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Additional Scoping Calculations of Tank 50 and Tank 48 Vapor Space Mixings

Si Young Lee
Richard A. Dimenna

October 2005

Westinghouse Savannah River Company
Savannah River National Laboratory
Aiken, SC 29808

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Abstract

Additional scoping calculations to address the mixing behavior in the vapor spaces of Tank 50 and Tank 48 and estimate maximum benzene concentrations have been completed by the solution method established in previous work. The analysis focused on changing the tank operating conditions to establish internal recirculation and changing the benzene evolution rate from the liquid surface. The calculations included nominal boundary conditions for air inlet and exhaust flows, recirculation flow rate, and benzene evolution rate. The calculations were based on prototypic tank geometry and nominal operating conditions as defined by the Closure Business Unit.

The results showed that the vapor space was fairly well mixed and that benzene concentrations were relatively low when forced recirculation was imposed. Because of the imposed boundary conditions, however, benzene concentrations were still about 25% LFL for these scoping calculations even for a well-mixed tank. In the absence of forced recirculation, the modeling results clearly indicated that benzene gas in the vapor space was stratified.

1. Introduction

Closure Business Unit Engineering has been evaluating flammability conditions in the vapor spaces of Tank 48 and Tank 50 in association with the safety analysis. In the previous work [1], Savannah River National Laboratory (SRNL) developed a computational model and made the scoping calculations to estimate the degree of benzene mixing and maximum benzene concentrations for nominal conditions of purge airflow and benzene evolution. In addition, a series of sensitivity analyses was performed to ensure that the scoping model could capture the necessary phenomena without introducing nonphysical behavior because of the numerical discretization. The present analysis used the same solution method established in that work.

The objective of the present work is to perform additional scoping calculations to evaluate the impact of internal gas recirculation and changes in the benzene evolution rate on local benzene concentration in the Tank 48 or 50 vapor space. The rate of benzene evolution from the liquid surface was lowered to a more realistic value than that used in the previous calculations. The purge air flow rate was also lowered commensurate with the reduced benzene generation. The calculations were performed to evaluate the degree to which forced internal recirculation would effect mixing of the purge air with benzene evolving from the liquid surface and prevent an unacceptable concentration of benzene from forming. The geometrical configurations for the vapor space with internal gas recirculation at the G-riser in Tank 50 are shown in Fig. 1.

A computational fluid dynamics (CFD) model was developed to evaluate air flow patterns and to estimate benzene concentration in the vapor space. The modeling domain represents the major features of Tank 50 or Tank 48 and includes the principal air flow ventilation path of the tank vapor space, the central concrete support column, and internal recirculation as shown in Fig. 1. The computational domains for the two cases shown in Figures 2 and 3 were developed based on the tank configurations shown in Fig. 1.

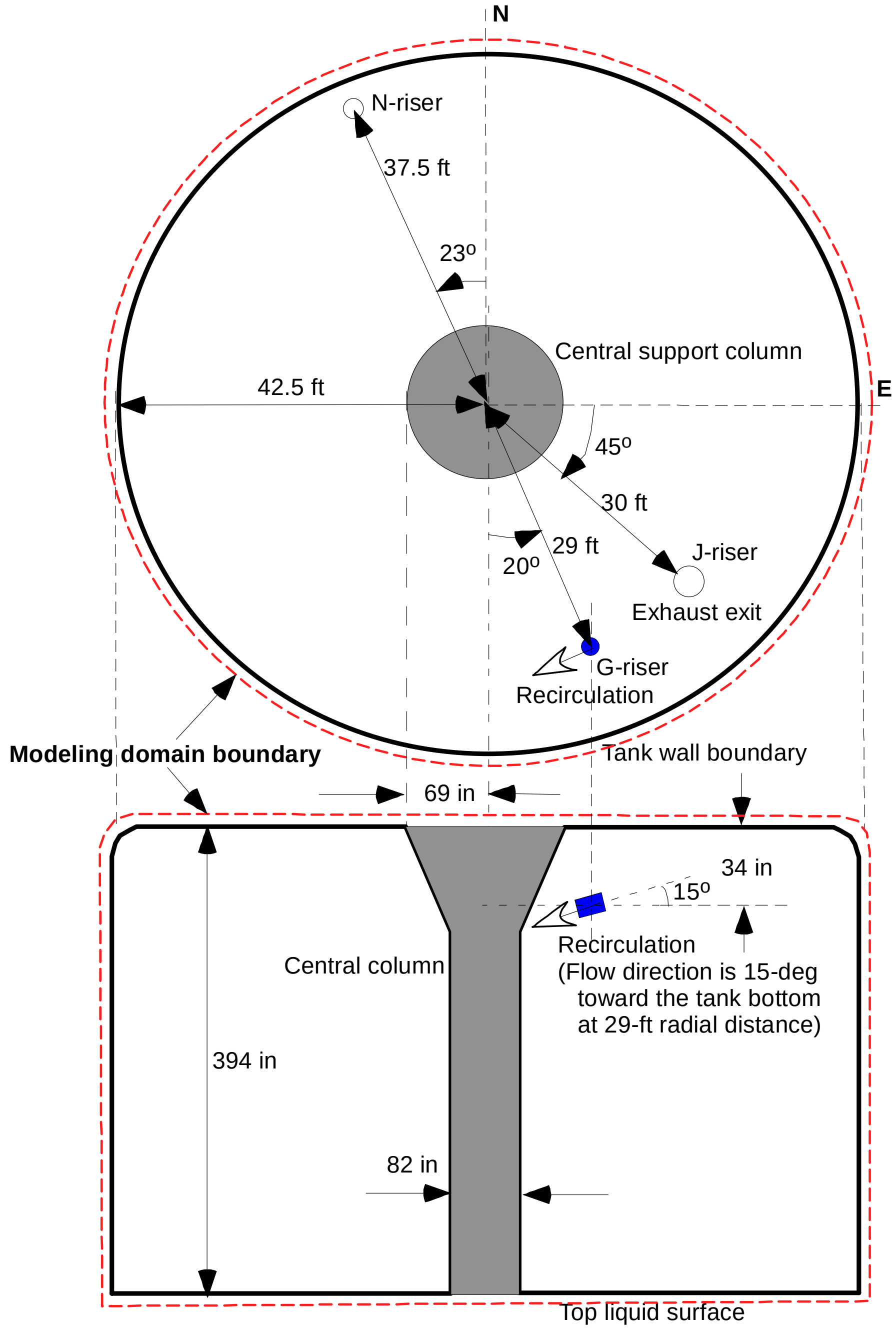


Figure 1. Modeling domain boundary used for the present scoping calculations

2. Modeling Approach and Analysis Method

A three-dimensional approach was taken to model the gas space of Tank 50 or Tank 48. A finite volume CFD code, FLUENT^{TM} [4], was used to perform the analysis. A standard two-equation, k-ε model, was used to estimate the gas turbulence. The circulation fan in the vapor space was modeled as a momentum source. Thus, the governing equations to be solved are composed of one mass balance, three momentum equations for the three-dimensional space, two turbulence equations, and one species transport equation for benzene gas. Forced recirculation was modeled as source term in the momentum equation. This solution method and the assumptions for the present calculations were established in the previous modeling task [1]. The computational domain boundary used for the present calculations is shown in Fig. 1.

Modeling assumptions for the scoping calculations are as follows:

- Single exhaust location from the vapor space
- Single gas injection location for a given calculation.
- Benzene evolution rate from the liquid space is constant and uniform.
- Cooling coils in the vapor space have no impact on gas flow patterns.
- Air leakage into the vapor space is negligible.
- Temperature is constant, so thermally driven convection can be ignored.
- No chemical reactions during the benzene transport and mixing process.
- Benzene gas is a dilute mixture component, so the mass diffusion coefficient is independent of gas composition.
- Target criteria for local benzene concentration will be provided by the customer organization. For the scoping calculations, 25% of local benzene LFL, 1.37 vol% benzene, is used as the target criterion.

Benzene mass fractions for the modeling cases are computed under steady-state operating conditions. The cases considered here and the material properties used for the calculations are shown in Table 1 and Table 2. All of the cases used a second order differencing scheme in order to minimize the numerical diffusion caused by the discretization.

The flow conditions for the vapor space are assumed to be fully turbulent since Reynolds numbers for the nominal 72 cfm air flow rate are in the range of 20,000 based on the inlet conditions of the 6-in nozzle. A standard two-equation turbulence model, the $k-\varepsilon$ model [4], was used since previous work [5] showed that the two-equation model predicts the flow evolution of turbulent flow in a large stagnant fluid domain with reasonable accuracy. A full three-dimensional representation of the entire gas space was used to capture significant circulation phenomena related to the turbulent behavior of the gas flow.

Air was used to simulate the purge gas in the vapor space. Although nitrogen is currently used as a purge gas in Tank 48, its flow pattern and mixing behavior are expected to be similar to those of air under the same operating conditions. The first case, Case-1, is the modified Tank 50 operating conditions with 150 cfm of forced recirculation. The second case, Case-2, is a sensitivity run of the previous Tank 48 model [1] with benzene generation rate changed as shown in Table 1. Detailed modeling domains of the two CFD models are presented in Figs. 2 and 3. Computational meshes for both cases are shown in Fig. 4. The meshes for the Case-1 model were larger than the Tank 48 model of Case-2 because of the larger modeling domain of the tank vapor space.

The major material and physical properties used for the calculations are listed in Table 2.

