Development of a novel model for emptying of a self-pressurising nitrous oxide tank

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Abstract. Self-pressurised, or vapour pressurised system is a system that maintains operational pressure in ambient conditions, with no need for additional pressurisation. An example of such system is a tank filled with nitrous oxide, which keeps pressure of 50.35bar at 20°C. Self-pressurised tanks are used in hybrid rocket engines, due to low weight and simple construction. At the same time, accurate prediction of the dynamics of these systems during emptying creates a significant challenge, due to occurrence of near equilibrium two phase flow and rapid changes in pressure and temperature. The authors have developed several numerical models with aim of capturing described phenomena. The development started with basic assumption of lumped parameters approach and using mass and energy balance equations. First model featured two elements, one for the investigated fluid and second for the tank walls, with assumption of fluid in equilibrium, having single pressure and enthalpy. Such approach, while capturing major trends, lacked accuracy. To order to improve it, fluid was divided into two separate elements, one with saturated vapour and the second with the two-phase mixture. This proved to be more useful for predicting mass flow, but still did not offer accurate results. Further development included treating both fluid elements as two phase mixtures, first being mostly vapour and the second being mostly liquid and required additional equation describing tank’s internal dynamics. Resultant model allows for significantly higher pressure prediction accuracy than previously and gives better prediction of parameters of fluid flowing out of the investigated tank.

1. Introduction
Nitrous oxide (N₂O) is a widely used substance across many fields. It finds usage in food industry as food additive [1], medicine as anaesthetic [2] and others. Due to widespread usage, it is easily available and relatively inexpensive. In rocketry, nitrous oxide is used as an oxidizer, mainly for hybrid rocket motors such as SpaceShipOne [3], or NASA Peregrine sounding rocket [4]. Ease of handling and non-toxicity are significant advantages over numerous toxic and difficult for usage rocket propellants, such as liquid oxygen requiring cryogenic temperatures, or highly toxic and corrosive dinitrogen tetroxide (N₂O₄). Nonetheless, key feature of dinitrogen monoxide is the high saturation pressure in ambient temperature, with saturated vapour pressure of 50.5bar at 20°C, rising with temperature up to 72.5bar at 36.4°C, which is it’s critical temperature [5].

Having high saturation pressure enables usage of a self-pressurising propellant tank configuration. Classic pressurised vessels require additional tank containing high pressure neutral medium, such as helium or nitrogen, which is gradually released into the pressurised vessel in order to maintain required pressure. Such configuration allows for fast emptying of pressurised tank due to low amount
of vapour in the evacuated fluid, which results in high outflow mass stream. It also allows for more steady conditions in reference to the case without additional high pressure source. At the same time, additional equipment required for pressurisation, including tank, valves and piping add mass and complexity, which have negative impact on overall efficiency of a rocket engine.

Selection of nitrous oxide as an oxidiser allows for using a self-pressurising configuration oxidiser feed system, therefore removing need for pressurisation equipment, reducing total mass and volume of the engine. While such solution is less complicated, different set of issues arises. Without additional high pressure medium, oxidiser tends to return to equilibrium between liquid and vapour through evaporation at interface, condensation and boiling. This process, while providing necessary pressure to force the outflow, causes the propellant to have significantly higher void fraction than in the pressurised case [6]. Moreover, increased amount of vapour impacts average fluid density and therefore limits outflow mass stream. Increased complexity of the phenomena occurring inside self-pressurising tank due to non-steady state and non-equilibrium conditions during emptying create need for detailed approach to modeling.

2. Theory and modeling

2.1. Experimental observations

Behaviour of nitrous oxide in a small scale self-pressurised tank was investigated in [7]. The authors used polycarbonate tubing as a transparent propellant tank, resulting in the test stand enabling pressure and temperature measurements, as well as optical access. High speed video recording allowed for detailed view of the tank emptying process, including observing changes in oxidiser state. The experiment included filling the tank with liquid propellant up to a given level of around 90% and allowing pressure to stabilise to pressure rate change lower than 0.1psi/s (689Pa/s).

In all recorded cases similar pattern emerges. Initially, all fluid is transparent and there is neither vapour bubbles visible in liquid nor condensation of liquid in the top, vapour part. As the outflow at the bottom of the tank starts, bubbles start to appear at the lower end of the tank and rise up to the boundary between bottom and top part. Clear division into two parts is visible from the point the vapour bubbles reach top surface of the liquid and stays visible throughout the whole process. Similarly, the apparent amount of bubbles in the liquid part seems to be stable during emptying. After liquid level gets lower, mist of condensed vapour becomes visible in the top part and stays visible until the end of the process.

