Numerical modeling of processes in water treatment plants as a basis for an optimal design
Sorin C. Ulinici, Grigore Vlad, Dumitru Vâju, Iosif Balint, Gabriela Băisan, Mihaela Hetvary

S.C. ICPE Bistriţa S.A., Bistrita, Romania. Corresponding author: S. C. Ulinici, sorin_ulinici@icpebn.ro

Abstract. Centrally supplied water for human consumption is subject to complex physico-chemical and biological treatment processes, from the source to the consumer. The degree of complexity for these processes depend both of the quality of the water source as well of the higher quality requirements imposed by regulations. The investment and operating costs of water treatment systems, as well as energy efficiency are also key factors in the selection of the applied technologies. The design of technological processes (related both of the capture and water conveyance as well of the water treatment plants) requires a complex engineering approach including specialties related to hydraulics, physical engineering, chemical engineering, electrical installations and industrial automation. The complexity and the interconnection degree of the involved processes (also the higher costs even in the pilot stage) determines the numerical modelling and simulation of processes as a mandatory stage in the design process with a major aim related to the evaluation of efficiency and operational costs and also risk assessment. The paper shows numerical modeling methodology used for the design of the technological processes for drinking water treatment, based on the Finite Element Method (FEM) for the numerical modeling of some specific processes (e.g. filtration/bio-filtration, ozonation, disinfection) and on a free software package (EPANET 2.0) developed by the Environmental Protection Agency U.S. (EPA) for the modeling of the hydraulics of the water treatment plants. Are also presented numerical models which were used as a design basis for some water treatment facilities already in operation.

Key Words: numerical modeling, water treatment, hydraulics, Finite Elements Method.

Introduction. Demographic evolution and the current industry development stage involve high consumption of natural resources (materials and energy). In this context, water has become a strategic resource. High consumption of water - speaking here both about consumption for drinking water needs and domestic needs and about the use for economic activities (industrial and agricultural) - determines the need for reconsideration of water resources considered in previous periods as non compliant or difficult to treat. The challenge of reuse and recycling of some wastewater categories determines the need to develop water treatment technologies that are suitable functionally and operationally efficient and also energy-efficient.

Technological design of the water treatment plants is a defining step in the process of implementation of a new investment or upgrading of existing capacities. Technological flows of the water treatment involve the concurrence of various processes of physical-chemical nature that are the object of specialties in various branches of science and technology (physics, chemistry, biology, mechanical and electrical engineering, industrial automation). Current status of technical and technological development, the complexity of addressed processes, involves as almost mandatory preliminary stage in the process of the technological design, development and implementation of numerical models for selected processes. There are three main motivations in the development and use of numerical models and simulators for technological processes of water treatment: implementation of new processes and optimization of investment costs, modeling and functional optimization (operational, of the energy consumption and maintenance procedures), implementation of procedures for managing the risk situations (defined as major faults or environmental hazard situations).

For a long period of time, engineering design was based on careful sampling and processing of empirical data. This information were often presented in the form of correlation tables or nomograms. The main difficulty relating to empirical data retrieved is the fact that they are applicable only to limited areas in relation to the scale of fluid velocity, temperature, time intervals or linear dimensions. When there is a need of designing large systems at real scale, empirical information should be collected on the basis of exploring of experimental models at the scale, information that is not easy to
obtain. This requires the development of scaling rules that would provide geometric, kinetic and dynamic similarities between laboratory-scale model and real scale model, requiring vast experience and a high level of ingenuity of the experimenters and designers. In the case of fluids dynamics such scale modeling are based on the physical visualization of sets of of some parameters (variations thereof), and also, are based on analytical solving of equations systems describing the basic phenomena.

Existing software packages for modeling and simulation of processes in water treatment plants offer, more or less, the same functionalities: design, process optimization, operator training, automation. Some also include investigating ways of the economic costs. They are generally similar in terms of their use. The interface allows the construction of its own model, having specified certain characteristics (in terms of raw water quality, implemented processes, etc.) required to achieve the simulation (Mandel et al 2008). Table 1 provides an overview of some of the simulators usually available.