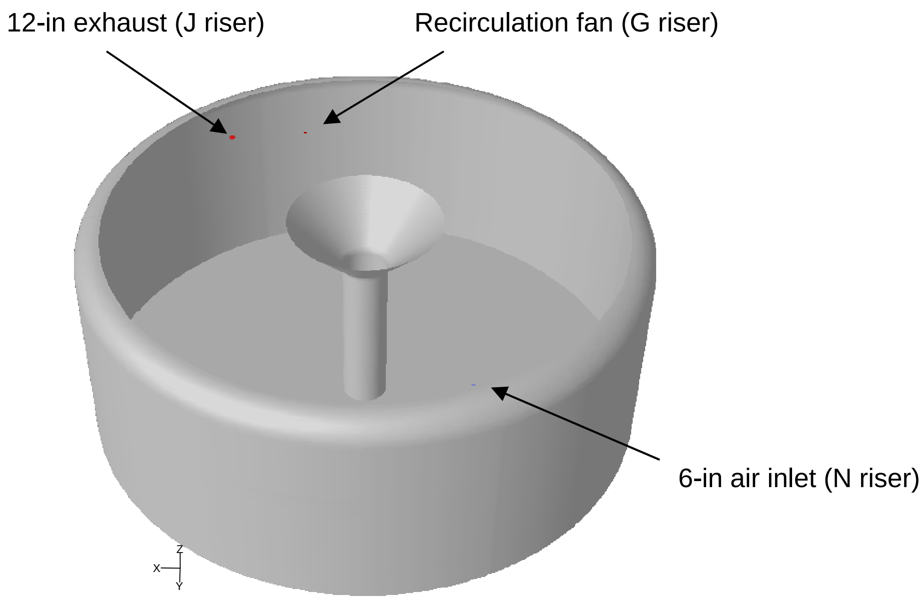
Table 1. Modeling conditions for the two cases considered in the calculations

Cases	Purpose	Air recirculation rate (ft^3/min) and location	Air inlet location (size)	Liquid level (in)	Air flowrate at inlet (ft^3/min)	Benzene generation (gm/min)
Case-1	To evaluate the mixing behavior in Tank 50	150 (4-in dia. pipe via G-riser)	N-riser (6-in dia.)	2	72	25
Case-2	To evaluate the Tank 48 sensitivity	No recirculation	N-riser (6-in dia.)	54	72	25

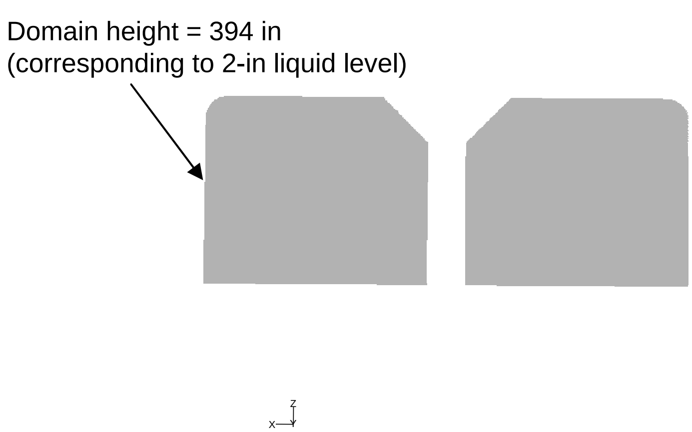
Table 2. Material properties and modeling conditions

Parameters	Input data
Air density	1.225 kg/m^3
Benzene vapor density	3.3 kg/m^3
Benzene molecular diffusion coefficient in air	8.8 x 10^{-5} m^2/sec [3]
Turbulent Schmidt number*	0.7

Note:*: Ratio of turbulent viscosity to mass diffusion

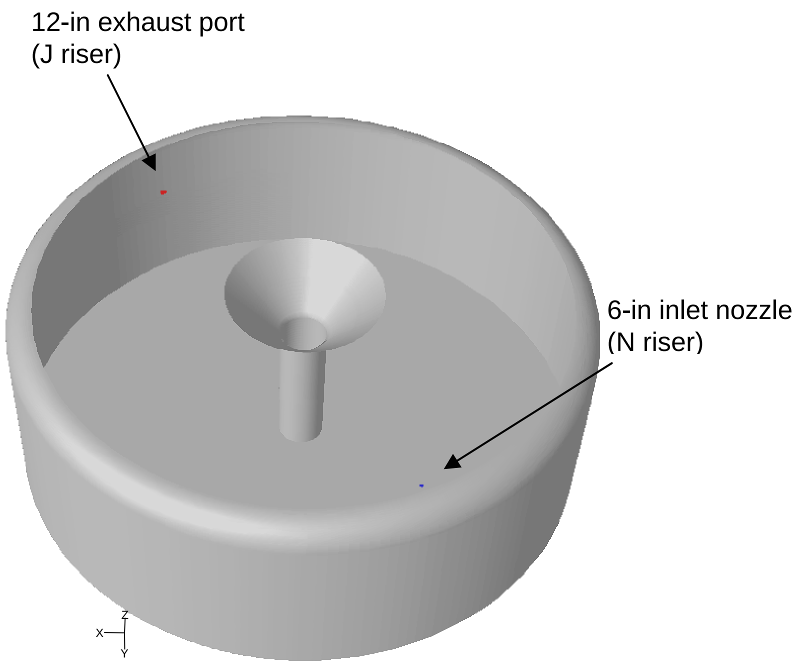


(Three-dimensional top view)

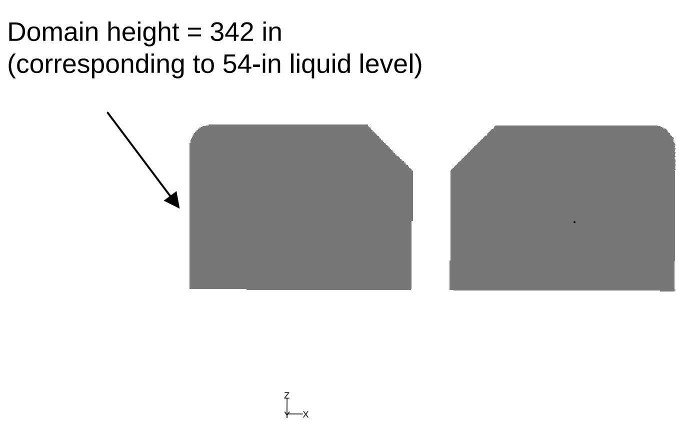


(Two-dimensional side view)

Figure 2. Computational domain as modeled for the calculations of benzene concentrations in the vapor space of Tank 50 (Case-1)

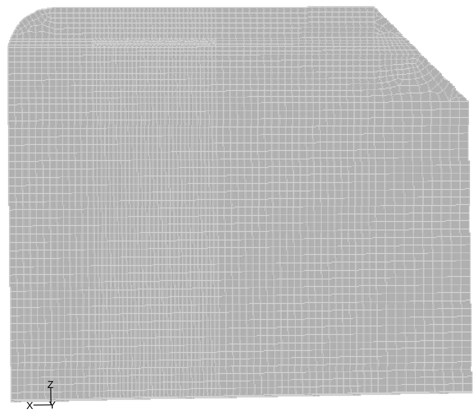


(Three-dimensional top view)

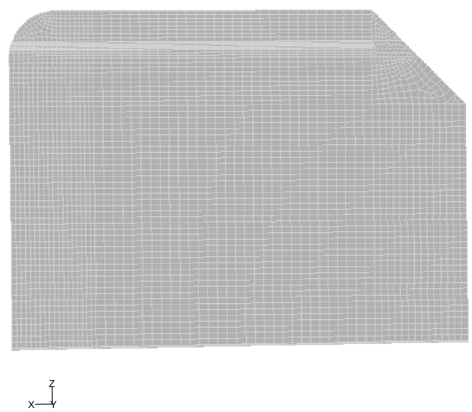


(Two-dimensional side view)

Figure 3. Computational domain as modeled for the calculations of benzene concentrations in the vapor space of Tank 48 (Case-2)



(Computational meshes for Case-1 on two-dimensional domain: 1.5-million total meshes)



(Computational meshes for Case-2 on two-dimensional domain: 1-million total meshes)

Figure 4. Computational domain meshes for the two cases considered in the analysis

3. Results and Discussions

The present models for the additional scoping calculations employed a three-dimensional CFD approach with two-equation turbulence model described in terms of turbulent dissipation and eddy diffusivity, referred to as k-ε model in the literature.[6] It assumed isothermal conditions for the gas medium so that natural convection was not included. The computational domains for the two cases considered here are shown in Figs. 2 and 3. The present model used two different meshes because of different modeling domain sizes. The computational meshes corresponding to the two-dimensional modeling domains are shown in Fig. 4.

The primary result of the work was an estimate of the maximum benzene concentration under the imposed operating conditions as shown in Table 1. The models actually compute benzene mass fractions. The benzene volume fraction is obtained by applying a gas density ratio of benzene vapor to air of about 2.7. Graphical results are presented in Fig. 5. Table 3 shows numerical values of the benzene volume concentration corresponding to benzene mass fraction. The benzene LFL concentration of 1.37 vol% corresponds to a mass fraction of 0.036.

<u>Case 1</u>: 150 cfm recirculation, 72 cfm purge air

Case 1 used 150 cfm forced circulation through a 4-in pipe 34 inches below G riser, 72 cfm air inlet flow the N riser and 25 gm/min benzene evolution from the liquid surface. The discharge velocity from the recirculation fan is about 8.75 m/sec. Figure 6 shows flow patterns and gas velocity distributions at the vertical plane crossing the recirculation region for Case-1. Flow patterns and benzene concentration distributions at the horizontal plane crossing the circulation region are shown in Fig. 7. The results indicate that the vapor space is well mixed except for the region near the air inlet of the N riser where the benzene concentration is low.

