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# Natural Convection Flow Pattern Analysis for a Large-Scaled Saltstone Facility

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## INTRODUCTION

Waste Solidification Engineering at Savannah River Site (SRS) has been evaluating the potential flammable conditions in the air space of Saltstone vault facility for the safety analysis. In order to help assess the potential for benzene layer formation on top of the grout, a computational model of the vault vapor space was developed to estimate the nature of air movement inside the vault. The vault geometrical configurations are shown in Fig. 1.

The vault has two breathing holes, which are located along the diagonally opposed location as shown in Fig. 1. The main objective of this work is to examine the gas motions inside the vapor space under the current vault configurations by taking a computational fluid dynamics (CFD) modeling approach [1]. The modeling domain of the present analysis is shown in Fig. 1. The modeling analysis was focused on the impacts of two breathing holes on the gas flow patterns due to the mass and energy exchanges between the cooler gas of the ambient air and the warmer space gas of the vault, especially, under hot summer conditions.

In this work two modeling cases were considered. One case represents the nominal reference conditions for the baseline analysis. The other is for the case with negative temperature gradient, that is, Saltstone vault has the inner roof surface temperature 5°C higher than the bottom surface of Fig. 1. The latter case corresponds to the potential bounding case in terms of flammable gas mixing, which is expected under the hot summer conditions.

A series of sensitivity calculations for different vapor space height and grout surface temperatures is also considered. The primary objective of this work is to examine the impacts of the gas flow patterns due to the changes of the vapor space height and grout surface temperature. The modeling results will assist in understanding the qualitative gas flow patterns within the vapor space of the Saltstone vault and ambient air circulation paths through the two ventilation holes under the potential operating scenarios. This paper will discuss the modeling and analysis results.

## DESCRIPTION OF THE ACTUAL WORK

A three-dimensional CFD approach was taken to calculate flow patterns for the gas flow patterns of Saltstone vault and to examine the qualitative air circulation paths between the ambient air and the vault space gas through two breathing holes located at the roof of the vault. The detailed dimensions and

geometrical information as modeled are presented in Fig. 1. A finite volume CFD code, FLUENT™, was used here in creating the modeling geometry and in solving the governing equations for the present work. A computational domain of the prototypic vault geometry was non-uniformly discretized by a non-orthogonal and hexahedral mesh for the numerical simulations. Final nodes of about 450,000 meshes were established from a mesh sensitivity analysis. The modeling calculations were performed using the following assumptions:

- Typical gas flow behaviors of the vapor space in Saltstone vault due to the temperature difference between the inner roof and top grout surface are similar to the one driven by the air movement.
- Air follows ideal gas behavior.
- Top grout surface corresponding to bottom surface in Fig. 1 is assumed to be flat.
- Ambient air temperature is assumed to be constant, and it is 41°C.
- The initial conditions for the vapor space are stagnant and the same as ambient temperature 41°C.

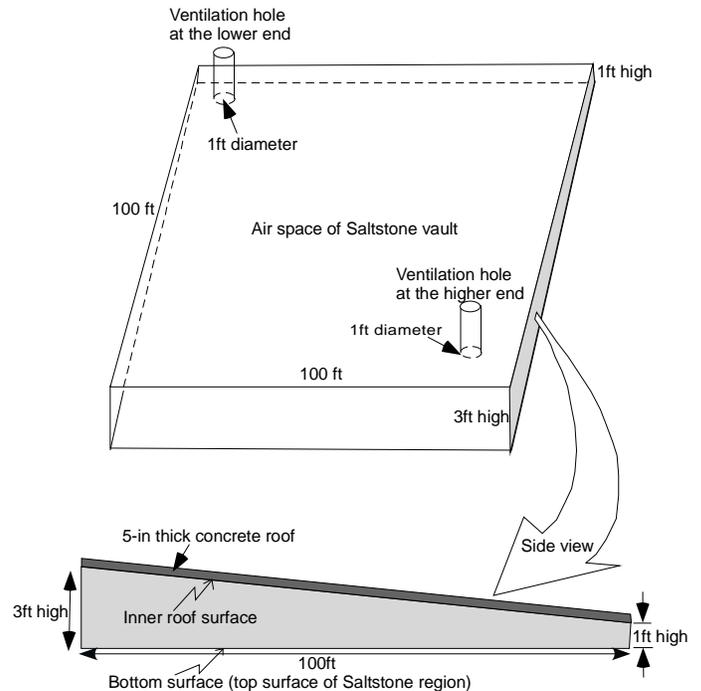


Fig. 1. Modeling domain of vapor space for Saltstone Vault facility used for the present work (1 ft = 0.3048m).

