Simulating a Nitrous oxide rocket engine run-tank

Introduction

This paper describes mathematical models of the emptying of a tank of saturated nitrous oxide that empties purely due to its self-pressure. This is sometimes called a 'Vapak' process (powered by vapour pressure alone).

Firstly, read our 'The physics of nitrous oxide' paper as it covers the processes we'll be modelling herein.

The mathematical model of the liquid phase emptying is based on a model of saturated propane emptying from a tank devised by Dr Bruce Dunn (Ref. 1). Aspirespace gratefully acknowledges the help we received from Dr Dunn in the preparation of our nitrous tank model.

The mathematical model of the vapour phase emptying is our own work.

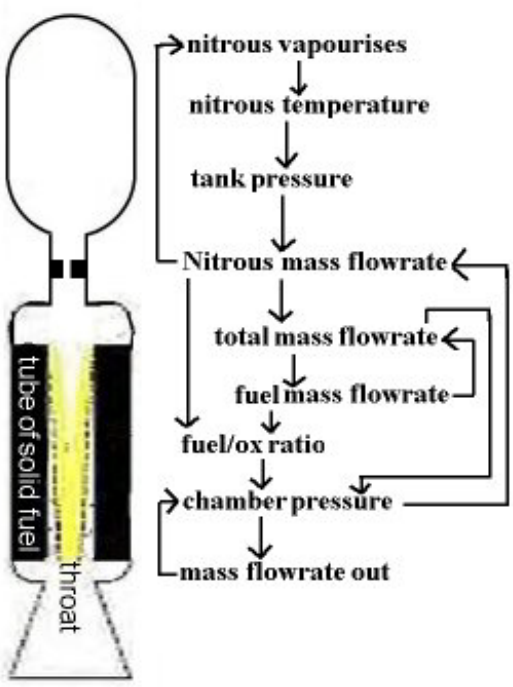
The nitrous rocket engine as a coupled system

The emptying process is iterative with time, and it's strongly coupled to the combustion chamber pressure.

Therefore, the simulation of the run-tank emptying has to be coupled to a simulation of the combustion chamber and nozzle throat of the rocket engine that it's feeding.

The ensuing feedback loops of a nitrous rocket engine emptying its liquid phase are as follows:

- Liquid nitrous flows out of the tank causing a drop in the level of the liquid nitrous. This causes an increase in the 'head space' (the volume at the top of the run-tank) of nitrous vapour above the liquid level.
- The nitrous vapour pressure drops due to this expansion.
- Some of the liquid nitrous then vaporises to try to raise the vapour pressure back up.
- The energy required to vaporise the liquid comes from the liquid itself, and so its temperature drops.
- This lower temperature lowers the tank pressure because vapour pressure is a function of temperature.



- The flow rate of nitrous out of the tank depends on the difference between the tank and combustion chamber pressure.
- The combustion chamber pressure depends on the fuel-to-oxidiser ratio, the gain of mass within the chamber (fuel flow rate + ox flow rate – flow rate out the nozzle), and the nozzle throat area.

1: A mathematical model of the liquid phase emptying

When the nitrous vapour expands due to the level of the liquid dropping, the pressure drops due to this expansion.

We don't need to know what this pressure drop is to model the tank emptying, instead we estimate how much mass $\Delta \boldsymbol{m_{vaporised}}$ of nitrous liquid has been vaporised (in one time iteration) in its attempt to raise the pressure back up again to as it was.

This is an iterative process; we pick an arbitrary non-zero value for $\Delta \boldsymbol{m_{vaporised}}$ to start with, and run with it: the program quickly converges on the correctly balanced value, staying with it as it changes during the tank emptying process.

The first step is to calculate the heat removed ΔQ from the liquid nitrous during its vaporisation:

$$\Delta \boldsymbol{Q} = \Delta \boldsymbol{m_{vaporised}}\, \boldsymbol{H_v} \quad \text{(equ. 1.1)}$$

where H_v is the enthalpy (latent heat) of vaporisation evaluated at the current nitrous temperature.

