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Full simulation of disinfection stage in a water recycling plant using low-cost, hybrid 3-dimensional computational fluid dynamics

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Abstract

Water purification is a crucial process in the operation of a municipality. Ensuring that water treatment plants are meeting regulatory requirements is a vital, but complicated and costly process. Because water treatment plant influent and effluent rates are demand driven, and vary both diurnally and seasonally, controlling flow rates for the disinfection stage can be challenging both operationally and economically. Thus, performing large-scale field experiments to verify water quality regulatory criteria such as modal transport time of conservative tracers in a chlorine disinfection contact tank under extreme operating conditions can range from difficult and costly to impossible. In this paper, a computational fluid dynamics (CFD) approach is used to verify the compliance of a water reclamation plant disinfection stage with respect to modal time. CFD allows a large parameter space to be tested without the need to build large physical models or taking functioning systems in a treatment plant offline. This can save facilities large amounts of time and money when designing, optimizing, and developing plants or checking compliance. This paper introduces a hybrid approach of computational analysis of a water reclamation plant's chlorine contact tank in Southern California. The method uses a hybrid approach which combines three-dimensional CFD with hydraulic grade line analysis of the open water surface. Verification cases were compared to experimental measurements at a functioning, full-scale plant with modal contact time differences below 15%. The method was then used to predict residence time distributions (RTDs) for cases which could not be artificially induced at the plant, but represented peak flow conditions that could be expected. © 2018 Water Environment Federation

Practitioner points

- The hybrid 3-dimensional CFD method allows low cost simulation of the disinfection stage.
- By using head loss calculations to properly define the water level at each section, a steady-state single phase flow simulation can be run in 3D without the need to scale down geometries.
- This allows for more accurate transport results and parameter studies.

Key words

computational fluid dynamics; chlorination; contact tank; disinfection; dispersion processes and models; flow-structure interactions; RANS models; three-dimensional models; wastewater treatment; water quality

Introduction

The proper treatment of municipal water is of utmost importance to our health and way of life. It is therefore critical to ensureall processes meet established governmental and regulatory guidelines. Sometimes, however, the tests required to prove difficult and costly because they involve challenging or unusual conditions such as extreme peak flow rates. In particular, this paper aims to provide a low-cost and accessible solution for disinfection stage studies. Section 60301.230 of California Title 22 Code of Regulations (2014) requires "disinfected tertiary recycled water" have a chlorine disinfection process with a minimum of 90 minutes of modal contact time at a peak dry weather design flow. To test compliance experimentally at field scale, at minimum, requires artificially raising throughput to peak design flow rates in the plant. This can be an expensive and prohibitive endeavor. This paper proposes a novel, economical computational fluid dynamics (CFD) approach, which can be used to test compliance or to design new facilities that will comply with regulations.

Computational fluid dynamics can be a powerful tool to model water treatment processes. While CFD was initially applied to solve problems in the aerospace, biomedical, and defense industries, it is also gaining popularity in simulating various water treatment processes (Brown & Salveson, 2006). Specific to disinfection, Greene, Farouk, and Haas (2004), Greene, Haas, and Farouk (2006) applied CFD to assess the effect of reactor configuration on the efficiency of chlorine disinfection. Wols et al. (2008) used CFD modeling to assess the residence time distribution during ozonation of drinking water. Tafilaku (2010) utilized CFD to optimize contact times during chlorination while also focusing on the formation of disinfection by-products. Xanthos, Ramlingam, Beckman, Deur, and Fillos (2013) studied the effects on mixing in water storage tanks caused by baffles, temperature gradients, and various design configurations through CFD modeling. CFD allows a large parameter space to be tested without the need to build large physical models or taking functioning systems offline for difficult or infeasible testing. This can save facilities large amounts of time and money when designing, optimizing, and testing plants to check compliance. However, adoption of CFD methods has been slow. This can be attributed in part to the shortage of CFD expertise in the water treatment field. More importantly, the relatively large scale of water treatment facilities relative to turbulent length scales makes computational analysis of plant facilities difficult as well as time-intensive and computationally intensive.

