Drinking Water Treatment Unit Processes: Computational Fluid Dynamics Modeling

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1 Introduction

An intricate understanding of the ways in which water flows has long been a goal of scientists and engineers. In treating large quantities of drinking water for municipal supply, this understanding of fluid mechanics is important to ensure the water is adequately treated in an energy- and cost-efficient manner. With the advent of computers and equation solving methods came the field of computational fluid dynamics (CFD). Some of the early efforts began in the 1960s, and commercial software packages became available around the 1970s [1]. CFD allows for a mechanistic understanding of fluid flow in intake structures, mixing vessels, reaction chambers, and distribution systems, giving practitioners the capability to optimize water treatment systems [2]. While CFD took hold in other engineering fields earlier than drinking water treatment [3], the instances of its use for plant design are increasing. This article aims to give an overview of the ways in which CFD analysis is being used for drinking water treatment plant design in the 21st century.

Drinking water treatment plants are built as combinations of various unit processes. In most cases, the subject of a CFD investigation is one particular unit process, rather than tackling several within the same model. Thus it is logical to break the treatment of this subject into the various unit processes of a conventional treatment plant, namely intake structures, rapid mix tanks, flocculation chambers, sedimentation basins, granular media filters, disinfection contact chambers, and distribution systems. Alternative unit processes will be discussed and compared to their closest analogs in the conventional train. Because the software is similar among the treatment types, it will be discussed at the outset.

2 CFD Software

It has been long understood that fluid dynamics problems require computational methods because of the nonlinear partial differential equations (PDEs) that govern their behavior [4]. Finding ways to solve these equations, such as finite difference and finite element methods, has been the work of mathematicians and physicists [5, 6]. Various software packages have been used for CFD modeling of modern drinking water treatment systems. These packages were developed over the years and the methods became more and more refined. Today their refinement continues. For commercial software, this progress is made possible through licensing fees that have grown along with the complexity of the software and the ease of use. However, an alternative model has emerged where users collaboratively develop open-source software packages. Instead of licensing fees, these open-source packages are sustained by the critical mass of users who contribute knowledge and code in an organic manner. The commercial software Fluent and COMSOL Multiphysics will be discussed here, being two of the more commonly employed commercial packages [7]. OpenFOAM will also be discussed, being the most common open-source package. Table 1 provides a summary comparison. This serves merely as an example of the wide variety of software available; a more extensive list can be found at the CFD Online website [8].

All software packages have three key components in common: the preprocessor, the solver, and the postprocessor [9]. Together these create workable systems that can be used to calculate and visualize fluid flow and mass transport phenomena. A key concept to understand CFD methods is that of a finite element: the idea is to take a shape (a tank, pipe, etc.) and divide it into many hundreds

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Table 1 Summary information for three of the more commonly used CFD modeling software packages.

Software name	Developers	Licensing model	Key features
Fluent	ANSYS	Commercial licensing fees	• Long history and strong reputation • Various historical packages now combined into one seamless user interface • Ease of use is increasing.
COMSOL Multiphysics	COMSOL Group	Commercial licensing fees	• Various CAE modules ("physics") designed to integrate with one another • Relatively easy for beginners to start modeling
OpenFOAM	OpenCFD and a Community of users	Open source	• Fully customizable and extendable because of open-source code • More difficult to use for beginners and nonprogrammers • Many examples are available in the online community

or thousands (sometimes millions) of smaller pieces, or elements. PDEs defining fluid flow (or other phenomena) are solved at each of those elements. This method was created to give computers a way to solve the PDEs that define the system [10]. The details of those solutions are typically hidden to the user, but a basic understanding of the approach is useful for enabling proper interpretation of the results [1]. The engineer thus has a powerful software tool for analyzing drinking water treatment plant unit processes.

2.1 Fluent

Fluent is a software package that is now developed and marketed by ANSYS. It is perhaps the most widely known and widely used package for CFD analysis in drinking water treatment plants. First introduced in 1983, the Fluent package was designed specifically with practicing engineers in mind, rather than being merely for researchers or computer scientists [11]. The Fluent solver historically needed another tool, GAMBIT, to create the finite-element mesh required as a preprocessing step. Recent improvements in the software provide the user with a complete package in one window on their computer screen, which streamlines the workflow [12]. A key advantage to Fluent is its long history of fluid mechanics analysis and development, which has refined the solver to enable quick convergence and credible results.

