CFD Modeling for Characterization and Optimization of
In-situ Ozone Treatment Performance

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ABSTRACT

To be effective, an ozone treatment process must provide optimal performance within the mechanical and operational constraints of a water or wastewater plant. The process of mixing an ozone sidestream Venturi injection (SVI) train into a plant’s bulk water flow is affected by a plant’s dynamic hydraulic operation. Complete mixing of the sidestream into the main flow significantly impacts ozone mass transfer. Computational fluid dynamics (CFD) is a modeling tool that can aid in diagnosing and correcting potential operational issues during the design-build process.

This paper summarizes two cases where CFD was utilized to rapidly diagnose, characterize and optimize an ozone SVI system. The first study reviews CFD modeling of a baffled ozone contact basin which utilized multiple SVI – Basin Nozzle Manifold (BNM) sets to allow for operational flexibility and turn down of the ozone system. BNM placement, gas mixing and distribution, and optimum operational sequence of the SVI-BNM sets are examined through CFD modeling. The second case study examines the optimization of mixing in a gravity-fed pipeline contactor where nozzle orientation, spacing and penetration were optimized to achieve the target coefficient of variation (CoV) without the added energy requirements and cost of using a full flow static mixer.
INTRODUCTION

Typically, water treatment and wastewater treatment plant designs, particularly from a fluid flow point of view, are done by civil engineers. The primary focus of their gas contacting designs is to approximate single phase (water) plug flow within the contact basin while minimizing pipeline and basin head loss and plant pump energy costs. Less common are tracer studies to calculate volumetric efficiency and contact times. In the absence of operational data, most calculations are based on assumptions of ideal flow conditions, which are uncommon to non-existent in most unit operations. Additional errors are introduced by assumptions that single phase flow (water) behaves similar to multiphase flow (gas and water). In reality, the behavior of gas-water multiphase flows can differ significantly. A single phase approach can completely misrepresent reality.

The Navier-Stokes equations are non-linear, partial differential equations. These equations are fundamental fluid flow equations which need to be solved to get flow fields, velocities, turbulence related information, pressures and so on. Computational fluid dynamics (CFD) comprises numerical methods and models designed to approximate a solution to the Navier-Stokes equations for any given flow domain. CFD is increasingly being utilized to design new plants and diagnose operational issues in environmental engineering in recent years (Do-Quang et al 1998).

Sidestream Venturi injection (SVI) is increasingly being selected as the preferred method for ozone gas dissolution (Rakness 2011, Crittenden et al 2012, Tchobanoglous et al 2002). In SVI ozone dissolution designs, ozone gas is mixed into the bulk water flow utilizing basin nozzle manifolds (BNM) in contact tanks or by mixing the SVI influent into the pipeline flow using a pipeline flash reactor (PFR). With both BNM and PFR methods of contacting, there is a fundamental need to have a clear understanding of multiphase hydrodynamics as a function of geometry, upstream and downstream conveyance, and specific ozone dosage. These factors, if not considered, can have an adverse impact on efficient mass transfer of ozone and can result in unstable residuals, poor mixing, and incomplete oxidation and disinfection.

This paper describes how a careful, iterative, multiphase CFD approach was utilized to optimize contacting and mixing in a BNM and a PFR.

BASIN NOZZLE MANIFOLDS IN A WATER TREATMENT PLANT

Background and CFD Modeling

The first case involves the Post-Ozone Contact Basin of a large municipal water treatment plant where sidestream Venturi injection (SVI) is utilized. Two-phase Venturi effluent is mixed with the bulk flow in the ozone contacting basin using subsurface jet nozzle manifolds located in a vertical water channel.
The following data was used as inputs for the CFD models.

**Case 1:** High flow rate, 4 Nozzle manifolds in operation.
- Channel Flow Rate: 17,500 m$^3$/hr
- Per injector Gas Flow Rate: 234.9 m$^3$/hr
- Per injector Water Flow Rate: 446 m$^3$/hr

**Case 2:** Low flow rate, 1 Nozzle manifold in operation.
- Channel Flow Rate: 8,750 m$^3$/hr
- Per injector Gas Flow Rate: 234.9 m$^3$/hr
- Per injector Water Flow Rate: 446 m$^3$/hr

The CFD modeling procedure is described very briefly here. The mixture model for multiphase flow (Manninen et al., 1996) was utilized in this case. The mixture model, an Eulerian-Eulerian approach was appropriate due to the low volume fraction of gas (<10%) (Brennen, 2005). Turbulent flow was modeled using a standard k-epsilon model (Lauder and Spaulding, 1974). A second order solution scheme was applied to the momentum equations and the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm (Patankar, 1980) was utilized. The mesh density was approximately 4 million hybrid tetrahedral and hexahedral cells. All piping was assumed to be constructed of stainless steel. Inlets were all modeled as mass flow inlets and the outlet was a pressure outlet.

