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COMPUTATIONAL FLUID DYNAMICS AND WATER QUALITY MODELING

OBLICZENIOWA MECHANIKA PŁYNÓW A MODELOWANIE JAKOŚCI WODY

Abstract: Modeling of water quality in distribution systems becomes nowadays a very popular tool applied in the processes of systems design and operation. Usually, according to everyday practice and literature reports, the chlorine propagation is one of the mostly reported subjects of modeling. Meanwhile, literature presents many examples of pollutants originated in polymer pipes' material seriously deteriorating the quality of water in distribution systems. In this case, the *computational fluid dynamics* (CFD) may be applied to numerical calculations of simultaneous transport of several organic and non-organic pollutants in drinking water supply systems constructed of metal or polymer pipes. This paper contains the presentation of recognized pollutants migrating to drinking water from plastic pipes, possibilities of CFD application to water quality modeling and basic set of necessary input data as well as range of simulation results. Advantages and disadvantages of CFD as a tool of water quality numerical assessment were also presented.

Keywords: water quality, numerical modeling, computational fluid dynamics, water supply systems

According to the rapid development of computing technologies and availability of various commercial and open source software modeling of water quality flowing through the distribution systems has recently gained wide popularity among scientists, designers and operators of water supply systems. Numerical simulations focused on water quality modeling allow to predict the propagation of selected pollutant, or several pollutants simultaneously, along the whole system of drinking water distribution in various operational conditions. The modeled pollutants of different kinds may enter the water distribution systems in the source (ie disinfectants) or in any given point of distribution system, including wall reactions or migrations from pipe material [1]. Thus, modeling of contaminants transport helps to understand the movement and behavior of pollutants resulting in possibility of proper network planning and management.

The initial water quality, after processes of treatment and disinfection may be changed due to different causes leading to its deterioration - oxygen decay, disinfectant decay, the formation of disinfection by-products (*trihalomethanes* THMs), change of color, smell and turbidity [2] as well as by leakage of organic or inorganic compounds from pipes materials during its contact with water [3-5]. The strict regulations concerning the proper level of disinfectant cause the necessity of studies and monitoring of chlorine propagation and decay along the drinking water distribution systems - the decay of disinfectant agent may result in the degradation of microbial conditions of water supply network, causing thus a possible risk to the consumers' health [6]. The recent literature studies show, however, that many different, organic and inorganic compounds creating possible danger to water quality (eg discoloration and fouling), customers complains as well as threats to public health may migrate from pipe material to drinking water during the distribution process

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through the water supply systems consisting of polymer pipes [3-5, 7, 8] - eg metals and heavy metals, organotins compounds, *volatile organic compounds* (VOCs) or thermal stabilizers such as Irganox 10XX series. The mentioned problem becomes more serious due to the rapid increase of polymer pipes (PE, PVC) application to construction of water distribution systems. Recent reports show that plastic pipes make up over 50% of all pipes installed worldwide [5]. In Poland approx. 70% of newly constructed pipelines are made of polymer pipes [9]. The most popular recognized pollutants originated from polymer materials migrating to drinking water and influencing its quality and organoleptic properties [4, 8, 10-12] are presented in Table 1.

Table 1

The most popular recognized pollutants migrating to drinking water from plastic pipes