We then calculate the temperature drop of the remaining mass of liquid nitrous in the run-tank m_{liquid} due to losing this heat:

$$\Delta \boldsymbol{T} = \frac{\Delta \boldsymbol{Q}}{\boldsymbol{m_{liquid}}\, \boldsymbol{C_{liquid}}} \quad \text{(equ. 1.2)}$$

where C_{liquid} is the Specific heat capacity of liquid nitrous at the current temperature.

We then subtract this temperature drop from the current liquid nitrous temperature to get a new lower liquid nitrous temperature.

The liquid density ρ_{liquid}, the vapour density ρ_{vapour}, and the vapour pressure (tank pressure) are now recalculated from tables of Nitrous properties based on this lower temperature.

Using this new tank pressure and the current combustion chamber pressure, the mass flow rate of liquid nitrous out of the tank $\dot{\boldsymbol{m}}_{\boldsymbol{liquid}}$ is now calculated, which is based on the flow through the rocket engine injector it feeds:

Injector mass flow rate

We want to calculate the mass flow rate of liquid propellant that will flow through an injector due to a pressure ΔP across it. Directly upstream of the injector face is the plumbing section known as the **injector manifold**.

We start with **Bernoulli's equation** (an energy equation which describes pressure as a form of potential energy and flow velocity as kinetic energy) for the flow of liquid from the injector manifold into the injector orifices:

$$\boldsymbol{P_{manifold}} + \frac{\boldsymbol{1}}{\boldsymbol{2}} \boldsymbol{\rho_{liquid}}\, \boldsymbol{V^2_{manifold}} = \boldsymbol{P_{orifice}} + \frac{\boldsymbol{1}}{\boldsymbol{2}} \boldsymbol{\rho_{liquid}}\, \boldsymbol{V^2_{orifice}} = \boldsymbol{constant} \quad \text{(equ. 1.3)}$$

As the liquid leaves the injector orifices, it breaks into droplets without changing pressure, so $P_{orifice}$ equals the combustion chamber pressure.

Substituting for the velocity *V* of the liquid from a rearrangement of the **mass continuity equation**:

$$\boldsymbol{V = \frac{\dot{m}_{liquid}}{A\,\rho_{liquid}}} \quad \text{(equ. 1.4)}$$

where $\dot{m}_{liquid}$ is the mass flow rate of liquid, *A* is the cross-sectional area of either the manifold or injector orifice, and ρ_{liquid} is the liquid density,

gives:

$$\boldsymbol{P_{orifice} - P_{manifold} = \Delta P = \frac{\rho_{liquid}\,\dot{m}_{liquid}^2}{2\,\rho_{liquid}^2}\left(\frac{K}{(N\,A_{orifice})^2} - \frac{1}{A_{manifold}^2}\right)}$$

$$\boldsymbol{= \frac{\dot{m}_{liquid}^2}{2\,\rho_{liquid}}\left(\frac{K}{(N\,A_{orifice})^2} - \frac{1}{A_{manifold}^2}\right)} \quad \text{(equ. 1.5)}$$

where *N* is the number of orifices.

Note the inclusion of a 'flow resistance coefficient' *K*, which is related to a traditional discharge coefficient as:

$$\boldsymbol{C_{dis} = \frac{1}{\sqrt{K}}} \quad \text{(equ. 1.6)}$$

As the static pressure of the Nitrous liquid drops as it passes through the orifices, it vaporizes. This means that what flows through the injector is a foam of liquid and bubbles - but mostly vapour - and so traditional tables of loss values or **discharge coefficients** don't work for this mixed fluid. You have to tailor this *K* coefficient until the time taken to empty the tank matches your own test firing results.