Installation concerns from the client required a specific design with manifolds perpendicular to the influent flow. Mazzei optimized this system by orienting all but the nozzles closest to the channel inlet to be counter-current to incoming flow by utilizing 45° elbows and varying the elevations of manifolds using a ‘staggered’ configuration to allow jetting flow from the nozzles to extend fully and not be obstructed/dissipated by the next nozzle manifold in close proximity, at the same elevation. This design is shown in Figure 1(a). This design, including optimal location of nozzle manifolds, was completed using CFD analysis and results showed good mixing, as shown in Figure 2.

In a later communication, Mazzei was informed that the engineering firm, due to head loss concerns, required an increase in the channel inlet height from 1 m to 2 m. This design is shown in Figure 1 (b). Intuitively, this change to the channel inlet height suggested that short-circuiting was likely to occur. Multiphase CFD modeling was conducted and this hypothesis was confirmed. It was determined that the original nozzle manifold layout and design would not provide sufficient mixing and contacting of the basin water with ozone gas as shown in Figure 3.
Figure 1. Basin nozzle manifold designs. (a) Original design, 1 m inlet. (b) Original design, 2 m inlet and (c) Optimized design, 2 m inlet.

Figure 2. Contours of dispersion of sidestream gas/liquid mixture, Design 1(a), Case 1.
Figure 3. Contours of dispersion of sidestream gas/liquid mixture, Design 1(b), Case 1

To meet the requirement of optimal mixing and mass transfer, while maintaining a 2 m height inlet, Mazzei performed extensive CFD analyses to arrive at an optimal design. The final design involved 4 vertically and horizontally staggered counter-current basin nozzle manifolds, and one co-current basin nozzle manifold. CFD results indicate improved mixing, as shown for Case 1 in Figure 4. Figure 5 depicts mixing for Case 2, the low flow rate point. This case utilizes only one manifold.

Figures 6 and 7 depict flow vectors for Design (b) and Design (c), respectively. Short-circuiting and poor volumetric efficiency is clearly apparent for Design (b). Design (c) shows improved mixing and swirl, which positively impact mass transfer efficiency.

With the aid of multiphase CFD analysis, Mazzei was able to provide the client with the optimal placement of BNM’s and provide nozzle sequencing and operation information for each ozone production design point. This CFD optimized gas mixing design ensures the SVI system will meet the ozone transfer target while providing the stable, dissolved ozone residual that is essential to control ozone production and calculate the disinfection Ct product.
Figure 4. Contours of dispersion of sidestream gas/liquid mixture, Design 1(c), Case 1

Figure 5. Contours of dispersion of sidestream gas/liquid mixture, Design 1(c), Case 2
Figure 6. Velocity vectors across a profile plan, Design 1(b), Case 1

Figure 7. Velocity vectors across a profile plan, Design 1(c), Case 1
PIPELINE CONTACTING IN A WATER TREATMENT PLANT

Background and CFD Modeling

To limit plant footprint and construction costs, the design team for the Buckingham WTP, located in Gatineau, Quebec, utilized a 100 meter length of 42" diameter HDPE (High-density polyethylene) pipe in place of a standard ozone contact basin for pre-ozone contacting of a 5,000 to 27,930 m³/d (1.3 – 7.4 MGD) raw water flow. To prevent deterioration of the HEDP pipe from ozone gas, ozone mass transfer and off gas removal was provided by GDT™ process ozone injection and degas sidestreams (Figure 8).

At low plant flows, a single GDT™ process sidestream was sufficient to treat the pipeline’s bulk water flow. At plant flow rates exceeding 14,000 m³/d (3.7 MGD), two GDT™ process trains were required to handle a maximum ozone production of 2.3 kg/h (122 ppd). To achieve the oxidation and disinfection goals of the pre-ozone system, it was essential to rapidly mix and disperse the sidestream dissolved ozone effluent into the bulk water flow to establish a stable dissolved ozone residual 5 meters downstream from the point of sidestream ozone addition. Consequently the ozone process design called for a dissolved ozone coefficient of variation (CoV) of 5 % at 5 meters downstream of the point of sidestream discharge into the pipeline flow. Figure 9 shows a photograph of the installation.

