Computer Simulation Helps Reduce Chlorine Concentration in Laboratory

Heejin Park, Ph.D., P.E.
hjpark@flonomix.com
Flonomix, Inc.

Computer simulation helped reduce the chlorine concentration in a laboratory to minimal levels while avoiding the expense and disruption of testing alternate exhaust systems.

Workers throughout a wide range of chemical processing industries are becoming more conscious than ever before of discharges that, although they fall within acceptable safety limits, cause annoyance and potential discomfort. The approach of redesigning process equipment in order to eliminate the discharges at the source is the ideal solution in the case where the process is being overhauled for other reasons, but is otherwise often too costly to consider. The more practical approach is usually to retrofit an exhaust system to the existing equipment to remove as much of the contaminants as possible before they are circulated through the plant. This approach, however, also has its challenges.

Facilities management planned to install an exhaust system to eliminate chlorine odor but were uncertain how the exhaust system should be configured to have the greatest impact. It would have been very expensive to install the exhausts in several different locations in order to see which configuration worked best. Hence the management hired Flonomix, Inc. to use computational fluid dynamics (CFD) to simulate the performance of the most likely design alternatives. The Flonomix engineers analyzed four different cases and found which one worked best. The chemical company installed the exhaust system based on these guidelines and discovered that the new system completely solved the problem.

Traditional approach involves cost and disruption

Exhaust system performance is highly dependent upon a number of variables such as the flow and pressure conditions inside the plant, the distribution of the various sources of contaminants, and the placement and capacity of the exhaust system. But it is impractical to measure the flow and pressure to any significant degree of accuracy, so the best that engineers can do in most cases is make a rough hand calculation or educated guess as to which configuration will work best. The accuracy of hand calculations is reduced by several factors. First, these calculations don't take the geometry of the structure into account. Second, they determine only average chemical concentrations but not the spatial distribution or gradients in the distribution, both of which are important.

The result is that engineers are unable to be certain about the performance of a prospective design until the ventilation system is installed and tested. Usually such a system is installed, the concentration of the contaminants is measured and the performance of the system is assessed. If the design does not meet the requirements, then it becomes necessary to perform a costly and, at times, disruptive series of experiments, modifying the design and evaluating its performance until the design criteria are satisfied.

Simulating airflow with computational fluid dynamics technique

CFD can dramatically improve this process by predicting airflow, pressure, and chemical concentrations throughout a region with a high level of accuracy. CFD uses numerical methods to solve the fundamental nonlinear differential equations that describe fluid flow (the Navier-Stokes and allied equations), for predefined geometries, boundary conditions, process flow physics, and chemistry. The result is a wealth of predictions for flow velocity, temperature, density, and chemical concentrations for any region where flow occurs. CFD is a very potent, non-intrusive, virtual modeling technique with powerful visualization capabilities. A key advantage of CFD is that engineers can evaluate the performance of a wide range of exhaust system configurations on the computer without the time, expense, and disruption required to make actual changes onsite. As the advances in HVAC/IAQ technology have developed dramatically during last decade, HVAC/IAQ design has required broader and more detailed information about the flow within an occupied zone. And the CFD technique meets this goal better than any other method, i.e., theoretical or experimental methods.