We've found that a good starting value for *K* is 2.0 for Nitrous oxide and other just-subcritical propellants. (Therefore $\boldsymbol{C_{dis} = \frac{1}{\sqrt{K}} = \frac{1}{\sqrt{2}} = 0.707}$)

Rearranging, and assuming that $A_{manifold}^2$ is 'infinitely' larger than (the square of) an injector orifice area gives:

$$\boldsymbol{\dot{m}_{liquid} = N\,A_{orifice}\sqrt{\frac{2\,\rho_{liquid}\,\Delta P}{K}}} \quad \text{(equ. 1.7)}$$

Grouping terms in this equation allows the entire injector plate to be described by a 'Loss factor', which we've found useful for comparison with actual injector flow test data:

$$\boldsymbol{\dot{m}_{liquid} = \sqrt{\frac{2\,\rho_{liquid}\,\Delta P}{F_{loss}}}} \quad \text{where} \quad \boldsymbol{F_{loss} = \frac{K}{(N\,A_{orifice})^2} = \frac{1}{(C_{dis}\,N\,A_{orifice})^2}} \quad \text{(equ.s 1.8)}$$

Alternatively, further rearrangement gives us the number of orifices required for a particular mass flow rate:

$$N = \frac{\dot{m}_{liquid}}{A_{orifice}\sqrt{\frac{2\,\rho_{liquid}\,\Delta P}{K}}}$$ (equ. 1.9)

Feed system

The feed plumbing between the run-tank and the injector manifold also suffers a loss, which needs accounting for.

Every feed system has its own geometry and loss characteristics: the differences between your static test stand plumbing and your flight vehicle's plumbing are so great that loss characteristics data from one cannot be used for the other. You need to calibrate both. We strive to keep the flight vehicle's plumbing losses as small as possible by minimising 'stuff' and by avoiding sudden changes in flow cross-sectional area.

The easiest way to model the feed system is to add an additional Loss factor. We can visualize the system of feed plumbing plus injector as two electrical resistors in series, where pressure drop acts as voltage drop, and Loss factor is the analogue of resistance:

$$I = \frac{V}{R} = \frac{V}{R_{feed} + R_{injector}}$$ is the electrical analogue of: $$\frac{\dot{m}_{liquid}^2}{2\,\rho_{liquid}} = \frac{\Delta P}{F_{loss}} = \frac{\Delta P}{F_{loss\_feed} + F_{loss\_injector}}$$

(equ.s 1.10)

ΔP is now the pressure drop between run-tank and combustion chamber:

$$\Delta P = \Delta P_{feed} + \Delta P_{injector}$$ (equ. 1.11)

Again, we're assuming that (the square of) one cross-sectional area is 'infinitely' larger than the other; in this case the run-tank versus the feed system plumbing.

$$A_{run-tank}^2 \gg A_{manifold}^2 \gg N^2 A_{orifice}^2$$ (equ. 1.12)

Using a Loss factor to describe the entire feed system avoids having to worry about all the changes in cross-sectional area along the test-stand plumbing.

Inside the run-tank

Having calculated the mass flow rate of liquid nitrous out of the tank, we can integrate it to get the mass that has left the run-tank over each time iteration ***dt***:

Liquid mass m_{liquid} has decreased by:

$$\Delta m_{liquid} = \int \dot{m}_{liquid}\, dt$$ (equ. 1.13)

And from the law of mass continuity, the total nitrous mass within the run-tank has also decreased by this amount.

The resulting new value for m_{liquid} is the mass of liquid that would now be in the tank if the nitrous didn't react to the expansion of the nitrous vapour and the ensuing drop in pressure. We'll designate this as $m_{liquid\_unphased}$:

$$\boldsymbol{m_{liquid\_unphased} = m_{liquid} - \Delta m_{liquid}} \qquad \text{(equ. 1.14)}$$

But the nitrous *does* react, both to the increase in nitrous volume and the drop in temperature. We now need to calculate how it responds:

The densities of the liquid and vapour are functions of temperature only, so the nitrous is forced to follow a run-tank internal volume formula:

$\boldsymbol{V_{vapour} + V_{liquid} = V_{tank}}$ or: $\boldsymbol{\frac{m_{liquid}}{\rho_{liquid}} + \frac{m_{vapour}}{\rho_{vapour}} = V_{tank}}$ (equ. 1.15)

Where ρ is density, m is mass.