Figure 8 shows that the recirculation fan rotates the gas clockwise. It also shows that the concentration gradient of benzene is very small within the vapor space, varying only by about 2% of LFL over the entire plane at the mid-elevation of the tank. This is consistent with previous results where the ventilation air inlet is located near the wall boundary and the air flow is injected into the vapor space azimuthally with a 15^o downward orientation toward the tank bottom, the same angle that was used for the forced recirculation flow. The calculation shows that gas movement in the wall boundary region is much stronger than in the region near the central column. The central region has higher benzene concentrations compared to the wall boundary region.

Fig. 9 shows the 72 cfm air flowrate through the 6-in inlet of N riser moving about 30 inches downward into the vapor space, and then changing flow direction into the rotational motion driven by the recirculation fan. Benzene concentrations corresponding to the flow patterns near the inlet region are shown in Fig. 10. The figure clearly shows that most regions surrounding the air inlet region have nearly-uniform concentrations of about 0.011 benzene mass fraction (28% LFL).

Air velocity distributions and benzene concentrations at the vertical plane crossing the center-line of the tank are shown in Figs. 11 and 12. The results show that benzene concentrations over the entire plane of the central region range from a minimum 25%

LFL to a maximum 34% LFL. It is noted that the heavier gas component of the air-benzene mixture is settled down over the slower region near the liquid surface as expected.

To put the calculated benzene concentrations in perspective, it is instructive to compare them with the concentration for a perfectly mixed vapor space. If the vapor space were perfectly mixed, the benzene concentration would depend only on the ratio of the benzene evolution rate to the purge air flow rate, or

$$C_{benzene\_perfectmixing} = \frac{\dot{m}_{benzene} / \rho_{benzene}}{q_{purgeair}}$$

For a benzene evolution rate of 25 gm/min, a density of 3.3 kg/m^3, and a purge air flow rate of 72 cfm, the perfect mixing benzene concentration is 0.372 vol%, or 27% LFL. The average benzene concentration in the vapor space cannot be lower than this value. The fact that the local concentrations calculated for the vapor space are close to this value indicates that the vapor space is fairly well mixed by the forced recirculation flow.

It is also instructive to note that the volume of the vapor space does not affect the perfect mixing concentration. Its only effect is on the time required to achieve a steady-state concentration. Therefore, the ratio of the benzene and purge air flow rates can be used as a quick assessment of the Fluent calculation.

Case 2: 72 cfm purge air, no forced recirculation

Case 2 has the same inlet flow and benzene generation rate as Case 1, but it has no forced internal recirculation. The computational domain is the same as the previous Tank 48 model, which has a vapor space height of 342 inches. Figure 13 compares the benzene concentrations between the two cases at a horizontal plane one meter above the liquid surface. The modeling results show that when the vapor space is ventilated only by 72 cfm air flow without any forced recirculation, the benzene gas is stratified near the liquid surface. Air velocity corresponding to 72 cfm flowrate via the 6-in inlet at the N riser is about 1.9 m/sec as shown in Fig. 14. The figure shows that the air flow penetrates into the vapor space about 6 feet below the N riser, and then dissipates into the surrounding stagnant vapor space. The benzene gas distributions near the inlet region are shown in Fig. 15. Figure 16 clearly shows that the benzene gas above the liquid surface in the tank is stratified except for the air entrance region. The 72 cfm air flow is not sufficient to mix the benzene gas in the vapor space.

The calculated results for the benzene concentration distributions at the vertical center plane of the tank are compared between the two cases in Fig. 17. Figure 18 compares these results using the same color scaling, which ranges from 28% LFL in dark blue to 41% LFL in red. It is noted that when benzene is perfectly mixed with air inside the tank gas space, its volume percent is about 0.37. This corresponds to about 27% LFL. Quantitative comparisons between the two results are made non-dimensionally along the vertical centerline in Fig. 19. This comparison is supported by a previous demonstration that the calculated results are not sensitive to the grid density used in the computational model. [1] The modeling results demonstrated that forced recirculation significantly improves the mixing characteristics in the vapor space.

The maximum benzene concentration for the case with internal recirculation is about 34% LFL. Maximum benzene concentration for the case with no recirculation is about 41% LFL. All the results considered here are summarized in Table 4. The calculation results show that neither case supports a target criterion of 25% LFL, or a benzene concentration of 0.34 vol%. These results are consistent with the previous calculations described in Reference 1.

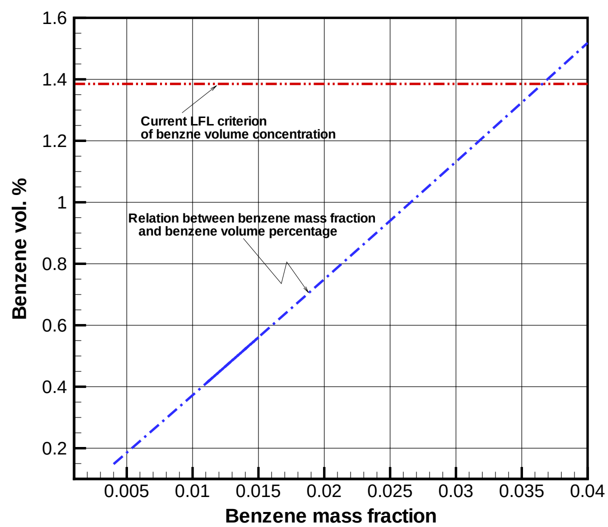


Figure 5. Benzene volume percentages for various benzene mass fractions

Table 3. Benzene volume percentages for various benzene mass fractions

C_6H_6 mass fraction	C_6H_6 vol.%	%LFL	C_6H_6 mass fraction	C_6H_6 vol.%	%LFL
0.0040	0.148	10.8	0.0150	0.560	40.9
0.0045	0.167	12.2	0.0200	0.750	54.7
0.0050	0.186	13.6	0.0250	0.940	68.6
0.0051	0.189	13.8	0.0300	1.132	82.6
0.0053	0.197	14.4	0.0350	1.325	96.7
0.0075	0.279	20.4	0.0362	1.370(LFL)	100
0.0100	0.372	27.2	0.0370	1.402	102
0.0104	0.386	28.2	0.0400	1.519	111
0.0110	0.410	29.9	0.0410	1.556	114
0.0123	0.459	33.5	0.0430	1.636	119

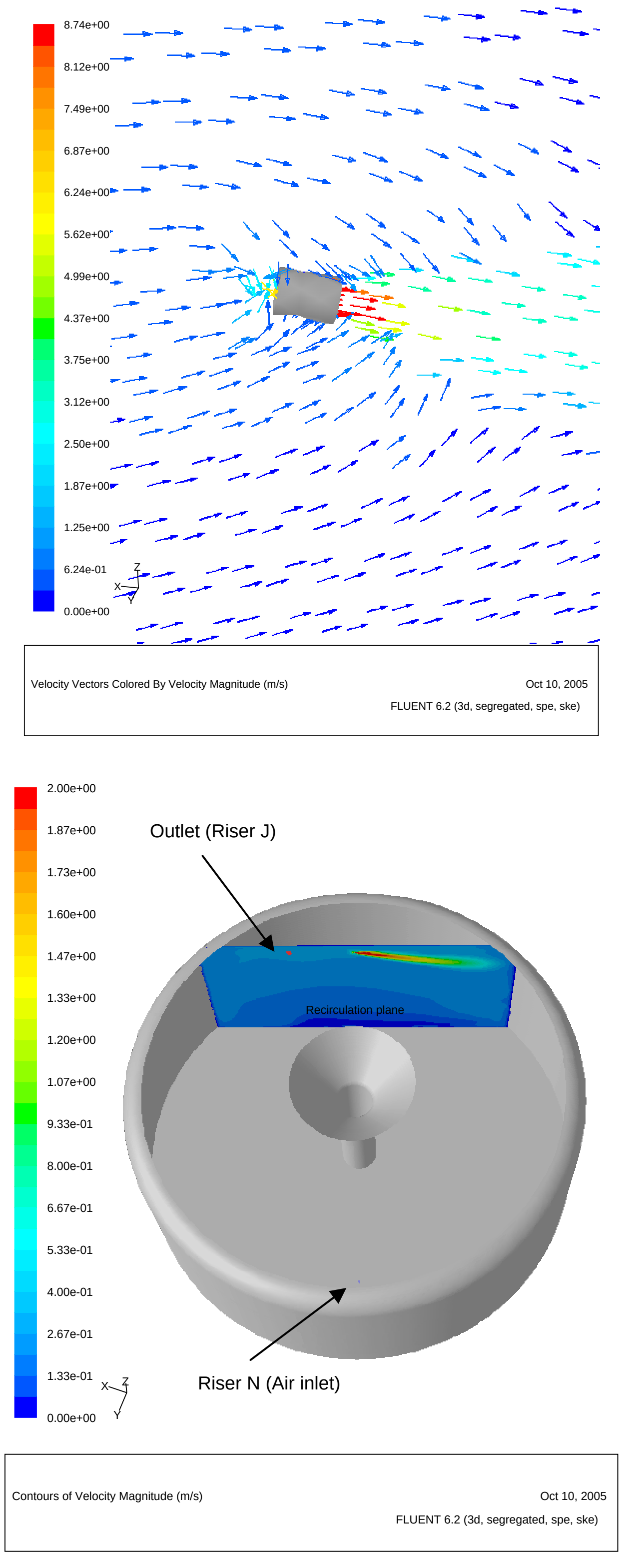


Figure 6. Flow patterns and contours for 25 gm/min benzene generation rate and 150 cfm air recirculation through 4-in pipe at the riser G plane of Tank 50 (Case-1)