2.2 COMSOL Multiphysics

The COMSOL Group company was founded in 1986 [13]. Their main product package, COMSOL Multiphysics, was released in 1998. The software is a package combining a variety of computer-aided engineering (CAE) applications, with CFD being one of the available modules. The focal point of COMSOL's approach is to provide a platform where different types of engineering problems (electromagnetics, acoustics, fluid flow, etc.) can be integrated; this is the genesis of the term "multiphysics." Drinking-water treatment plant designers may focus on the CFD module available in COMSOL's package, but may also benefit from modules like Chemical Reactions as add-ons to the strict CFD results.

2.3 OpenFOAM

Among open-source software, one of the best-known tools is OpenFOAM, an acronym for Open source Field Operations and Manipulations [14]. The successful development of the tool is fostered because a company, OpenCFD, has the development of OpenFOAM as its mission [15]. They released OpenFOAM version 1.0 in 2004 and their continuing goal is to make this CFD tool freely available and open-source to the broader engineering community. OpenFOAM is primarily a Linux-based system, but Windows versions have been available since at least 2015 and Mac versions since 2016. The user experience with OpenFOAM is not as seamless as with commercial software like Fluent and COMSOL Multiphysics, but the absence of licensing fees, the momentum of adoption by many users, and the continuing organized product development make this software attractive.

3 Conventional Treatment Train

Several unit processes constitute the conventional drinking water treatment plant treatment train. They are discussed here in the order that water flows through the facility.

3.1 Intake Structures

While not a unit process that provides treatment, intake structures are integral components of a water treatment plant; they are the infrastructure that delivers raw source water from a lake, reservoir, or river, to the plant. Their designs are often unique from plant to plant, based on the topography of the ground under the source water. Some intake structures are designed to selectively withdraw water from different elevations in a reservoir based on water quality [16]. The intake structure is essentially a frame or building that houses pumps that push water up a gradient to the plant.

Manufacturers design and test their pumps using a test bed at their manufacturing facility. That test bed usually has fairly ideal conditions for fluid flow, such that the pump will not experience vortices or swirling flow at the intake point and will not be starved of feed water. When the pump is taken to the field, it will operate best if it experiences the same (or similar) conditions. If vortices or starvation occur, the pump may vibrate or wobble in an unexpected manner, wearing out its bearings and seals, or possibly causing cracks or other mechanical failures [17]. The goal of CFD for modeling intake structures, then, is to ensure that the water flow through the structure and around the intake point of the pump has little or no vortex mixing and sufficient flow for proper pump performance. Figure 1 shows a 2D view of an idealized intake structure. Though swirling flow can be seen in the corners of the structure, those are low-velocity flows that do not interfere with the higher-velocity main stream entering the pump housing.

Fluid flow in intake structures is turbulent, driving CFD modeling into the turbulent regime. Adequately modeling these structures remains a field of active development because the erratic nature of turbulent fluid flow is difficult to handle via computer models. In fact, many design firms continue to contract with companies who build and test scaled physical models of intake structures. The physical models are trusted more than computational models since the physical models inherently capture all the nuances of the flow; it is actual fluid flowing through physical structures, just at a smaller scale. CFD modeling is gaining ground in its ability to capture those physical nuances. For example, some CFD work using new methods to calculate vortex shedding has exposed unintended vortex formation in intake structures where previous codes failed. There may be a future day when physical models are no longer needed because computational models provide all the needed information, though some feel that CFD is complementary to experimental and analytical work, not a replacement for it [9].

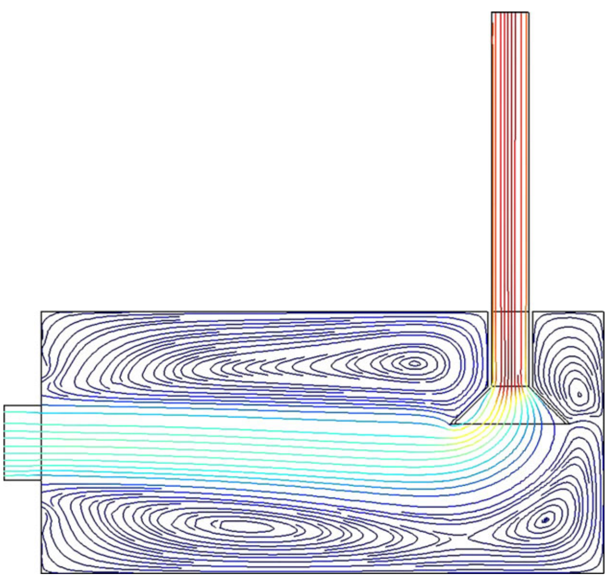

Figure 1 2D CFD model of the basic components of a raw-water intake structure showing high-velocity streamlines in red and low-velocity streamlines in dark blue or black.