<table>
<thead>
<tr>
<th>Software package</th>
<th>Developed by</th>
<th>Highlights-Strengths</th>
<th>Disadvantages / Weaknesses</th>
<th>Implemented models</th>
</tr>
</thead>
<tbody>
<tr>
<td>EPANET</td>
<td>EPA-USA</td>
<td>Friendly interface, suitable for extended hydraulic simulation</td>
<td>Does not allow modeling and investigation of individual processes</td>
<td>- Hydraulic models for networks and distributed processes - Models of reaction in volume and at contact surfaces Semi-empirical relations</td>
</tr>
<tr>
<td>OTTER</td>
<td>WRc</td>
<td>Easy to use for FORTRAN users familiar with FORTRAN /C/C++</td>
<td>Slow running</td>
<td>Semi-empirical relations</td>
</tr>
<tr>
<td>Stimela</td>
<td>TU Delft</td>
<td>Online access</td>
<td>Simple model of oxidation Results untested at real scale</td>
<td>Semi-empirical relations, Mechanistic correlations</td>
</tr>
<tr>
<td>Metrex</td>
<td>Duisburg University</td>
<td>Particles removal</td>
<td>Requires long periods for calibration</td>
<td>USEPA correlations</td>
</tr>
<tr>
<td>Watpro</td>
<td>Hydromantis</td>
<td>Disinfection of DBP-s</td>
<td></td>
<td></td>
</tr>
<tr>
<td>WTPmodel</td>
<td>USEPA</td>
<td>Removal of NOM and DBP-s</td>
<td>Limited domain</td>
<td>Empirical relations</td>
</tr>
</tbody>
</table>

This paper proposes a different approach to modeling and simulation of the processes in water treatment plants, involving the development of the numerical model on two levels: modeling of individual processes and technological modeling (hydraulic and operational) of the flow. The first level allows advanced modeling of established processes, modeling of new processes in order to develop and implement them, modeling of active elements of specific equipment. The second level was set on integration of individual processes in the global model of the plant, for operational simulation, optimization of energy costs and also, operational and for assessment of specific scenarios. The approached modeling methodology didn't has as final goal the development of a new software package for commercial use, but the development of the necessary structure to approach complex, particular, models with use in industrial research activities, development and technological design of water treatment plants. The necessary technical support to develop the presented models was provided by the use of specific software media for modeling of multiphysics processes using finite elements method (COMSOL Multiphysics) and of a processes simulator and hydraulic networks (EPANET-US EPA).

**Numerical modeling methodology.** The main purpose of the numerical models developed and presented in this paper refers to their use as tools for simulation and virtual testing of processes in water treatment stations in order to develop new technologies and for optimal technological design. Intended purpose involves the development of numerical models for both unitary processes involved in water treatment
technology and for the entire technological process, focusing on basic hydraulic component.

Considering the above, the methodology used has implicated the structuring of modeling process on two main levels: numerical modeling of unitary processes and equipment and technological modeling, focusing on hydraulic component for the entire flow treatment. Structuring of the model is schematically shown in Figure 1.

Figure 1. Numerical modeling methodology.
**Numerical modeling of unitary processes and of the equipment.** Unitary processes from water treatment flow imply, mainly, the concurrence of complex processes of physical and chemical nature. We talk about physical processes, related to gravitational sedimentation, filtration and adsorption, processes of contacting gas/liquid (involving biphasic flow processes), separation processes in electric and magnetic field. Processes of chemical nature involve, in particular, reaction systems in various configurations and the most various environmental conditions. There is a major interdependence between these categories of processes. It is enough to consider, for example, the ozonation processes that involve carrying out chemical reactions in biphasic environments (gas/liquid) or the treatment processes in the field of UV radiation involving both direct disinfection processes, photolysis processes or photocatalysis processes. In conditions of the presence of bio filtration stages, for example, physical and chemical processes are doubled by the concurrence of biological processes related to the conduct of the bacterial metabolism of populations present in the bio filters’ support environment.

