Is your tank inert? A study into the challenges of ensuring inert atmospheres

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Flow-through purging with an inert gas is a common method of explosion prevention where flammable materials are stored or used. Technical guidance is available to assist engineers in defining appropriate purging protocols. However, this typically assumes that the purge gas has a similar density to the air in the vessel and is rapidly mixed into the bulk. The most common purge gas, nitrogen, is 3.5% less dense than the air it is commonly used to displace. Under certain circumstances this is enough to allow stratification of the purge and bulk gases, which leads to ineffective purging of the vessel.

We have used simulation of a manufacturing vessel to show the flow conditions required to achieve adequate purging according to the guidance. Laboratory tests were conducted to demonstrate both effective and poor purging. A correlation is provided to assist engineers in defining suitable inerting protocols based only on equipment geometry and purge gas properties.

Keywords: flow-through purging; nitrogen, explosion prevention

Introduction and background

Despite decades of experience to draw from, it is an unfortunate reality that fuel/air explosions have still not been eliminated from the process and related industries. Techniques for explosion prevention are well known (removal of ignition sources, removal of oxygen by providing an inert atmosphere). This paper details investigations into the efficiency of flow-through purging which is used to provide an inert atmosphere in vessels which are unsuitable for other purging techniques such as pressure or vacuum swing and displacement inerting. This unsuitability is typically due to inadequate mechanical strength or a requirement to keep the vessel dry before filling.

Despite the ubiquity of flow-through purging in certain sectors, the literature is sparse in this area. Technical guidance documents have been published in many parts of the world including Europe (CEN, 2006) and the USA (NFPA, 2019). However, these are much broader documents covering the many types of inerting, and flow-through purging typically only merits a short section with an associated calculation for ideal scenarios.

A significant challenge in producing technical guidance is that it is impossible to cover all scenarios and plant designs. The guidance commonly makes allowance for this by providing 'safety factors' which may be varied depending on the equipment scale, design and operating characteristics. An example is the European guidance (CEN, 2006) which provides a method of calculating the time required to reduce the oxygen concentration to a specified level by flow purging

$$t = F\,\frac{V}{Q}\,\ln\left(\frac{C_i - C_0}{C_i - C_f}\right) \qquad (1)$$

Where t = time required for purging

F = safety factor

V = system volume

Q = inert gas flow

C_f = required final oxygen concentration after purging

C_i = oxygen concentration of inert purge gas (commonly set as zero)

C_0 = initial oxygen concentration in vessel (typically 21%)

t, F and V need to be in consistent units. Care should be taken with the concentration definitions as some authors exchange the *i* and *0* subscripts.

The calculation relies on the purge gas having a 'similar' density to the air being removed. 'Similar' is not defined, though the examples suggest that nitrogen is considered to be of a similar density to air. It also assumes that the vessel is always well mixed, so the outlet concentration is the same as the average concentration inside the vessel. The safety factor F can be calculated if the oxygen concentration can be measured at multiple points inside the vessel. Otherwise, it should be chosen between 2 and 5 depending on the system geometry: 2 if the inlet and outlet are diametrically opposite and 5 if they are not. 'Diametrically opposite' is not defined and it is not clear whether this definition includes the common configuration of ports on opposite sides of the roof of a vessel or storage tank. The guidance allows for a reduced safety factor where the inert gas is injected at high velocity (>10 m s^{-1}).

- Virtually no guidance is offered for cases which lie outside the ideal conditions:
- No allowance is made for the variation of air or purge gas density with temperature.

- Gas injection velocities below 10 m s^{-1} are not discussed
- Only a single example of plug-flow purging with a dense gas is referenced.

The current study was initiated after a manufacturing team requested assistance from our group to confirm whether their planned purging protocol was adequate. Since the tank geometry was relatively simple it was possible to set up a computational model which captured all the important aspects of the system, including spatially distributed flows, temperatures and densities. The model showed that the purging protocol was adequate and a safety factor of 2 was sufficient. However, it was noted that certain changes would lead to inadequate purging: reducing the purge flow by 50%, increasing the inlet diameter by 50% or increasing the purge gas temperature by 10 °C would each cause stratification of the gas flow. In some cases, purging would not be adequate even with a safety factor of 5. Modelling of a second vessel confirmed that certain configurations could lead to unexpected and unsafe outcomes. A theoretical investigation was conducted to provide additional understanding.

Numerical analysis of plumes with negative buoyancy

Several of the simulations showed well-defined plumes which projected downwards into the tank before turning and rising back towards the outlet. The plume depth was determined for a series of simulations and found to be directly proportional to the inlet flowrate for a fixed inlet diameter. This matched well with the results of Turner (Turner, 1966) who demonstrated that plume depth was related to a momentum flux and a buoyancy flux. These results have been reformulated (Williamson ert al, 2008) in terms of Froude and Reynolds numbers:

$$Fr = \frac{U_0}{\sqrt{R_0 \sigma}} \qquad (2)$$

$$Re = \frac{U_0\, R_0}{\upsilon_0} \qquad (3)$$

U_0 is the mean flow velocity through an inlet of radius R_0. The Froude number is based on a 'reduced gravity' term, σ:

$$\sigma = g\,\frac{\rho_i - \rho_0}{\rho_0} \qquad (4)$$

where ρ_i and ρ_0 are the densities of the purge gas and the air being purged and g is the acceleration due to gravity (9.81 m s^{-1}). Note that the plume depth will change during purging as the composition and density of the bulk gas change.