2.2. Literature approach

In literature, there are various theoretical approaches to modeling self-pressurising tank. Most share some basic assumptions. Common technic chosen is to describe the system using lumped parameters method, with number of nodes or elements chosen accordingly to assumptions about state of the fluid. Furthermore, fundamental equations used are similar, being mass and energy balance equations for the selected fluid nodes.

One of the used method is to assume that tank is filled with mixture staying in a homogeneous equilibrium, therefore using a two lumped parameter nodes for the propellant, one for saturated vapour and the second for saturated liquid, resulting in two differential equations of state of the fluid and two equations for the heat transfer between each of fluid element and appropriate tank wall segment. The equations are solved to obtain total propellant mass and energy as well as tank wall temperatures. Such model was developed and used by [8] and is described herein as the Equilibrium Model.

Other solution involves dividing the medium into non-saturated parts, such as [9], referred herein to as the ZK model. The two nodes describe vapour and liquid respectively and allow for temperature difference, therefore introducing heat transfer between phases. The same time, authors assumed the same pressure for both elements, resulting in a model featuring 4 differential equations, 2 for mass of vapour and liquid and 2 for their respective energies.

Referenced models share similar approach to heat transfer. Convective heat flux from ambient air to tank walls and from walls to fluid is calculated for both Equilibrium and ZK models. Conductive
heat transfer between tank wall element in contact with vapour and the wall element in contact with liquid is also taken into account. For the ZK model, heat flux between two fluid elements is also considered.

2.3. Novel model development

The authors herein chose lumped parameters method for development of novel models. Furthermore, all models share similar equation of state, namely writing density of the nitrous oxide as a function of pressure $p$ and enthalpy $h$, $\rho = \rho(p,h)$. To calculate density and its derivatives in wide range of parameters it is specified as a function of saturated liquid density $\rho_{\text{liq}}^{\text{sat}}(p)$, volumetric liquid fraction $\alpha_{\text{liq}}(p,h)$, saturated vapour density $\rho_{\text{vap}}^{\text{sat}}(p)$ and volumetric vapour fraction $\alpha_{\text{vap}}(p,h)$ per formula

$$\rho(p,h) = \alpha_{\text{liq}}\rho_{\text{liq}}^{\text{sat}} + \alpha_{\text{vap}}\rho_{\text{vap}}^{\text{sat}}$$

(1)

Functions $\rho_{\text{liq}}^{\text{sat}}(p)$ and $\rho_{\text{vap}}^{\text{sat}}(p)$ were approximated using thermodynamic properties calculated by NIST Refprop library [5].

2.3.1. Single Node Equilibrium model. Initial approach included substantial simplification of the investigated phenomena, namely assumption that the whole volume of fluid is homogeneous therefore it might be represented by a single, non-saturated node. Similarly, whole propellant tank walls were assumed to be in the same temperature. Simplified, graphic representation of this model is shown by Figure 1. To unambiguously describe this system two unknowns are needed for the fluid and one, temperature, for the tank walls. For the fluid, pressure and enthalpy were chosen. The system of equations solved, equations (2-4), consists of fluid mass (equation 2) and energy (equation 3) balances and additional energy balance for the walls (equation 4). This model is referred to as Single Node Equilibrium (SNE)

\[
\begin{align*}
V \frac{dp}{dt} &= -m_{\text{out}} \frac{d}{dt}h \\
V \frac{d(h)}{dt} &= -m_{\text{out}}h + Q \\
m_wC_w \frac{dT_w}{dt} &= -Q
\end{align*}
\]

(2)
(3)
(4)

where $V$ is tank volume, $m_{\text{out}}$ is outflow stream, $h$ is enthalpy, $Q$ is heat flux between fluid and tank wall, $m_w$ is tank wall mass, $C_w$ tank’s heat capacity and $T_w$ tank’s temperature.

![Figure 1. Simplified schematic of the Single Node Equilibrium model](image)

2.3.2. Phase Interface Model with saturated upper element. Based on the first results, more detailed approach was used, by designating two separate nodes for fluid and third node for tank walls. Based on this method, two separate models were created, sharing most of the structure, although with differences in assumptions and equations. Common features include usage of mass and energy balance equations for both fluid elements as well as heat transfer calculation method. Both models are referred
to as Phase Interface Models, with first version featuring saturated top element and the second non-saturated top element, or PIM-sat and PIM-unsat respectively.