The flow conditions for the vault operations are assumed to be fully turbulent since Reynolds numbers for typical operating conditions are in the range of 24,000 based on the inlet conditions of the ventilation hole. A standard two-equation turbulence model, the  $\kappa$ - $\varepsilon$  model [2], was used since previous work [3] showed that the two-equation model predicts the flow evolution of turbulent flow in a large stagnant fluid domain with reasonable accuracy. This model specifies the turbulent or “eddy” viscosity  $\mu_t$  by the empirical equation.

$$\mu_t = \left( \frac{C_\mu \rho_f k^2}{\varepsilon} \right) \quad (1)$$

In eq. (1)  $C_\mu$  is an empirical constant, and  $\rho_f$  is gas density. In the present calculations,  $C_\mu$  is 0.09 [2]. Thus, the turbulent viscosity is computed by solving two transport equations for  $k$  (turbulent kinetic energy) and  $\varepsilon$  (rate of dissipation of turbulent energy). The governing equations to be solved for the present work are composed of one continuity equation, three momentum equations for the three component directions ( $x$ ,  $y$ , and  $z$  directions), one energy equation, and two constitutive equations for the turbulence descriptions. The detailed descriptions for the governing equations and computational methods are provided in the previous work [1]. The model is a full three-dimensional representation of the entire gas space to capture significant phenomena related to the turbulent behavior of gas flow evolution in a large-scaled Saltstone vault.

Air was used to simulate the gas in the vapor space within the vault, assuming that it would give an acceptable representation of the flow patterns. Governing equations for the entire computational domain were solved with FLUENT<sup>TM</sup> for two different cases in a transient simulation mode. They are the baseline reference and the bounding cases as described in the previous section. The modeling conditions for the nominal baseline case are summarized in Table 1. As shown in the table, boundary conditions for two ventilation holes of the vault system were set as 250 Pa gauge pressure since the amplitude of the sinusoidal pressure oscillations due to diurnal temperature variations is set at 2.5 mbar about the mean pressure of 1,103 mbar [4].

The key areas in the present analysis such as the turbulence and natural convection behaviors were benchmarked against the literature and theoretical results [1,3] in order to demonstrate the adequacy of the software for the vault model since the modeling results are to support a safety significant calculation.

Finally, the benchmarked modeling equations were applied to the Saltstone vault model using the computational domain as shown in Fig. 1. Design and modeling conditions for the baseline calculation are presented in Table 1.

Table 1. Reference modeling conditions used for the baseline calculations in the present modeling analysis.

Parameters	Baseline conditions
Modeling domain size (see Fig. 1)	100ft x 100ft x 1 ft (lower end) x 3 ft (higher end)
Roof thickness	5 inches
Ambient temperature	105F (41°C)
Initial gas temperature for vapor space	105F (41°C)
Bottom surface of domain (see Fig. 1)	158F (70°C)
Solar heat flux	400 W/m <sup>2</sup>
Ventilation hole	250 Pa (2.5 mbar) gauge pressure
Ventilation hole diameter	1 ft
Chimney height of ventilation hole	4 ft
Primary cooling mechanism	Natural convection

## RESULTS AND DISCUSSIONS

The present model employed two-equation turbulence described in terms of turbulent dissipation and eddy diffusivity, and ideal gas law was used in association with natural convection mechanism for the entire computational domain as shown in Fig 1.

