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JOURNAL ARTICLE

Computer Simulation Demonstrates Mixing Speed in Vapor Space to Regulatory Authorities

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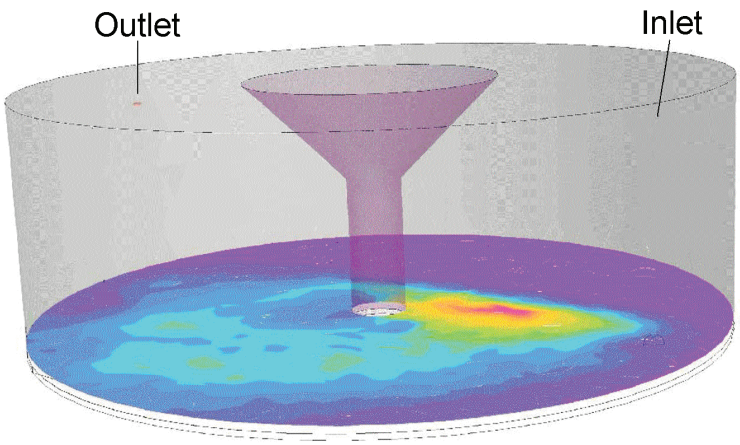
Computer simulation helped Westinghouse Safety Management Solutions (WSMS) engineers demonstrate that benzene mixing within a large vapor space at the top of a liquid-filled tank would be fast enough to prevent the formation of a significant volume of this gas above the lower flammability limit (LFL). This issue arose in the licensing of a nuclear waste processing unit that produced benzene as a byproduct. While experimental methods could only measure benzene concentration at a few discrete points, computational fluid dynamics could predict values throughout the vapor space as a function of time. The analysis correlated well with physical measurements.



CFD image showing contours of benzene mole fraction at 2 minutes

Westinghouse Safety Management Solutions is a wholly owned subsidiary of Westinghouse Savannah River Company (WSRC). WSRC is the prime contractor for the DOE Savannah River site in Aiken, SC, and performs all types of safety work for the DOE facilities around the country.

Waste Processing

A nuclear waste processing facility under development at the Savannah River Site is designed to remove radioactive cesium 137 from solution by adding tetraphenylborate (TPB) in order to produce cesium tetraphenylborate, which precipitates out of the solution. The precipitate slurry is filtered and sent to another plant where it is vitrified. The remaining liquid has relatively low radioactivity so it can be processed using less expensive methods.

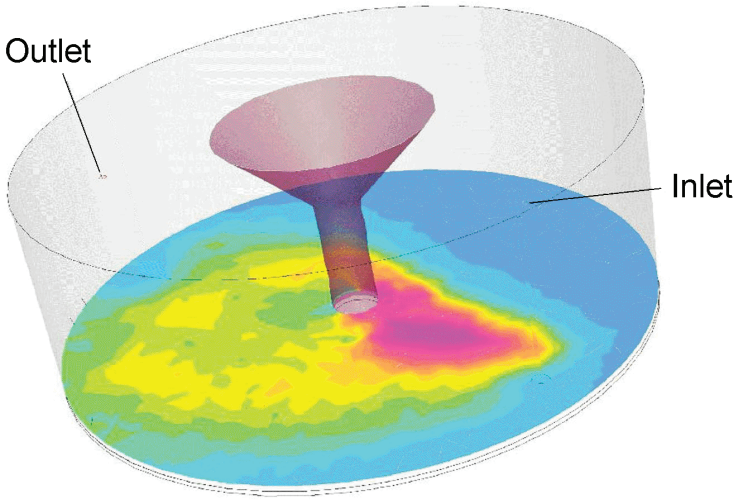
The TPB added to the tank is subject to radiolytic, thermal, and chemical degradation. One of the products of this degradation is benzene. In order to eliminate the slightest possibility of a fire in the tank, both oxygen and fuel control are exercised. Oxygen control is maintained by a nitrogen purge in the vapor space above the liquid. At the same time, the

concentration of benzene in the vapor space must not reach a value that would support combustion at any location.

The tank is 85 feet in diameter and 33 feet high. The liquid depth at the end of a precipitation cycle is approximately 4 feet, so there is 29 feet of vapor space. A column 6.75 feet in diameter at the base is centered in the tank and used for structural support. The top of the column consists of a conical section with horizontal and vertical sides 12 feet in length. The tank contains a 12 inch diameter outlet in the top surface, positioned 225^{o} counterclockwise from north. The nitrogen purge is located 36 ft. from the axis of the unit, 340^{o} counterclockwise from north. The nitrogen purge is a 1-inch diameter inlet pipe with an orientation of 15^{o} downward below the top surface, tangential to a circle at this radius, and pointing in a counterclockwise direction. The tank contains cooling coil loops that consist of a large number of 2 inch pipes spaced approximately 3 ft. apart and oriented in a vertical direction.