First model was designed to test the assumption of saturated top element, with non-saturated bottom element. To incorporate this assumption into 5 equation approach, it was assumed that top, mostly vapour element, is in quasi-saturated state, governed by relaxation of mass void fraction. Starting from equation (5)

$$\frac{dY_{up}}{dt} = -\frac{Y_{up} - \bar{Y}_{up}}{\theta}$$

where $Y_{up}$ is a mass void fraction in the upper part. Mass void fraction in general is defined by equation (6)

$$Y = \frac{m_{up}}{m_{total}}$$

$\bar{Y}_{up}$ is an assumed level of void fraction (equal to 1 in case of saturated conditions) and $\theta$ being relaxation time constant, authors were able to arrive at more general equation of mass balance for the top element, equation (7)

$$\frac{dm_{up}}{dt} = -\bar{m}_{up} - m_{up}$$

with $m_{up}$ being upper node mass and $\bar{m}_{up}$ being mass derived from assumed level of void fraction. Using this implicit definition of top element saturation level allowed not only for testing assumptions of fluid staying in saturated state but also allowed for numerical experiments with various variants of assumed void fraction and various time scales of the process. Very small scales of $\theta$ allow to emulate essentially immediate return to saturated state from any deviations. Furthermore, using relaxation parameter proved to be useful for usage in two-phase models [10]. Remaining equations of the PIM-sat are

$$\frac{dV_{up} \rho_{up} \left(p\right) h_{up}^{sat}}{dt} = -\dot{m}_{up-bot} h_{bot}^{sat} + \dot{Q}_{up}$$
$$\frac{dV_{bot} \rho_{bot} \left(p\right) h_{bot}}{dt} = -\dot{m}_{up-bot} - \dot{m}_{out}$$
$$\frac{dV_{bot} \rho_{bot} \left(p\right) h_{bot}}{dt} = -\dot{m}_{up-bot} h_{bot}^{sat} - \dot{m}_{out} h_{bot} + \dot{Q}_{bot}$$
$$m_{w} C_w \frac{dH_{sat}}{dt} = -\dot{Q}_{up} - \dot{Q}_{bot}$$

where $V_{up}$, $\rho_{up}$ and $h_{up}$ are volume, density and enthalpy of the upper part respectively, $\dot{m}_{up-bot}$ is mass stream between the upper and bottom part, $\dot{Q}_{up}$ and $\dot{Q}_{bot}$ are heat fluxes between upper or bottom part of fluid and corresponding part of tank wall and $V_{bot}$, $\rho_{bot}$ and $h_{bot}$ are volume, density and enthalpy of the bottom element. Graphic representation of the PIM-sat model is presented by Figure 2.

![Figure 2. Simplified schematics of the Phase Interface Model with saturated top element](image-url)
2.3.3. **Phase Interface model with non-saturated upper element.** Second variation of 5 equation model is presented in simplified manner by Figure 3. This model uses straightforward mass balance equation for the top element, equation (12),

\[
\frac{dV_{up}\rho_{up}(p,h)}{dt} = \dot{m}_{up-bot}
\]

and remaining equations are

\[
\begin{align*}
\frac{dV_{up}\rho_{up}(p,h)h_{up}}{dt} &= \dot{m}_{up-bot}h_{sat} + \dot{Q}_{up} \\
\frac{dV_{bot}\rho_{bot}(p,h)}{dt} &= -\dot{m}_{up-bot} - \dot{m}_{out} \\
\frac{dV_{bot}\rho_{bot}(p,h)h}{dt} &= -\dot{m}_{up-bot}h_{sat} - \dot{m}_{out}h_{bot} + \dot{Q}_{bot} \\
\dot{m}_w C_w \frac{dT}{dt} &= -\dot{Q}_{up} - \dot{Q}_{bot}
\end{align*}
\]

![Figure 3. Simplified schematics of the Phase Interface Model with non-saturated top element](image)

Selected equations were supplemented by source term for mass transfer between the nodes, heat transfer and outflow. In terms of heat exchange, all three presented newly developed models use nucleate boiling heat stream formula for liquid or mostly liquid elements, i.e. total volume in the Single Node Equilibrium model and bottom node in the both 5 equation models. Heat flux per unit area is defined by equation (17) according to [11]

\[
\dot{Q} = \mu_i h_{lg} \left[ \frac{\varphi(\rho_l - \rho_v)}{\sigma} \right]^{\frac{1}{2}} \left( \frac{C_p l \Delta T}{C_f h_{lg} p r_l^2} \right)^3
\]

where \(\mu_i\) is dynamic viscosity of the fluid, \(h_{lg}\) is latent heat, \(g\) is gravity constant, \(\rho_l\) and \(\rho_v\) are liquid and vapour densities, \(\sigma\) is surface tension, \(C_p l\) is heat capacity of the liquid, \(\Delta T\) is temperature difference between liquid and wall, \(Pr_l\) is the liquid Prandtl number and \(C_{sf}\) and \(n\) are model parameters.