In terms of numerical modeling of these various categories of processes, both at qualitative and, especially, quantitative level, the support is provided by the existence of mathematical models based on descriptions that use systems of differential equations with partial derivatives. Solving these systems of equations provides the main characteristics of interest in evaluating these processes. Unfortunately, it is almost impossible using of analytical mathematical tools in addressing these complex systems of equations. Our approach is based, therefore, on the numerical solving of such systems, the selected method being the one using finite elements method (FEM), a suitable one for approaching of multi-physical systems, mainly due to the existence of adequate software environments. Considering the particularities of the processes addressed, there were used numerical modeling methods related to computational modeling of processes in fluid environments (Computational Fluid Dynamics - CFD). History of numerical modeling methods related to systems with fluid components - CFD (Computational Fluid Dynamics) began in the 70s of the last century, combining the methods from physics, mathematics and computational technique, in order to simulate the behavior of systems involving fluid phases. The evolution of CFD techniques and applications is closely related to the evolution of computer technology and of software environments, especially focused on the development of computer networks and distributed processing of the data (Blazek 2001).

The implementation of CFD modeling is based mainly on the implementation of transport equations: transport of mass, momentum conservation law, energy conservation law. Based on tensorial formalism, the basic equations used can be described easily in the Cartesian space (Date 2005). For the particular implementation of our models, it was used the Comsol Multiphysics software package (Comsol 2012).

**Modeling of integrated processes and hydraulic systems.** The unitary processes addressed in the first stage of numerical modeling are integrated into the general hydraulic model of the water treatment plant. Technological flow involves the integration of the peculiar unitary processes that optimally provide the achievement of the performance criteria imposed both by entire treatment process, by energy efficiency and operational efficiency, as well as by investment costs of the future project implementation.

The basic criteria for selection of methodology, methods, numerical modeling software environment of general hydraulic flow in treatment plant were, mainly the following: flexibility, accessibility (related to software environment), the possibility of portability of the models and the degree of configurability (involving mainly the possibility of up-grading of the initial models from carrying out their reassessment processes).

For modeling of integrated hydraulic processes it was used the EPANET package, developed by National Risk Management Research Laboratory from USA-EPA (USA-Environment Protection Agency) (Rossman 2000). This software package contains advanced facilities of hydraulic modeling of pressurized hydraulic networks systems, at the same time with modeling facilities related to the reaction rate of treatment chemical agents, and, although not for direct modeling of technological hydraulic systems, it can
be adapted for this purpose (Ulinici et al 2010). The hydraulic modeling software package (EPANET) is used worldwide to design water distribution networks and to optimize their operation, up to a complete integration with SCADA systems (Worm et al 2008). However, in the current EPANET library, the elements that describe the hydraulic properties of some water treatment units are missing. These elements have been developed and integrated by us, based on modeling of unitary processes performed in the first stage.

**Results and Discussion.** The development of numerical models related to unitary processes and particular configurations of these processes for particular stages of water treatment, using CFD and FEM principles were presented in detail, in some previous papers. Thus, in terms of modeling of water ozonation processes, it was presented a contact and reaction biphasic pattern in the bubble column, the model being experimentally verified and its results were the basis for the design of some concrete configurations for ozone treatment of the water (Ulinici et al 2013). This model allowed the evaluation of dissolved ozone concentration in the reaction tank and its dynamic evolution depending on the main technological parameters of the process (injection rate, ozone concentration, pressure in the system, fluid flow). Output data of the model were used as input parameters of the hydraulic model of the whole treatment process. Also, it was developed a model for the treatment reactor with circulating flow of water under pressure in order to use UV radiation in disinfection processes and in initiation of photolysis reactions in the presence of ozone, in water treatment processes (Ulinici et al 2011). Output data (concentration of dissolved reactive depending on the intensity of UV radiation, average reaction rates) were also used for technological design of the UV reactors depending on the flow and physical characteristics of the environment (e.g. turbidity). Modeling results of the unitary process were used in the integrated hydraulic model. The next section shows the basic aspects of modeling for a multimedia filtration stage and adsorption in pressurized filter, in the presence of dissolved ozone.