The resulting changes in the proportions of the two phases can then be calculated by rearranging this equation:

$$\boldsymbol{m_{liquid} = \rho_{liquid}\left(V_{tank} - \frac{m_{vapour}}{\rho_{vapour}}\right)} \qquad \text{(equ. 1.16)}$$

substituting equation 1.14:

$$\boldsymbol{m_{liquid} = \rho_{liquid}\left(V_{tank} - \frac{(m_{total} - m_{liquid})}{\rho_{vapour}}\right)} \qquad \text{(equ. 1.17)}$$

collecting terms:

$$\boldsymbol{m_{liquid}\left(1 - \frac{\rho_{liquid}}{\rho_{vapour}}\right) = \rho_{liquid}\left(V_{tank} - \frac{m_{total}}{\rho_{vapour}}\right)} \qquad \text{(equ. 1.18)}$$

dividing by ρ_{liquid}:

$$\boldsymbol{m_{liquid}\left(\frac{1}{\rho_{liquid}} - \frac{1}{\rho_{vapour}}\right) = \left(V_{tank} - \frac{m_{total}}{\rho_{vapour}}\right)} \qquad \text{(equ. 1.19)}$$

gives:

$$\boldsymbol{m_{liquid} = \frac{\left(V_{tank} - \frac{m_{total}}{\rho_{vapour}}\right)}{\left(\frac{1}{\rho_{liquid}} - \frac{1}{\rho_{vapour}}\right)}} \quad \text{and} \quad \boldsymbol{m_{vapour} = m_{total} - m_{liquid}} \qquad \text{(equs. 1.20)}$$

We'll designate this new volume-adjusted value as m_{liquid_new}.

From mass continuity, the discrepancy between m_{liquid_new} and $m_{liquid\_unphased}$ has to be the mass of Nitrous that has been vaporised by the phase changes:

$\boldsymbol{m_{vaporised} = m_{liquid\_unphased} - m_{liquid\_new}}$ (equ. 1.21)

Now, previous incarnations of our tank-emptying software model used simple integration rather than Trapezoidal integration and this running $m_{vaporised}$ calculation was unstable. We therefore had to numerically stabilise it, with a filter known as a first-order time lag.

Providentially, it transpired that the real-world nitrous vaporisation process isn't instantaneous, and a time lag of about 0.15 seconds gives a good match with our run-tank test data.

So this time lag remains:

$$\boldsymbol{time\_constant} = \frac{\Delta t}{0.15}$$

$$\boldsymbol{A} = \boldsymbol{m_{liquid\_unphased}} - \boldsymbol{m_{liquid}}$$

$$\boldsymbol{B} = \boldsymbol{B_{t-1}} + \boldsymbol{time\_constant}\,(\boldsymbol{A} - \boldsymbol{B_{t-1}})$$

$$\boldsymbol{m_{vaporised}} = \boldsymbol{B}$$

(equ.s 1.22)

With this new running value for $m_{vaporised}$ we can proceed to the next time iteration, and begin the calculation loop again.

N.B. Bear in mind that this model is an approximation only. Occasionally, the model goes awry just as the last of the liquid nitrous is emptying. Add the following check to catch this, and use it to trigger engine burnout:

if ($\boldsymbol{m_{liquid\_new}} > \boldsymbol{m_{liquid\_unphased}}$) then trigger burnout.

