An improved approach for tank purge modeling

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Many launch support processes use helium gas to purge rocket propellant tanks and fill lines to rid them of hazardous contaminants. As an example, the purge of the Space Shuttle’s External Tank used approximately 1,100 kg of helium. With the rising cost of helium, initiatives are underway to examine methods to reduce helium consumption. Current helium purge processes have not been optimized using physics-based models, but rather use historical ‘rules of thumb’. To develop a more accurate and useful model of the tank purge process, computational fluid dynamics simulations of several tank configurations were completed and used as the basis for the development of an algebraic model of the purge process. The computationally efficient algebraic model of the purge process compares well with a detailed transient, three-dimensional computational fluid dynamics (CFD) simulation as well as with experimental data from two external tank purges.

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1. Introduction and background

PURGING rocket propellant tanks with helium is done to ensure that contaminant gases or water that may become a hazard during flight are removed from the tank prior to filling with propellant. For example, residual nitrogen or water may freeze and solidify when brought into contact with cryogenic propellants such as hydrogen or oxygen. Catastrophic damage may occur, if rocket engine’s turbomachinery would ingest solid nitrogen or water particles. A commonly used purge gas is helium because of its lower boiling point, 4.22 K at 1 atm, than any liquid propellant [1]. The low boiling point is important since the introduction of cryogenic liquids will not cause helium to solidify, unlike many of the contaminants, which a purge is attempting to replace. With the cost of helium continuing to rise, initiatives undertaken are to attempt to reduce the amount of helium used in a tank purge process, while still ensuring complete compliance with purging criteria [2].

An example of a process that uses a significant amount of helium is the purge of the Space Shuttle External Tank (ET) prior to the introduction of propellants, although what follows will be true for propellant tanks used on the next generation of rockets as well. At the conclusion of the purge process, samples taken would analyze the relative humidity of the gas mixture inside of the tank. If the purge is successful, the gas remaining in the tank will have a relative humidity below a critical threshold thus ensuring that only acceptable levels of residual water remain inside the tank. Additionally, the amount of nitrogen or other contaminant gases monitored to ensure that these gases are at acceptable levels.

The purge flow rate and purge time for the ET are not currently based on any detailed models to optimize the process, but rather on loose historical ‘rules of thumb’. Additionally, within the literature, there does not appear to be any type of systematic study for providing basic guidelines of purge characteristics of tanks and lines and

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purging of tanks or lines is currently limited to using one of two methods:

1. Advanced modeling, such as computational fluid dynamics (CFD) of purge performed on each tank or line. An overly conservative estimate of purge time and gas replacement volume based on the experience and data from prior tank purges.

Any new model used to predict the success of a purge process or employed to minimize the use of helium must successfully predict the level of relative humidity and contaminant gases left inside of the propellant tank after the purge. In order to develop a physics-based model of the tank purge process a generic tank created which is much similar to the ET and displayed in Fig. 1.

The tank mimics features of the ET including the overall height to diameter ratio, gas inlet and outlet geometries, and anti-vortex baffle system located at the base of the tank. Unlike the actual ET which has a series of stiffener rings located along the inside diameter of the tank, the tank used for this study has a smooth inner wall.

The tank purged in the vertical orientation done with helium introduced at the top inlet through a radial diffuser. The helium displaces the gas within the tank and the resulting mixture of gas forces through the outlet. Examining two limiting cases of tank purging allows for approximate minimum and maximum expected purging times to be determined.

1. The minimum expected purge time for a cylindrical tank at a constant pressure is: when, the purge gas at the inlet, enters the tank with no mixing, no molecular diffusion, and acts as the face of piston, which forces the tank gas through the outlet located at the bottom of the tank. The minimum purge time for the geometry

![Fig. 1. Generic tank geometry mimicking key features of the ET](image-url)
shown in Fig. 1 and given by Eq. (1) is approximately 1,200 s.

$$t_{\text{min}} = \frac{\pi HD^2}{4Q_i}$$

(1)

2. An estimate for the maximum purge time occurs when the purge gas completely mixes with the tank gas and the mixture exits through the outlet. To predict the tank time for the perfectly mixed scenario, a numerical code iteratively solves the governing differential equations for the concentration of gases inside the tank. This model takes into account the inlet flow rate of purge gas, the complete mixing of purge and tank gases, changes in pressure inside the tank and finally exit mass flow rate of the tank gases for a given exit area. For the geometry shown in Fig. 1 the completely mixed purge time is approximately 10,000 s.

Fig. 2 shows the examples of these two limiting cases modeled using computational fluid dynamics (CFD), with a tank initially filled with nitrogen and using helium as a purge gas. The top row of pictures shows nitrogen mole fraction contours during a low flow rate purge, in which the helium forms a ‘piston’ face on top of the nitrogen and pushes the tank gas out of the exit without creating a swirling, mixed flow, i.e. the purge and tank gases remain separated throughout the purging process. This case tends to lead to shorter purge times and minimal use of helium purge gas. However, purging too slowly allows for molecular mixing via diffusion to take place and thus increases the actual purge time above a perfectly non-mixed case.