Metal stabilizers		Lead, organotins compounds, cadmium
Antioxidants		Irganox 1010, Irganox 1035, Irganox 1076, 2,6-di- <i>tert</i> -butyl-4-methylphenol (BHT)
Products degradation of antioxidants used in polymer production		4-ethylphenol, 4- <i>tert</i> -butylphenol, 2,6-di- <i>tert</i> -butyl- <i>p</i> -benzoquinone, 2,4-di- <i>tert</i> -butylphenol, 3,5-di- <i>tert</i> -butyl-4-hydroxystyrene, 3,5-di- <i>tert</i> -butyl-4-acetophenone, 3,5-di- <i>tert</i> -butyl-4-hydroxyacetophenone, 1,5-bis(<i>tert</i> -butyl)-4-(2-carboxyethylidene)cyclohexa-1,4-dien-6-on, 3-(3,5-di- <i>tert</i> -butyl-4-hydroxyphenyl)methylpropanoate, 3-(3,5-di- <i>tert</i> -butyl-4-hydroxyphenyl)propanoic acid
VOCs	Esters	Butylacetate, ethylhexanoate, hexylacetate, propylhexanoate, butylhexanoate, ethyloctanoate, hexylhexanoate, hexamethylbutanoate, isobornylacetate, ethyldecadienoate, 2,2,4-trimethyl-1,3-2,2,4-TPD
	Aldehydes	Nonanal, decanal
	Ketones	2-decanon, 2-undecanone, 2-dodecanone
	Terpenoids	Alpha-pinene, delta-carene, limonene, alpha-terpinolene, alpha-farnesene
	Aromatics	Benzene Ethylbenzene, <i>m</i> - and <i>p</i> -xylene, <i>o</i> -xylene, styrene, isopropylbenzene, <i>n</i> -propylbenzene, 1,3,5-trimethylbenzene, 1,2,4-trimethylbenzene, <i>p</i> -isopropyltoluene, naphthalene

Nowadays, the EPANET-based (by EPA, USA) chlorine propagation modeling, as the main disinfectant applied worldwide, is very popular and is being reported frequently [13-20]. Usually, the following set of assumptions is required: distribution network is consisting of sources, pipes and nodes; flow directions in pipes are fixed, all hydraulic parameters and chlorine concentration in all outer sources are known [17]. Usually, the obtained results cover predicted chlorine concentrations in modeled systems nodes and pipes. However, these models have many disadvantages limiting the proper assessment of water quality in distributional systems (eg in some EPANET-based models propagation of studied pollutant may be studied only in system nodes) or just limiting their usage only to small networks as well as, which seems to be fairly important, simulating changes of narrow group of pollutants of in fixed hydraulic conditions [2] - these may not be problematic for engineers and network operators but may be insufficient for more complicated hydraulic analyses.

Computational fluid dynamics and water quality modeling

More precise numerical calculations of water quality inside distribution systems covering different, not only chlorine, pollutants propagation in various, dynamic flow conditions (laminar or turbulent), chemical reactions inside the water body with different kinetic rates as well as migration of organic and non-organic compounds of pipe material to water are possible when the *computational fluid dynamics* (CFD) methods are applied [eg 10, 21].

The development of CFD was started in the first two decades of XXth century and it has recently reached high popularity, due to the rapid development of computational techniques. The CFD is now being applied in many branches of science and technology, from dynamic hydraulic of water supply and sanitation systems, water and wastewater treatment [22-24] to food industry [25], different technological processes [26], heating and ventilation [27, 28] and modeling of flow in rivers [29]. This popularity is reflected by availability of many open source and commercial CFD software.

One of the most popular commercial CFD software applied to water quality calculations is FLUENT developed by Fluent Inc., which was required by Ansys in 2006. Since then Fluent is a part of ANSYS engineering modeling software package. FLUENT was frequently reported as a successful tool in various simulation calculations of fluid flow [25, 29-32].

Fluid flow modeling in CFD is based on the following governing equations [29, 33]:

Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \text{div} \rho \mathbf{u} = 0$$

For incompressible fluid flow:

$$\text{div} \rho \mathbf{u} = 0$$

Conservation of momentum

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i$$

Navier-Stokes:

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial p}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i$$

where: ρ - fluid density, t - time, u - velocity, \mathbf{u} - velocity tensor, $\boldsymbol{\tau}_{ij}$ - stress tensor.

These equations, with the proper set of computational simplifications, boundary conditions and support of numeric techniques provide for comprehensive modeling tool for various laminar and turbulent, compressible and incompressible fluid, steady state and transient fluid (gas, liquid or multi-phase) flows analyses.

Qualitative calculations in CDF covering transport and mixing of reactive and non-reactive chemical species are usually based on the conservation equations of considered species. The mentioned equation general form for i species may be presented as follows [34]:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla(\rho \bar{u} Y_i) = -\nabla \bar{\mathbf{J}}_i + R_i + S_i$$

where: Y_i - local mass fraction of i species, $\bar{\mathbf{J}}_i$ - vector of diffusion flux of species i , R_i - production rate of i species by chemical reaction, S_i - creation rate of i species by addition from dispersed phase or any other possible source.