Nitrous roulette

We've recently added a new precursor to the above tank-emptying model, attempting to model those bipropellant engines that use the nitrous vapour pressure to pressurise the fuel tank via a (hopefully) impermeable piston or bladder. This precursor accounts for the effective rate of increase of the nitrous run-tank volume as a volumetric flow rate of liquid fuel is expelled from *its* run-tank:

$$\left(\frac{\boldsymbol{dV}}{\boldsymbol{dt}}\right)_{\boldsymbol{ox\_tank}} = \dot{\boldsymbol{V}}_{\boldsymbol{fuel}} \quad \text{where:} \quad \dot{\boldsymbol{V}}_{\boldsymbol{fuel}} = \frac{\dot{\boldsymbol{m}}_{\boldsymbol{fuel}}}{\boldsymbol{\rho}_{\boldsymbol{fuel}}} \qquad \text{with } \rho \text{ being density.} \quad \text{(equ.s 1.23)}$$

This is time-integrated to get the current oxidiser run-tank volume to feed into the above tank-emptying model:

$$\boldsymbol{V_{ox\_tank}} = \int \left(\frac{\boldsymbol{dV}}{\boldsymbol{dt}}\right)_{\boldsymbol{ox\_tank}} \boldsymbol{dt} \quad \text{(equ. 1.24)}$$

We don't as yet have test data from firings of such biprops so this precursor isn't yet validated.

2: A mathematical model of the vapour-only phase emptying

After all the liquid nitrous has run out of the run-tank, there will still be some vapour remaining. Even if you started with a tank completely full of liquid, some vapour will be created as the tank empties.

This vapour is dense enough for combustion and so produces thrust, though it burns fuel-rich (too little oxidiser), and this 'vapour-only' phase doesn't last long.

From our test-firing data, we've learned a few surprising things about this 'vapour-only' phase of combustion:

1) It transpires that the pressure loss that occurs as the vapour flows through the injector orifices is identical to when the liquid was flowing through it (the *K* coefficient is the same). This proves that the liquid vaporises almost completely to vapour inside the orifices, assuming that you use numerous small orifices as we did.
2) The vapour emptying out of the run-tank can be modelled as an Isentropic process. That means that very little energy is wasted (increase of entropy) during the emptying, and no heat is transferred from the tank walls to the vapour.
3) Therefore the **vapour pressure** and temperature drop rapidly as the tank empties and the vapour expands.
4) The vapour is not an **ideal gas**. Intermolecular forces (the forces between the vapour molecules) are noticeably at work, so nitrous vapour expands differently to that of an ideal gas.

With the above in mind, a simple mathematical model can simulate the tank emptying of nitrous vapour, which is now described:

Historically, we modelled the vapour-only run-tank emptying process as a classic Isentropic process, but fudged to account for the **real gas** behaviour of the nitrous vapour; this appeared to work as it matched our test-data very well.

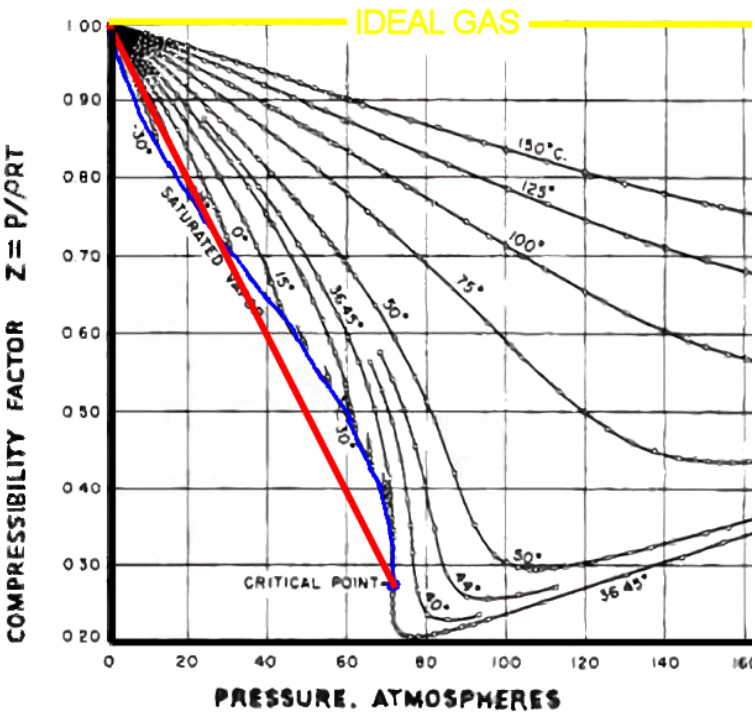
To our relief, Ref. 5 confirms that this approach was valid, and suggests new parameters to generalise the isentropic parameter γ, albeit requiring hard-to-obtain thermophysical data.