The bottom row of pictures in Fig. 2 shows a purge using a much higher flow rate of purge gas. The high flow rate purge gas enters the tank through the radial diffuser and quickly forms vorticies, which mix the two gases together within the tank. This mixing is detrimental because it then takes an enormous supply of helium to purge the tank to satisfactory levels. These two illustrative cases show that to purge tanks in the least time with the least use of helium, an optimal flow rate of purge gas is to be determined. A full 3D transient computational fluid dynamics (CFD) simulation of the purging process incorporating all essential physics using this tank was completed and discussed in Section 5.

2. Computational modeling

In order to develop an accurate, quick turnaround-time tank purge process simulation tool, a systematic and detailed numerical survey was performed in order to better understand the underlying physics of purge behavior. These studies elucidated key aspects associated with the purge process. Simulation performed used
commercial computational fluid dynamics (CFD) code ANSYS FLUENT (version 6.3). Gambit (version 2.4), preprocessor for FLUENT used to create and mesh geometries. A large number of simulation were run in two-dimensional configuration while some three-dimensional simulation were run to account for obstructions in the model, such as stiffener rings or baffles located within the tank. The computational model used a double precision-pressure based implicit solver with a species model. Second order discretization used for density, momentum, species components, and energy calculations. Grid density and time-step size sensitivity study performed to ensure that the solution was capturing essential spatial and temporal features associated with the purge process. A grid resolution study was completed to ensure grid independence in the solution.

Fig. 3. Binary Vs. multi-component diffusion comparison.

Fig. 4. Purge models of, (left) inlet, (right) purge layer encounter with obstruction and outlet.
Viscosity and diffusion models examined prior to performing the parametric study. A full multi-component model option for diffusion is only available with the laminar viscous model. Two purge simulations performed were with binary diffusion that only differed by the viscous model employed. Results showed 6.3% percent difference between the laminar and turbulent models. The laminar flow model selected was because of this level of agreement and because of the low flow speeds involved (Re of the inlet helium flow was 142). A test concerning the behavior of binary and multi-component diffusion was performed and the results shown in Fig. 3. In all cases, the inlet gas is helium. The tank gas for the binary case was pure nitrogen. In the multi-component cases, the tank gas was standard air with the given humidity levels. Standard air was assumed to contain only nitrogen, oxygen, argon, and the necessary amount of water vapor for the given humidity level.

The difference in starting density relates to the chosen starting tank purge gas and is not due in any manner to the actual purge. From the figure, it is evident that the overall behavior of all the cases is remarkably similar. Most of the differences simply relate to different starting density, so binary diffusion option is preferred to allow for shorter simulation times.

3. Numerical modeling of tank purge processes

For a numerical model of a tank purge, the physical processes taking place can be broken into three sections:

1. Introduction of the purge gas through an inlet.
2. Formation of a purge layer and interaction with tank wall obstructions (such as baffles or stiffener rings).
3. Exit of the contaminant and purging gas mixture through the tank’s outlet.

Each section was independently analyzed using a parametric set of computational fluid dynamics (CFD) simulations to explore different tank geometries and sizes, purge flow rates, purge gas conditions (temperature and pressure) and initial composition of contaminant gases within the tank. For the inlets in this section, an axial inlet was used to make the models more generic than those associated with a specific radial inlet diffuser. Fig. 4 shows the modeling approach for each section of the purge.

Table 1 presents a summary of the simulations performed. For each case, the helium purge gas inlet velocity is uniform across the inlet diameter, and the helium temperature and total pressure are 300 K and 1 atm, respectively. The tank initially is completely full of dry nitrogen (no water) and with binary diffusion enabled.

The individual obstruction and outflow simulation sets can merge to form a single simulation set because an exit located at the bottom of the tank is analogous to an obstruction. Table 1 also presents a summary of the obstruction and exit simulation cases performed. The cases performed were using laminar flow models with the tanks oriented vertically.

3.1. Inlet behavior of purge gas

The behavior of the incoming purge gas may introduce large levels of mixing with gases contained in the tank. These re-circulating flows rapidly mix the purge gases with the tank gases, which make the tank more difficult to