Unstructured code

The tank was modeled with the FLUENT CFD code from Fluent Incorporated, Lebanon, New Hampshire. Westinghouse engineers selected this software package because it dramatically reduces the amount of time required to model complicated geometries such as this tank. FLUENT is a state-of-the-art computer program that uses pressure-based finite volume methods to solve fluid flow and energy equations. FLUENT utilizes an unstructured grid to provide truly automatic mesh generation. This means that once the surface is defined, the grid can be generated with little or no user intervention. FLUENT also has a solution-adaptive grid capability, which allows the user to refine the grid after a preliminary calculation in regions with large gradients, in order to achieve a higher level of accuracy. Fluent is the world's largest CFD software provider with over 1000 users.



CFD image showing contours of benzene mole fraction at 14 minutes

The unstructured meshing approach made it quite simple to model the tank despite its complex geometry and large variations in length scale - an 85 foot tank diameter containing a 1 inch diameter inlet nozzle. The unstructured approach facilitates the construction of finite volumes in the computational domain because it provides an easy transition from a region where a fine mesh is required to a region where a coarser mesh can be used. The tank cooling coils were not explicitly modeled, but their presence was accounted for by frictional losses to the flow field in the form of a momentum sink. The automatically generated mesh consisted of approximately 17,000 finite volumes. This mesh was later refined to accommodate changes in the location of the benzene source and to support sensitivity studies.

Boundary conditions

Nitrogen is introduced into the tank from upstream ambient vaporizers. The nitrogen flow rate is specified using a dynamic pressure at the inlet that generates the correct mass flow rate. The ventilation outlet from the tank is assigned a static condition of atmospheric pressure. This treatment results in a small positive pressure in the tank. Despite the fact that the actual tank has a small negative pressure to prevent leakage, the small positive pressure in the CFD simulation has no effect on the calculated flow field in the tank. Benzene release into the vapor space was modeled as a volumetric source from a single layer of cells centered about the location of a

pump at the bottom of the tank. The pump is used in the processing of the liquid, when benzene is most likely to be released into the vapor space.

One of the main purposes of the analysis was to demonstrate that the model was capable of reproducing the large concentration gradients of benzene in the vapor space that were typical of one particular pump run. In that case, pump operations were resumed after a quiescent period of 61 days. During earlier pump operation, benzene release rates on the order of 50 to 100 grams per minute had been observed. It was recognized that the long quiescent period could lead to larger release rates, so only a single pump was employed. The pump was shut down after 14 minutes when multiple high benzene concentration readings were detected. Measurements were taken at five minute intervals from two sample ports located 18 inches above the liquid surface. Based on these readings, the average benzene release rate was calculated to be 1.6 kg per minute during the 14 minutes of pump operation.

Analysis cases

Four analysis cases were formulated to simulate the pump run with large benzene concentrations. All four cases used benzene release rates to match the calculated release rate of 1.6 kilograms per minute for 14 minutes. An additional 16 minute period with no benzene release was included for a total duration of 30 minutes. The four cases were developed to evaluate specific modeling methods. Case 1 used a fairly large volume containing a minimum number of computational cells to represent the benzene source. No adaption was done. In Case 2, the mesh was refined in the vicinity of the source to explore the effects of source layer thickness on benzene concentration. The purpose of Case 3 was to investigate the impact of several changes in the benzene release parameters that could affect the benzene distribution. The radius of the source zone was increased from 30 ft. to 40 ft. The source was ramped up linearly for the first minute of the analysis and ramped down over the last two minutes of the release period. Case 4 was designed to show the effect of further reductions in source layer thickness and grid refinement on the resulting benzene concentration in the bulk vapor space. The layer of cells directly above the liquid was split and additional mesh refinement was carried out in the bulk vapor space.

Good correlation

The calculated concentration gradients for all cases were in general agreement with the experimental results. In particular, both analytical and experimental results showed the presence of large gradients near the surface of the liquid and in the vapor sampling location 18 inches above the liquid surface. These results demonstrated that CFD analysis is capable of reproducing the general behavior observed in the tank with large benzene release rates. The minor differences between the calculated and measured benzene concentrations at the measurement locations were judged to be due primarily to the simplifying assumptions made in the release characterization in the model.

Further analysis of the vapor space gradients showed that mixing was occurring at a sufficient speed to avoid dangerous benzene concentrations under the current assumptions for the maximum benzene release rate. This application demonstrates that CFD can accurately model the vapor space mixing characteristics while providing considerably more data than can be obtained from physical testing at a far lower cost and leadtime.