For turbulent jets (Re > 2400) and Fr > 3, the plume depth was found to depend only on the Froude number and inlet radius:

$$z = 2.4\, Fr\, R_0 \qquad (5)$$

This can again be reformulated in terms of physical variables:

$$z = 2.4\, U_0 \sqrt{\frac{R_0}{\sigma}} \qquad (6)$$

Simulation of purging flows

Model configuration

Purging flow simulation was performed using the COMSOL Multiphysics® simulation environment. Of particular importance is the ability to model how the gas density varies with both the temperature and average molecular mass. The following modules were selected to fully describe the problem:

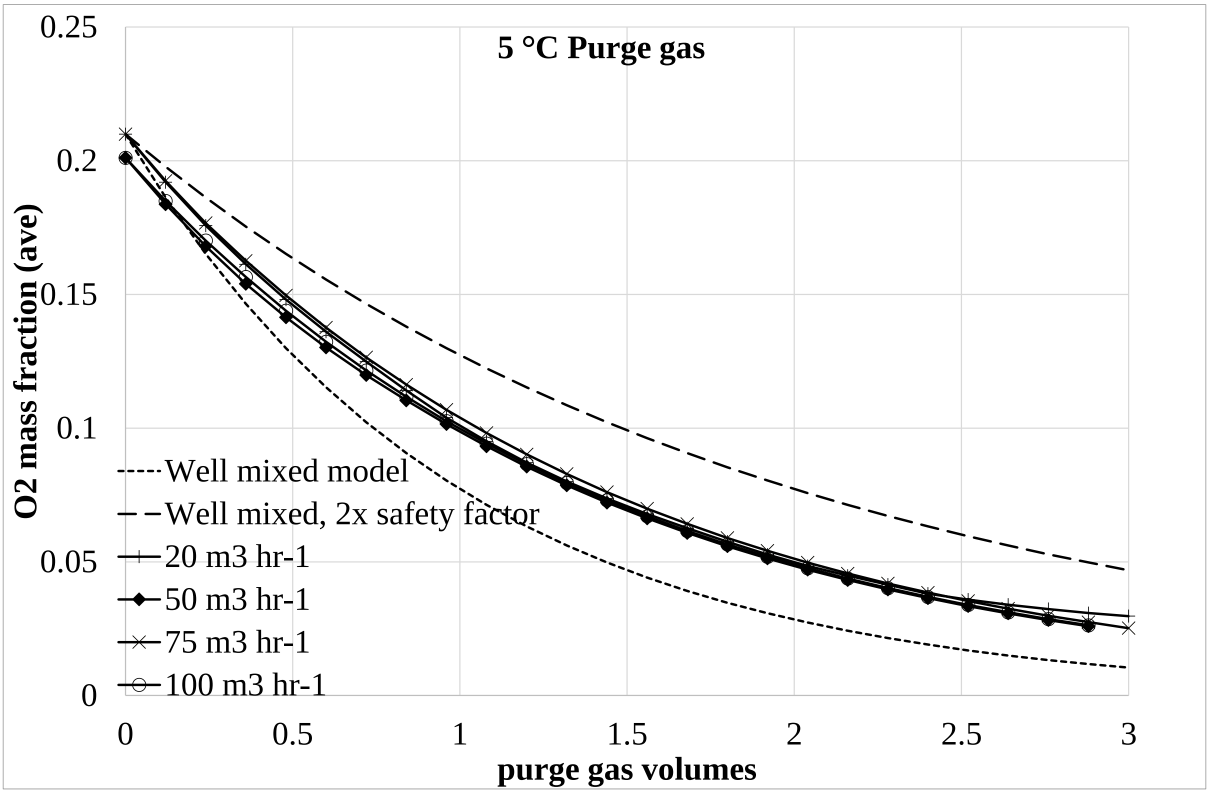
- Turbulent flow using the low Reynolds number k-ε formulation with wall distance initialisation. This was considered to be the most appropriate turbulence model
- Transport of concentrated species - captures the spatial variability of the gas composition and the average molecular mass
- Heat transfer in fluids - captures the spatial variability of temperature within the system and its effect on density
- Reacting flow Multiphysics coupling – ensures that the density change due to changes in average molecular mass are fed back to the turbulent flow module
- Non-isothermal flow Multiphysics coupling – ensures that the density change due to changes in local temperature are fed back to the turbulent flow module

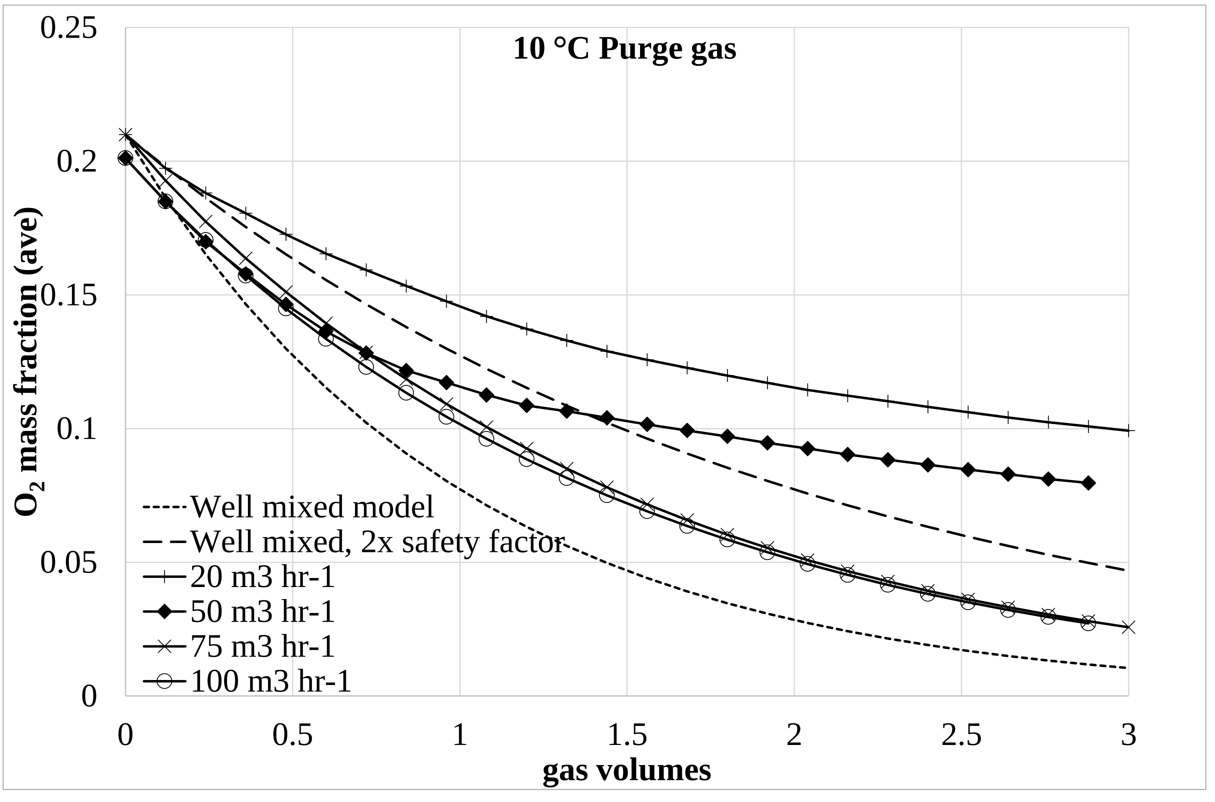
All simulations in the current study were performed at atmospheric pressure, though the model is also constructed to allow for pressure variance.