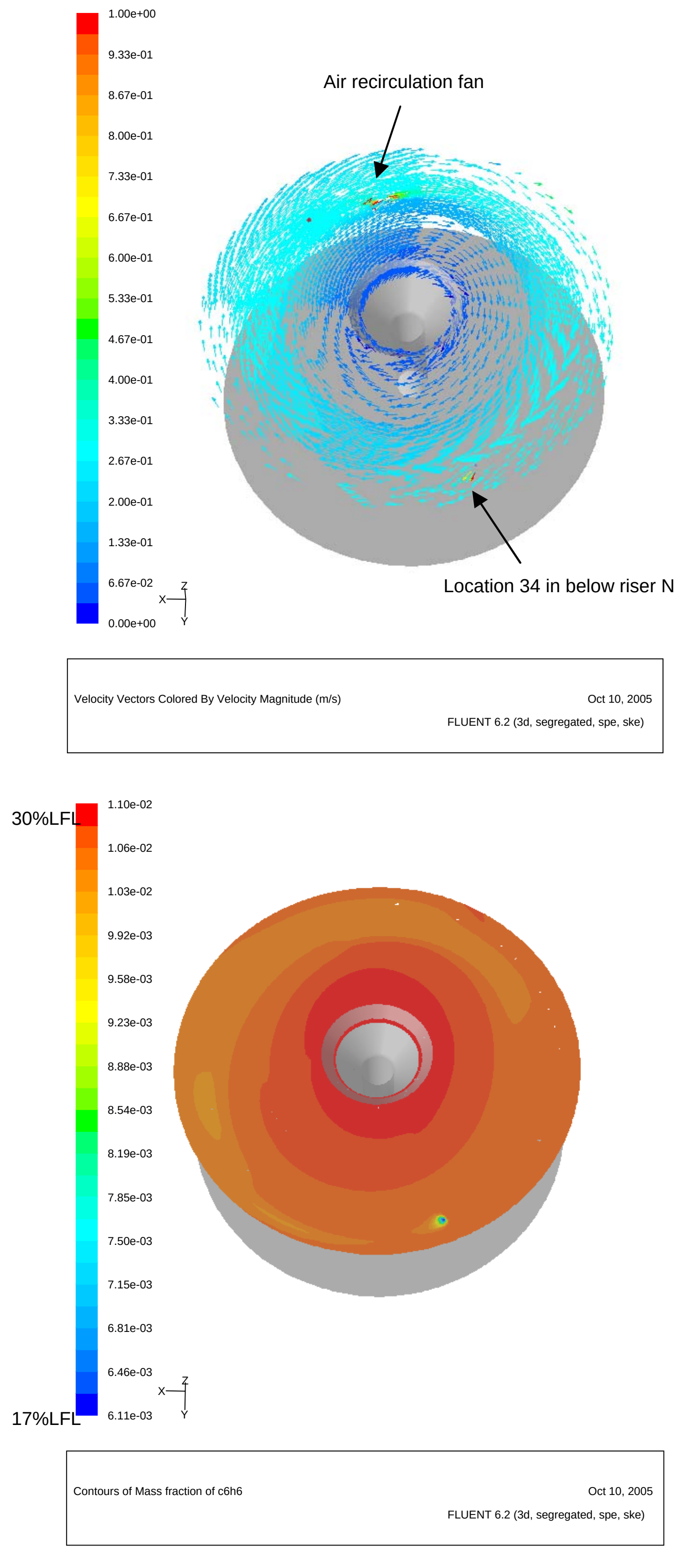


Figure 7. Flow patterns and benzene concentrations at the horizontal plane crossing the air recirculation fan region in Tank 50

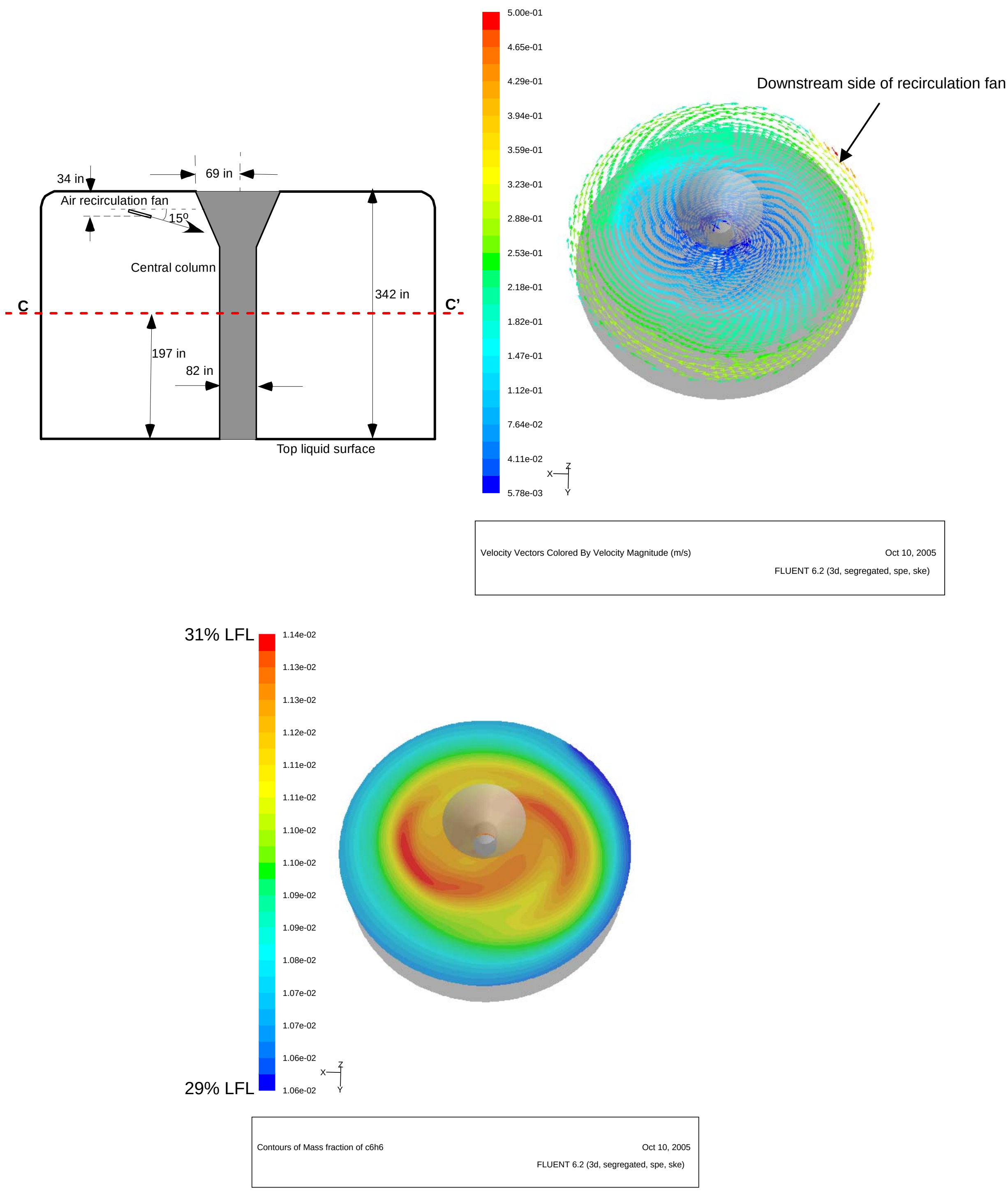


Figure 8. Flow patterns and benzene mass fraction distributions under 150 cfm air recirculation through G riser at the mid-elevation plane of Tank 50 crossing the line C-C' (0.0362 mass fraction corresponds to 1.37 C6H6 vol%)