Heat flux from outside environment is calculated using natural convection, assuming tank is not insulated and ambient air has temperature of 20°C.

For outflow calculations, Dyer model was used, according to [12], which formulates the flow as a combination of two elements, one accounting for homogeneous, fully two phase flow and second describing single phase incompressible flow, as described by equation (18)

\[
\dot{m}_{out} = C_d \left[ \frac{1}{1+k} \dot{m}_{SPI} + \left( 1 - \frac{1}{1+k} \right) \dot{m}_{HEM} \right]
\]

where \(C_d\) is dimensionless discharge coefficient dependant on injector, \(k\) is a parameter dependant on upstream, downstream and vapour pressure. Two mass flow components are defined as

\[
\dot{m}_{SPI} = A_{inj} \sqrt{2\rho_{upstream} \Delta P}
\]

\[
\dot{m}_{HEM} = A_{inj} \rho_{downstream} \sqrt{2(h_{upstream} - h_{downstream})}
\]
where $A_{inj}$ is injector area, $\Delta P$ is pressure difference across injector and $\rho$ and $h$ are upstream or downstream densities and enthalpies.

### 3. Numerical results

Experimental pressure and temperature plots documented in [7] were compared with results obtained from three newly developed models. The test results are included to provide reference and not to measure accuracy. In this work, authors chose to explore relations between models and parameters rather than accurately predicting process outcome. In order to achieve higher accuracy, several model constants could be adjusted.

First, SNE model is presented. Figure 4a and 4b show pressure and temperature history plots versus experimental data. Plot 4c shows nitrous oxide mass time history and plot 4d presents global, volumetric void fraction, defined as ratio of vapour volume over total tank volume.

![Figure 4](image)

**Figure 4.** Pressure (a), temperature (b), liquid and vapour mass (c) and volumetric void fraction (d) plots from SNE model

Numerical results from the first model present typical results obtained from equilibrium model, similar in character to [8]. Changes in presented parameters are smooth and there are no oscillations. Initially, behaviour of all shown variables is nearly linear which is followed by increased rate of changes. Pressure and temperature drop steadily, as well as liquid mass within control volume. Volumetric void fraction increases significantly over duration of the process, which is associated with increased mass of vapour in the tank. According to final amount of oxidiser mass, tank was not completely drained, with both liquid and vapour present.

On the Figure 5, results from model with forced saturated state of the upper element, or PIM-sat, are shown. Trends and values similar to those from previous model can be observed. At the same time, this model gives more insight into behaviour of the bottom part of the tank due to with possibility of calculating mass of vapour present in form of bubbles, which is defined as mass void fraction of the bottom element. It can be observed that, unlike other selected parameters, mass void fraction stabilises in the later phase of the process and seems to be constant after initial rise. It is noteworthy that similar effect, namely stabilisation of bubble content, was observed in the transparent tank experiment [6].
Figure 6 summarises results from the third, PIM-unsat model, featuring two unsaturated fluid elements. Adding an assumption of a non-saturated upper element significantly changes behaviour of the solution. First, rate of emptying is significantly increased in reference to previous models, which might be observed by increased slope of pressure and temperature curves as well as bottom mass curve. All bottom mass is either drained or transferred to upper element before 4 seconds of the process, while previously, the bottom element mass has not been completely reduced during 5 seconds of the simulation. The same can be deduced from global volumetric void fraction plot, which shows that the upper element accounts for the whole volume. According to mass plots, it is clear that a significant portion of bottom mass is transferred into upper part, with intensity of that process increasing with decreasing amount of bottom mass. At the same time, mass void fraction of the upper node reaches a minimum of approx. 0.17, which corresponds to 17% of vapour phase and 83% of liquid phase by mass, in the upper node. While assessing quantitative accuracy of this numerical result is difficult, it appears to qualitatively conform to experimental results, where a nitrous oxide fog was observed within upper element of the tank.

Figure 5. Pressure (a), temperature (b), upper and bottom mass (c), global volumetric void fraction and bottom mass void fraction (d) plots from PIM-sat model
Figure 6. Pressure (a), temperature (b), upper and bottom mass (c), global volumetric void fraction, upper and bottom mass void fractions (d) plots from PIM-unsat model

Figure 7 presents comparison between two settings of the Dyer outflow model parameters, namely product of injector area $A_{inj}$ and discharge coefficient $C_d$. For the high flow setting product value is equal to $8 \times 10^{-6}$ m$^2$ and for the low flow it is $6 \times 10^{-6}$ m$^2$. It can be observed that increasing flow rate accelerates rate of emptying and shifts the whole process in time, therefore accurate selection of both outflow model and its parameters is of crucial importance.