The vessel being simulated is 5.2 m tall and 2.4 m in diameter with standard torispherical heads at both ends. The total volume is approximately 21 m^3. The inlet is a 3" nozzle near the periphery of the top head and the vent is a 6" nozzle in the centre of the top head. The vessel is filled with dry air at 15 °C at the start of the simulation and the purge gas is pure nitrogen. The purge flow rate and temperature were varied as part of the investigation. The simulation time was set to be equivalent to 3 tank volumes of purge gas. According to equation (1), a fully mixed system with a safety factor of 1 would reach 1% oxygen after 3 gas volumes.

Simulation results

Figure 1 shows the evolution of average oxygen concentration as determined from the various simulations. In each plot, the purge flow is varied between 20 and 100 $m^3\ hr^{-1}$. The 3 plots show purge gas temperatures of 5, 10 and 15 °C respectively. The well-mixed model from equation (1) is also plotted, both with and without a safety factor of 2.





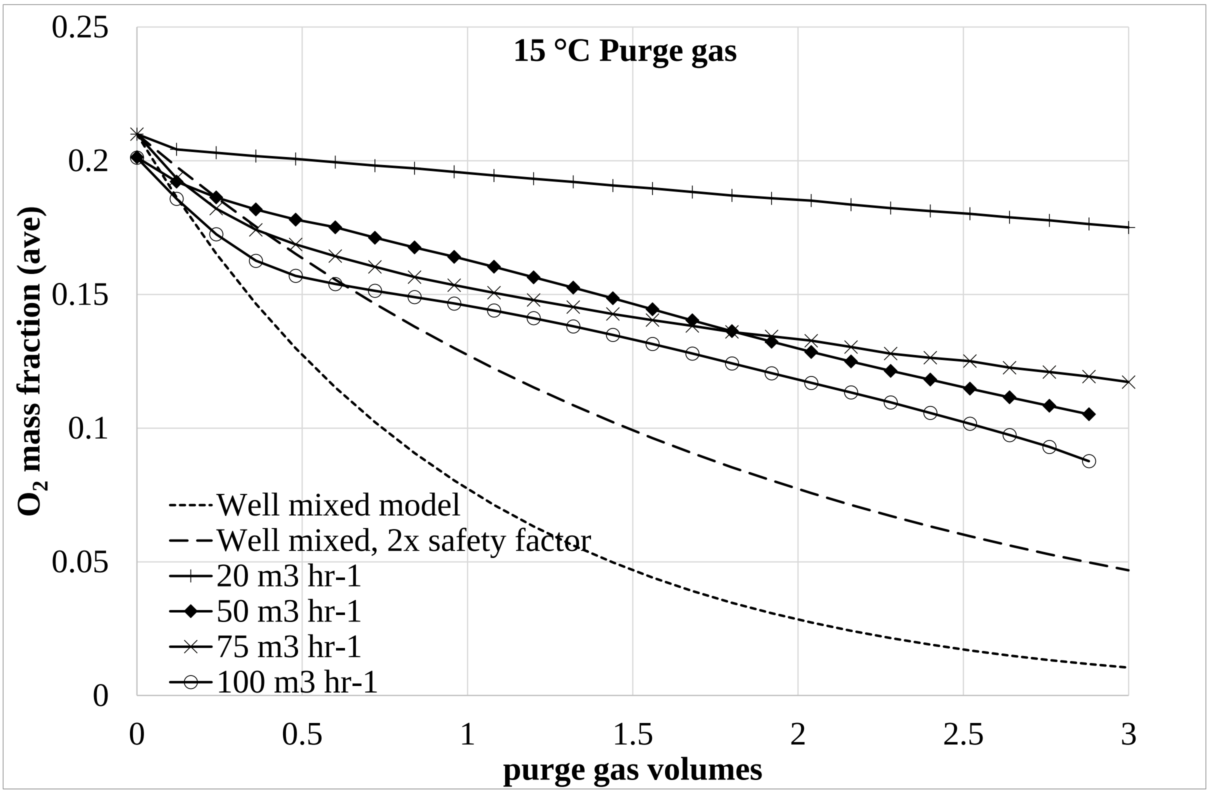


Figure 1. Evolution of the simulated average oxygen mass fraction as a function of the cumulative volume of purge gas. The 4 marked lines on each plot denote different volumetric flow rates. Each plot shows a different purge gas inlet temperature. The initial vessel contents temperature was 15 °C.

At 5 °C, the volumetric flow rate has no discernible effect on the evolution of the oxygen level. The overlaid curves lie between those for the well mixed model (equation (1)) and the well mixed model with a safety F factor of 2. We can estimate an F factor of approximately 1.4 for the simulations. F is not equal to unity because the system is not ideally mixed. A circulating flow is developed in the vessel, with a slightly higher oxygen concentration in the centre of the vessel than at the periphery. The vent flow is therefore at a lower concentration than the average in the vessel, leading to a value of F which is more than 1.