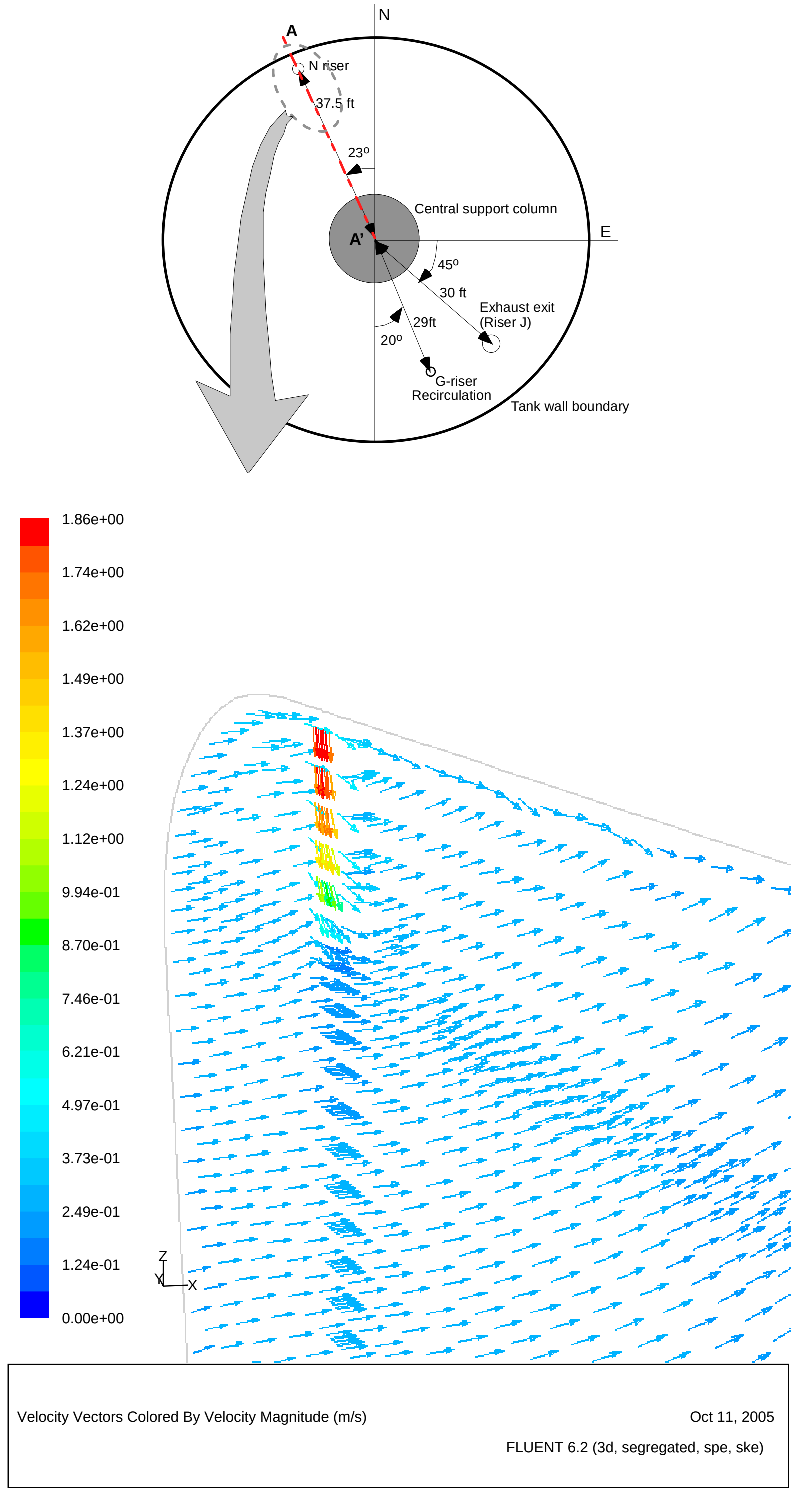


Figure 9. Flow patterns under 150 cfm air recirculation through G riser at the vertical plane of Tank 50 crossing the line A-A'

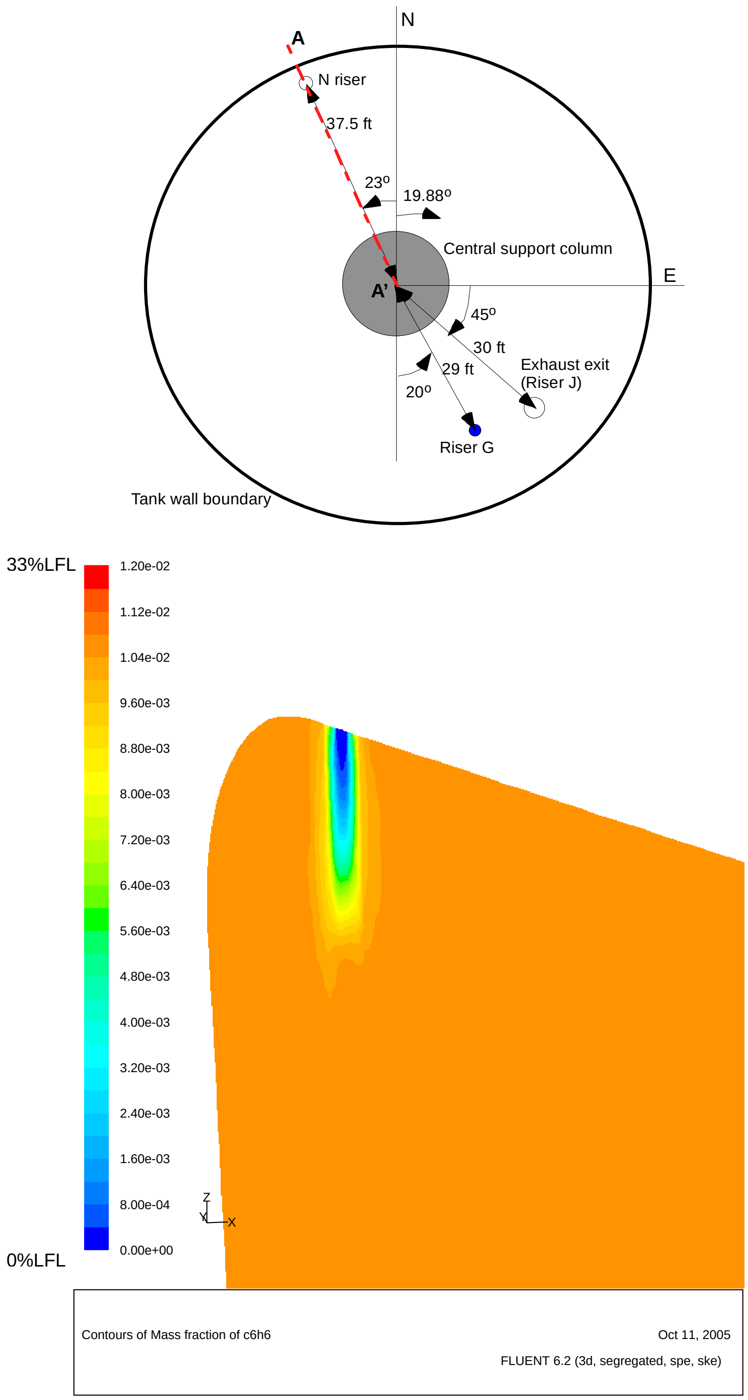


Figure 10. Benzene mass fractions under 150 cfm air recirculation through G riser at the vertical plane of Tank 50 crossing the line A-A' (0.0362 mass fraction corresponds to 1.37 C_6H_6 vol%)

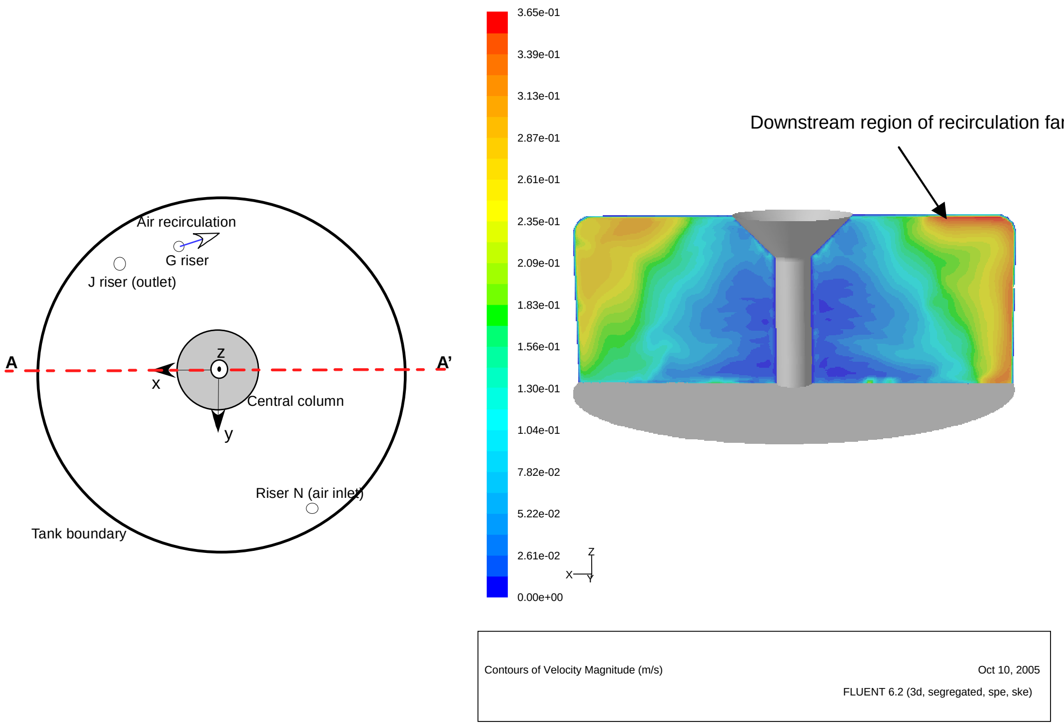


Figure 11. Air velocity distributions at the vertical plane crossing the center-line of Tank 50 (Case-1).