There are several factors which make simulating an entire full-scale disinfection stage challenging. The size of the chlorine contact tanks requires a large computational grid with numerous cells (on the order of 1e+6 to 1e+7 elements). The concentration of cells must be higher in areas with large velocity gradients. This high concentration requirement is compounded by the fact that the chlorine contact tank is typically an open channel system. Water levels can vary with flow rates, so high vertical resolution is necessary near the top of the tank's water surface. UV disinfection studies such as Huang, Brouckaert, Pryor, and Buckley (2004) can model only flow without regard for diffusion of scalar as is necessary for chlorine disinfection. Compared with flow velocity simulations, this scalar transport simulation is the more time-consuming of the two components of modeling contact tank flow dynamics. Some previous methods for decreasing the large computational load include 2D models, laminar flow models, neglected diffusion, or drastically reduced model size (Khan, Wicklein, & Teixeira, 2006; Kim, Stoesser, & Kim, 2013; Templeton, Hofmann, & Andrews, 2006). The proposed method does not necessitate any of those compromises. Zhang et al. performed simulations of Ozone contactor (2013) and baffled contact tanks (2016) using the Reynolds-averaged Navier-Stokes (RANS) equations. However, both these studies were for scaled models <11 m in the longest dimension. Notably, they also were closed tanks with no free surface, which is unusual in chlorine disinfection. Angeloudis, Stoesser, Gualtieri, and Falconer (2016) used RANS simulations to study contact tank design variations on performance also with a scaled model. Their computational work was validated against a scale-model experiment. This scale model was studied in Angeloudis, Stoesser, Falconer, and Kim (2015), which concluded, "hence, the absolute disinfection performance for a given contact time should only be examined at full-scale conditions since only then scaling effects of hydrodynamics, surface roughness and contact time are absent." This is due to the necessity of full-scale dimensions to match both the Reynolds and Froude numbers.

The current work uses a full-scale model of a real-world water recycling plant chlorine contact tank and corresponding tanks and piping which comprise the disinfection stage. The approach adds the complexities of size, as well as well-to-pipe transitions, pipe-to-well transitions, sluice gates, and weirs. The presented method allows all these complexities to be included, while still performing simulations in a short amount of time on a standard office workstation PC. The low-cost hybrid, three-dimensional CFD method uses hydraulic grade line analysis and preliminary flow studies to simplify the scalar transport modeling. This method has its own complexities, but allows calibration against field studies and simulation of multiple scenarios at many flow rates in short time periods with little or sacrifice of model accuracy.

Case description

The current study focused on estimating the residence time of a conservative nonreactive tracer (scalar) in a serpentine chlorine contact tank under steady-state flow condition. The regulations require the use of conservative tracers instead of reactive tracers to facilitate the determination of modal times. Calculations of modal times are necessary to ensure the chlorine contact tank effluent meets the applicable recycled water regulations. The hybrid approach in question will produce a residence time distribution for each flow rate and water depth condition in the tank. Thus, the residence time distributions can be temporally integrated to calculate modal times for the different steady-flow simulations of interest.

Disinfection stage geometry

Three parallel chlorine contact tanks, each with three serpentine passes and fed by a single inlet channel, are used for the chlorine disinfection step after primary treatment, secondary treatment, and filtration to produce high-quality recycled water. Together, the three chlorine contact tanks total roughly 100 m long by 20 m wide with depths ranging from 4 to 7 m depending on flow conditions. The tanks are shown in Figure 1. After filtration, the water is pumped into the filter effluent channel, which is equipped with a large mixer. This is the point of addition of the nonreactive tracer or scalar in lieu of the usual chlorine injection. Downstream of the channel, the

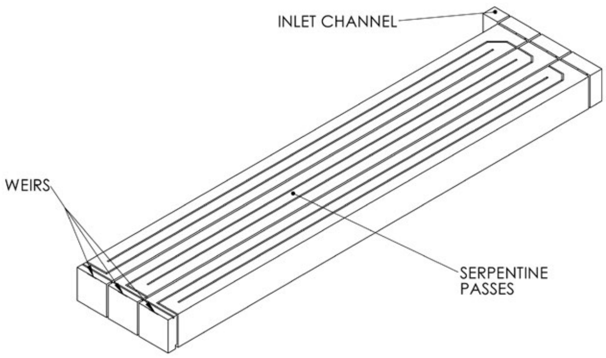

Figure 1. Chlorine contact tanks at water reclamation plant.

effluent travels through a long pipe into an inlet channel. From this channel, there are three adjustable sluice gates which flow into three separate chlorine contact tanks. The water in each of the three tanks flows through the three serpentine passes before exiting over the final weir of each tank. Aside from the weirs, two of the tanks have bottom outlets for separate recycled flow extraction. The interior geometry from the mixer to the contact tank weirs is modeled carefully following the dimensions and details provided in the engineering drawings for the treatment plant.