<table>
<thead>
<tr>
<th>Case</th>
<th>H (m)</th>
<th>d_o or d_e (m)</th>
<th>D (m)</th>
<th>d_o/D or d_e/D</th>
<th>U_i (m/s)</th>
<th>Re_i</th>
<th>Fr_i</th>
</tr>
</thead>
<tbody>
<tr>
<td>17</td>
<td>0.152</td>
<td>0.076</td>
<td>0.152</td>
<td>0.9</td>
<td>0.0152–0.152</td>
<td>17–170</td>
<td>0.141–0.141</td>
</tr>
<tr>
<td>18</td>
<td>0.152</td>
<td>0.038</td>
<td>0.152</td>
<td>0.7</td>
<td>0.0152–0.152</td>
<td>13–133</td>
<td>0.014–0.141</td>
</tr>
<tr>
<td>19</td>
<td>0.152</td>
<td>0.102</td>
<td>0.152</td>
<td>0.5</td>
<td>0.0152–0.152</td>
<td>9–95</td>
<td>0.014–0.141</td>
</tr>
<tr>
<td>20</td>
<td>0.305</td>
<td>0.076</td>
<td>0.152</td>
<td>0.9</td>
<td>0.0152–0.152</td>
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<td>0.0152–0.152</td>
<td>9–95</td>
<td>0.014–0.141</td>
</tr>
</tbody>
</table>

Table 1
Overview of numerical simulations sets.
purge, and consequently higher purge gas flow rates do not necessarily lead to faster times for a purge. For the current analysis, it is more accurate to have the inlet gas avoid creating any macroscopic vortex development. This criterion ensures that the purge and tank gases remain in distinct layers defining a boundary between the purge and tank gases that will be referred to simply as the layer. It is this layer that acts as a piston face to displace the existing tank gases with purge gas. For the inlet velocities shown in Table 1, the Reynolds number based on inlet diameter ranged from 21 to 947, with the intent of introducing a laminar jet of purge gas into the tank. Using data obtained from the simulations shown in Table 1, modified Reynolds and Froude numbers identified were necessary to characterize the inlet purge gas behavior.

For jets issuing into a quiescent ambient of the same fluid, the Reynolds number is useful to determine when turbulent mixing is important. For the purge scenarios examined in this work, the purge gas is different from the tank gases and a modified Reynolds number was developed. A Reynolds number which uses the density of the inlet gas, the viscosity of the tank gas, and the inlet diameter as the characteristic length is valuable in predicting turbulence for cases where the diameter ratio \((d_i/D)\) is greater than 0.6. In this case, the modified Reynolds number needs to be less than 350 to prevent strong turbulent mixing. For smaller diameter ratios, this number was not that relevant. However, the Reynolds number does not account for buoyant interactions between different purge and tank gases, and therefore another non-dimensional number is required.

A modified Froude number, which is the ratio of inertia of the inlet jet to gravitational force, was useful to characterize the results of the inlet simulations. The appropriate velocity is the average velocity across the inlet plane, which scales based on the diameter ratio \((d_i/D)\) is given in Eq. (2).

\[
Fr_i = \frac{U_i (d_i/D)}{\sqrt{g(\pi/4)D_i^2}}
\]  

(2)

This number proved to be effective for determining if a given purge scenario produces an unacceptable level of vortex development. The value of \(Fr_i\) has to be less than 1 in order to avoid turbulent behavior and is usually restricted to about 0.75. The smaller the value becomes, the more well behaved the jet will be.

The buoyancy of the incoming jet relative to the tank gas governs the details associated with the formation of the layer. To highlight various aspects of layer formation, Fig. 5, shows mole fraction contour of nitrogen (in red) with a helium jet (in blue) with a \(Fr_i\) near the imposed 0.75 limit issuing into a tank filled with nitrogen, which corresponds to case 10 in Table 1. The initial penetration of the laminar jet to some depth into the nitrogen is based on the momentum of the incoming gas as well as the buoyancy force opposing the inlet gas motion (Fig. 5a).

The maximum penetration depth achieved is when these forces balance. The inlet gas fills a hemispherical region with a radius equal to the penetration depth, which for the conditions examined in this study is on the order of the inlet diameter, \(d_i\).

The jet core near the inlet plane begins to spread along the inlet plane wall (Fig. 5b) for the cases when a lighter gas issues into tank with a heavier gas. As the core spreads the volume of the trapped gas increases, thereby increasing the buoyancy forces and the inlet gas moves back toward the inlet increasing the speed at which the core continues to spread. Core spreading continues until the inlet gas impacts the outer wall of the tank (Fig. 5c).

The buoyant gas then behaves in an oscillatory manner similar to a mass-damper system. Samples of velocity centerline profiles in the tank at various times highlight this behavioral characteristic. Fig. 6 shows profiles of axial velocity normalized by inlet velocity \((U/U_i)\) versus penetration distance into the tank normalized by tank diameter. Each line represents a different time in the simulation and the collection of lines highlights the behavior of the lighter helium gas with the nitrogen gas. In Fig. 6a, the centerline velocity penetrates smoothly into the tank with time. In contrast, Fig. 6b exhibits an oscillatory behavior that is characteristic of most buoyant jets as shown in Fig. 5b and c. This is because the volume flow rate of the helium was large enough to penetrate rapidly into the nitrogen in the vertical direction without first displacing most of the nitrogen in the radial direction. The feedback of the nitrogen pushing back on the helium jet produces an oscillatory motion, which creates the oscillatory velocity profiles. Despite the highly erratic motion the system eventually damps enough (as the helium fills radially) to begin to form a smooth layer as shown in Fig. 5d and e. Simulations performed with radial diffusers also exhibited these general physical features in large tanks.