3.2 Rapid Mix

Every water plant requires some sort of chemical addition to allow for proper removal of contaminants. In a conventional treatment train the first chemicals that are typically added are a coagulant and an alkaline agent. The alkaline agent is needed because the coagulant usually reacts with water to decrease the pH; the alkaline chemical helps maintain the pH in the correct range for downstream flocculation. Alum is the most common coagulant and sodium hydroxide or lime are typically used as alkaline agents. These chemicals need to be mixed thoroughly into the water and the rapid mix tank is the unit process to achieve that mixing. The tank is often square in plan view, and the water depth is similar to the width, creating a roughly cubical water volume (though many plants deviate from this). An impeller is inserted with its shaft vertical and a motor drives the impeller from above. Radial-flow impellers with a disk and six rectangular vanes are common, though impellers with other numbers and shapes of vanes, or axial flow directions are sometimes used.

The place where CFD modeling is beneficial in rapid mix tank design is in assisting to understand the details of the mixing environment. A perfect mixing tank would have no regions of low flow (dead zones) [18] and all the fluid within the tank would feel the same velocity gradient (often referred to as the G value, with units of s^{-1}). Along the same lines, every parcel of water entering the tank should have the same residence time, so as to achieve a constant GT value, which is the unitless product of G value and residence time. In practical treatment plant design, varied flow rates or footprints within the plant mean that rapid mix tanks may not perform ideally. CFD modeling can be used to verify whether dead zones occur and whether the mixing intensity is sufficiently distributed throughout the tank [19]. If the design proves to be underperforming, the mixer can be resized or baffles can be placed within the tank to alter fluid flow. Proper placement of the baffles can be educated by running CFD simulations for various placement locations and comparing the results *in silico* before expensive physical installations are needed.

The flow regime in a rapid mix tank is highly turbulent, necessitating turbulence models in the CFD environment [20]. Successful models are those that can adequately capture the intense shearing created where the tips of the impeller vanes meet the water. Swirling flow within the reactor will mean the water feels less shear than if it were able to remain stagnant. The CFD model can compare the swirling flow velocity to the impeller velocity to give a proper shear rate. It has been suggested that calculating the shear via modeling, and integrating that over the three-dimensional reactor volume is more appropriate than using the standard G-value calculation, which incorporates an empirical impeller constant. The impeller constants were found for known reactor geometries and baffle configurations and often fail when new geometries/configurations are used. CFD, then, can assist designers if they are willing to move beyond conventional design practice.

3.3 Flocculation

After introducing coagulant in the rapid mix tank, time is needed for the coagulant to (i) form precipitates upon reaction with hydroxide ions, and (ii) interact with particles, organic matter, and planktonic organisms, to form large flocs. This is achieved in the flocculation basin. Conventional flocculation basins are designed with two or three cells; the first cell has a higher mixing intensity than the second, and the second has a higher mixing intensity than the third (if present). This "tapered flocculation" provides a more intense mixing environment when flocs are forming and a gentler environment when the flocs have already formed; gentler mixing means less shear and breakup of the already-formed flocs. Mixing in flocculators can be done with either vertical or horizontal impellers or paddles.

Flocculation design benefits from CFD analysis in much the same way as the rapid mix unit process. Flocculation uses the same conventional design principles of G value and GT value. The mixing intensity is greatly reduced (lower G value) and the contact time is increased, but this is still a turbulent process [21]. CFD can help designers understand mixing, minimize dead zones, and ensure the water does not short-circuit around the mixing paddles [22]. Rotational flow is a common problem, so CFD can give information about baffle placement to mitigate the rotation. Distinct from rapid mix, an important consideration in flocculation is the desire for even and normalized flow as water moves into the flocculation basin and as it moves from one chamber to the next. Baffle walls are used to renormalize the flow and CFD can give insight into whether the baffle walls are functioning well. For example, if the paddle motion in the first chamber is pushing water more forcefully through the bottom of a baffle wall than through the top, CFD can help identify this and the mixing paddles or baffle wall can be redesigned.

3.4 Sedimentation

The purpose of creating large flocs in the flocculation unit process is so that they will settle out readily in the sedimentation basin. Sedimentation basins are usually the same width as the flocculation basins, separated by only a baffle wall. Unlike the previous unit processes, the goal of sedimentation is to have as little mixing as possible. Water is intended to move quiescently from the beginning of the basin to the end, where it gently pours over launders with weirs that assist in mitigating turbulence at the exit.