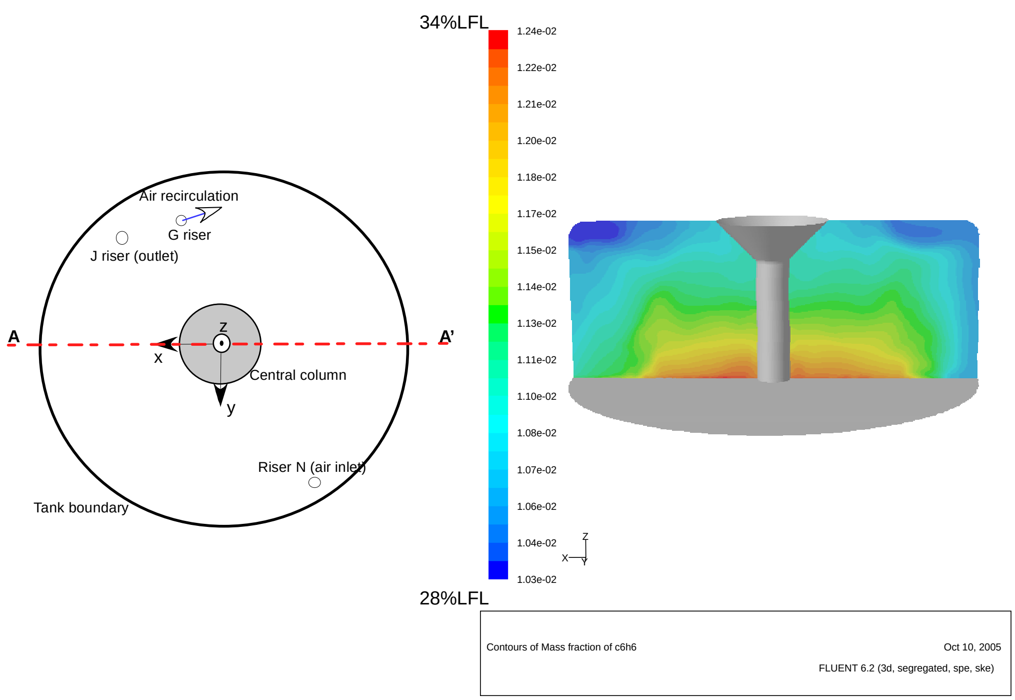
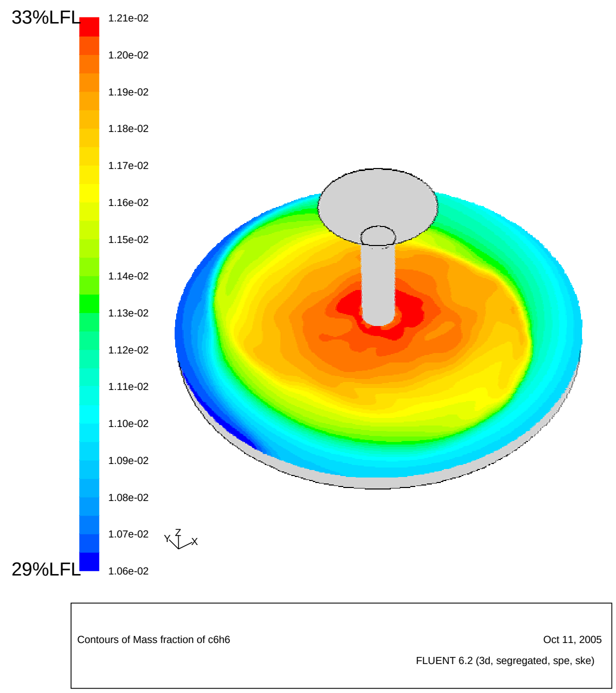
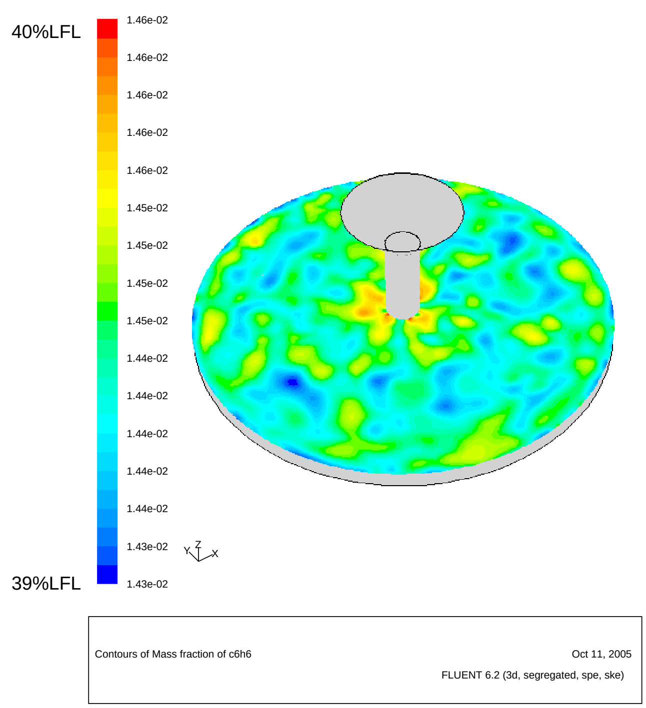


Figure 12. Benzene mass fraction distributions at the vertical plane crossing the center-line of Tank 50.



(Case-1: 72 cfm airflow and 25 gm/min benzene generation rate with air recirculation)



(Case-2: 72 cfm airflow and 25 gm/min benzene generation rate with no air recirculation)

Figure 13. Comparison of benzene mass fractions between the two cases at 1-m elevation above the liquid surface

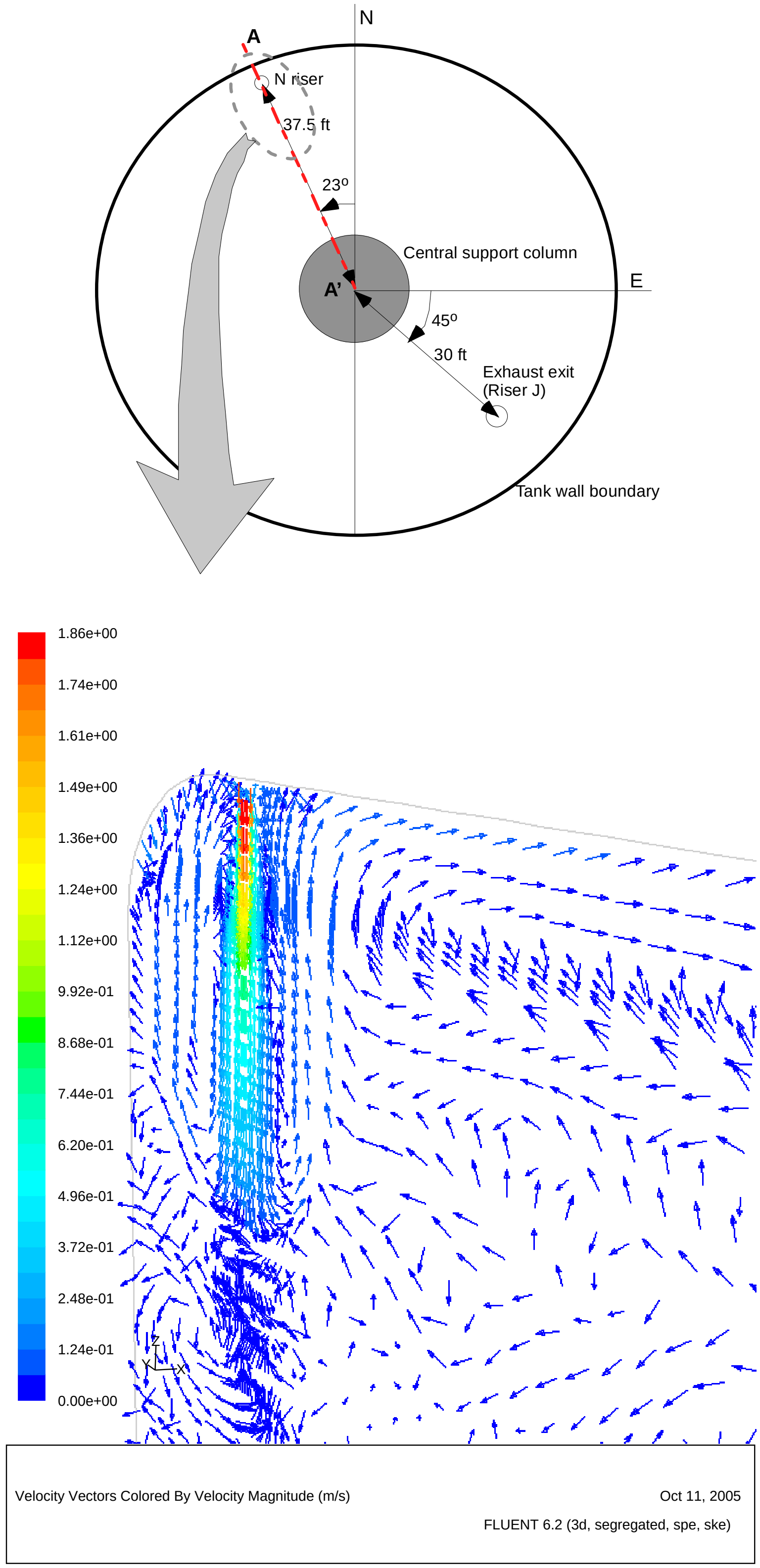


Figure 14. Flow patterns under 72 cfm air inlet flow through N-riser with no air recirculation at the vertical plane of Tank 50 crossing the line A-A'