![Fig. 5. Nitrogen mole fraction contours \((d_i/D=0.25)\), Case 10.](image-url)
A criterion to determine the layer formation location is determined from the simulation data set. A layer forms when the average absolute value of the slope of the 50% nitrogen mole fraction surface is less than 10, but this criterion can be adjusted to give more or less conservative estimates of layer formulation location. Large slope values indicate extreme wave action in the layer (Fig. 6b), while lower values indicate a relatively flat layer (Fig. 6a). The thickness and formation time are functions of the layer formation location.

3.2. Steady layer behavior of purge/tank gas

A study of the purge flow behavior revealed with appropriate flow rate a piston-face shape layer ultimately forms, which then pushes the tank gas through the outlet. Molecular diffusion taking place during layer motion is symmetric and perpendicular across the layer. The layer velocity during this steady region is a function of the inlet flow rate and tank diameter. The layer velocity mentioned here refers only to the velocity of the layer center since the velocities of the outer regions depend on their local diffusion rates as well as the center velocity.

3.3. Outlet behavior of tank gas

Most of the turbulent behavior caused by an outlet occurs downstream of the outlet plane. However, the vortices generated around the circumference of the tank exit can trap a portion of the remaining tank gas. A modified Froude number for the outlet, given in Eq. (3), is to characterize the importance of the vortex entrapment of tank gases.

\[
Fr_e = \frac{U_L (D/d_e)}{\sqrt{g (\pi/4) d_e}} \tag{3}
\]

\[
U_L = \frac{U}{D} \left( \frac{d_e}{D} \right)^2 \tag{4}
\]

This parameter correlates with the size of the shear layer formed at the exit plane of the tank. It is this shear layer, which provides the mechanism for transporting any trapped tank gas above the exit plane out of the tank.

3.4. Quantification of layer thickness and diffusion

Section 4. will detail the development of an algebraic model of the tank purge process using the results of the computational fluid dynamics (CFD) cases developed in Section 3. Before the development of algebraic model, two metrics need to be accessed, which are vital to describe a purge process and they are quantification of layer thickness and diffusion. The mole fraction of the inlet gas determines the layer thickness, with the 50% mole fraction being the center of the layer. Layer thickness ranges include 75–25% inlet gas fraction, 85–15% inlet gas fraction, and 90–10% inlet gas fraction with the layer being symmetric about its center. The layer thickness quantified by \( P_l \) is the difference between the two fractions representing the edges of the layer. Using the combinations listed above, \( P_l \) would be equal to 0.5, 0.7, and 0.8, and can range from any number between 0 and 1, with 0 indicating no layer and 1 implying an infinitely thick layer.

The layer thickness as defined must then be incorporated into an expression of generic diffusion growth. Fick’s law predicts that the growth rate of the diffusion layer is proportional to the square root of the product of time and the binary diffusion coefficient. A general expression for the layer thickness, \( TH(t) \), as a function of \( P_l \) and Fick’s law is given in Eq. (5)

\[
TH(t) = f(P_l) \sqrt{D_{AB} t} \tag{5}
\]

Using values of \( TH(t) \) from the numerical model, the functional form involving \( P_l \) with values with constant \( D_{AB} \) and over the same time interval would force all of the curves with differing \( P_l \) onto a single curve. The necessary multiplication factors were then curve fit with respect to \( P_l \) in order to obtain the parameter necessary to complete the thickness growth equation. The result is Eq. (6) and the usage of this equation is throughout the algebraic
model developed in Section IV.

\[
TH^*(t) = \left( \frac{3.422}{D} \right) \left( \frac{P_i}{(1-P_i)^{0.17437}} \right) \sqrt{D \Delta t} \tag{6}
\]

This equation specifies layer thickness growth due to diffusion as a function of time in units of outer diameters (D) and thickness fraction parameter.

4. Development of reduced order algebraic tank purge model

This section uses the results of the computational fluid dynamics (CFD) studies completed in Section III to develop a simplified algebraic model capable of replicating the tank purging process. Algebraic models developed are for the inlet, layer, and exit flows and then combined into a single model.