The flow conditions for the Saltstone vault facility are assumed to be fully turbulent since Reynolds numbers for typical operating conditions are in the range of  $2 \times 10^4$ . A standard two-equation turbulence model, referred to as  $k$ - $\varepsilon$  model [2], was used since benchmarking results against the literature data [5] showed that the model predicts turbulent flow evolution in a large fluid domain with reasonable accuracy. The benchmarked model was applied to the Saltstone vault geometry for the transient assessment of the gas flow patterns inside the vapor space of the vault region using the potential boundary conditions.

The present work considered two cases for the estimations of the flow patterns within the vapor space. One is the baseline reference case as provided in Table 1. The other is for the negative temperature gradient between the roof inner and top grout surface temperatures intended for the potential bounding condition. For this case, wall temperature of the inner roof is assumed to be 5°C higher than that of the bottom surface for the vault air region shown in Fig. 1. Pressures at both holes are assumed to be maintained as 250 Pa gauge pressure given by the literature data [4]. As the initial conditions for the present transient simulations, the vapor space is assumed to be stagnant at ambient temperature 41°C.

The transient results show that maximum temperature of the roof inner wall is still about 10°C lower than the top Saltstone grout surface temperature, which is provided as 70°C boundary condition shown in Table 1. This case corresponds to positive temperature gradient between the roof inner and top grout

surface temperatures. The flow pattern results confirmed the air circulations through the two holes. It is noted that the ambient air of about 41°C comes into the gas space through the lower end hole, and after it is heated up to 64°C at 7 hours transient time, it comes out of the vault via the higher end one.

Density distributions along the diagonal plane crossing the two ventilation holes confirm that heavier (cooler) air comes into the hole located near the corner of the lower end region. Temperature distributions at the entire plane crossing the middle elevation of the vapor space are shown in Fig. 2. Density distribution patterns are very similar to the temperature distributions, showing the local cell patterns. These results are consistent with the literature information [6,8]. The velocity flow pattern results at the mid-plane of the vault vapor space show that the flow patterns consist of small cells like honeycomb as the ambient cooler air gets heated up during the residence time inside the vault. Maximum speed of air movement is at the two ventilation holes of the vault, and it reaches about 1.2 m/sec. Detailed results are shown in Fig. 3. Positive velocity in the figure indicates the gas flow leaving the vault vapor space through the ventilation hole.

As the second case, the potential negative temperature gradient is considered as the bounding case. This case corresponds to the case that the inner roof surface temperature is higher than the top grout surface temperature. The negative temperature gradient case has 5°C difference between the top and bottom surfaces of the domain as shown in Fig. 1. The results show that the vapor space near the lower end region gets heated more quickly than the higher end region since the heat transfer mechanism at early transient period is controlled primarily by the conduction mode. During the first 90-second transient period, it is shown that the gas contained inside the vapor space of the vault is breathing out through both of the two holes because of the dominant gas buoyancy. When the transient time reaches about 3 minutes, the ambient air starts to flow into the vapor space of the vault via the lower-end hole and to flow out through the higher-end hole. As shown in Fig. 4, the air circulation patterns are formed through both ventilation holes. It is noted that flow patterns for this case are very similar to those of the first case, the positive temperature gradient.

The work presented here considered two cases for the estimations of the flow patterns within the vault vapor space. One is the reference baseline case. The other is for the negative temperature gradient between the roof inner and top grout surface temperatures intended for the potential bounding condition. The flow patterns of the vapor space calculated by the CFD model demonstrate that the ambient air comes into the vapor space of the vault through the lower-end ventilation hole, and it gets heated up by the Benard-cell type circulation before leaving the vault via the higher-end hole.

The conclusive flow patterns of the vapor space obtained by the CFD modeling results are summarized in Fig. 5 in a qualitative way, which is consistent with the literature information [8]. Table 2 summarizes the quantitative results for the air flow rate coming into the vapor space through the ventilation hole near the lower end of the vault under the two modeling conditions considered in this work.

