WATER water everyhere

AND MAKING IT FIT TO DRINK

Amsterdam Water Supply (AWS) of the Netherlands produces some of the cleanest drinking water in the world using an environmentally benign ozone disinfection approach. To clean up the 100 million cubic meters per year they handle requires giant turbulent disinfection reactors. COMSOL Multiphysics simulations help AWS researchers Dr. Jan Hofman and colleagues fine tune what happens inside these big rigs.

BY LEIGH SOUTTER

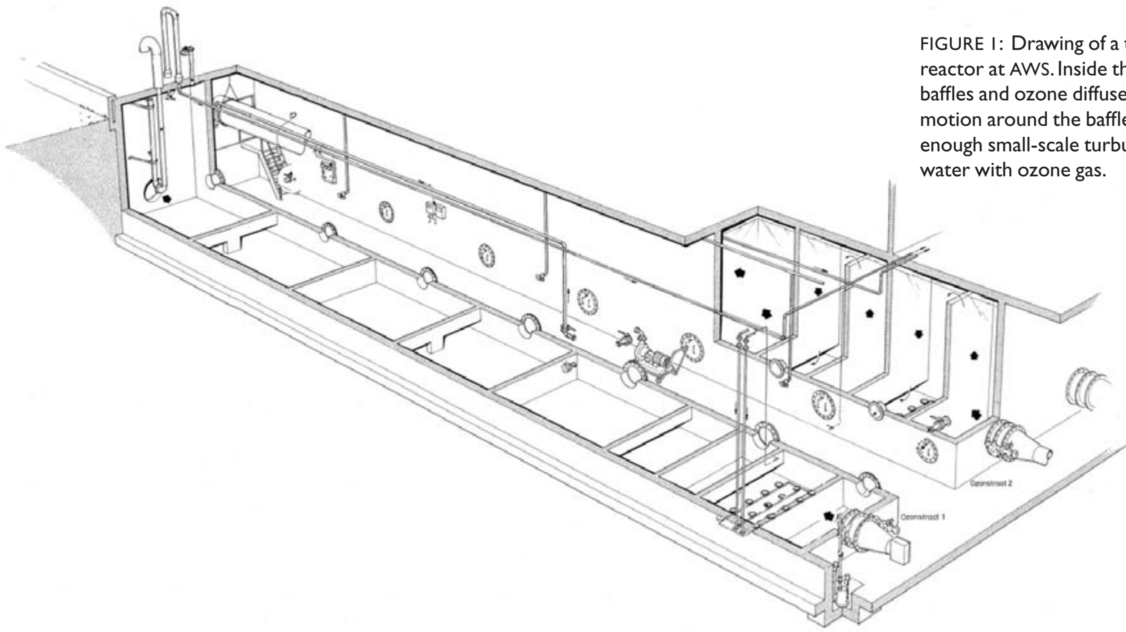

FIGURE 1: Drawing of a turbulent ozone reactor at AWS. Inside the reactor are baffles and ozone diffusers. Water motion around the baffles produces enough small-scale turbulence to mix water with ozone gas.

Ozone reactions are the primary disinfection step at AWS (Figure 1). Conventional chlorine disinfection produces unwanted byproducts: a chemical soup containing trihalomethanes, haloacetic acids, and chlorite. These compounds require such a slate of monitoring and mitigation measures that it begs the question of whether the cure is worse than the pollution. For its part, ozone transforms organic substances, pathogenic organisms such as viruses and bacteria, and pesticides into benign substances that subsequent treatment steps can filter off. Considered perhaps the most environmentally feasible tool to disinfect water at large scales, ozone (O_3) is a pure oxygen molecule with an extra oxygen atom attached. Inherently unstable, it readily drops one oxygen atom to react with micropollutants. It reverts to oxygen in minutes, so the unused ozone vanishes without trace. COMSOL Multiphysics simulations make it easy to avoid or remedy the one byproduct that ozone reaction produces, bromate.

It begins as Alpine runoff

AWS transforms water from the Rhine River into potable water for approximately 800,000 people in Amsterdam and surrounding areas. The Rhine River begins in the Rheinwaldhorn glacier in Switzerland and flows to the North Sea. Along the way, the river collects runoff from the dense cities, open fields, and vast farms it passes.

The 14 steps of the purification process at AWS distill into three main phases. The initial phase removes solid particles through coagulation and settling plus filtration in the Amsterdam dunes and man-made sand filters. The next phase targets various micropollutants using ozone in a turbulent reactor, water softening, and biologically activated carbon filtration. In the final polishing phase the water passes through a string of fine filters before going to consumers.

FIGURE 2: Dr. Jan Hofman stands near a flow-meter station at the header of the turbulent ozone reactor at Amsterdam Water Supply. His team positions flow meters such as these at various locations inside its water-treatment facility. Dr. Hofman and other AWS engineers use COMSOL Multiphysics to fill in the gaps between their sparse measurements.

The ozone-approach proves especially effective for AWS. It significantly raises the plant's disinfection capacity since the ozone-treated water is so pure it requires no chlorination. In fact, last year AWS received an honor for providing the highest quality drinking water in the Netherlands.

In a turbulent reactor

At its treatment plant in Leiduin, AWS operates five turbulent ozone reactors in parallel. Water coming from earlier filtration steps feeds into a header system (Figure 3), which mixes the incoming water and distributes it to multiple turbulent reactors

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FIGURE 3: In the header assembly for the turbulent ozone reactors, filtered water passes through large pipes and empties into a long conduit or header roughly 1 m in diameter. The header mixes the filtered water and feeds it into the turbulent ozone reactors through relatively small pipes or "streets."

through pipes known as "streets." Inside a reactor, water winds around partial walls or baffles to create turbulent flow. The turbulence mixes the water with ozone gas that enters through diffusers just long enough to inactivate micropollutants. Then the water leaves the reactor through a pipe, and the remaining purification steps filter off or otherwise remove the reacted pollutants.