4.1. Inlet model development

This section details three quantities that are all associated with the inlet flow: layer formation location, time, and thickness. In order to compute the layer formation location, two parameters need to be determined. The first parameter referred to as the inlet representative velocity, \(U_i\), quantifies the oscillatory behavior of the purge gas for a range of inlet conditions (shown in Fig. 6). This parameter takes into account the various turbulence effects associated with different \(d_i/D\) ratios and is a scaled version of the average inlet velocity. A higher \(U_i\) indicates that the layer forms further into the tank. Eq. (7) is a curve fit of \(U_i\) computed as a function of \(U_i\) and \(d_i/D\). The details of the curve fit process are in [3].

\[
U_i = \frac{U_i}{(\frac{d_i}{D})^{2}} \left[ (\frac{d_i}{D})^{0.675} + (\frac{d_i}{D})^{7.75} + 0.18 (\frac{d_i}{D})^{3.5} \left( \frac{1}{1-(d_i/D)} \right)^{0.405} \right]^{-1} \tag{7}
\]

The second parameter needed for the estimation of the layer formation location is the penetration depth of the inlet gas \(Z_p^*\). This parameter determines if a layer forms at the end of the oscillatory period or if the jet penetrates deep enough into the tank gas that the oscillations dampen prior to reaching that location. The equation for \(Z_p^*\) was derived from a balance of inlet pressure against the buoyancy force generated due to the volume of the enclosed buoyant gas. The result of this balance is Eq. (8).

\[
Z_p^* = \left( \frac{1}{D} \right) \left[ \frac{\rho_i D_i^2}{2g(\rho_e - \rho_i)} \right] \tag{8}
\]

From the computational fluid dynamics (CFD) simulations, when the oscillatory behavior of the inlet purge gas dampens out, the layer formation location is determined in comparison to computed \(U_i\) from, Eq. (7) and a curve fit of the relationship gave the layer formation location independent of penetration depth. If the depth of the penetration affects the layer, it adds to the curve fit result with a scale factor. This scale factor allows for the concurrent behavior of oscillations and penetration with the oscillatory effect relating to the size of the penetration depth column using \(d_i/D\). As a result, Eq. (9) is a piecewise equation that varies depending on the relationship between \(Z_p^*\) and the exponential curve fit of layer formation location.

\[
L_f^* = \begin{cases} 
Z_p^* + 0.05e^{0.428U_i} \sqrt{1 - \frac{d_i}{D}} & Z_p^* > 0.05e^{0.428U_i} \\
0.05e^{0.428U_i} & Z_p^* < 0.05e^{0.428U_i} 
\end{cases} \tag{9}
\]

The second quantity in this analysis is layer formation time based on the normalized fill rate per unit depth described in Eq. (4) and the layer formation location, \(L_f^*\) and given by Eq. (10).

\[
t_f = \frac{L_f^* D}{U_i(d_i/D)^2} \tag{10}
\]

This expression assumes symmetric mixing which means that while some of the tank gas displaces upstream, a similar amount of inlet gas has moved further downstream and thus the amount of gas required is roughly equal to the amount needed to fill the entire volume above the layer formation location.

The third quantity is layer formation thickness, which depends on macroscopic mixing phenomenon between the inlet purge gas and tank gas as well as the molecular diffusion between these two gases. The effect of macroscopic mixing assessed was by examining the computational fluid dynamics (CFD) cases with no diffusion. Relevant variables were examined and a following parameter was identified, \(L_f^*(U_i^2 D t_i (d_i/D)^{0.8} (D)^{-0.8})\), which was plotted versus the computational fluid dynamics (CFD) layer formation thicknesses for four different \(P_i\) values.
The results were curve fit and given in Eq. (11).

\[
TH_{L,ND}^* = L_0^* \left[ \frac{U_T^* D t_i(d_i/D)}{D} \right]^{0.8} \left[ \frac{3.422}{5.75} \left( \frac{P_i}{(1-P_i)^{0.17433}} \right) \right]^{0.8} 
\]

(11)

This curve fit is a scaled version of the generic thickness curve described in Eq. (6). Fig. 7 shows a side-by-side comparison of layer thicknesses with and without the effects of molecular diffusion. The impact of molecular diffusion may be significant, for example, at 3 s the layer with diffusion is approximately twice as thick as the no diffusion model.

Qualitatively the general shapes of the layer are the same without and with diffusion and hence the layer formation locations are essentially identical.

To include the effects of molecular diffusion on layer formation thickness, a layer formation time constant was ascertained from a curve fit of the time constant and the representative curve and ascertainment with the no-diffusion model.

The results were curve fit and given in Eq. (11).

\[
\tau_L = t_L \left( 1 + \frac{d_i}{D} \right)^4
\]

(12)

Eq. (12) is from the layer formation time from Eq. (10) and using the time constant and the representative curve in Eq. (6) the additional thickness of the layer generated by diffusion can be accounted for using Eq. (13).

\[
TH_{L,D}^* = \left( \frac{3.422}{5.75} \right) \left( \frac{P_i}{(1-P_i)^{0.17433}} \right) \sqrt{D_{AB} \tau_L}
\]

(13)

Diffusion is an additive process and thus the macroscopic mixing thickness computed in Eq. (13) would add to the molecular diffusion thickness computed in Eq. (11) to produce the layer formation thickness, shown in Eq. (14).

\[
TH^*_m = \frac{3}{4} TH_{L,ND}^* + \frac{1}{2} TH_{L,D}^*
\]

(14)

Eq. (14) without the constant scale factors on the two input thicknesses ignores the concurrent growth due to mixing and diffusion, which can hamper diffusion effects depending on the particular geometry during the wave action. Layer thickness due to molecular diffusion depends on current thickness of layer and as such, a thicker layer grows slower. This effect is incorporated into Eq. (14) using scale factors computed using a curve fit from computational fluid dynamics (CFD) simulation data. Fig. 8 shows the plot of Eq. (14) for four different values of \( P_i \) and its accuracy.

