced by many factors and it is virtually impossible to take them all into account.*

*Nevertheless there are models available that in one hand consider all the significant factors and in other hand are not too bulky enabling quick calculations with the computing power available in most labs. However additional efforts are needed to compare models and check reproducibility of results obtained with different models and various packages of simulation software. The present paper makes an attempt to compare results obtained with the help of Fortran IMSL library and Epanet-MSX software.*

*A mathematical model describing growth of bacteria in water distribution pipes has been proposed by Zhang et al (2004). In the present paper the equations of the model were solved by means of Fortran IMSL library for a straight pipe. The same model excluding the dispersion term was used in Epanet-MSX environment. The results were compared.*

*It has been found that the results obtained with IMSL library agree well with the results of Epanet-MSX software. The results indicate that the dispersion term may not be significant in some cases.*

**Juhna T., Kolyshkin A., Nazarovs S., Rubulis J. Применение IMSL библиотеки и среды Epanet-MSX для моделирования размножения бактерий в водопроводных системах**

*Распространение бактерий в водопроводных сетях исследовалось многими авторами. Были произведены попытки разработать модель, описывающую рост бактерий в трубах подачи воды, которая позволяла бы также определить влияние различных факторов на размножение бактерий. Однако существуют некоторые трудности, препятствующие разработке подобной модели. На размножение и распространение бактерий влияют многие факторы. Все факторы, производящие какой-либо эффект на рост бактерий, практически невозможно учесть полностью.*

*Несмотря на это, существуют модели, которые, с одной стороны берут во внимание все параметры, имеющие наиболее значительное влияние на развитие бактерий, но с другой стороны достаточно компактны и не требуют больших вычислительных мощностей для их использования. Однако, необходимы дополнительные исследования, направленные на сравнение результатов, полученных с помощью различных моделей и повторяемость результатов, полученных путем использования разных программных пакетов. В данной работе сделана попытка сопоставить результаты моделирования с помощью программы Epanet-MSX и результаты решения уравнений той же самой модели с помощью библиотеки Fortran IMSL.*

*Математическая модель, описывающая рост бактерий в водопроводных сетях была предложена в работе Zhang et al (2004). В данной же статье уравнения вышеупомянутой модели были решены с помощью библиотеки Fortran IMSL. Те же самые уравнения, исключая лишь описывающий дисперсию член, были использованы в программе Epanet-MSX. Было произведено сравнение полученных результатов.*

*Полученные результаты свидетельствуют о том, что решение, произведенное с помощью библиотеки Fortran IMSL, хорошо согласуется с результатом моделирования в среде Epanet-MSX. Это также указывает на то, что дисперсия в некоторых случаях не имеет принципиального значения.*