There is no way to look inside a turbulent reactor when it is working, so until now AWS engineers deduced the operation from scattered measurements. They collect velocity data using flow meters and sample concentrations. They also examine time tracers en route from inlets to outlets to ascertain mixing and residence times. With simulations, Dr. Hofman and his colleagues fill in the gaps with models of turbulent flow as well as chemical transport and reaction. According to Dr. Hofman, "The COMSOL Multiphysics environment is so easy to understand and use, it didn't take long before several of us could model with it and collaborate."

Once the simulation matches collected data, the team iteratively changes and solves the tested model to find retrofits that improve how the reactor and header assembly perform. As Dr. Hofman explains, "Our simulations of the reactors and header assembly save us tremendous amounts of money and time. Because we test our ideas on a computer, we don't waste manpower or material costs on trial-and-error retrofits. Besides, the modeling results come in handy when we report to government officials."

Mapping the flow field

A turbulent reactor at AWS resembles a maze about the size of a house—it's a big concrete structure with baffles that divide the space into room-sized compartments. The reactor in Figure 1 is 40 m long, 5 m high, and has seven compartments of varying width created by baffle spacing. Filtered river water enters the reactor and winds around baffles until it exits through a pipe.

In this reactor, a flowmeter straddles the fourth U-turn, taking samples in the gap between the fifth baffle

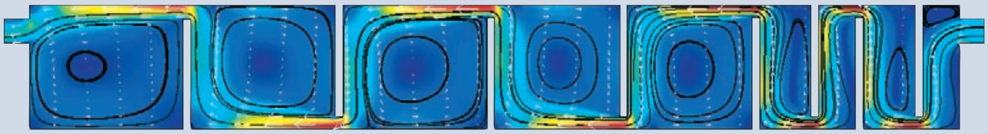

FIGURE 4: COMSOL Multiphysics results show the velocity field inside the turbulent reactor. The water speeds up in the U-turns between the baffle ends and the reactor walls, but it slows and even recirculates over the rest of the reactor. The velocities crossing the narrow passage in the middle of the reactor are very close to the flow-meter measurement of 0.17 m/s found in the actual reactor.

and the reactor wall. For the flow component of his models, Dr. Hofman uses the k-ε Turbulence Model application mode. To get a fast, accurate solution, he uses the parametric solver to obtain and solve for better and better initial pressure and velocity fields. The results almost exactly match the flow-meter velocity of 0.17 m/s towards the middle of the reactor (Figure 4).

With a working flow model, the team switched gears and began tracer experiments. They injected fluoride at the inlet and measured the concentration as it passed through the outlet. Comments Dr. Hofman, "The fluoride works well as a tracer because it travels with the water but does not react with the ozone. We modeled the tracer movement by adding convection and diffusion inside the existing model file. Then we got the average outlet concentration at each time using the integration tools, and the model matches the concentrations we measured." He elaborates, "Because the COMSOL Multiphysics model did such a nice job of matching the experimental data, we could rely on it to rethink the reactor design and achieve greater uniformity in the flow field."

Eliminating bromate production

Accurate estimates of the flow field are critical for managing the ozone disinfection that Dr. Hofman and his colleagues model (Figure 5). As he explains, "Once we know how long the water spends in the reactor and where it flows, we fine tune the reactor and diffuser setup so that the contaminants stay in contact with the ozone for just the right amount of time and not long enough for bromate to form."

The researchers started modeling complex chain reactions beginning with bromide and ozone using the prewritten COMSOL Multiphysics example "Turbulent Ozone Reactor" for a simple reaction chain with a flawed reactor design. According to Dr. Hofman, "What-if modeling on simple reactors with obvious design flaws such as this one gave us intuition when we began investigating ozone reaction in our real reactors. It was so easy to open the model and change it. We used it to see how certain baffle arrangements and diffuser setups limit bromate production. Now we use an altered version of the model to simulate real reactor geometries."

Taking it to the next level

Dr Hofman continues, "Being able to set up computational fluid dynamics models quickly and easily proves invaluable to understanding processes inside the ozone reactors, optimizing them in existing reactors, and also designing new ones."

One way the team will take its modeling to the next level is by adding bubbly flow. The ozone comes in as a jet of bubbles that eventually dissolves into the water. This means that near the diffuser there actually are two phases: ozone gas and water. Dr. Hofman elaborates, "Extending our model to 2-phase turbulence will let us examine how the ozone bubbles disturb the flow field and determine whether the dissolving of the bubbles affects the chemical reactions."

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His team is also adding 3D models to investigate other purification steps including a fluidized bed water-softening reactor. Says Dr. Hofman, "When we started the modeling for the real reactors, we focused on 2D simulations. But when the 3D turbulence application mode appeared in an earlier update, we added the *z*-direction to our models." ■

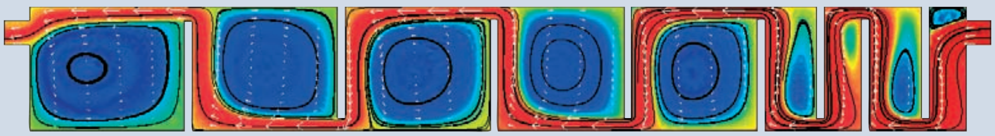

FIGURE 5: This COMSOL Multiphysics plot gives a snapshot of ozone concentrations in the turbulent reactor. AWS uses results like these to position ozone diffusers that improve the ozone mixing.