**CFD modeling of unitary processes. Multimedia filtration and adsorption process in systems with dissolved ozone.** Numerical modeling of multimedia filtration and adsorption processes in systems with chemical reactions involves the concurrence of two categories of processes: (1) Hydraulic processes, including fluid flow through porous media and (2) Mass transport processes with chemical reactions (diffusion, convection, chemical reactions). The fluid flow in porous media, in specific conditions of analysis, can be described by the Brinkman equations, where momentum transport within the fluid due to the shear stress is required to be taken into account. Physical properties of the fluid, such as density, viscosity and pressure, are defined as volume averages corresponding to the volume unit of the pores. Thus defined, they show relevant physical parameters that can be experimentally measured, being presumed of having continuity with the corresponding parameters of the adjacent free flow. The flow rates are defined as a volume average, which correspond to an average volume unit including both the pores and the matrix. They are sometimes called Darcy velocities, defined as flows per unit of cross section. Flow in porous media is described by a combination of the continuity equations and of momentum equation, equations that form the system of Brinkman equations (Le Bars and Worser 2006):

\[
\frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla \cdot (\rho \vec{u}) = Q_{br}
\]

(1)

\[
\frac{\partial}{\partial t}(\varepsilon_p \vec{u}) + \nabla \cdot (\vec{u} \nabla \rho) = - \nabla p + \nabla \cdot \left[ \frac{1}{\varepsilon_p} \left\{ \mu (\nabla \vec{u} + (\nabla \vec{u})^T) - \frac{2}{3} \mu (\nabla \cdot \vec{u}) \right\} \right] - \frac{\rho}{\varepsilon_p} + Q_{br} \vec{u} + F
\]

(2)

where:
- \( \mu \) - dynamic viscosity of the fluid (kg/(m·s));
- \( \mathbf{u} \) – velocity vector (m/s);
- \( \rho \) – density of the fluid (kg/m³);
- \( p \) – pressure (Pa);
- \( \varepsilon_p \) – porosity;
- \( k \) – permeability of the porous medium (m²);
- \( Q_{b7} \) – mass source or mass flow (positive and negative) (kg/(m³·s))

Influence of the gravitational force and of other forces can be represented by the general term force \( F \) (kg/(m²·s)). The value of the concentration \( c \) of the dissolved ozone will be obtained based on an equation of non-conservative convection – diffusion, of transport, for the ozone dissolved in water:

\[
\frac{\partial c_{O3}}{\partial t} + \nabla \cdot (-D \nabla c_{O3}) = R - \nabla \cdot (c_{O3} \mathbf{u})
\]  

where: \( D \) – diffusion coefficient of the ozone solubilized in the fluid medium (scalar or tensorial). In the case of turbulent flow, intervenes the turbulent diffusion coefficient;

\( R \) – reaction rate. In this case, this rate includes gas/liquid mass transfer term (ozone entering in solution) and terms of decomposition and of reaction with pollutants for ozone already dissolved in liquid.

In our case, the model was developed in order to assess the qualitative and quantitative pressure drop depending on water flow, structure and configuration of multimedia filter layers. Also, the model was developed in order to estimate the rate of recombination reactions of the dissolved ozone in the multimedia filter, in the presence of a layer of activated granular carbon.

Numerical modeling of the filter used a two-dimensional model that allowed an adequate representation of a bio filter structure at real scale. Due to the complexity of the mathematical system of partial differential equations, modeling of a 3D field, in this context, involves significant computational resources that are not always proportional to the degree of accuracy of the solutions obtained. Dimensional structure of the modeled domains is shown in Figure 2, the geometrical and physical characteristics of the layers are shown in Table 2.

Figure 2. Structure of the modeled domains.
Numerical modeling was made based on the Brinkman equations and mass transport equations, being made using the finite element method (FEM - Finite Elements Method) to solve systems of equations in specific domains, the implementation being done using the COMSOL Multiphysics 3.5.1. package.