Method

The method presented here uses a hybrid approach which combines three-dimensional CFD with hydraulic grade line analysis. By using energy loss (head loss) calculations for open channel hydraulics, boundary conditions for the water surface are set under steady-state flow conditions. Thus, simulations which do not neglect turbulence or diffusion and that are manageable on a regular PC workstation can be run. Fully modeled residence time distributions can be produced in under 4 days on a computer with a 4-core processor (<400 CPU-hours).

The hybrid approach is introduced in calculating the water depths in the separate tank sections. To prevent the simulation from having to account for water depth variations and calculate the corresponding surface levels along the entire open channel system, the models are cut to match the computed water levels calculated through analysis of energy losses (head loss) before the simulation begins. The resulting spatially varied water surface profile calculated for each flow rate represent the model's boundary condition for the free surface. This surface is then modeled as a wall with zero shear. With a known steady flow rate, water surface elevations can be calculated for weirs, passes, and other hydraulic structures. For example, the water surface elevations for weirs are calculated based on weir characteristics and flow rate. The hydraulic grade line for the contact tank passes, which are gravity-driven, are determined by using frictional losses and appropriate minor losses obtained from the literature for each hydraulic structure. For instance, the conveyance method is used to calculate friction slopes in the tanks. In this case, the head loss due to friction in the tanks is less than 1e-4 m per pass. Minor losses in the elbows are calculated using a $K_L = 1.5$ loss coefficient. Because the overall slope of the water surface is practically negligible in the contact tanks, the contact tank is modeled with a flat surface. The next loss scenario is through the sluice gate. The loss in the gate is calculated with a minor loss coefficient of $K_L = 2$. The height of the water surface in the model in the upstream inlet channel is then raised above the level of the downstream contact tank by an amount equivalent to the calculated head loss through the sluice. To prevent a sudden jump in height, a smooth, sloped surface is introduced to the transition region between the inlet channel and contact tank when the sluice gate is not fully submerged. This transition region is roughly four times the water depth of the sluice gate's weir crest. Hazen-Williams (or alternatively Darcy-Weisbach) calculations are used to find the head loss in the pipe upstream of the inlet channel. This head loss calculation then gives the height for the filter effluent channel where the chlorine is introduced. The hydraulic grade line profile obtained from the energy loss calculations for the pipe, channels, weirs, and other hydraulic structures matches well with calculations performed by the agency that designed and operates the treatment plant.

Model simplification

The model described above was simplified slightly for faster computation. The full model included the 3 × 8 plywood baffles which support the walls between the serpentine channels. The simplified model replaces the baffled walls with slightly thicker walls which have the same thickness as the baffles. Mesh refinement is also necessary near all wall surfaces and corners. Because of the large number of baffles and the resulting increased surface area, the baffles added a very large number of elements to the mesh. Due to the large size of the treatment tank, the number of elements in the simulation mesh was already exceedingly large for a single processor computer. By eliminating the baffles, the mesh size was drastically reduced with little effect on fidelity. Velocity field comparisons between the model which included these baffles and a model with the thicker walls showed very limited variation. The original and modified geometries are shown in Figure 2. A comparison of velocity fields between the two cases for a representative plane is shown in Figure 3. This figure shows that the regions between the baffles have insignificant velocities. Replacing

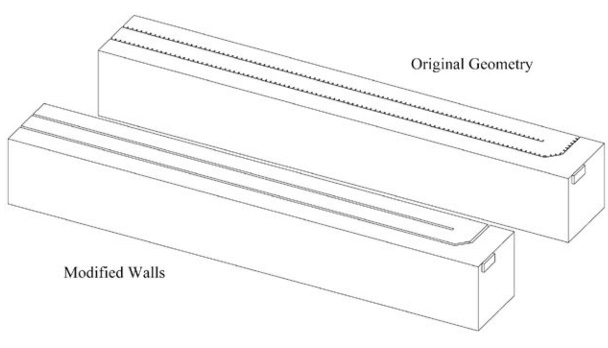

Figure 2. CAD model simplification by replacement of 3 × 8 supported walls (top) with thicker walls (bottom).

these "dead zones" with solid material does not affect the main flow regions.