Though this unit process is the simplest yet encountered in the conventional train, and traditional engineering design is usually adequate, CFD analysis can be useful in two ways: (i) CFD can help detect dead zones where water age will become extreme, since the basins are often quite large, and (ii) as the basin fills with settled flocs, the flow paths can become altered, causing the basin to perform differently than its intended design. A common location for dead zones is near the outlet of the rectangular basins (Figure 2). Launders are often designed to protrude from the end wall into the basin. Water can rise and pour into the launders well before it reaches the wall, leaving the bottom corner of the wall as a dead zone. CFD analysis can help identify such dead zones and assist in launder or baffle placement to decrease the effect [23].

An interesting aspect of sedimentation basin analysis is the study of both the fluid flow as well as the particle deposition, which is also a fluid-mechanics phenomenon. Goula et al. [24] studied sedimentation using Fluent software. The fluid flow was solved first, then the particles were treated separately from the flow, which was an efficient computational technique. This is a common theme in not just sedimentation analysis but in CFD in general: some physical processes need to be solved simultaneously because they affect one another, but when the phenomenon can be separated and solved one after the other the computational approach is simplified.

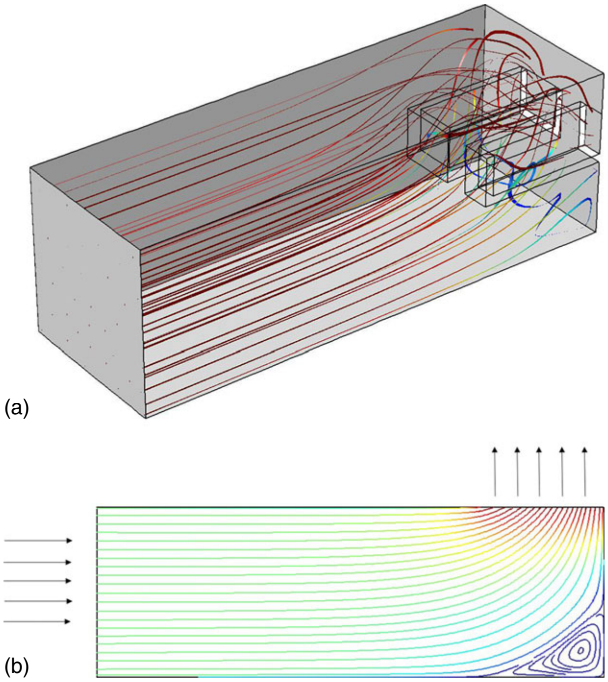

Figure 2 Two rectangular sedimentation basin (clarifier) models showing (a) a 3D view of flow over submerged launders and (b) a 2D view of flow over weirs at the top right surface. These models have an idealized inlet from a baffle wall at left. An eddy, or dead zone, is apparent at bottom right.

3.5 Granular Media Filtration

After sedimentation in a conventional treatment, train is granular media filtration. The most common media is a combination of sand and anthracite coal. Sand is denser than anthracite, so when the filter is backwashed (which it periodically must be) the sand settles fastest and falls to the bottom, leaving the anthracite as the top layer. The anthracite is selected to have a larger particle size than the sand, which means it will capture larger flocs near the top of the bed. This protects the smaller sand from becoming plugged too quickly, and thus the full bed depth can be better utilized. The sand and anthracite are held by underdrain blocks having small pores such that water can pass, but the granular media cannot. A system of troughs, inlet pipes, and outlet pipes allows for the granular media filter to toggle between active filtration and backwash modes. Air scour is typically employed to enhance the backwash and clean the media thoroughly.

Analysis of granular media filters by CFD usually operates on two size scales: the entire filter can be modeled at large scale, or the interstices of the sand/anthracite grains can be modeled at small scale. When using a large-scale filter model the sand/anthracite bed usually must be considered as a continuum of porous media. Darcy's law (or equations of similar construct) can be employed to account for head loss in the filters, which increases as the filters collect material and the Darcy permeability decreases. These kinds of models require empirical data on plugging in order to simulate the real system.

CFD models of flow through porous media on the micrometer to millimeter scale can be useful for understanding finer details of porous media behavior [25]. For example, this kind of analysis reveals that most flocs are not collected because of a straining mechanism where the flocs cannot physically enter the pore space. Rather we learn that flocs and other particles do enter the pore space but are retained on the sides of the granular media through electrostatic and/or van der Waals forces. The typical design engineer would not use such detailed information since she/he would rely on vendors and prior practice to choose media, but refinement of our basic understanding of the performance of filters via CFD modeling leads to improvements in media selection to find those with optimal characteristics.