### Table 2

<table>
<thead>
<tr>
<th>Domain</th>
<th>Description</th>
<th>Height [m]</th>
<th>Porosity ε&lt;sub&gt;p&lt;/sub&gt;</th>
<th>Permeability [m&lt;sup&gt;2&lt;/sup&gt;]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Free volume (strainers filter - output)</td>
<td>0.3</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>Coarse grained sand, D = 4÷6 mm</td>
<td>0.1</td>
<td>0.3</td>
<td>1 x 10^-7</td>
</tr>
<tr>
<td>3</td>
<td>Average grained sand, D = 2÷4 mm</td>
<td>0.1</td>
<td>0.39</td>
<td>1 x 10^-9</td>
</tr>
<tr>
<td>4</td>
<td>Fine grained sand, D = 0.8÷1.2 mm</td>
<td>1</td>
<td>0.43</td>
<td>1 x 10^-9</td>
</tr>
<tr>
<td>5</td>
<td>Activated carbon (CAG)</td>
<td>0.5</td>
<td>0.64</td>
<td>5 x 10^-12</td>
</tr>
<tr>
<td>6</td>
<td>Mosaic (gravel)</td>
<td>0.2</td>
<td>0.25</td>
<td>1 x 10^-7</td>
</tr>
<tr>
<td>7</td>
<td>Free domain (input volume)</td>
<td>0.8</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

For the ozone reaction rate (upon decomposition) there were used different reaction rates for various geometrical domains. In the geometrical domain where activated carbon is present, are involved adsorption and reaction processes of the ozone followed by decomposition processes. Practically, it is a reaction system of the ozone in the multi-stage environment: gas, liquid, solid (heterogeneous catalytic decomposition). This reaction kinetics can be described by a Langmuir-Hinshelwood equation. The reaction rate can be approximated with sufficient accuracy for practical cases as a reaction pseudo-rate of order 1 in relation to the concentration of dissolved ozone (Beltran et al 2002). If for decomposition in an aqueous medium, at pH values slightly above 7 we can use coefficients of reaction rate with values of 0.4•10^-3 s<sup>-1</sup> (Mizuno et al 2007; Mizuno & Tsuno 2010) in case of adsorption on activated carbon processes we can use coefficients of the rate (pseudo-rate of order 1) with values of up to 8•10^-3 s<sup>-1</sup> (Beltran 2004). Water flow at the filter entry was considered to be Q=10 m<sup>3</sup>/h. For the flow considered, pressure drop in the vertical section of the filter is shown in Figure 3. For an entry concentration of the dissolved ozone of 0.4 g/m<sup>3</sup>, modeling results are presented hereinafter. It is observed the high pressure drop on activated carbon layer and a high pressure gradient on this layer.

![Figure 3. Pressure drop on the filter layers.](image-url)
In Figure 4 is shown the variation of concentration of ozone in filtering layers. It is observed a high concentration of ozone at the entrance of filter, this concentration decreasing dramatically after the layer of activated carbon.

Analysis of the evolution of dissolved ozone concentrations in the filter, in the transitional regime, was made for time intervals of 100s, 400s, 600s, 800s and 1200s from the injection of water with concentration of dissolved ozone in the upper part of the filter. In Figure 5 is shown the variation in time of the concentration of dissolved ozone in the radial section of the filter, at a height of 2 m.

![Figure 4](image1.png)

**Figure 4. Variation of ozone concentration in filter layers.**

![Figure 5](image2.png)

**Figure 5. Variation in time of concentration of dissolved ozone at H = 2 m.**
The model developed for multimedia filtration system and adsorption in media with concentrations of dissolved ozone allows developing of the technical design specifications, especially for systems with bio filtration, systems where concurrence of advanced oxidation processes with the bio filtration processes must operate on well defined media, a concentration over a certain level of the dissolved ozone being possible to lead to inhibition of bacterial growth, and consequently, to "defusing" of the filter.

Numerical modeling of unitary stages allows addressing of the technological design stage of the treatment processes with a significant reduction in the time required for this stage and providing of coherent input data for the development of dynamic models needed to implement automation algorithms for processes.