Mesh generation

Once the model for each case is complete, meshing is conducted in ANSYS Meshing. A tetrahedral mesh is created with inflation layers on each wall surface. This mesh is generated automatically by the software with the sizing set to "fine" and no additional sizing criteria. Additional sizing restrictions are then placed near any area of increased pressure or velocity gradient. Examples of such areas include the weir exit, each area of turning in the contact tanks as well as the turn of the water into the weir, the entrance and exit areas of the sluice gates, and the inlet and exit areas of the feed pipe. Cells with above 95% skewness are identified and corrected before moving on to the next step. Once the mesh is of sufficient quality, it is imported into ANSYS Fluent. Within Fluent, the mesh is converted from tetrahedral to polyhedral elements. A sample section of the converted mesh is shown in Figure 4. This conversion significantly decreases the number of elements in the mesh and decreases computational time. Studies such as Spiegel et al. (2011) have shown that polyhedral meshes have no additional error compared to tetrahedral meshes. The final mesh had roughly 2×10^6 elements with slight variations depending on the weir height of each case.

Boundary and initial conditions

When the mesh passes a final check for quality, boundary conditions are implemented. The inlet is prescribed a flow rate, while the outlet is given an atmospheric boundary condition. A 12% turbulence intensity is prescribed at the inlet to account for the effects of the mixer. The pressure at the weir exit is allowed to vary as long as the average pressure (gauge) at the water surface is zero (i.e., atmospheric). No-slip conditions are given to the walls. As stated earlier, energy loss calculations are used to determine the hydraulic profile for each steady flow rate simulated. However, the question of what boundary condition to give the water surface arises. The flow is gravity-driven. Nonhydrostatic pressure variations are minimal in the flow. A pressure condition would seem logical, however would allow for flow to leave the computational volume. This would add complexity and allow errors. Additionally, low-pressure

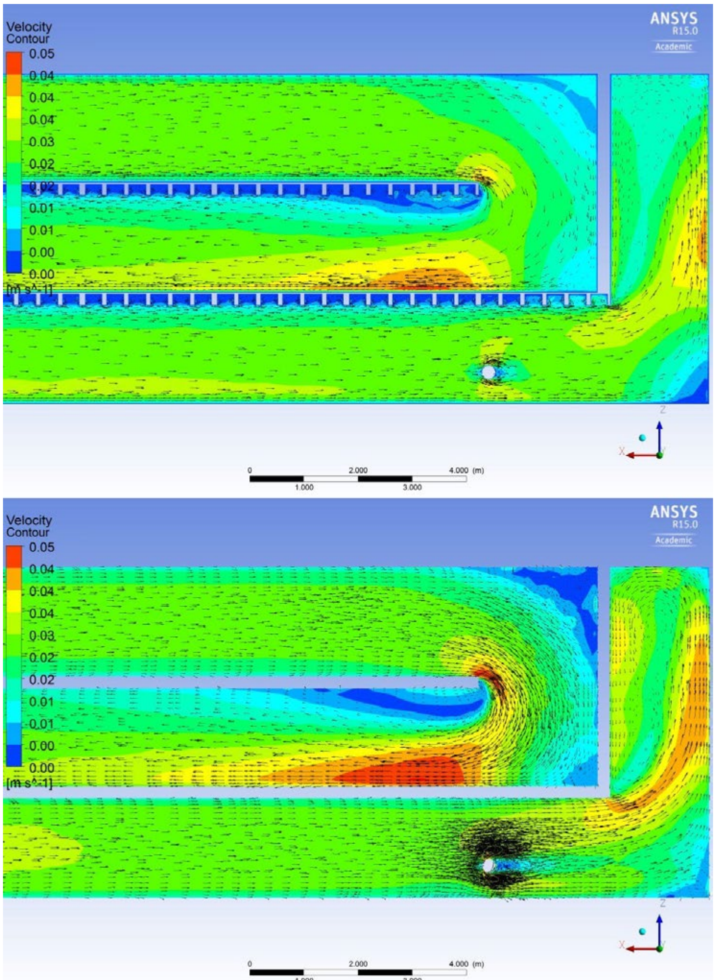

Figure 3. Computational fluid dynamics velocity magnitude results for 3 × 8 supported walls (top) versus thicker walls (bottom).