Modeling the laboratory

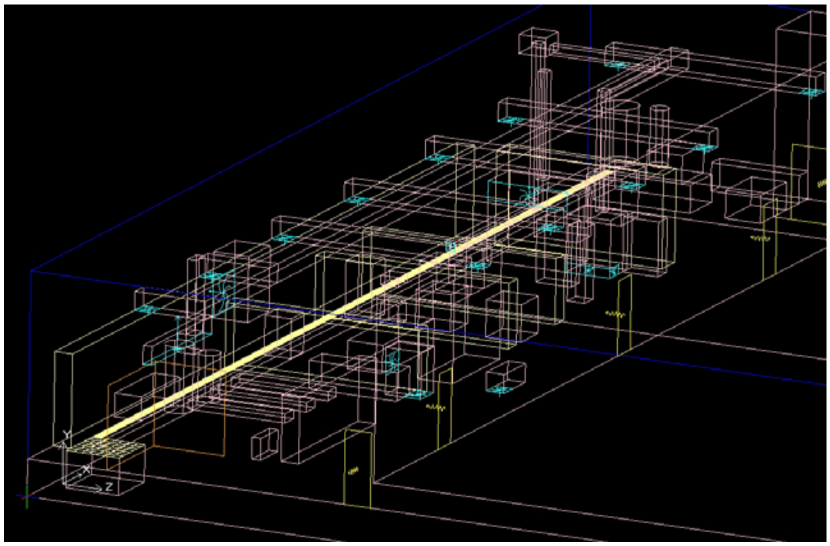

Figure: Overall view of the chemical lab under consideration

On this project, the engineers worked with floor plans provided by the chemical laboratory, direct measurements and observations, and photos taken in the lab. The computational domain covered an area 131 feet long, 24 feet high, including 4 feet under the floor (sump and trench area), and 126 feet deep. They created a CFD model that used about 850,000 cells to reproduce the geometry of open space within the plant. The model took about 10 hours to solve on a personal computer with dual 1.7GHz Xeon processors and 2 GB Ram. An air balancing report was provided by Pro Control that measured air moving in and out of the laboratory at various locations. The boundary conditions were created based on this report. Chlorine sources were located in the sump area, trench area, and on the surface of three tanks. The laboratory itself provided measurements on the volume of chlorine emitted by the various sources in the plant. The values for chlorine were not accurate enough to determine absolute values for chlorine concentration but were sufficient to meet the objectives of this study by determining the relative performance of various design alternatives. A conventional k-ε turbulence model was used.

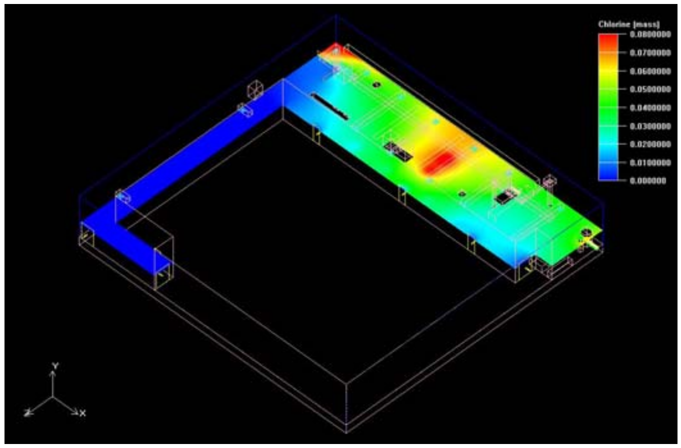

Figure: Chlorine concentration at an elevation of six feet without any modifications.

The Flonomix engineers decided to focus first on the sump and trench, which were the largest sources of chlorine, so they turned off the other sources of chlorine in the model. Based on experience, the chemical company's engineers suggested two exhaust system configurations, which they thought had the best chance of succeeding in this difficult area of the problem. Each configuration used four 200 cfm exhausts for the trench and one for the sump. In the first case, the exhausts were located under covers that were positioned on top of the trench and sump, while in the second they were located above the trench and sump covers. The consultants then ran the simulation and generated color-coded plots that showed the concentration of chlorine predicted by the simulation throughout the plant at a height of four feet, six feet, and eight feet. The results of these simulations showed that placing the exhausts two feet above the tanks provided superior results.

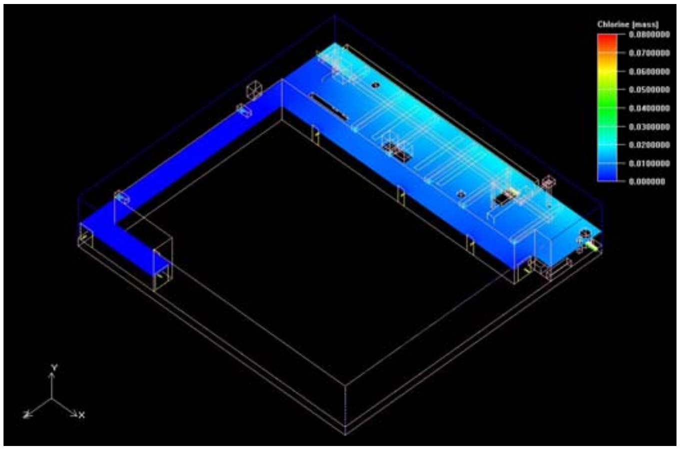

Figure: Chlorine concentration at an elevation of six feet,
with exhausts located under the sump and trench covers.

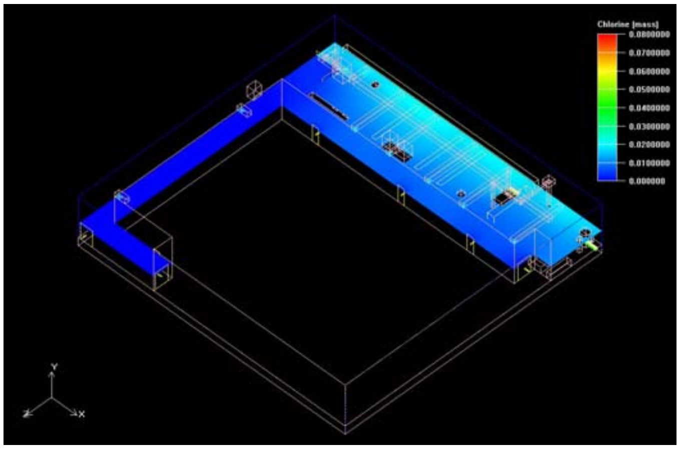

Figure: Chlorine concentration at an elevation of six feet
with exhausts located above the sump and trench covers.