Thus, the CFD calculations of multiple species transport and mixing in different flow conditions reflect convection, diffusion and reaction sources for each component species. The involved chemical reactions of transporting, mixing and migrating may occur in the bulk phase of fluid, on pipe/tank walls or particle surfaces as well as in porous media. So the most important advantages of CFD application to modeling of water quality in distribution networks should be now visible - the wide choice of pollutants, possibility of simultaneous calculations of multiple chemical processes occurring in water body and on pipe walls as well as in porous filtering bed, concentration of studied pollutants may be observed in any, freely selected, points of studied water system.

Usually, to apply CFD to engineering calculations the *finite element method* (FEM) or *finite volume method* (FVM) is required. Thus, the standard regime of the above-mentioned techniques is enabled: preparing the spatial mesh of finite elements/volumes and assignments of medium parameters, initial and boundary conditions in pre-processor, numerical calculations in model processor (solver) and results viewing and exporting in postprocessor. The appropriate skills represented by software users are required. Generally, CFD software is not suitable for beginners - some level of experience in computer modeling in FEM or FVM is necessary.

Below, in Table 2, the exemplary necessary set of basic input data for flow and species transport-mixing model as well as the possible results of calculations by commercial software Ansys, Fluent [34, 35] are presented.

Table 2

Input data and calculation results of CFD

Input data		Results
Material properties	Flow inputs	
Density, molecular weights Viscosity Mass diffusion coefficients-Fickian or full multicomponent diffusion User defined scalar diffusivity, isotropic or anisotropic	Flow type: laminar/turbulent, single or multiphase flow, turbulences model and its input data, Transport equations Source and sink terms Species transport type: mixing or non-mixing, species volumetric reactions Constant or time and space dependant boundary conditions: inflow, outflow and wall: mass flow, pressure gradient or distribution, temperature, velocity distribution, species inlet mass fraction, wall surface reactions	Pressure and velocity of flow distribution, Mass and mole fraction of species, Concentrations and molar concentrations of species distribution, Laminar and effective diffusion coefficient of species, Kinetic and turbulent rate of reaction

Summary and conclusions

The presented literature review shows a high potential of CFD application to water quality in distribution systems modeling. One may compute different scenarios, from the

simplest ones (eg non-mixing transport of species in simple system) to the most complicated cases (eg mass transport of n-species with volumetric and wall surface reactions inside the complex distribution systems). The presented above advantages of CFD application allow numerical modeling of probably all engineering cases and problems encountered in practice. The popularity of CFD modeling among water distribution systems' designers and operators may be limited by its disadvantages: usually complex structure of open source software, high cost of commercial programs, required experience in data management and simulation calculations, high system and hardware requirements, full range of necessary input data (in dependence to the level of problem simplification). Nonetheless, the CFD's capabilities and range of possible application make it a worthy tool in modeling of water quality in distribution systems.

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OBLICZENIOWA MECHANIKA PŁYNÓW A MODELOWANIE JAKOŚCI WODY

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Abstrakt: Modelowanie parametrów jakości wody w systemach dystrybucji jest obecnie stosowane zarówno w procesie projektowania, jak i w eksploatacji sieci wodociągowych. Najczęściej stosowanym w modelowaniu wskaźnikiem jakości wody w sieci jest rozkład chloru. Badania literaturowe wskazują, iż istnieje duża grupa zanieczyszczeń pogarszających jakość wody, a pochodzących z materiału przewodów. W celu numerycznego określenia transportu tych zanieczyszczeń w sieciach wodociągowych wykonanych z różnych materiałów może być zastosowana obliczeniowa dynamika płynów (CFD). W artykule przedstawiono najczęściej identyfikowane w wodzie zanieczyszczenia pochodzące z materiału przewodów wykonanych z tworzyw sztucznych, możliwości zastosowania CFD do modelowania jakości wody oraz niezbędne w tym celu dane wejściowe. Przedstawiono także wady i zalety CFD jako narzędzia do modelowania zmian jakości wody w sieciach.

Słowa kluczowe: jakość wody, modelowanie numeryczne, obliczeniowa dynamika płynów, sieci wodociągowe