At 10 °C, the curves for 75 and 100 $m^3 hr^{-1}$ follow a similar trajectory to the 5 °C curves. However, the 20 and 50 $m^3 hr^{-1}$ curves deviate from ideality. As suggested by the analysis above, this is due to reduced momentum in the inlet jet which leads to poor mixing of the jet with the bulk gas.

At 15 °C where the purge gas is at the same temperature as the air in the vessel, the deviation from ideality becomes even more pronounced. At 20 $m^3 hr^{-1}$, it is unlikely that the vessel would be adequately purged even if an F factor of 5 was used, although this extended time period was not explored in the simulations.

Graphical results

A useful benefit to numerical simulations is the ability to visualise flows that cannot be observed physically. Figure 2-4 below shows a selection of the simulated processes. The results are shown after 1.5 volumes of purge gas to allow time for concentration disparities to become visible. The shading indicates the oxygen concentration and the arrows show the flow direction and magnitude.

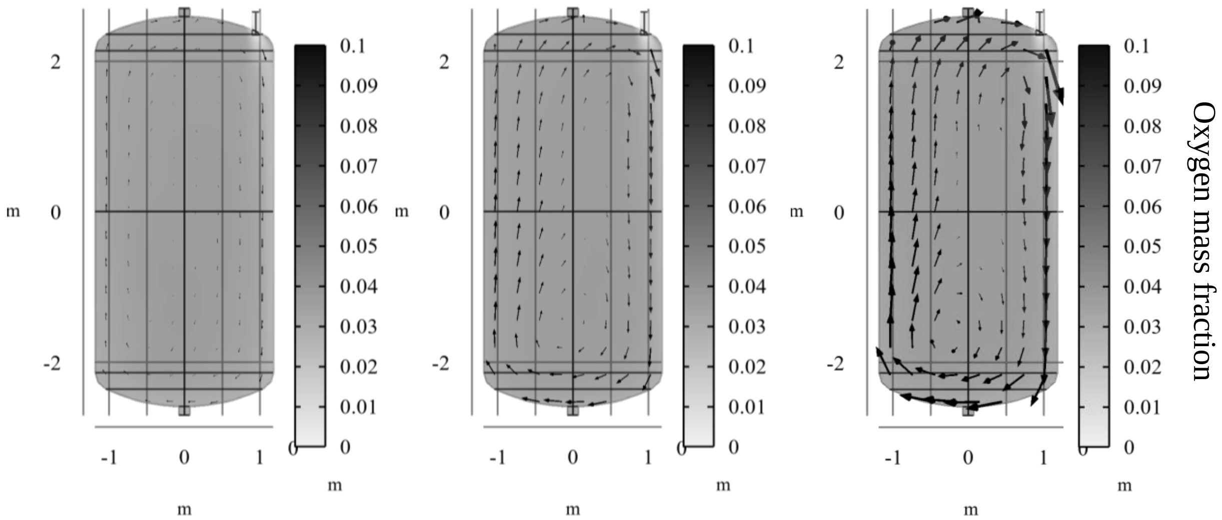


Figure 2. Simulated oxygen mass fraction (grey scale bar) after 1.5 volumes of purge gas introduced at 5 °C. Volumetric flow rates are 20 $m^3 hr^{-1}$ (left), 50 $m^3 hr^{-1}$ (centre), 100 $m^3 hr^{-1}$ (right).

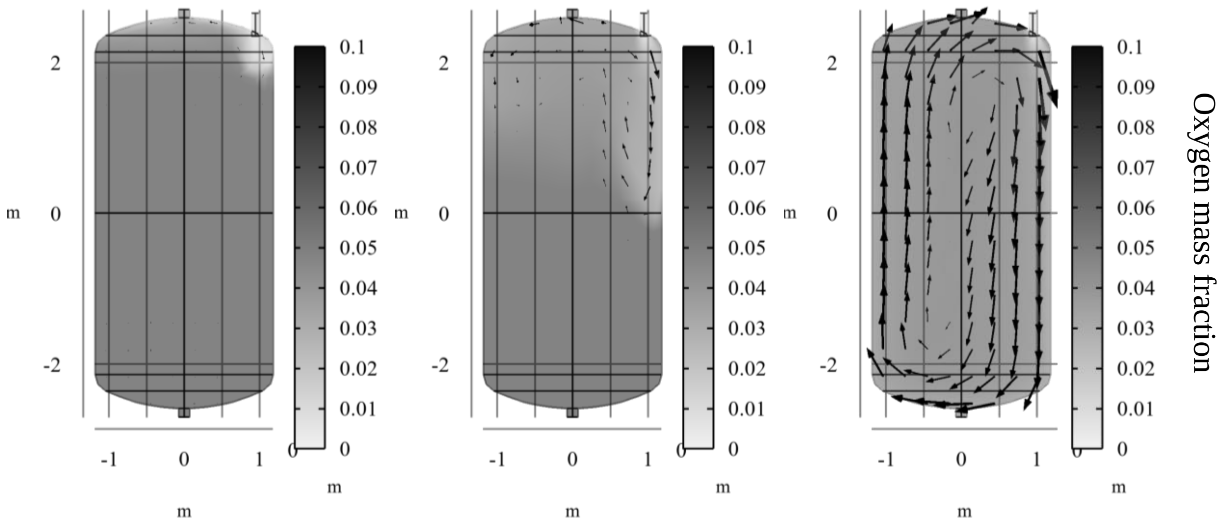


Figure 3. Simulated oxygen mass fraction (grey scale bar) after 1.5 volumes of purge gas introduced at 10 °C. Volumetric flow rates are 20 $m^3 hr^{-1}$ (left), 50 $m^3 hr^{-1}$ (centre), 100 $m^3 hr^{-1}$ (right).