3.6 Disinfection

Despite the multipronged approach of coagulation/flocculation, sedimentation, and filtration in a conventional train, disinfection is needed. Some number of pathogens that may be present in the source water can escape the prior unit processes and must be eliminated (or deactivated) in the disinfection step. The most common disinfectant is chlorine, delivered via chlorine gas (Cl_2) or hypochlorite (OCl^-). Other disinfectants include chlorine dioxide, chloramines, and ozone. Regardless of which chemical is used, there must be adequate contact time between pathogens and disinfectant for the pathogens to be eliminated.

The question of adequate contact time is the crux of the reason that disinfection is the domain of CFD analysis more than any other unit process in the conventional train. Studies often focus on defining the actual residence times, or residence time distributions, in disinfection clearwells [26]. In the United States, contact time is written into drinking water legislation in the form of the CT concept. This stipulates that the disinfectant concentration multiplied by the contact time results in the disinfection credit a plant achieves. A minimum disinfection credit must be achieved based on source water quality and the nature of the unit processes. Engineers must validate their designs to show that the contact time is adequate.

Contact time in disinfection goes beyond the traditional residence time concept of chemical engineering. Regulations use the t_{10} time, which is the time elapsed before ten percent of a pulse tracer has left the disinfection contact chamber. This ensures that at least 90% of any pathogens in the water have been exposed to the disinfectant (at its design concentration) for the time required to achieve inactivation. Determining the t_{10} for a given reactor requires a detailed understanding of fluid flow. Regulators will accept a variety of methods for determining t_{10}, with the gold standard being a tracer test.

CFD modeling can replace the tracer test, at least in the design phase. Regulators will often accept modeling results, assuming they can be sufficiently validated using best practices employed at other plants where tracer tests were performed. For the disinfection case, Navier–Stokes equations describing fluid flow must be augmented with convection–diffusion equations to capture mass transport. Fortunately, the two sets of equations need not be coupled (which would require more computational resources). The fluid flow equations can be solved first, then the convection–diffusion equations can be solved.

Most of the CFD problems described above for other unit processes can be adequately understood using steady-state analysis. The same is true for the fluid-flow portion of the disinfection problem, but a time-dependent study is required for the convection–diffusion part of the study. This is needed because the investigation *in silico* is analogous to the real tracer study: a dye or other detectable, conservative tracer is added as a pulse to the inlet pipe of the contactor and its concentration is measured over time while it leaves the reactor. The computational simulation mimics this approach and the simulated tracer concentration is recorded while the calculations proceed. A residence time distribution function and a cumulative residence time distribution function can be generated, from which the t_{10} value can be extracted. Performing these computational experiments during the design phase of a treatment plant can give design engineers confidence that their disinfection unit process will receive regulatory approval.

3.7 Distribution

As with the intake structure, which was the first "unit process" explored in this article, the last topic discussed here as part of the conventional treatment train – distribution – does not have a treatment goal. Instead, the goal of the distribution system is simply to deliver water to customers; however, distribution systems are places where chemical reactions and biological activity continue to occur, and large sums of energy are spent in delivering water. CFD analysis can assist in optimizing distribution systems to provide the best water quality for the lowest resource expenditure [27].

Storage tanks are a key part of the distribution system and one where CFD models can be helpful. A poorly designed storage tank will have a simple design with one pipe serving as inlet and outlet. This is adequate from a water volume perspective, but in many cases, it will mean that the last water that entered the tank will be the first to leave, because the most recent water is nearest the entrance, and thus nearest the exit, the two being the same. CFD analysis can educate design engineers about using alternate inlets and/or outlets in the tank to ensure that the oldest water leaves the tank first when the tank is being drawn down during peak demand. More proactive methods, like jet-mixing, have also been analyzed by CFD [28].

Another area of concern with storage tanks is disinfection by-product (DBP) formation, such as trihalomethanes and haloacetic acids. Several of these compounds are semi-volatile, so they can be partially removed from the water through aeration or spraying. Storage tanks can be outfitted with aerators or sprayers that operate continuously or intermittently. CFD analysis can assist in locating these devices at the best place in the tank to achieved maximum removal. Capturing the two-phase flow of bubble delivery can also be attempted to help understand which aeration rates and bubble sizes would be most effective with the smallest energy penalty. Two-phase flow problems are challenging in CFD, but adequate techniques are finding their way through the research community and into practice.

4 Alternative Unit Processes

Aside from the conventional treatment train, other unit processes have become popular for drinking water treatment when special needs exist. They are discussed here in the context of CFD analysis and compared to their analogous conventional unit processes.