The precision in final layer formation thickness depends on accurately identifying the initial thickness. When attempting to minimize purge times, this is a conservative computation because it over-predicts the size of the mixing region in most cases.

4.2. Steady layer model development

This section details the progress of the layer as it moves through the tank. In most of the purging scenarios, the inner circumference of propellant tanks are lined with obstructions (shown in Fig. 4) such as baffles and stiffener rings. This section also assesses the impact of these obstructions on the steady layer development. Two quantities fully describe the steady layer as it moves through the tank and then an additional two quantities characterize obstruction effects on the steady layer development. The first sets of quantities are steady layer velocity at the centerline of the tank (axial direction) and a diffusion time constant for the beginning of layer motion. The additional quantities needed to quantify the effects of having obstruction in a tank is the diameter ratio of the obstruction diameter to the outer diameter and the location below the inlet plane of the obstruction \( H_o^* \), which is in units of outer diameters (D's).

Steady velocity at the center of the tank is from a constant pressure and temperature requirement that the volume flow of the inlet gas be equal to the volume displacement of the tank gas. It is this requirement that leads directly to Eq. (4) which defines the velocity of the center of the layer.

The diffusion time constant for the beginning of layer motion gives the amount of time required for a sharp interface between the inlet purge gas and tank gas to become the thickness solved for at the end of layer formation. This allows the thickness to continue to grow due to diffusion from its current state. Rearranging Eq. (6) gives the diffusion time constant (for time, \( \tau_{m} \), and the thickness value in the new equation would be the layer formation thickness from the preceding sub-section.

Steady layer motion is a combination of the quantities defined above along with the fundamental equations of motion. Eq. (15) is the equation for layer location as a function of time, while, Eq. (16) is the thickness equation as a function of time and solved consecutively or as a system. Layer location \( L_m^* \) in Eq. (15) is measured in units of outer diameters (D's) from the inlet plane.

\[
L_m^*(t + \tau_L) = L_0^* + \overline{U}^*_L t
\]

(15)

\[
TH_m^*(t + \tau_L) = \left( \frac{3.422}{D} \right) \left( \frac{P_i}{(1-P_i)^{0.17433}} \right) \sqrt{D_{AB}(\tau_m + t)}
\]

(16)

In order to compute the effect of a given obstruction, the model assumes that the obstructions are sufficiently
The difference between obstruction position if no obstruction had been present.stant (time constant at the obstruction, a measured post-obstruction time constant) and the expected time constant (\( \tau_p \)) at the post-obstruction position if no obstruction had been present. The difference between \( \tau_p \) and \( \tau \) is \( \tau_+ \). For different values of \( \tau_o \) the ratio of the additional time constant to the time constant at the obstruction is found to be roughly a constant. The relationship shown in Eq. (17) is with \( G \) being a constant for each obstruction diameter and velocity combination.

\[
\frac{\tau_+}{\tau_o} \approx G(d_o, \omega L)
\]  

(17)

The above relation showed some deviation for larger velocities or larger obstructions, which cause heavy mixing prior to the obstruction plane. A modified Froude number, Eq. (18), similar to the one used in inlet model development was useful to characterize the amount of mixing that a given obstruction would cause to a layer.

\[
Fr_o = \frac{\omega L (D/d_o)^{3/2}}{\sqrt{g(\pi/4)d_o}}
\]

(18)

In order to prevent significant mixing, \( Fr_o \) needs to be less than 0.5 for accurate prediction by this algebraic model. This value is from computational fluid dynamics (CFD) simulations, which showed macroscopic turbulence at the higher \( Fr_o \) values, which would impact the layer before the obstruction plane. Plots of the time constant ratio values in Eq. (17) versus different obstruction parameters and a curve fit of those plots identified the relationship given in Eq. (19).

\[
P_o = \frac{\sqrt{d_o/D}}{U_L^n}
\]

(19)

Plotting this parameter against the values of Eq. (17) gives a curve of the data. Fig. 9 shows the plotted data points as well as the curve fit.

The curve fit has a relatively small error if the value of \( P_o \) is greater than 15. This requirement is quantitatively similar to \( Fr_o \) being less than 0.5. Both parameter restrictions prevent heavy mixing and trapped purge gas accumulation as well as reduce the error inherent in this computation. Using the curve fit from Fig. 9, an equation for \( \tau_+ \) based on known constants previously measured or calculated as well as the curve fit constants forms Eq. (20).

\[
\tau_+ = (\tau_o) \left[ \frac{\sqrt{d_o/D}}{29.458(U_L)]} \right]^{-1/0.89}
\]

(20)

The additional thickness resulting from the obstruction can remain in this form or altered to an actual thickness value using Eq. (6), which, then adds to the layer when the layer center is at the location of the obstruction. This introduces a discontinuity at each obstruction and by adding the additional thickness in a functional manner around the obstruction rectifies the discontinuity. The work, however, to define the necessary function was not undertaken in this analysis.