Figure 7. Pressure (a) and void fraction (b) plots from the high flow parameter settings versus pressure (c) and void fraction (d) plots from the low flow parameter setting
4. Conclusions
Available data, both experimental and numerical, show that the investigated problem has nonlinear and complex character, which creates a challenge for accurate numerical modelling. The authors have tested three different lumped parameter models, each featuring different set of assumptions taken and equations solved. The results obtained show that Single Node Equilibrium model, using single lumped parameter node for the investigated fluid, gives similar results to the Phase Interface Model with saturated upper element, which uses two parameter nodes. At the same time, division of the studied medium into two distinct elements allows for more detailed description of the process, giving access to additional information, such as fill level or amount of vapour within liquid. Transition from more rigid model, upper element saturated state, toward more general, non-saturated upper node, or PIM-unsat model, proved to have a significant impact on the results. With all boundary conditions remaining unchanged, the rate of tank emptying was increased greatly, according to sharper decrease in pressure and earlier point where all of bottom element mass is expended. This effect might be directly attributed to allowance for non-saturation conditions within the upper node, due to mass transfer from bottom to upper element which was enabled to greater extent by allowing presence of liquid within both elements.

It is noteworthy that presented results were not aimed to achieve high accuracy with chosen experimental data. Instead, the experiment was used as a reference point which helped to anchor the models to the actual process and facilitate comparison between models. The main goal of this study was investigation of differences in behaviour between models in order to look for the models which offer best qualitative representation of the process of emptying of a self-pressurised nitrous oxide tank. To achieve high accuracy and ability to correctly predict experimental results with numerical models it will be required to carry out tuning of the model parameters, such as outflow mass stream function constants or coefficients used for calculating mass transfer between the elements.

Furthermore, outflow mass stream proved to be a crucial parameter determining time scale of the whole process, which calls for closer investigation and more detailed modeling in future works.

References
[1] ***World Health Organization 2011 Evaluation of certain food additives and contaminants, technical report series
[2] Korttila K, Östman P, Faure E, Apfelbaum J L, Prunskis J, Ekdawi M and Roizen M F 1990 Randomized comparison of recovery after propofol-nitrous oxide versus thiopentone-isoflurane-nitrous oxide anaesthesia in patients undergoing ambulatory surgery, Acta Anaesthesiologica Scandinavica 400-403
[3] Erickson K 2008 Advanced TSTO Vessel Design for Safe and Inexpensive Human Orbital Access, AIAA SPACE 2008 Conference & Exposition
[4] Zilliac G, Waxman B, Evans B, Karabeyoglu A and Cantwell B 2014 Peregrine hybrid rocket motor development, 50th AIAA/ASME/SAE/ASEE Joint Propulsion Conference 2014, pp 1-17
[5] Lemmon E, Huber M and McLinded M 2010 NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties (REFPROP), Version 9.0, National Institute of Standards and Technology
[6] Zimmerman J, Cantwell B and Zilliac G 2012 Initial experimental investigations of self-pressurizing propellant dynamics, 48th AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit
[7] Zimmerman J, Waxman B, Cantwell B and Zilliac G 2013 Comparison of Nitrous Oxide and Carbon Dioxide with Applications to Self-Pressurizing Propellant Tank Expulsion Dynamics, 60th JANNAF Propulsion Meeting, pp 1-22
[8] Zakirov V and Li L 2005 1-D. Homogeneous Liquefied Gas Self-Pressurization Model, European Conference for Aerospace Sciences (EUCASS), pp 1-7
[9] Zilliac G and Karabeyoglu M 2005 Modeling of Propellant Tank Pressurization, 41st
[10] Bilicki Z, Kardaś D and Michaelides E 1998 Relaxation Models for Wave Phenomena in Liquid-Vapor Bubble Flow in Channels, *Journal of Fluids Engineering* 369-377

[11] Bergman T, Lavine A, Incropera F and Dewitt D 2011 *Introduction to Heat Transfer*, Sixth Edition, Wiley & Sons, pp 620-628

[12] Dyer J, Doran E, Dunn Z, Lohner K, Zilliac G and Cantwell B 2007 *Modeling feed system flow physics for self-pressurizing propellants*, Collection of Technical Papers - 43rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference, pp 6835-6847