Evaluating conditions with all sources on

With this key point established, Flonomix engineers moved on to evaluate the effects of adding the other sources. They positioned exhausts under the covers of the sumps and trenches, the design that was shown to be best from the earlier simulation. Then they added additional 400 cfm exhausts above the three tanks while varying the gap between the top of the tank and the exhaust at 2 feet and 4 feet. The results of these simulations showed that placing the exhausts two feet above the tanks provided superior results.

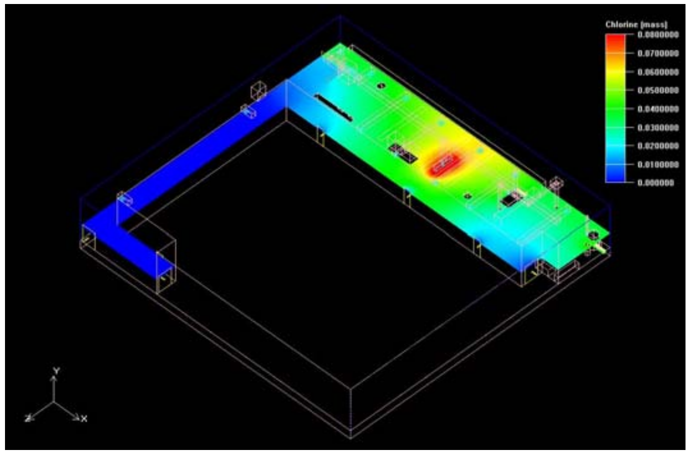

Figure: Chlorine concentration at an elevation of six feet with all sources considered and exhausts placed 4 feet above tanks

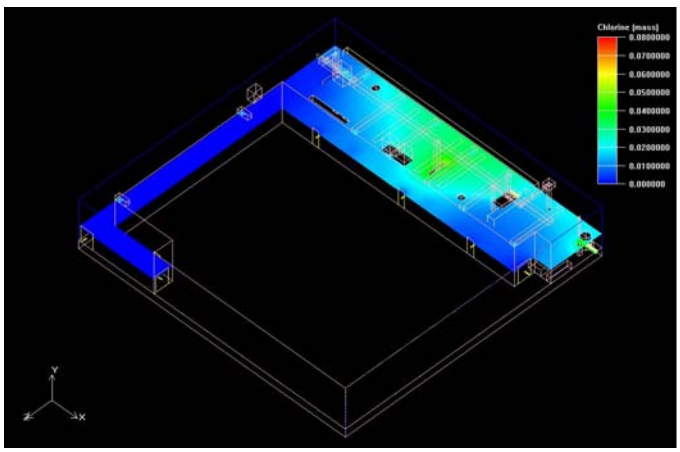

Figure: Chlorine concentration at an elevation of six feet with all sources considered and exhausts placed 2 feet above tanks.

In their final report, the consultants recommended that the exhausts be positioned two feet above the surfaces to maintain chlorine concentration at minimal levels as predicted by the simulation, with the sump and trench exhausts located under the covers and the tank exhausts. The color graphic output provided by the simulation made it relatively easy to make the case for the optimized design to laboratory management. Having a validated design provided confidence that the new configuration could be installed without the need for downstream changes that would have otherwise increased the cost and disruption involved in the changes. When the new exhaust system was installed, reports from the site indicated that workers could no longer smell chlorine in the plant. The laboratory management believes that they have successfully accomplished their objective of reducing chlorine concentration to unobjectionable levels at the lowest possible cost.

About the author:

Dr. Hee-Jin Park has been leading Computational Fluid Dynamics (CFD)/R&D division at Flonomix, Inc. He has extensively applied computational airflow simulation techniques to various HVAC/IAQ applications, fire protection analysis, and toxic chemical spreading simulation for last 15 years. He also has researched on advanced HVAC systems including thermal displacement ventilation and adapted computational simulation as a tool to verify the effectiveness of displacement ventilation system. He published numerous technical papers and has been frequently invited for presentation of his work at various technical conferences in his fields. He holds a bachelor degree from Seoul National University and a master degree from Korean Advanced Institute of Science & Technology (KAIST) and a Ph.D. from University of Michigan (Ann Arbor) in mechanical engineering. He is a registered professional engineer in Minnesota and an active member of ASHRAE.

Contact Flonomix at: Phone 503-648-0775. Email: hjpark@flonomix.com.