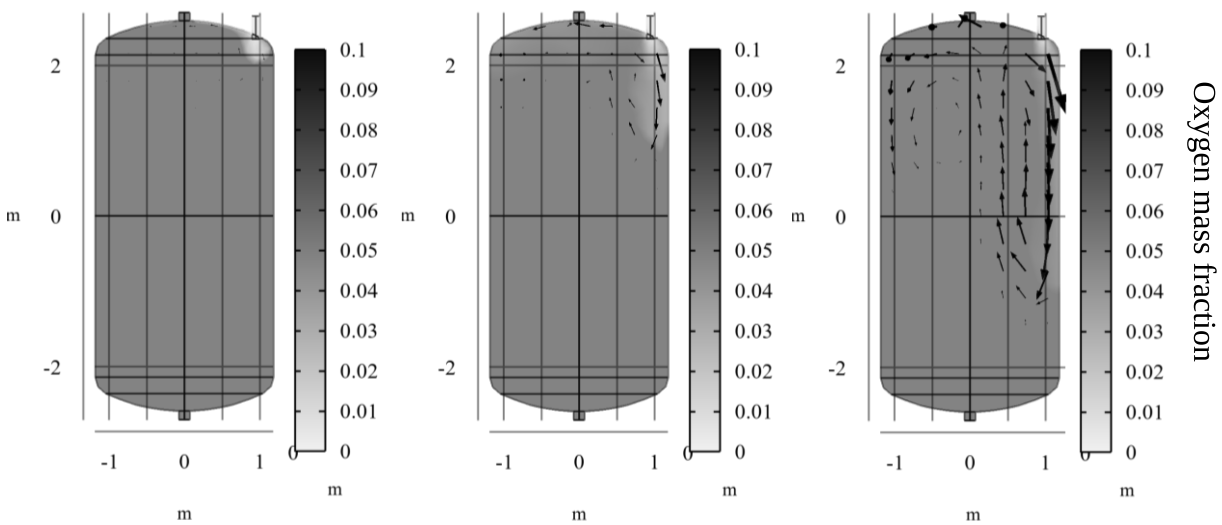


Figure 4. Simulated oxygen mass fraction (grey scale bar) after 1.5 volumes of purge gas introduced at 15 °C. Volumetric flow rates are 20 $m^3 hr^{-1}$ (left), 50 $m^3 hr^{-1}$ (centre), 100 $m^3 hr^{-1}$ (right)

From Figure 2, it can be seen that introducing the purge gas at 5 °C (i.e. 10 °C colder than the air in the vessel) leads to good mixing and a distint circulatory flow within the vessel. This is because the nitrogen is slightly denser than the air in the vessel. There is thus no buoyancy force acting to turn the flow upwards towards the vent.

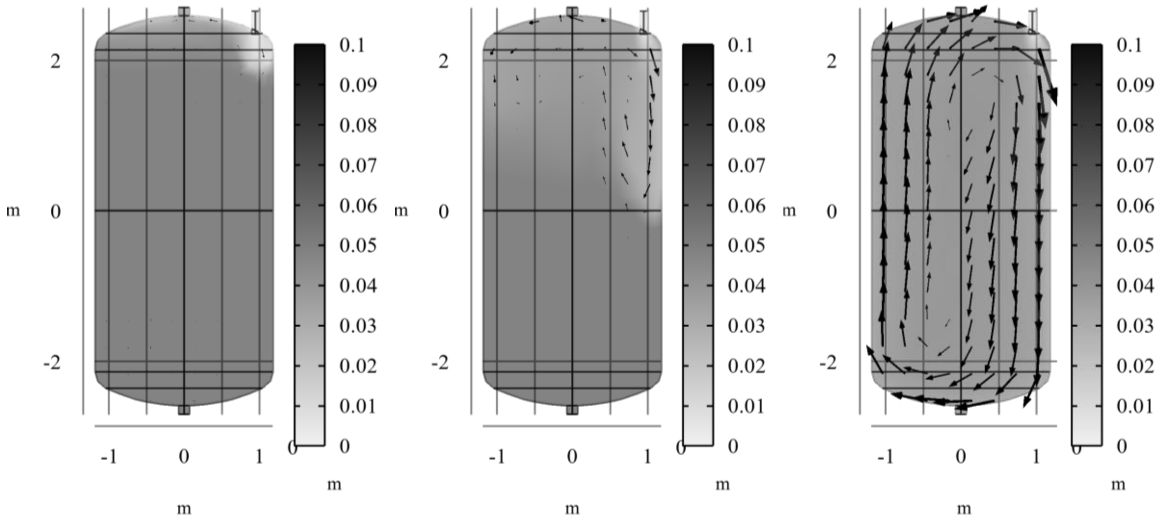
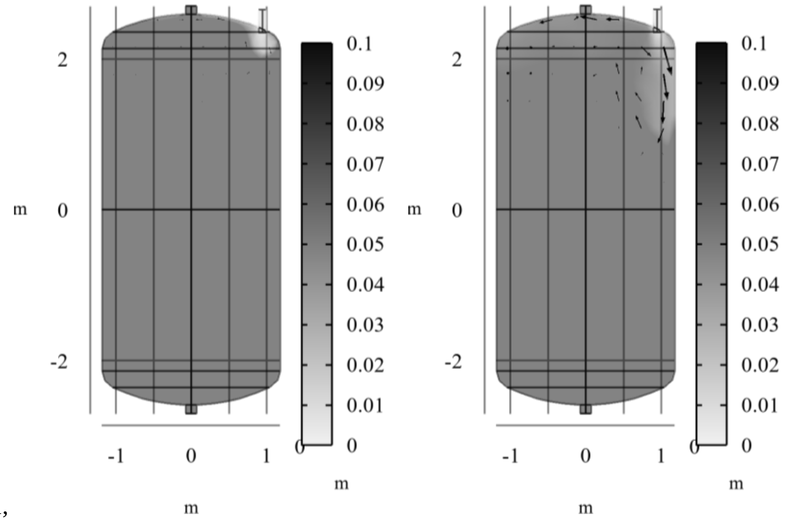
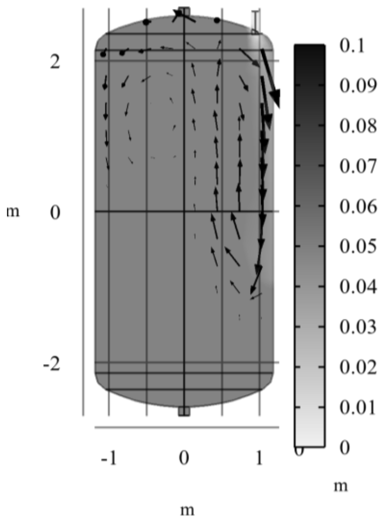


Figure 3 shows good mixing at 100 m^3 hr^{-1} flow, but slower inlet velocities lead to the formation of visible plumes which only penetrate part way into the vessel. This agrees with Figure 1 which showed that the vessel was well-mixed only at flow rates of 75 and 100 m^3 hr^{-1}. As anticipated from equation (6), the plume depths appear to be proportional to the inlet flow rate.