4.3. Outlet model development

The difference between obstruction and outlet geometries is the location of data collection, as highlighted in Fig. 4. The outlet data collection is at the obstruction plane because of the behavior downstream of the outlet is of no consequence to the purge procedure. \( Fr_e \), which is identical to \( Fr_o \), has the same maxing restriction, which is \( Fr \) needs to be less than 0.5 for the model to be accurate. This is due to the fact that the long-term entrainment of tank gas in the vortex regions surrounding the exit is not modeled.

Each purge case required two modeling approaches. In the first model, the exit diameter of the tank \( (d_e) \) is equal to \( D \). In the second model, the exit diameter \( (d_e) \) is treated as an obstruction \( (d_o) \) in which the resulting additional thickness is added prior to the exit plane. The two different model approaches for each purge case were plotted along with the computational fluid dynamics (CFD) results at the exit plane. Examination of the plot lead to an insight of the total additional obstruction thickness that would add to the layer before it reaches the exit plane. A sample of these results provided in the left side of Fig. 10a, which has an outlet diameter ratio of 0.5 but a value of 0.576 for \( Fr_e \). This case is extreme example as it is on the edge of the acceptable \( Fr_e \) range and shows the largest difference in curve shape.

As a note, the motion of center layer accelerates at the outlet plane. However, to maintain simplicity of the algebraic model, this center layer motion is not considered. This is a reasonable assumption because if there is no motion then the model will be a conservative estimate.

---

**Fig. 9.** Obstruction effect with curve fit.
of the actual values. To reconcile this center layer change with the obstruction results, it is prudent to assume that the center of the layer accelerates through the obstruction and then slows during the mixing downstream. This would provide for the zero net change in center layer location seen in the obstruction data sets.

A quantity was needed to explain the difference in curves between the simulation results and model results in Fig. 10a, while making sure it would be an overall conservative estimate. A reasonable quantity developed is from the adjusted average of the two simulation approaches discussed in the earlier paragraph. This average is from the value of Fr_e and a representative equation, shown in Eq. (21) with K being a representative parameter.

\[
K = \frac{K_{No_e} + Fr_e(K_e)}{1 + Fr_e}
\]  

(21)

Using Eq. (21), any variable as a function of time is from the results of both the model run without an outlet and the model run with the full obstruction treatment. The solution from this blend is in Fig. 10b alongside the original model data from which the blended solution is computed.

5. Full purge model validation

This section compares the model developed in Section 4 against experimental data acquired from the purging of two ET hydrogen tanks at the NASA Kennedy Space Center [4]. This section also compares the model and experimental data with a detailed transient three-dimensional computational fluid dynamics (CFD) simulation.

A standard helium ET purge occurs after an initial nitrogen gas purge, however, prior to the helium purge the outlet of the tank is open to the ambient and air can intrude into the ET while inspections occur. Helium purge gas enters the tank through the inlet diffuser and the tank gases exit through the outlet port. This purge lasts approximately 1 h and uses about 1,100 kg of helium.

The data collected during this purge are used to assess the performance and accuracy of the models. Measurements of exiting gas concentration are acquired using a Portable Refrigerant Leak Indication System (PReLiS), which is a single quadrupole mass spectrometer system. A capillary tube located just outside of the outlet port samples the gas concentration at 14 s-intervals [4]. Experimental data for purges of two different ET purges were acquired on December 15, 2007 (ET 125) and on April 8, 2008 (ET 128). At the conclusion of this helium purge the outlet port is covered with a flange which has a 1 in. diameter hole and additional purging takes place. The purge continues until a 1.5–2.5 psig pressure builds up within the tank, after which the helium inflow stops but the 1 in. outlet port remains open to ambient for about 10 min to vent. The outlet port is then closed and the tank is pressurized with helium to about 8.5 psig.