**Hydraulic modeling of water treatment systems.** For hydraulic modeling of technological flows it was used EPANET package developed by the National Risk Management Research Laboratory within USA-EPA (USA - Environment Protection Agency) (Rossman 2000). This software package contains advanced facilities for hydraulic modeling of pressurized networks systems, simultaneously with modeling facilities related to the reaction rate of chemical treatment agents and, although not directly intended for modeling of technological hydraulic systems, it can be adapted for this purpose (Ulinici et al 2010). EPANET, as it was originally conceived, allows running of simulations for hydraulic systems, with water quality assessment facilities, for extended periods of time, and for complex networks. Regarding the hydraulic modeling capabilities, these include: virtually unlimited dimensions of the modeled network, calculation of pressure loss in networks using multiple models (Hazen-Williams, Darcy-Weisbach), modeling of pumps with constant or variable speed, assessment of cost elements. A characteristic of this program is given by the capability of the user to include its own hydraulic circuit elements, with well-defined particular characteristics, which can describe individualized processes and technological equipment. This last facility has been extensively exploited by us. Thus, results of numerical modeling performed for particular processes and water treatment stages (using finite elements modeling, for which an example was presented in the previous section) were used as input data to define the technological blocks integrated in the general hydraulic model developed in EPANET.

In this section are presented the models of two complete water treatment processes, corresponding to specific applications. The first application refers to a water potabilization plant including ozonation technologies in pressurized multimedia contact and filtration system. The second application consists of an extensive system, including a system of well water pumps with the corresponding network pipes, a pressurized multimedia filtration system and deferrization with pyrolusite on catalytic bed. Both applications include facilities for pumping and storing of water volumes. Table 3 presents an inventory of the main categories of modeled technological items and hydraulic circuit elements, which have been integrated into the global model.

<table>
<thead>
<tr>
<th>Cat. No.</th>
<th>Item category</th>
<th>Model source</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Valves, pipes, controls</td>
<td>EPANET</td>
</tr>
<tr>
<td>2</td>
<td>Pumps</td>
<td>EPANET</td>
</tr>
<tr>
<td>3</td>
<td>Tanks volumes (buffer tanks and storage tanks)</td>
<td>COMSOL (CFD, FEM)</td>
</tr>
<tr>
<td>4</td>
<td>Pressurized filters</td>
<td>COMSOL (CFD, FEM)</td>
</tr>
<tr>
<td>5</td>
<td>Pressurized filters with adsorption (GAC, pyrolusite)</td>
<td>COMSOL (CFD, FEM)</td>
</tr>
<tr>
<td>6</td>
<td>Ozone injector and static mixer</td>
<td>Integration in EPANET</td>
</tr>
<tr>
<td>7</td>
<td>Water / ozone contact and reaction vessel (including degassing system)</td>
<td>Integration in EPANET</td>
</tr>
</tbody>
</table>
Ozone water treatment plant model. Simplified flow diagram of ozone water treatment plant is shown in Figure 6. Raw water is taken from a raw water storage tank ($V = 300 \text{ m}^3$) through a group of feed pumps, and introduced in the treatment flow. Ozone is injected into the flow through a Venturi injector, into a by-pass circuit. The mixture of the two phases (gas/liquid) is provided through a static mixer. Mass transfer between gas phase and liquid phase is provided in a contact and reaction vessel fitted on the upper side with an automatic degassing valve to remove excess of undissolved gas. In the technological process, after the contact and reaction vessel is introduced a multimedia filtration stage, which includes an adsorption bed with granular activated carbon (GAC). After filtration stage, water is stored in a buffer tank with a volume $V = 20 \text{ m}^3$, from where water is taken through a booster pump group and circulated to the storage tank with a volume $V = 100 \text{ m}^3$, at an upper hydraulic level. From the storage tank, the water is distributed to consumers through a gravitational distribution network. Nominal treatment flow rate of the station is $Q=20 \text{ m}^3/\text{h}$.