4.1 Static Mixers

While the rapid mix tanks discussed earlier are generally understood to be the conventional process for mixing in drinking water treatment plants, static mixers are an alternative that have been implemented fairly widely. The "static" term in the name refers to there being no moving parts in this unit process; vanes protrude from the walls of a pipe and cause turbulence as water moves through, but the vanes themselves do not change position (Figure 3). This feature of having no moving parts constitutes the main advantage of static mixers over rapid mix tanks. Static mixers require much less maintenance than the motors and impellers used for rapid mixing.

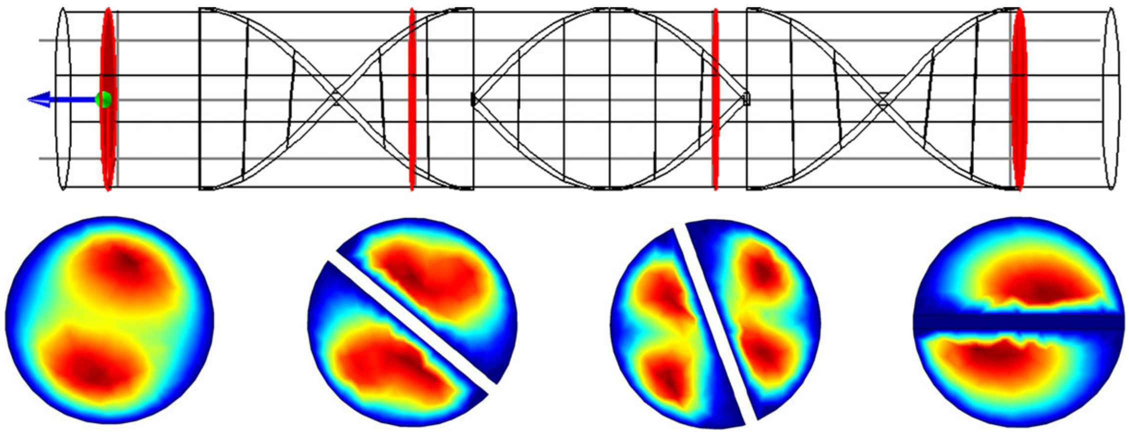

Figure 3 Static mixer CFD model. Vanes protrude into the water flow; they do not move (are static), but increase turbulence as water passes around them. The bottom circular images are cross-sectional cuts taken at the locations denoted with red in top image. Hot spots of fluid flow are shown by the dark red of the color flood and low-velocity regions are shown in blue.

Another key selling point of static mixers is their reduced energy consumption. The device must provide adequate mixing, which is easy to achieve if enough vanes are included to cause a very tortuous fluid path. Modeling can elucidate pockets of reversed flow and can help observe longitudinal vortices characteristics of mixing [29]. But the pressure drop from inlet to outlet in the mixer needs to be kept at a minimum to reduce energy costs. CFD modeling of various static mixer designs can be used to find optimal geometries that provide good mixing, in terms of high average velocity gradients, with reduced pressure drop.

A key disadvantage of static mixers is that their mixing intensity decreases when flow rate decreases. Most drinking water treatment plants operate at lower flow rates than their design since the plants are built with extra capacity to accommodate future population growth. For rapid mix tanks, the impeller speed does not have to be reduced when the flow slows, so the mixing intensity can remain high; static mixers do not have that capability. Modeling the mixers in CFD allows designers to test the design *in silico* and discover whether the mixer will be adequate if the treatment plant is operated at lower capacity. Engineers can decide, for example, to install two smaller static mixers (rather than one large one) so that a mixer can be taken offline and all the flow directed to the remaining unit. The velocity through the remaining mixer will be high enough to maintain mixing intensity. CFD analysis is a useful design tool to assist in making this sort of decision.

4.2 Reverse Osmosis and Nanofiltration

A water treatment technology that has seen rapid development and adoption over the past few decades is the use of membranes for removal of salts and other small-molecule contaminants like those found in wastewater. Reverse osmosis (RO) is the predominant term used for these processes. Nanofiltration (NF) is a term introduced later to denote a membrane process that is quite similar in materials and form factor as RO, but with a membrane that allows more monovalent (e.g. sodium and chloride) salt passage while maintaining good rejection of divalent salts (e.g. calcium and carbonate). NF has overtaken ion exchange as the technology most commonly recommended for water softening at the treatment plant scale. For CFD analysis, RO and NF can be safely discussed together; the only difference between the two is that water flux and salt passage will be higher through the NF membrane. The same CFD models used for RO can be used for NF, as long as the boundary conditions at the membrane wall are adjusted.