As anticipated by Figure 1,



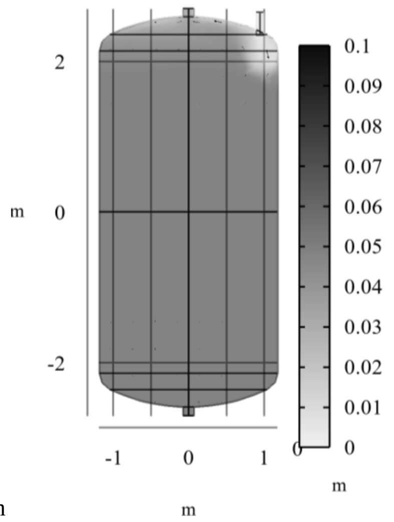


Figure 4 shows plumes being generated at all flow rates. As with

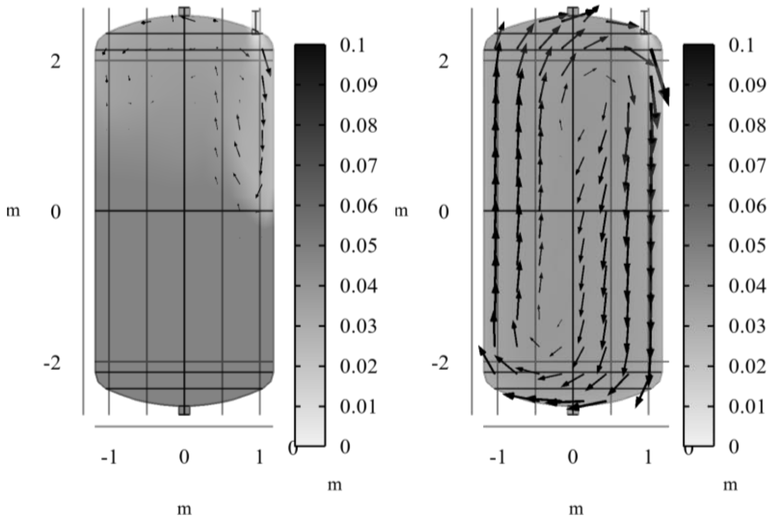


Figure 3, the plume depths are roughly proportional to the inlet flow rates.

We can use equation (6) to calculate the expected plume depth for each of the above conditions and compare with the vessel height. Note that for the 5 °C inlet, since the purge gas is more dense than the bulk, σ becomes negative. Equation (6) therefore cannot be applied as the imaginary root has no physical meaning. The physical result is that the plume depth effectively becomes infinite as the dense purge gas sinks below the bulk air. As can be seen from Table 1, the only combinations for which the calculated plume depth is greater than the vessel height (5.2 m) are those with 5 °C inlet and the 10 °C processes with inlet flows of 75 and 100 $m^3\ hr^{-1}$. This matches with the data from Figure 1. The calculated plume depth at 15 °C inlet and 100 $m^3\ hr^{-1}$ flow is only slightly smaller than the vessel height. However, even in this case the mean oxygen concentration after 3 tank volumes is still approximately 8%.

Purge temperature °C	**Purge flow $m^3\ hor^{-1}$**	**σ $m^2\ s^{-1}$**	**calculated depth m**	**simulated depth m**
5	20	-0.002	∞	∞
5	50	-0.002	∞	∞
5	75	-0.002	∞	∞
5	100	-0.002	∞	∞
10	20	0.171	1.41	0.7
10	50	0.171	3.53	2.7
10	75	0.171	5.30	>5.2
10	100	0.171	7.07	>5.2
15	20	0.338	1.00	0.5
15	50	0.338	2.51	1.95
15	75	0.338	3.77	2.9

15	100	0.338	5.02	3.7

Table 1. Calculated and simulated plume depths for each of the simulated cases.

It can be seen from Table 1 that the calculated and simulated plume depths are correlated. This is shown in Figure 5 below. A least squares linear regression fit through the origin shows that the correlation is better when the plumes are larger. This is potentially due to difficulties in identifying the exact extent of the plume from the visualisation plots exemplified in Figures 2-4 above. The slope of the best fit line is approximately 0.75. This deviation from unity was not anticipated and is currently unexplained.

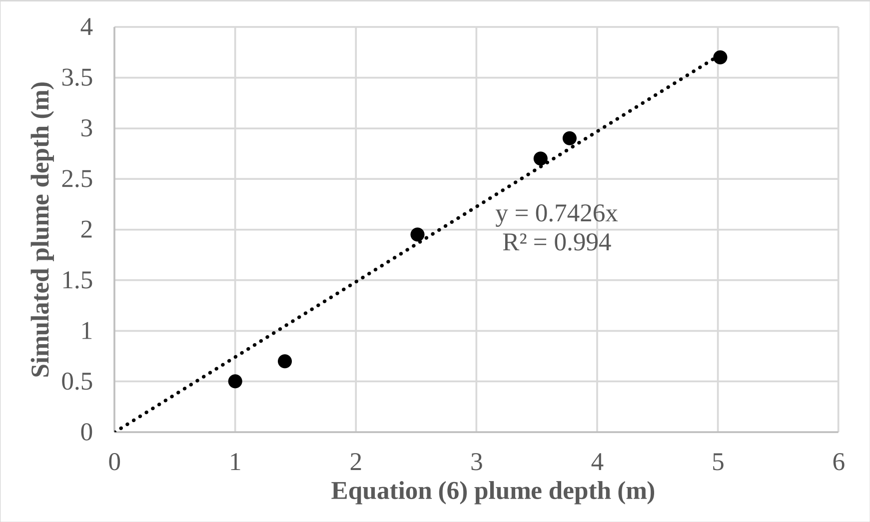


Figure 5. Correlation plot for simulated and calculated plume depths.