The network related to the EPANET model of the technological flow is shown in Figure 7. The flow rates related to hydraulic routes and in junctions ozone concentrations (for an output of ozone generator $Q=200 \text{ g O}_3/\text{h}$) are complying with the color scale from the attached legend. The two multimedia filters operate in parallel, the total flow rate of the treatment plant being equally divided. Although the analysis performed was an exhaustive one, we will present, punctually, the considerations of interest related to concentrations of ozone in the system. In Figure 8 are represented ozone concentrations modeled in the main junctions of the network, when achieving the stationary regime, in parametric representation depending on ozone production of generator. The values of ozone concentrations at the multimedia filter output constitute a measurement of development of advanced oxidation processes in the volume of the adsorption bed from multimedia filter, in the presence of dissolved ozone. In Figure 8 is represented the concentration of dissolved ozone at the multimedia filter output, depending on the
thickness of activated carbon adsorption bed, depending parametrically on the ozone generator output.

Figure 7. EPANET network of the treatment flow model.

Figure 8. Variation of ozone concentrations in junctions of interest, in stationary regime.

In diagram from Figure 8 is observed a steep variation of ozone concentration on the portion of static mixer, situation that corresponds to mixing of main water flow with the flow coming from the Venturi injector. Also, ozone concentrations at the multimedia filter output depend significantly on the thickness of activated carbon bed from the filter. Direct oxidation and ozone disinfection reactions occur, mainly, in the volume of the contact and reaction vessel. Activated carbon adsorption bed from filter multimedia favors the advanced oxidation reactions, generated by $^\bullet \text{OH}$ radicals, generated at the liquid/solid interface in the granular bed. From technological point of view, high ozone concentrations are desirable to be obtained in the reaction vessel volume, in the filtering
layer being generated a negative concentration gradient. The hydraulic levels are represented on diagram from Figure 9 (in meters, in relation to the level of the treatment plant, considered at zero level).

![Figure 9. Ozone concentration at filter output depending on the CAG filter bed thickness.](image)

The treatment/deferrization plant model. Simplified P&ID diagram of the treatment plant is shown in Figure 10. Section of raw water supply and feeding network of treatment system include a set of 13 drilled wells, arranged on an extended catchment front, with piping lengths that reach a total value of 3750 m. Hydrodynamic level of wells varies from -13 m and -23 m in relation to ground level, the necessary pumping rates ranging between 11 and 16 m³/h for each of the wells.

Due to high concentrations of Fe from the raw water (> 200 µg/L) treatment system is provided with a stage of multimedia filtration on sand bed and on catalytic bed with pyrolusite. Water flow rate of treatment plant is $Q_{w} = 320$ m³/h, in this context, the multimedia filters battery consisting of two filtering modules. Each module consists of a total of four filters with the diameter $D = 1600$ mm and useful height $H = 2400$ mm. To conduct the catalytic oxidation processes, it is provided a pre-chlorination stage with gaseous chlorine placed before the catalytic bed filters. After filtration is provided the remnant water disinfection with gaseous chlorine, the storage tank with the volume $V=1000$ m³ being also the reaction and contact tank. Water distribution is provided by the group of distribution pumps P1, P2 and P3.

Given the expansion of treatment system including raw water feeding network, treatment plant, storage tank and system of distribution pumps, EPANET model is presented in two sections: section of wells and raw water feeding network (Figure 11) and section of treatment plant (Figure 12). Given the existence of an extended number of punctual catchment sources (such as catchment from groundwater sources), it is difficult to calculate the pumping needs. This task is greatly facilitated by the use of modeling of catchment system in EPANET.

In order to determine the pumping needs for catchment fronts, pumps capacities are determined depending on characteristics of wells and configuration of the total hydraulic network.

To select the pump that equip wells within the catchment fronts of the groundwater, the flow rate value is given by the flow capacity of the well indicated by the hydro-geological survey and pumping height is determined based on hydraulic calculations prepared for the entire groundwater catchment system.
Figure 10. Simplified P&ID diagram of the process.

Figure 11. EPANET model network of the raw water supply area.

Pumping height is given by the difference between the piezometric level achieved in the front of the well and hydrodynamic level of the groundwater in the well, according to the formulas:

\[ H_p^i = C_p^i - C_{i,NHS} \ [m] \]  \hspace{1cm} (4)

\[ C_p^i = C_{R,max} + \sum_{h_r} \ [m] \]  \hspace{1cm} (5)
where:
- $H_p^i$ - pumping height of the submersible pump that equips well $i$;
- $C_p^i$ - piezometric level in front of well $i$;
- $C_{NHd}^i$ - hydrodynamic level of the water in well $i$;
- $h_r$ - pressure loss calculated for the catchment and feeding system of the groundwater from the well to the storage tank.