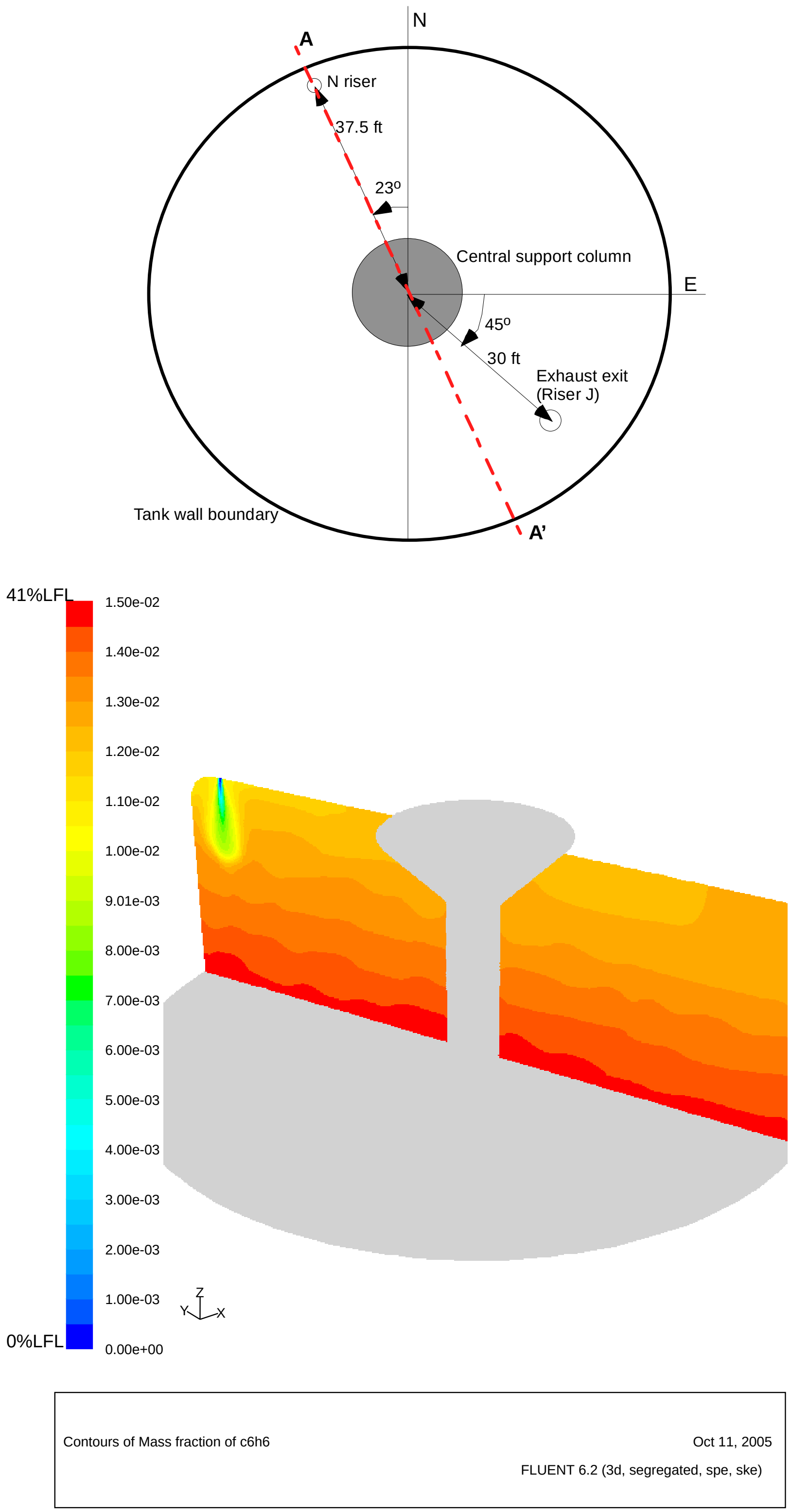
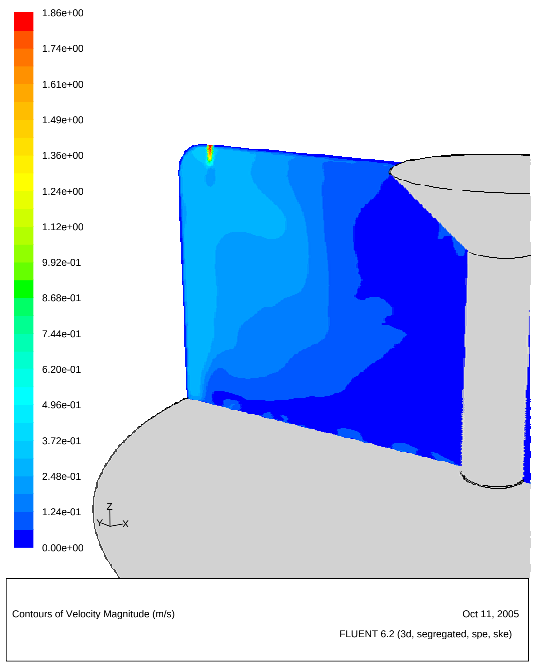
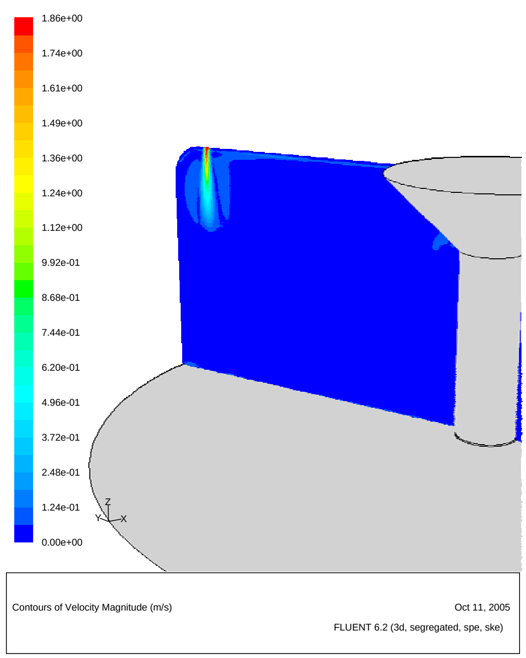


Figure 15. Benzene mass fraction distributions under 72 cfm air inlet flow through N-riser with no air recirculation at the vertical plane of Tank 50 crossing the line A-A' (0.0362 mass fraction corresponds to 1.37 C6H6 vol%)

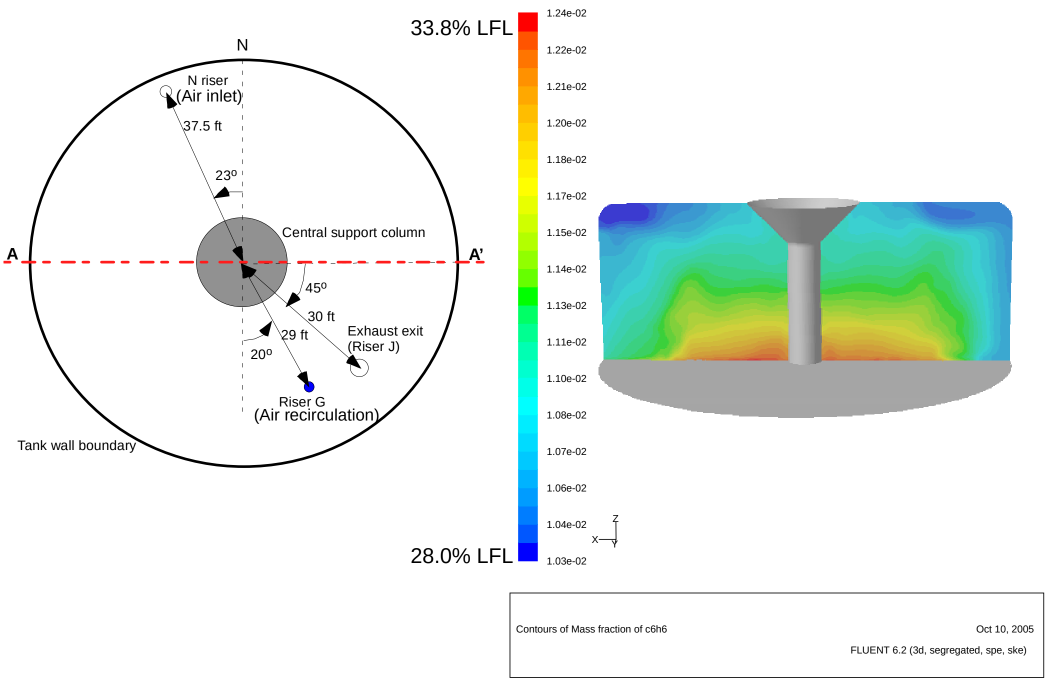


(Case-1: 72 cfm airflow and 25 gm/min benzene generation rate with 150 cfm air recirculation)

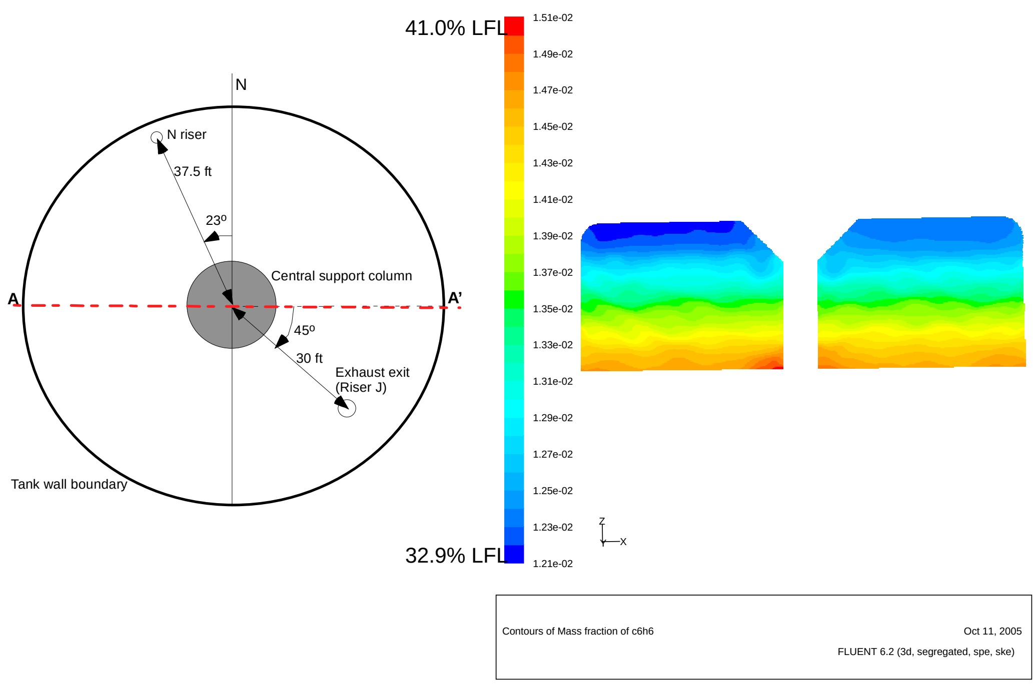


(Case-2: 72 cfm airflow and 25 gm/min benzene generation rate with no air recirculation)