Model validation

It has not yet proved possible to validate the inerting model on plant scale equipment. However, small-scale tests have been performed which show consistency with the model despite the challenges of modelling gas jets at smaller scales.

Experimental setup

A glass vessel which was an almost exact 10:1 scale-down of the manufacturing vessel was selected for this work. The internal diameter was 0.240 m for the main part of the vessel and 0.225 m for the section above the external jacket. The overall internal height was 0.515 m to the inside of the lid, resulting in a total volume of approximately 21.3 L. A nitrogen supply was connected through a port on the lid via a Bronkhorst EL-flow Sselect flow controller. Two delivery tubes were available, with 3.5 and 6.0 mm nominal bore. The inlet port and tubing were inclined towards the centre of the vessel at approximately 3° to the vertical and this was reflected in the model.

An outlet port on the vessel lid was connected to a LuminOx oxygen sensor (SST Sensing Ltd, Coatbridge, UK) before being vented to atmosphere via a fume cupboard. Monitoring of the oxygen levels inside the vessel was not possible using this equipment, so the model was configured to output the mean oxygen concentration at the outlet. This was compared with the data supplied by the oxygen sensor.

Experimental results

The first experiment used the 3.5 mm i.d. inlet tube. A purge gas flow rate of 1.0 L/min was used. The purge gas temperature remained stable at 19.0 ± 0.5 °C during the experiment. The vessel temperature started at 21.6°C and gradually fell to 20.2 °C during the experiment. Figure 6 below shows the gas composition at the vent sensor as a function of time. The experimental data correlates well with the well-mixed model plot, decreasing slightly faster than expected. This is probably due to the vessel having a slightly lower volume than calculated from the measured dimensions. Adjusting the volume to 20.0 L in equation (1) gives an even better fit to the experimental data.

Surprisingly, the plume depth calculated using equation (6) is only 0.30 m, which is less than 60% of the vessel height. In this case we would expect the vessel to be only partially inerted. This is in agreement with the simulation which showed that the vessel only reached 5% oxygen concentration after 3 volumes of purge gas. The experiment reached this concentration after 1.5 volumes. A likely explanation for the difference is that the small diameter (3.5 mm) and moderate velocity (1.7 m s^{-1}) of the inlet jet leads to more mixing with the bulk than would be expected for larger diameters and/or slower flows.

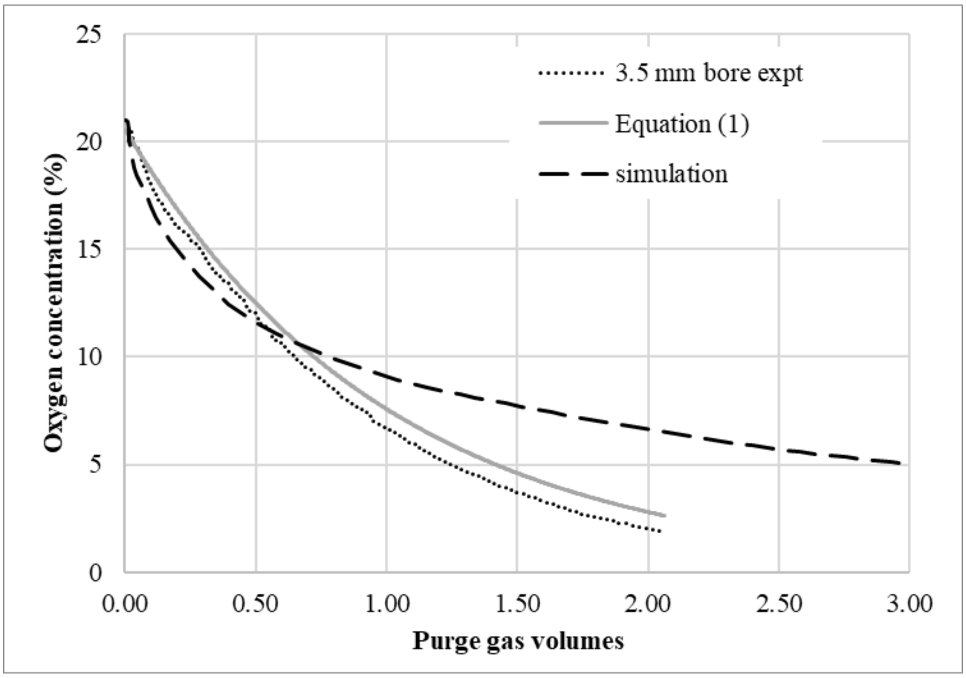


Figure 6. Evolution of vent gas composition for 3.5 mm i.d. inlet tubing. The well-mixed model of Equation (1) is also plotted for comparison.

A second experiment was performed using a 6 mm internal diameter inlet tube. The vessel and nitrogen temperatures were within 1 °C of each other. In this case, the calculated plume depth is only 0.13 m and poor mixing is anticipated. The results are shown in Figure 7 below.