![EPANET model network of water treatment plant.](image)

Figure 12. EPANET model network of water treatment plant.

Water flow rates of treatment plant routes and hydraulic levels of the station network nodes are also shown in Figure 12.

One of the main challenges in technological design of water treatment systems and plants is the energy optimization of the system. The largest consumers of energy in the system are the pumps, both pumps in the feeding system, pumps in the technological treatment system, as well as pumps that provide the necessary pressure on distribution network. Numerical modeling of the treatment system enables accurate estimation of energy consumption with the pumping systems (Figure 13).
Conclusions. Technological design for water treatment plants is an adaptive process, heavily dependent on conditions imposed: the quality and flow of the water source, the limitations imposed by the legal norms of water quality, technical and economic limitations (at investment and operational level). Unitary processes, part of the technological processes for water treatment are various. Their composition, configuration and parameters are constantly evolving. The need to reduce time cycle and costs needed for design, along with the desire to increase the quality and accuracy of technical solutions offered on the market, require the almost mandatory option of introduction in the technological design practice of the stage of modeling and numerical simulation of component processes and of technology for water treatment. Modeling and numerical simulation of processes and technologies involving interdisciplinary approaches differ drastically from regular CAD processes. If the latter are based on software implementations of procedures and execution blocks that are well defined, numerical modeling and simulation of processes seem mainly creative, often being complementary with performing of experimental activities.

Numerical modeling methodology presented in this paper has imposed the interdependent approach of two conceptual levels: the modeling of component unitary processes and the integrated process, with a focus on hydraulic component. Modeling of unitary process approach presented in this paper was based on the numerical implementation of models from physics, chemistry and biotechnology. It has been used the multiphysics formalism based on mathematical description of phenomena and processes using coupled differential equations systems. For numerical solving of these systems it was used the finite elements method (FEM) using COMSOL Multiphysics software package.

Modeling and simulation of integrated processes were based on using a free distribution software package, developed by the American Environmental Protection Agency (EPA- USA). The initial purpose of this software was the modeling of networks for water supply and distribution. The use of this package has been adapted for our purpose by customizing some elements and component blocks, using as input data the results obtained from previous modeling of unitary processes.

The models presented in this paper mainly come to exemplify the general methodology approach. In particular, these models have real projects in the "background", the results obtained from numerical modeling and functional simulation
being the foundation for elaboration of technical specifications for the development of new equipment configurations and unitary processes, or they provide a basis for execution projects of well defined investment.

The usefulness of the approach presented is obvious, the development and the expansion of the models presented provide support for development of useful work instruments, both in the field of development and application of complex technologies for water treatment and also in the field of strictly technological design.

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Authors:
Sorin Claudiu Ulinici, S.C. ICPE Bistriţa S.A., Parcului Street no. 7, 420035, Bistriţa, Romania, e-mail: sorin_ulinici@icpebn.ro
Grigore Vlad, S.C. ICPE Bistriţa S.A., Parcului Street no. 7, 420035, Bistriţa, Romania, e-mail: vlad@icpebn.ro
Dumitru Vâju, S.C. ICPE Bistriţa S.A., Parcului Street no. 7, 420035, Bistriţa, Romania, e-mail: icpebn@icpebn.ro
Iosif Balint, S.C. ICPE Bistriţa S.A., Parcului Street no. 7, 420035, Bistriţa, Romania, e-mail: icpebn@icpebn.ro
Gabriela Băisan, S.C. ICPE Bistriţa S.A., Parcului Street no. 7, 420035, Bistriţa, Romania, e-mail: icpebn@icpebn.ro
Mihaela Hetvary, S.C. ICPE Bistriţa S.A., Parcului Street no. 7, 420035, Bistriţa, Romania, e-mail: icpebn@icpebn.ro

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