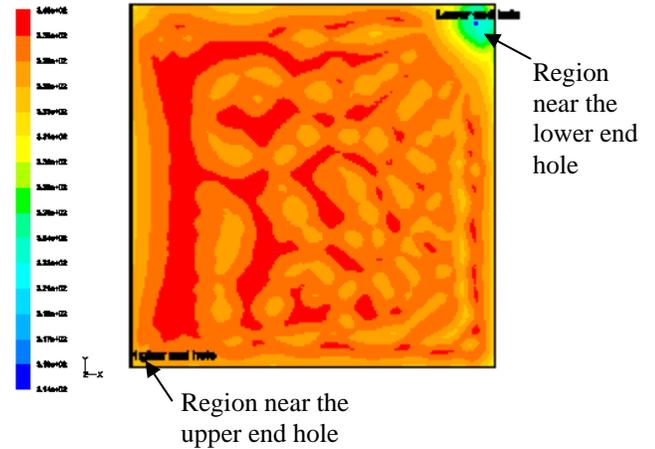


Fig. 2. Temperature distributions at the mid-plane of the gas space showing the honeycomb-type heat transfer at t = 7 hours (Red and blue regions are 67°C and 41 °C, respectively)

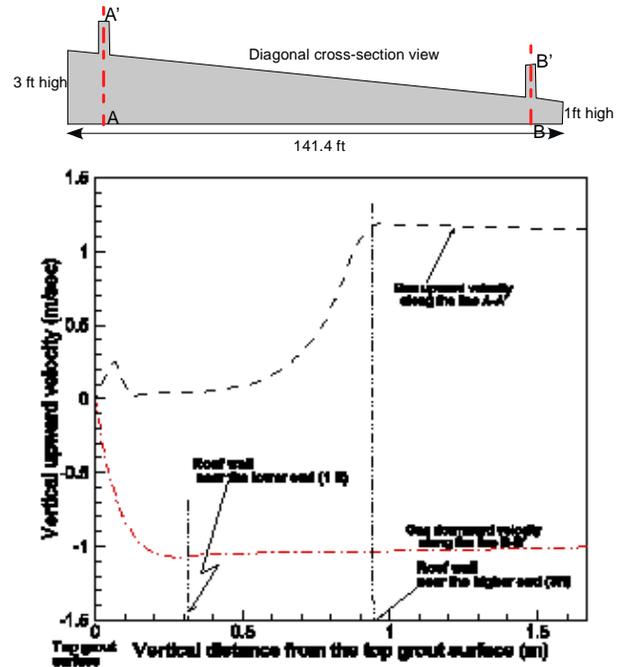


Fig. 3. Gas upward velocity profile along the vertical lines A-A' and B-B' of the two ventilation holes indicating that the lower end hole has downward airflow patterns under the baseline case

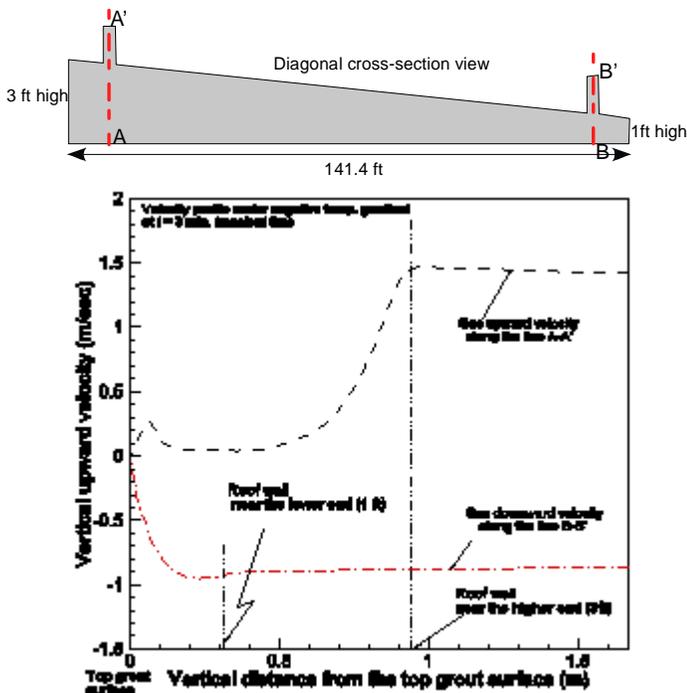


Fig. 4. Gas upward velocity profile along the vertical lines A-A' and B-B' of the two ventilation holes under the negative temperature gradient between the inner roof and top grout surface at 3-min. transient time, noting that the lower end hole has the gas flow patterns switched from the upward flow of the 90-second transient to the downward one of the later transient