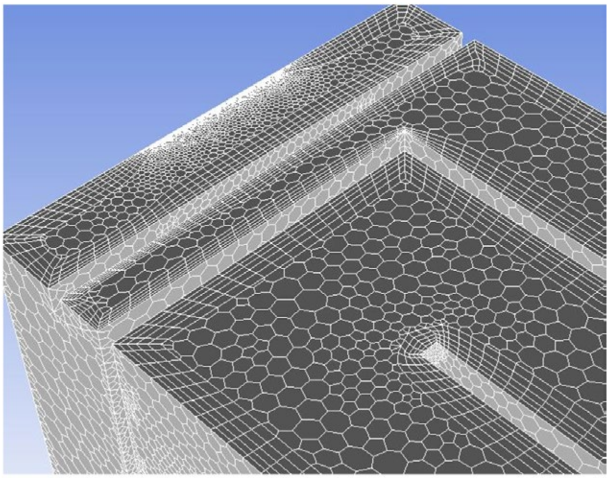

Figure 4. Close-up of contact tank outlet of final polyhedral mesh (converted mesh) with inflation layers along all walls.

regions would introduce new fluid to the volume. The conditions for this inflow would have to be known. To simplify the simulation, a symmetry condition is used on the water surface. This boundary condition type allows flow along the surface to flow tangent to the surface with zero shear stress. This eliminates the possibility of fluid entering or leaving the volume and allows easier convergence. For some cases, only one contact tank was modeled. The geometry upstream of the contact tanks was all retained. Mass flow conditions are applied to the other two sluice gates, and equal flow is assumed between the tanks.

For scalar simulations, an initial condition of zero scalar is implemented in the flow field. The flow field and turbulence values are the converged solution of the flow simulation. Scalar is introduced at a constant rate at the inlet plane.

Simulations

Flow simulations are run using ANSYS Fluent to solve the Reynolds-averaged Navier-Stokes equations (RANS) using the k-epsilon turbulence model. Second-order discretization is used to solve for a steady-state flow field. Scalar transport is modeled in a transient simulation also in Fluent. Once the flow field is solved, the frozen flux condition is implemented. Because the scalar transport does not affect velocity values, there is no need to recalculate the velocity and turbulence values at each time step. A turbulent Schmidt number of 0.9 was used. Time steps of 0.25 s are used after a convergence study showed no change in results using finer increments of time.

Results and Discussion

Simulations consist of a two-stage process. First velocity data are obtained from the model and inspected. The flow fields are observed for discontinuities, and mass flow rates at each transition are monitored to confirm conservation of mass. Contours of velocity magnitude for a representative case are plotted for planes in the middle chlorine contact tank in Figure 5. These planar velocity fields show the behavior of the fluid as it passes through the serpentine channels. The importance of a 3D model is immediately appreciated in the entrance region, with the high-speed flow near the bottom of the tank. This is also seen in the last passage as the exit geometry effects are evident upstream of the weir. Figure 6 shows the progression of the scalar within the chlorine contact tank at two different time steps. Again, vertical asymmetry can be seen, with most of the tracer staying near the surface as it enters the contact tank.

Verification of model

Initial trials were run with steady-state flow rates equal to those in experimental cases tested at the water reclamation plant. The flow-through curves (FTC) of the simulation data were