Much of the CFD literature on RO and NF seeks to answer questions about salt buildup on the membrane surface, called concentration polarization. This is a dynamic process that does not involve adsorption of the salts to the surface, but rather the buildup occurs because salts are pulled toward the membrane and cannot pass through. Once the flow ceases, the salts diffuse back into the feed water. Understanding concentration polarization is important because the membrane feels the osmotic pressure of the salt nearest its wall. If that concentration is elevated, water passage through the membrane is diminished. To minimize concentration polarization, feed water is swept through the channel tangential to the membrane surface. Turbulence promoters are used, in the form of spacers that also have the function of keeping the membrane leaves separate from one another. Figure 4 shows a CFD model of a portion of a typical feed spacer in RO/NF. Regions of higher velocity are observed where water flows over

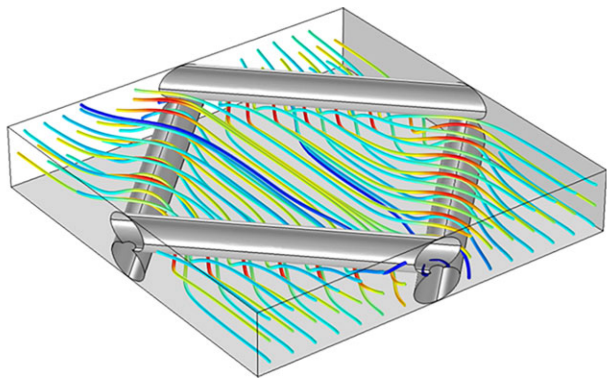

Figure 4 Simulation of fluid flow around a conventional, net-style mesh spacer typical for RO and NF applications. Flow paths are shown with red indicating higher velocity and blue indicating lower velocity.

and under the spacer filaments. The spacers also cause water to change its angle of attack, because of the 45° configuration of the filaments. An interesting aspect of CFD for spacer analysis is that the repeating geometry of the spacer allows an assumption of "periodic fully developed" flow [30]. Instead of running a model that incorporates many small filaments in the geometry, the model can include only one repeating unit. This vastly increases the speed at which models can be solved.

Understanding concentration polarization and the fluid dynamics around spacers leads to the next important question in RO and NF: fouling. Fouling is the buildup of material on the membrane that (unlike concentration polarization) does not diffuse away when water flow ceases. Organic matter in feed water, such as humic acid, polysaccharides, or proteins, is usually the first to adsorb to a membrane, and thus constitutes a conditioning film that is the basis for subsequent foulant development. Bacteria attach and replicate on the membrane, creating thick and persistent biofilms; these biofilms are a common cause of headaches for RO/NF operators. Another cause of concern is scaling, defined as the precipitation of salts such as calcium silicate on the membrane surface. Scaling is most common in softening and brackish-water desalination where high recoveries (e.g. higher than 80%) are pursued. Recovery is defined as the amount of clean water obtained compared to the amount of feed water brought into the system. Recoveries in seawater desalination are limited to about 50% because of the high monovalent salt concentrations, thus scaling is not as common in seawater RO.

Fouling presents a particular challenge in CFD modeling because the water flow is affected by the foulant buildup. In most of the other unit processes of drinking water treatment, tank and pipe dimensions remain constant and thus the CFD model can study fluid flow in a constant geometry. In the case of fouling, the geometry of the boundaries to fluid flow is changed dynamically as parts of the membrane are blocked and some open areas of the spacer are plugged. Accounting for this dynamic geometry change to adequately build fouling models is an open area of research in CFD.

An important question asked in CFD models of RO/NF processes is with respect to spacer design. New spacer geometries are sought to diminish concentration polarization and decrease fouling while at the same time not exacerbating pressure drop. Achieving both objectives is not easy since features that cause more mixing in a system usually also cause greater pressure drop. Also, features that cause mixing tend to be locations where the channel is blocked, dead zones are formed, and foulants can accumulate. Spacer designs must achieve mixing while also allowing for fairly open flow regions. CFD models can be used to find such designs, such as spacers that create sinusoidal flow patterns that have shown promise in recent work [31].

4.3 Ozonation

While chlorine has a long history of use as the primary disinfectant in water treatment, ozone is an alternative that now has an established foothold in the field. Ozone is a more powerful disinfectant than chlorine and can inactivate pathogens at lower temperatures. Ozone can also be used for other purposes, like removing the taste-and-odor compounds geosmin and 2-methylisoborneol (MIB). It can be combined with hydrogen peroxide for advanced oxidation that can remove many emerging contaminants that are difficult to remove by other means.