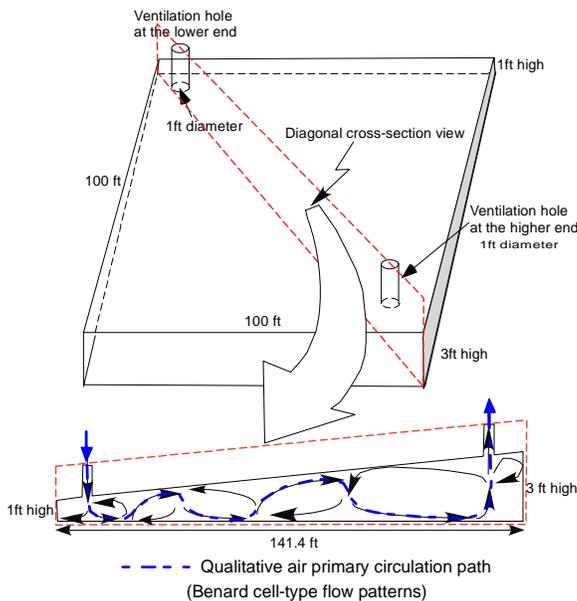


Fig. 5. Qualitative gas circulation patterns obtained by the present CFD modeling calculations for the vapor space of Saltstone vault, showing that the ambient air comes into the vapor space of the vault through the ventilation hole located near the lower end

Table 2. Quantitative results for the established air flow rate coming into the vapor space through the ventilation hole near the lower end of the vault under the two modeling conditions considered in the present work

Cases	Average air velocity coming into the vapor space within the vault	Air flowrate coming into the vapor space via the lower inlet hole (1-ft diameter)
Positive temperature gradient*	0.66 (m/sec)+	760 gpm
Negative temperature gradient**	0.56 (m/sec)+	648 gpm

Note:\* Baseline modeling conditions as provided by Table 1  
 \*\* Modeling conditions for 75°C roof inner temperature and 70°C bottom surface temperature under the same modeling domain as the baseline case  
 + Average flow velocity ( $V_{avg}$ ) was computed by averaging local velocity  $v$  over the ventilation hole area ( $A_{hole}$ ) by eq. (2) :

$$V_{avg} = \frac{1}{A_{hole}} \int_{A_{hole}} v dA \quad (2)$$

## REFERENCES

1. S. Y. Lee, "Computational Fluid Dynamics Model for Saltstone Vault 4 Vapor Space", WSRC-TR-2005-00288, Rev. 0, July 2005.
2. W. P. Jones and P. E. Launder, "The Prediction of Laminarization with a Two-Equation Model of Turbulence", *Int. J. of Heat and Mass Transfer*, Vol. 15, pp. 301-314, 1972.
3. S. Y. Lee, R. A. Dimenna, R. A. Leishear, D. B. Stefanko, "Analysis of Turbulent Mixing Jets in a Large Scale Tank", *ASME Journal of Fluids Engineering*, Volume 130, pp. 011104, 2008.
4. Auer, L. H., Rosenberg, N. D., Birdsell, K. H., and Whitney, E. M., "The effects of barometric pumping on contaminant transport," *J. Contam. Hydrol.*, Vol. 24, pp. 145-166, 1996.
5. Nielsen, P. V., Restivo, A., and Whitelaw, J. H., "The Velocity Characteristics of Ventilated Rooms", *J. of Fluids Engineering*, Vol. 100, pp. 291-298, 1978.
6. Bird, R. B., Stewart W. E., and Lightfoot, E. N., *Transport Phenomena*, John Wiley & Sons, New York, 1960.
7. *FLUENT6.3*, Fluent, Inc., 2012.
8. J. P. Holman, *Introduction to Heat Transfer*, Hemisphere Publishing Co., New York, 1969.