Measurements from nitrogen concentration from the ET 125 and ET 128 purges are shown in Fig. 11. The two purges were completed on different days with somewhat different set volumetric helium purge flow rates. Initial data from the measurement suggested a volumetric flow rate (2675 standard cubic feet per minute), a revised estimate was provided later suggested a volumetric flow rate of 1.35 m³/s (2859 cubic feet per minute), The purpose of the data is to show approximately how long it takes to purge the ET with helium and the general shape of the nitrogen mole fraction at tank exit port as a function of time. The top plot shows nitrogen mole fraction at the exit port of the tank during the first 1,800 s (30 min) of the purge process. At around 1,100 s a steep drop-off in nitrogen concentration is observed which is when the bulk of the nitrogen has been displaced from the tank by the incoming helium gas. The middle plot shows a zoom-in of the nitrogen mole fraction at tank exit port as a function of time. The top plot shows nitrogen mole fraction at the exit port of the tank during the first 1,800 s (30 min) of the purge process. At around 1,100 s a steep drop-off in nitrogen concentration is observed which is when the bulk of the nitrogen has been displaced from the tank by the incoming helium gas. The middle plot shows a zoom-in of the nitrogen mole fraction at tank exit port as a function of time. The top plot shows nitrogen mole fraction at the exit port of the tank during the first 1,800 s (30 min) of the purge process. At around 1,100 s a steep drop-off in nitrogen concentration is observed which is when the bulk of the nitrogen has been displaced from the tank by the incoming helium gas. The middle plot shows a zoom-in of the nitrogen mole fraction at tank exit port as a function of time. The top plot shows nitrogen mole fraction at the exit port of the tank during the first 1,800 s (30 min) of the purge process. At around 1,100 s a steep drop-off in nitrogen concentration is observed which is when the bulk of the nitrogen has been displaced from the tank by the incoming helium gas. The middle plot shows a zoom-in of the nitrogen mole fraction at tank exit port as a function of time.
particularly valuable to assess the levels of nitrogen contaminant gas still left within the tank after a majority of the nitrogen has been displaced.

Fig. 11 shows the comparison of the measured nitrogen mole fraction versus the model developed in Section 4. This model was performed with a volumetric flow rate of helium of 1.18 m$^3$/s (2500 standard cubic feet per minute), which was an approximate historical average of purge flow rates used on numerous ET purges. As can be seen from the figure the model prediction of N$_2$ mole fraction versus time agrees with the overall trends seen in the measured data. Furthermore, the model also shows the rapid depletion of nitrogen from the ET between 1,050 and 1,200 s. It is interesting to note that this agrees well with the very simple estimate made in Eq. (1) for the no-mixing case. However, the no mixing estimate cannot predict the details of the shape shown in the figure and simply predicts an abrupt exhaustion in N$_2$, rather than the exponential shape shown in Fig. 11.

Fig. 11 also shows results of detailed transient three-dimensional computational fluid dynamics (CFD) simulations using the geometry shown in Fig. 1. Fig. 1 shows the computational domain for computational fluid dynamics (CFD) simulation, with a close up of inlet diffuser and outlet port boundary in the domain. The model uses an inlet volumetric flow rate of 1.18 m$^3$/s, which is the same as the flow rate used in the model. To examine the sensitivity of the purge process to the volumetric flow rate used, a second simulation was completed using 1.416 m$^3$/s (3000 cubic feet per minute).

The results show that the model is accurate for this system to within $<5\%$ of purge time on either data curve. The algebraic model did not consider the effect of interior stiffeners and small geometric obstruction within the tank because of their relatively small effect on overall purge behavior. The inlet diffuser area would map to a circular inlet at the top of the tank. The same method would map the exit tube at the bottom the tank. The overall length would decrease so that the total volume of the cylindrical model is the same as the pill shaped hydrogen tank.

While the overall trend of the purge appears to be similar, there is still an error of about $5\%$ in different portions of the purge curve. This maximum $5\%$ error is a resulting miscalculation of up to 90 s on the 30-minute purge. The errors are particularly noticeable in the inlet and exit regions because this is where the concentrations change the slowest. Fig. 11 highlights this fact by picture in bottom showing the region of the purge where the mole fraction of tank gas changes from nitrogen to helium. The initial change in concentration and the final change in concentration from nitrogen to helium is lot slower than overall change in concentration. The model is effective even with tanks that are much different scales than the test cases.

6. Conclusions

Current work objective is to use a systematic approach to purge modeling. Purge modeling was decoupled into three sub-components. Purge inlet was analyzed first. Its general behavior was studied and conclusions were drawn concerning overall inlet trends. Simulations were then run and a sub-model was developed to describe the results. Steady layer motion and diffusion were then studied. They were then combined into a comprehensive
sub-model that matched their behavior. Next, obstruction flow and, similarly, outlet flow were examined. Another set of simulations was run and sub-models were composed that conformed to the results. Once the sub-models were completed, they were combined into the full model. Finally, the full model validity was demonstrated against independent data.

Importance of Reynolds and Froude non-dimensional parameters in successfully describing the mixing characteristics of purge flow is stressed. An algebraic model was developed and validated with experimental data that accurately characterized complete purge behavior. A modified Froude number for each flow geometry was found to be the most successful single parameter for characterizing general purge mixing behavior. The model is most accurate when dealing with purges that heavily rely on steady layer motion and have low turbulence.

Future studies will focus on using a purge gas flow rate schedule which begins the purge with a low flow rate when first introducing purge gas into the tank to minimize mixing and once the layer has been formed and begins to move away from the inlet flow rates can be increased to decrease purge time and minimize diffusion contact time between purge gases and tank gases across the layer.

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References