The questions that CFD can help address the ozone unit process are similar to those for traditional disinfection. Though the system is turbulent [32], ozone works best when the hydrodynamics approach plug-flow conditions because adequate react time is needed. Typical contactor designs have over-under baffles that cause water to flow up, down, and up again in a serpentine manner. This contrasts with side-to-side serpentine channels typical for chlorine disinfection because ozone is introduced as a gas, with bubbles rising through the water; having a vertical baffle configuration lends itself to taller tanks that allow more distance for ozone mass transfer as the bubbles rise through the water. Analysis of these contactors by CFD allows for an understanding of how the water behaves as it moves over and under the walls of the serpentine contactor. A common result for such contactors is swirling fluid flow or dead zones in the corners (Figure 5). Additional baffles can be

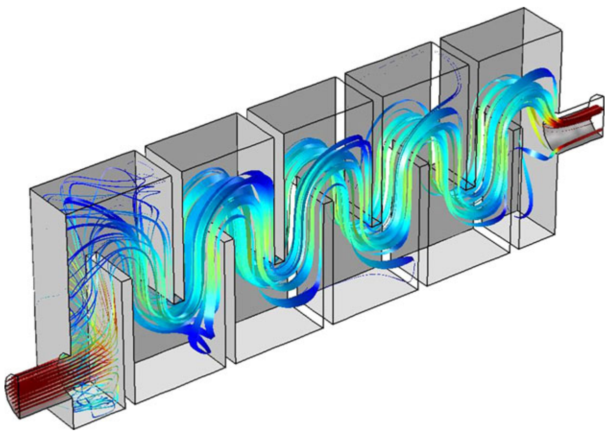

Figure 5 Cutaway view of an ozone contactor with streamlines showing fluid flow over and under baffles. These 3D streamlines are set to follow the main flow paths; the corners between baffle walls and side walls that have no streamlines are relatively dead areas with little velocity.

inserted to reduce the flow, but another approach is to be prescriptive with the width of the channel (i.e. the distance from one wall to the next). CFD analysis has shown that that width is an important determinant of whether eddies will form or not.

5 Considerations for Effective CFD Modeling

A common concern in CFD modeling projects is the question of whether the computer-generated results are realistic or diverge from reality. Ideally, every model would be validated through laboratory or field experiments, but cost and time preclude this approach. It is common that the first few iterations of a modeling effort result in spurious data that the user must identify and correct. A robust approach for ensuring model accuracy is to run a control model that has a known analytical solution. For example, the velocity field for laminar flow through a circular tube has an analytical solution in the Hagen–Poiseuille equation [18]. A modeler can begin with this simple circular tube and verify the results using the analytical solution, then add geometrical complexity to their model.

Another important consideration is mesh sensitivity. This arises because every model is built on an array of finite elements in a geometrical arrangement; this is the mesh. The position and density of the elements are selected by the modeler, usually through an automated subroutine in the software package. Fluid flow and mass transport in the physical system being modeled should not be dependent on the location of the mesh elements. A user should run several iterations of their model, adjusting the density of the mesh with each iteration. When different mesh arrangements result in the same overall fluid flow and mass-transport results, the user gains confidence that the model is accurate; the results are said to be mesh independent.

Perhaps the most robust method (other than physical experiments) for validating CFD models is a collaborative approach where two modelers tackle the same problem and compare their outputs. If the results disagree, the modelers can identify whatever assumptions or parameters were not common, then work together to converge on the most appropriate model setup to give consistent results. Because several software packages are now available, using more than one package is also a viable strategy. When the two packages yield the same fluid flow solution, the users gain a great deal of confidence that their results are valid.

6 Summary

This article looked at a conventional drinking water treatment plant through the lens of CFD modeling. Less-conventional unit processes were also mentioned. Some fluid flow questions – and the resulting answers – are common in several unit processes. For example, the concept of preventing or minimizing dead zones or eddies is common to flocculation basins, sedimentation tanks, disinfection contactors, and ozonation processes. The idea of understanding velocity gradient, or the magnitude of shear imparted by mixers, was common to rapid mix tanks and flocculators. There is a clear conceptual connection between static mixers employed for bulk fluid at the head of the plant and the much-smaller-scale membrane spacers in RO/NF: both provide mixing, but both need to be optimized to minimize pressure drop while accomplishing the mixing task. CFD analysis gives designers a useful tool for trying out new designs *in silico* before taking those designs to the plant for construction. Or for already-constructed plants, CFD provides a means to troubleshoot problems with fluid flow and test out various remediation strategies. While most published papers deal with individual unit processes and employ commercial codes, the advent of open-source codes and repositories of solved models is creating new opportunities for broader penetration of CFD into drinking water treatment plant engineering practice.

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