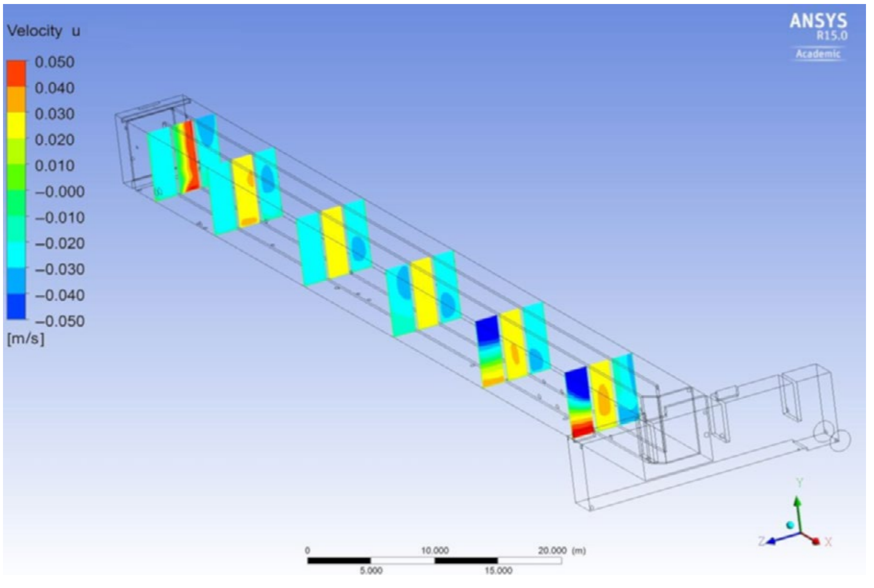

Figure 5. Cut planes with contours of streamwise velocity for center chlorine contact tank.

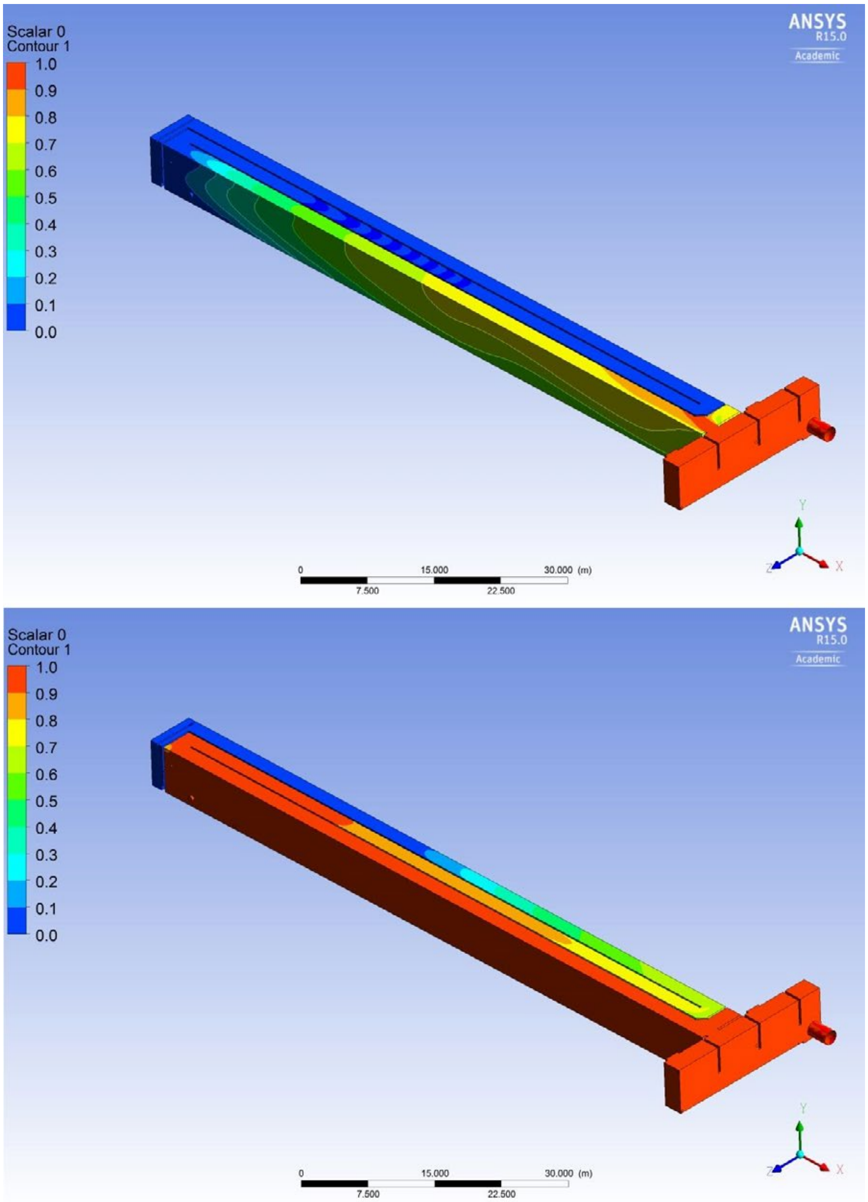

Figure 6. Scalar diffusion shown through scalar concentration contours for early (top) and mid (bottom) flow times.