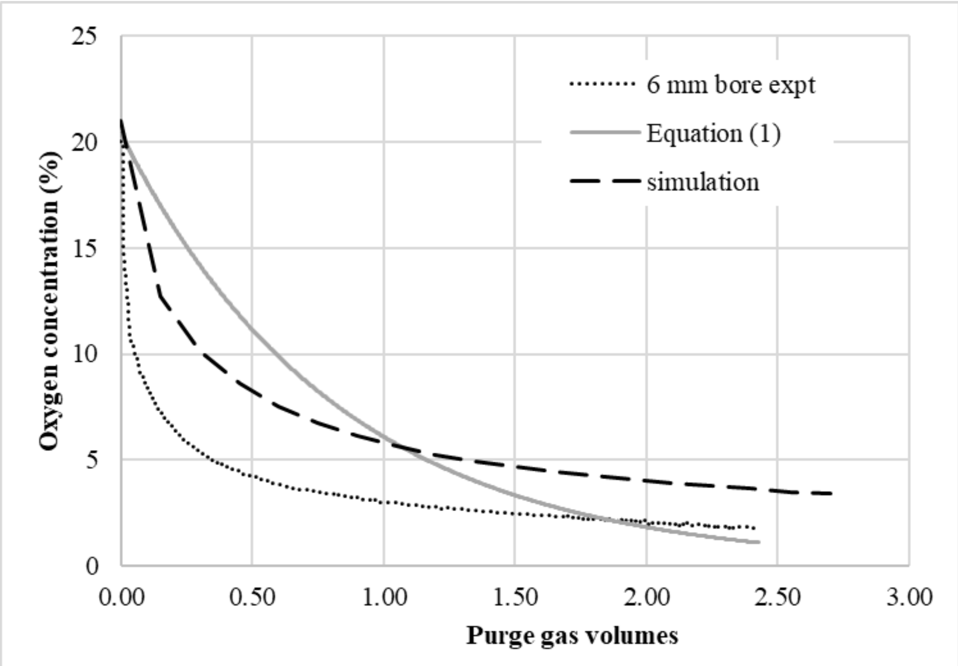


Figure 7. Evolution of vent gas composition for 6 mm i.d. inlet tubing. The well-mixed model of Equation (1) and the model simulation are also plotted for comparison.

In contrast to the previous case, the experimental data do not fit with the well-mixed model from Equation (1). Instead, there is an initial rapid drop in the oxygen concentration at the vent, followed by a long tail of slightly raised oxygen concentration. The rapid drop is indicative of bypassing, where nitrogen from the inlet passes to the vent while undergoing little mixing with the bulk. This can be seen in the example image shown in Figure 8. After 0.6 volumes of purge gas, the lower third of the vessel remains above 20% oxygen while the oxygen concentration is between 0% and 7% across the top third of the vessel.

The plume can be seen in Figure 8. It extends approximately 0.12 m below the inlet, which in this case is at the top of the 20 mm cylindrical port. This is in excellent agreement with the 0.13 m which was calculated above.

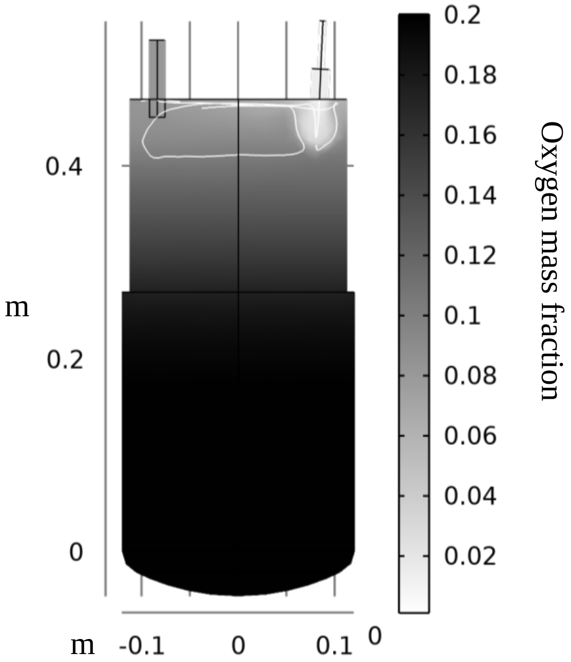


Figure 8. Oxygen concentration within the simulated vessel after 0.6 volumes of purge gas have been introduced. The inlet is the narrow tube at the top right. The vent is at the top left. The scale shows oxygen concentration and an example streamline is shown.

It should be noted that the model only gives an approximate match to the vent concentration profile. However, it does give a much better match than the well-mixed model. The visualisation in Figure 8 shows that the model is capturing the main effect of the bypassing which is believed to be responsible for the rapid drop in outlet concentration. This gives us a good deal of confidence in the model even though we have not yet been able to validate it at plant sale.

Future work

It has not yet proved possible to validate the simulation method against measured data at the large scale. Work is ongoing in this area and we look forward to being able to being able to provide an update to this paper. The model has also been extended to allow the simulation of pressure- and vacuum-swing purging, which is outside the scope of this paper. We hope this will form the basis of a separate publication.

Summary

International guidance on flow-through inerting of vessels provides an inerting time calculation based on the assumption that the vessel is well mixed. One requirement for this assumption to be true is that the gas in the vessel and the purge gas are of similar density. Specifically, the guidance assumes that the densities of air and nitrogen are sufficiently similar.

Fluid dynamics modelling has demonstrated that the well-mixed model is unsuitable to ensure that vessels are always adequately purged. This is mainly due to the difference in density between air and nitrogen. In particular, cases were observed where the inlet plume of purge gas did not reach the bottom of the tank. This resulted in stratification of the gas in the tank, with only the upper portion achieving the required oxygen level. The lower section retained a significant amount of oxygen, often 2-3x what would have been predicted using the well-mixed model.

Comparison of the simulations and theoretical calculation of nitrogen plume depth gave a convincing correlation. The simulation model has yet to be validated by measurements of oxygen levels in commercial scale equipment. However, the small-scale experimental results gave a qualitative match to the vent concentration profile and the visualisations showed the expected bypassing between inlet and vent.

The authors recommend that process engineers responsible for defining equipment inerting procedures should satisfy themselves that the process they intend to use will result in good mixing between the purge gas and the air to be removed from the vessel. In order to do this, they need to be able to calculate the plume depth, which requires understanding of the inlet geometry as well as the flow rate and temperature of the purge gas. If this information is not available, the progress of inerting processes should be monitored using (as a minimum) an oxygen sensor on the vent line, and ideally a flow meter. A rapid reduction in the oxygen concentration in the vent is indicative of bypassing which could potentially lead to unsafe conditions inside the vessel. In extreme cases, increasing the safety factor may still not be sufficient to ensure adequate purging.

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