The initial design considered the use of a static mixer in the 42” pipeline to blend the sidestream ozone effluent into the bulk water flow. However, because raw water was gravity fed into the pipeline contactor, the allowable pipeline pressure loss at the point of sidestream mixing was limited to only 1 mm of water column at the peak design flow. Analysis by the design team showed that a commercially available static mixer could not meet the required CoV of 5% across the pipeline flow range at the stringent pressure loss requirement.

In place of a static mixer, the design team selected a Pipeline Flash Reactor (PFR) to blend and mixed the GDT sidestreams’ effluent into the pipeline bulk water flow. Multi-phase Computational Fluid Dynamics (CFD) modeling and analysis was added into the project’s submittal requirements to confirm that the PFR design would meet the dissolved ozone CoV and gas mixing pressure loss targets.

CFD analysis was conducted in order to demonstrate that the discharge of the GDT™ sidestream into the Mazzei PFR design produced a “well mixed” condition in the downstream pipeline. The effectiveness of mixing flow was determined by calculating the downstream coefficient of variation (CoV) to represent a homogeneously mixed system. The CoV was not to exceed ± 5% prior to the outlet of the simulated pipeline for the following two scenarios.

- Case 1: High flow rate (27, 930 m³/day), 4 nozzles in use.
- Case 2: Low flow rate (5000 m³/day), 2 nozzles in use.
Figure 8. Typical GDT process schematic.

Figure 9. PFR installation, Buckingham WTP.
Figure 10 depicts the optimal PFR design for both high-flow and low-flow cases for this specific plant. The length of the PFR is 48 inches. The extent of the computational domain is illustrated in the figure below. All piping was assumed to be constructed of stainless steel. All other modeling methodology and model selection is the same as described in the previous section.

![Diagram of PFR design](image)

**Figure 10. Recommended PFR Design: Alternating nozzles with Nozzle Set #1 protruding into mainline flow. Pipeline length for simulation: Inlet defined at 60 inches upstream of PFR, Outlet defined at 173 inches downstream of PFR**

For all cases, the primary phase refers to the water in the main pipeline and the secondary phase refers to the ozonated and degassed water entering through the nozzles. The temperature is assumed to be 25°C.

**Case 1: High flow rate (27,930 m$^3$/day), 4 nozzles in use**

Figures 11 and 12 depict plan and profile views of contours of volume fraction of phase 2 plotted on a central axial plane. Both cases show that the CoV remains within the target range of ± 5%.
Figure 11. Case 1 - Plan view of computational domain. Contours of volume fraction of the secondary phase are clipped to the defined “well-mixed” range [μ - 0.05 μ, μ + 0.05 μ].

Figure 12. Case 1 - Profile view of computational domain. Contours of volume fraction of the secondary phase are clipped to the defined “well-mixed” range [μ - 0.05 μ, μ + 0.05 μ].

Case 2: Low flow rate (5000 m³/day), 2 nozzles in use

Mass flow rates were provided for at the inlets of the main pipes and the nozzles. The modeling inputs are as follows:

- Main Water Mass Flow Rate: 127.5 lb/s (916.7 GPM)
- Per-Nozzle Water Mass Flow Rate: 18.97 lb/s (136.4 GPM)
- Number of Nozzles On: 2

Figures 5 and 6 depict plan and profile views of contours of volume fraction of phase 2 plotted on a central axial plane. Both cases show that the CoV remains within the target range of ± 5%.
Figure 13. Case 2 - Plan view of computational domain. Contours of volume fraction of the secondary phase are clipped to the defined “well-mixed” range $[\mu - 0.05 \mu, \mu + 0.05 \mu]$.

Figure 14. Case 2 - Profile view of computational domain. Contours of volume fraction of the secondary phase to the defined “well-mixed” range $[\mu - 0.05 \mu, \mu + 0.05 \mu]$.

Multiphase CFD analysis demonstrates that the Mazzei PFR design produces a “well mixed” condition in the downstream pipeline under both high flow rate and low flow rate conditions. Based on startup results and communication with Buckingham WTP since installation, this PFR has been functioning successfully; providing a stable dissolved ozone residual at a high ozone transfer efficiency.

CONCLUSIONS

This paper described two SVI ozone contacting applications where multiphase CFD was utilized for optimizing mixing – a basin nozzle manifold system and inline contacting using a pipeline contactor. CFD modeling was successfully utilized to analyze multiple physical configurations in order to accommodate plant hydraulic constraints. In the case with basin manifolds, CFD modeling provided crucial information regarding sequencing and operation of specific manifolds at specific treatment flow rates. In the case with pipeline contacting, CFD modeling confirmed
that a targeted homogenous mix can be obtained with careful design of a pipeline flash reactor, chosen here in lieu of a static mixer by the clients.

REFERENCES