compared to these experimental results for verification. Six cases were tested. The main result of interest was the modal transport time of the scalar. The maximum discrepancy in modal times between the simulations and experiments for all tested cases was 15%, while the minimum error was 1%. Model errors may be compounded by sources of error in the experiment which include the flow rate measurements (with meter uncertainties of ±5% or higher not uncommon), unsteadiness in the flow rate of the experiments (standard deviations of 5%–8% of average flow rate), low recovery rate of dye in the experiments (20%–50%), and errors due to the fluorometer used in the field to measure the dye tracer.

Results for two trial cases are shown in Table 1 and Figure 7. The authors would like to note that no tuning was conducted to obtain these results. Trials 1 and 2 had similar flow rates of 0.87 and 0.91 m^3/s, respectively. However, trial 2 had 0.16 m^3/s of water drawn for use as recycled water, resulting in less flow over the weir and lower water levels in the tanks. Trial 1 did not have any flow diverted from the weirs. One-third of the total flow passed through each serpentine passage. Reynolds number based on hydraulic diameter through the serpentine passages was roughly, $Re = 9 \times 10^4$. Trial 1 had a modal time 13% greater than the experimental value from the full-scale tests at the plant. Trial 2 had a modal time 11% greater than the experimental value. Median and modal contact times were both greater for the computations than experiments, leading to larger model baffling factor values. However, the Morrill Dispersion Index was similar

Table 1. Comparison of experimental and computational test case conditions and results for trials 1 and 2

	TRIAL 1		TRIAL 2	
	EXPERIMENTAL	COMPUTATIONAL	EXPERIMENTAL	COMPUTATIONAL
Conditions (MGD)				
Average effluent	19.8	19.8	20.80	20.80
Average flow/CCT	6.6	6.6	6.93	6.93
Std. Dev. CCT flow	1.1	0.0	1.30	0
Contact time (min)				
Theoretical	188	188	180	180
T10	129	148	140	150
Median	152	167	169	180
T90	203	220	217	229
Mode	**137**	**155**	**151**	**168**
Efficiencies				
Baffling factor	0.73	0.82	0.84	0.93
Mode/theoretical	73%	82%	84%	93%
T10/theoretical	69%	79%	78%	83%
T90–T10	74	72	77	79
Morrill Dispersion Index	1.57	1.49	1.55	1.53

Note. Modal contact times are in bold.