Figure 16. Comparison of gas velocity distributions at the vertical plane crossing the gas inlet through G-riser between the two cases under the same color scaling system

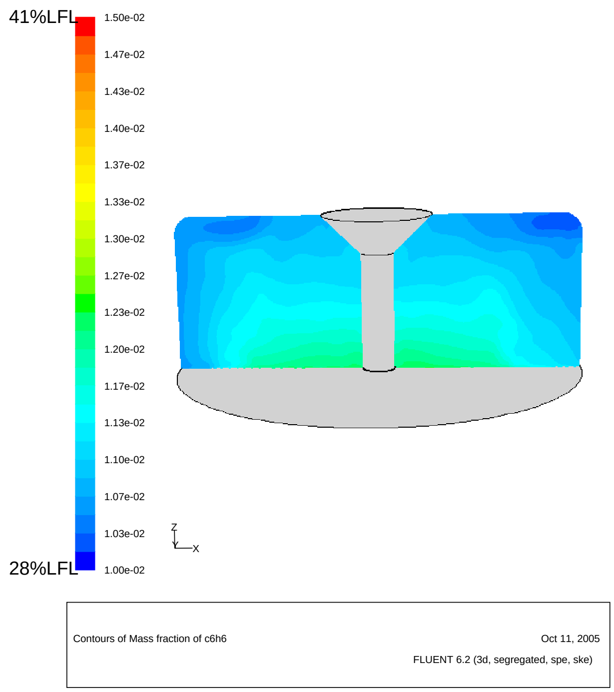


(Case-1: 72 cfm airflow through N-riser with 150 cfm air recirculation via G-riser under 2-in liquid level)

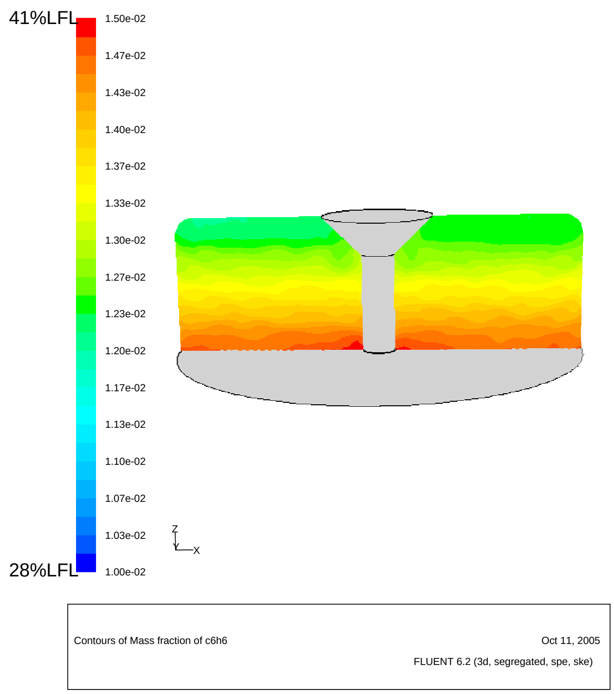


(Case-2: 72 cfm airflow through N-riser with no air recirculation under 54-in liquid level)

Figure 17. Comparison of benzene concentrations of the tank vapor space between the two cases at the vertical plane crossing the centerline A-A'.

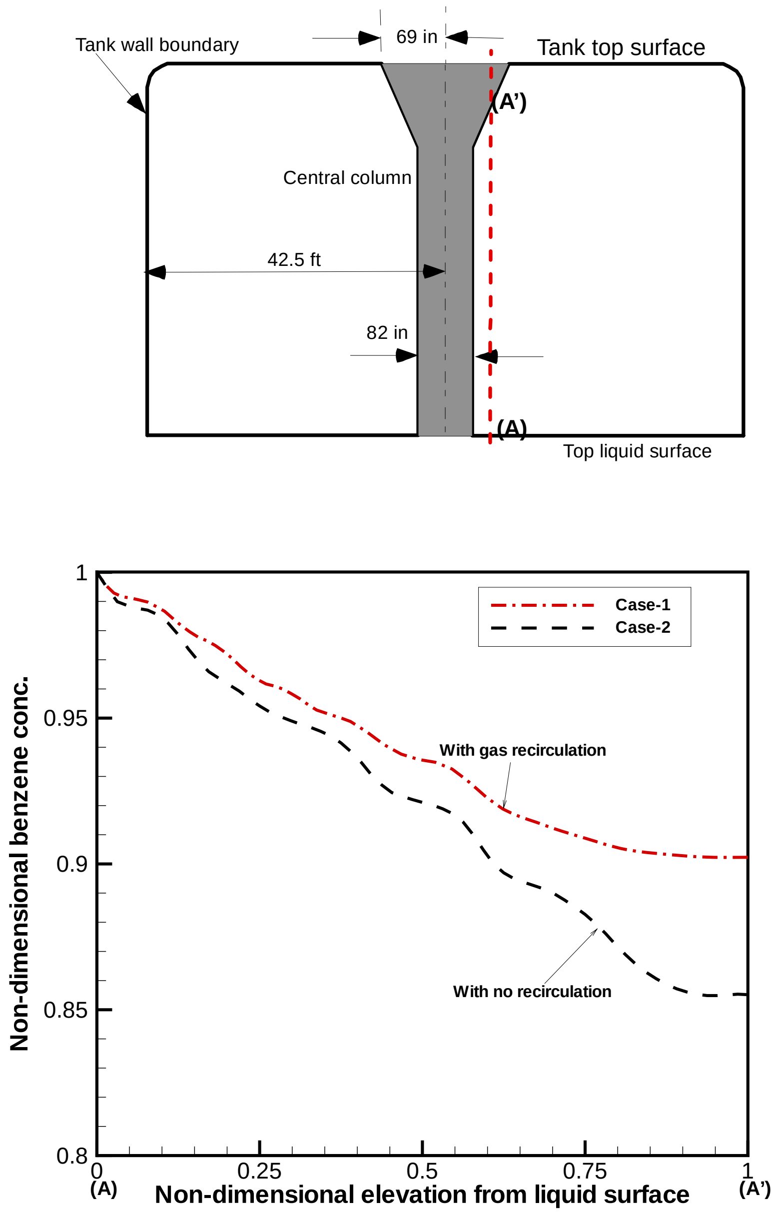


(Case-1: gas recirculation)



(Case-2: no gas recirculation)

Figure 18. Comparison of benzene concentrations of the tank vapor space between the two cases at the vertical plane crossing the centerline under the same color scaling.



$$Non-\dim ensional\,elevatiion = (local\,elevation\,along\,the\,line\,AA')/(total\,vapor\,space\,height\,along\,the\,line\,AA')$$

$$Non-\dim ensional\,benzene\,conc. = (local\,benzene\,conc.)/(\max.benzene\,conc.)$$

Figure 19. Non-dimensional benzene concentrations along the non-dimensional vertical line A-A' for the two cases considered in the analysis

Table 4. Summary of the calculated results for the cases considered in the present study

Cases	Air recirculation rate (ft^3/min)	Air inlet location (size)	Air flowrate at inlet (ft^3/min)	Benzene generation rate (gm/min)	Max. benzene conc. (vol. %)	% benzene LFL value*
Case-1	150 (via G riser)	N riser (6 in)	72	25	0.46	34
Case-2	0	N riser (1 in)	72	25	0.56	41

Note:* % LFL value is based on benzene LFL of 1.37 vol.% at 25°C.

4. Summary and Conclusions

The previous CFD model developed for the Tank 48 scoping analysis was applied to the estimation of maximum benzene concentration for the vapor space inside Tank 50 and Tank 48. The model used a three-dimensional momentum-species transport coupled approach. The flow conditions are assumed to be fully turbulent since Reynolds numbers for typical operating conditions are in the range of 20,000 to 70,000 based on the inlet conditions of the air purge system. A standard two-equation turbulence model was used.

Additional sensitivity calculations included a reduced benzene evolution rate, reduced air inlet and exhaust flow, and forced internal recirculation. The calculations were based on prototypic tank geometry and nominal operating conditions.[1, 2] Detailed cases considered in the additional calculations are provided in Table 1.

The flow patterns in the vapor space demonstrate that with internal recirculation through a 4-in pipe near the G riser and 72 cfm ventilation air entering the tank through the 6-in N riser, the vapor space is fairly well mixed. For the same 72 cfm air inlet flow but without forced recirculation, benzene gas is stratified. The modeling results showed that benzene concentrations were relatively low for typical operating configurations and conditions. The maximum benzene concentration for the case with internal recirculation is about 34% of an assumed LFL value of 1.37 vol% benzene. Maximum benzene concentration for the case with no recirculation is about 41% LFL. The results show that neither case supports a target criterion of 25% LFL, or 0.34 vol.% benzene.

5. References

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