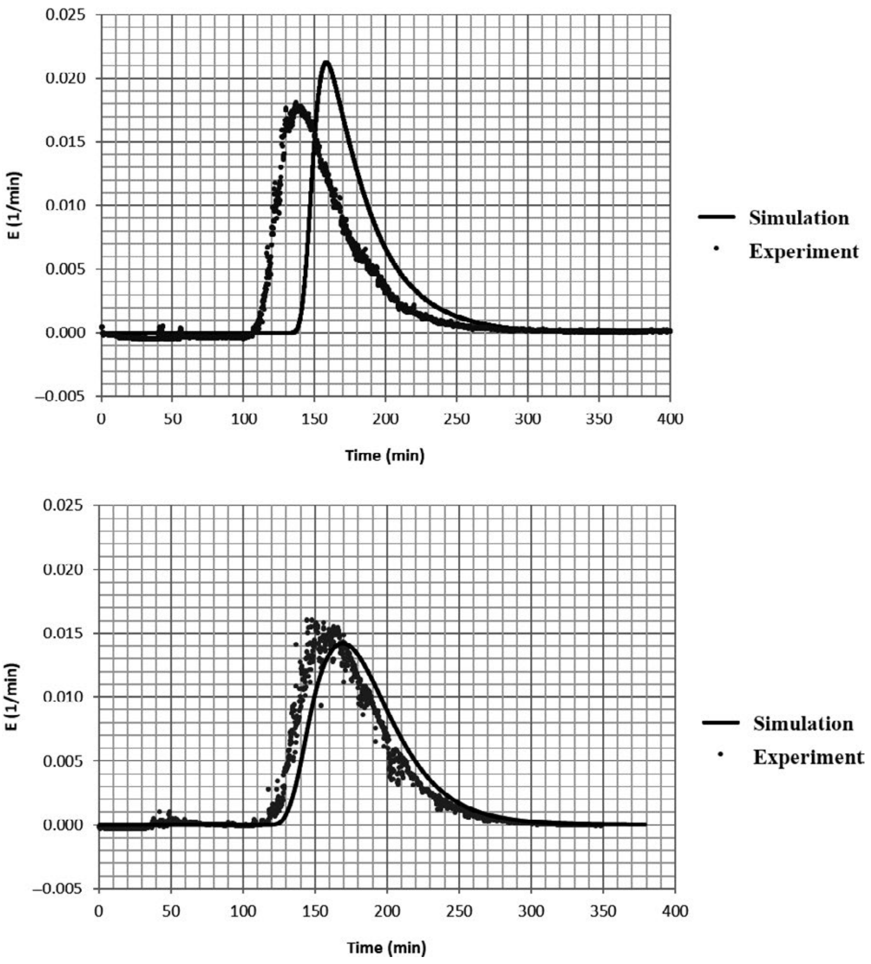

Figure 7. Flow-through curve comparisons for trial 1 (top) and trial 2 (bottom).

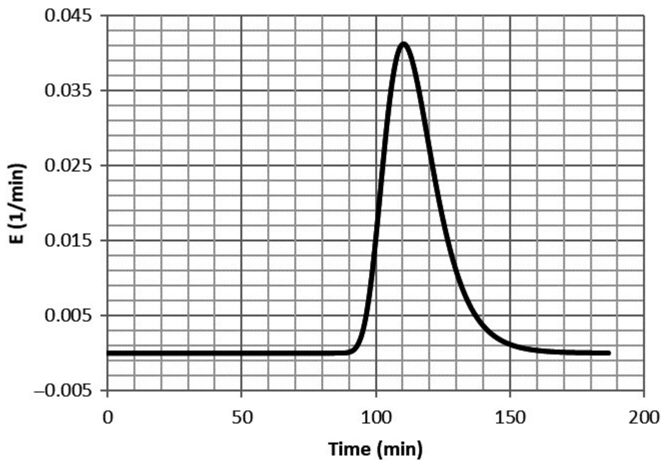

Figure 8. Predicted flow-through curve for hypothetical extreme flow case.

between the computations and experiments. There was minimal difference in either trial in elapsed time between the passage of 10% of introduced scalar to passage of 90%. The increased travel time of the simulations is most likely due to the geometry modifications. The introduction of thick dividing walls versus a thin wall with support beams increases the shear stress experienced by the fluid. The authors believe that the differences between the simulations and the experiments are acceptable given the complexities of the physical system and field data uncertainties.

Predictive modeling

Having shown that the model meets experimental data to an acceptable degree, a simulation was run to model a case which could not be completed experimentally without unreasonable cost and downtime of the facility. This case involved a lowered tank level (which can occur during periods with low influent flows) and maximum output capacity of recycled flow. The flow-through curve for this case is shown in Figure 8. The results for this predictive case show the recycled flow complying with the California Title 22 requirement of a minimum of 90 min of modal contact time at a peak dry weather design flow.

Conclusions

The verification cases prove that the hybrid modeling approach presented in this work can accurately model the entire disinfection stage of a water reclamation plant in a reasonable timeframe without the need for large computer servers. A single workstation ran all the cases tested in under 7-day real time. The verification cases all showed results within 15% of the experimentally collected modal times. By using this model and the method described, simulations can be run to test the plant under conditions which would be impossible or very costly to test in the real world. For example, peak flow conditions are often difficult to test in a real-world plant. Using a computer model to simulate different conditions removes the need for manipulation of the real physical system, which includes waiting, system downtime, unsteady flow conditions, other challenges, and yet provides a useful tool to determine whether the chlorine contact tanks are operating satisfactorily and meeting regulatory requirements.

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