Our pragmatic approach involved data that we *did* have, such as Nitrous oxide's **Compressibility factor** (Z). Its graph is shown here:

Our sims show that the nitrous vapour travels up the blue-coloured **saturated vapour** line as it empties from the run-tank and loses pressure.

We can approximate this vapour curve as the straight line (coloured red) running from the **Critical point** up to the point (0,1) at zero pressure.

Thus, the compressibility factor can be modelled essentially as a linear function of tank **vapour pressure**.



We begin the vapour-only phase-emptying model by snapshotting the compressibility factor just as the liquid phase has run out.

Then we calculate the mass flow rate of nitrous vapour out of the tank using equations 1.8, but working with vapour instead of liquid. The loss coefficient *K* in equations 1.8 remains the same though.

Both the nitrous mass within the run-tank, and the run-tank internal volume, are known at each time iteration, so we calculate their quotient, which is the current nitrous vapour density:

$$\boldsymbol{\rho_{nitrous}} = \frac{\boldsymbol{m_{nitrous}}}{\boldsymbol{V_{run-tank}}} \quad \text{(equ. 2.1)}$$

Next, the vapour emptying can be approximated as an Isentropic process. The inter-relationships between *P, T*, and ρ for an isentropic process are the standard Isentropic equations:

$$\frac{\boldsymbol{dT}}{\boldsymbol{T}} = \left(\frac{\boldsymbol{\gamma-1}}{\boldsymbol{\gamma}}\right)\frac{\boldsymbol{dP}}{\boldsymbol{P}} = (\boldsymbol{\gamma-1})\frac{\boldsymbol{d\rho}}{\boldsymbol{\rho}} \quad \text{or:} \quad \frac{\boldsymbol{T_2}}{\boldsymbol{T_1}} = \left(\frac{\boldsymbol{P_2}}{\boldsymbol{P_1}}\right)^{\frac{\boldsymbol{\gamma-1}}{\boldsymbol{\gamma}}} = \left(\frac{\boldsymbol{\rho_2}}{\boldsymbol{\rho_1}}\right)^{\boldsymbol{\gamma-1}} \quad \text{(equ.s 2.2)}$$

where γ is the ratio of specific heats which has value 1.3 for nitrous vapour (averaged over the subcritical temperature range of interest).

We'll take state 1 as the 'old' values from the previous time iteration, and state 2 as the current time iteration.

Starting with the equation for a **real gas**:

$\boldsymbol{P = Z\rho RT}$ (equ. 2.3)

Then:

$\frac{P_2}{P_1} = \left(\frac{Z_2}{Z_1}\right)\left(\frac{\rho_2}{\rho_1}\right)\left(\frac{R_2}{R_1}\right)\left(\frac{T_2}{T_1}\right)$ (equ. 2.4) where R is the specific gas constant for nitrous.

If we assume that R doesn't notably change with time, then $R_2 = R_1$ and that term drops out.

Using equ.s 2.2 to substitute density for temperature gives:

$\frac{P_2}{P_1} = \left(\frac{Z_2}{Z_1}\right)\left(\frac{\rho_2}{\rho_1}\right)\left(\frac{\rho_2}{\rho_1}\right)^{\gamma-1} = \left(\frac{Z_2}{Z_1}\right)\left(\frac{\rho_2}{\rho_1}\right)^{\gamma}$ (equ.s 2.5)

Rearranging equ. 2.3 for temperature similarly gives:

$\left(\frac{T_2}{T_1}\right) = \left(\frac{P_2}{P_1}\right)^{-1}\left(\frac{Z_2}{Z_1}\right)^{-1}\left(\frac{\rho_2}{\rho_1}\right)^{-1} = \left(\frac{\rho_2}{\rho_1}\right)^{\gamma}\left(\frac{Z_2}{Z_1}\right)^{-1}\left(\frac{\rho_2}{\rho_1}\right)^{-1} = \left(\frac{Z_2}{Z_1}\right)^{-1}\left(\frac{\rho_2}{\rho_1}\right)^{\gamma-1}$ (equ.s 2.6)

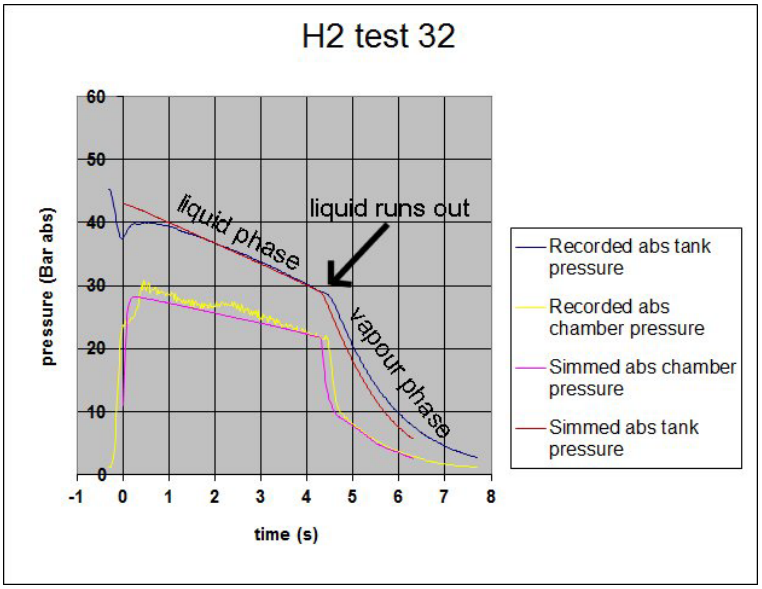
There is one problem though: we need to calculate Z_2 in equ.s 2.4 and 2.6, but this depends upon P_2, the vapour pressure at time 2, which we calculate *after* calculating these equations.

So we need to resort to recursion: we continuously re-calculate a 'running' Z_2

based on the previous time iteration's tank pressure.

3: Sim results

When coupled to a sim of the combustion chamber, the results of the above tank emptying simulation models give a good match with our experimental test-firing data:



Glossary:

Bernoulii's principle: Is just a statement of the Law of Conservation of Energy couched in fluid dynamic terms, and is expressed by his equation:

$$\boldsymbol{P + \frac{1}{2}\rho V^2 = constant} \quad \text{or:} \quad \boldsymbol{\Delta P = -\frac{1}{2}\rho \Delta V^2}$$

where *P* is pressure, ρ is density, and *V* is flow velocity.

Drag: (archaic: 'air resistance') is the retarding force experienced by bodies travelling through a fluid (gas or liquid).

Injector manifold: the section of plumbing immediately upstream of the **injector plate.** This is usually a divergent section in order to raise the (subsonic) flow pressure.

Injector plate: the section of combustion chamber wall incorporating the injector orifices.

Isentropic process: a physical process (such as an expansion) that occurs without change in flow Entropy. Whilst this doesn't happen in reality, many gas processes are *almost* Isentropic.

Mach number: The vehicle's airspeed *V* (or the local airspeed around a nose or fin) compared to the speed of sound '*a*' in the atmosphere:

$$\boldsymbol{M = \frac{V}{a}}$$

Mass continuity equation: describes the Law of mass continuity applied to the flow through a pipe. If we measure the flow of fluid mass passing any particular point along the pipe which has cross-sectional area *A*, then:

$$\boldsymbol{\dot{m} = \rho A V}$$

where $\dot{m}$ is Newton's fluxion symbolism for $\frac{dm}{dt}$, the time rate of change of mass, known as the **mass flow rate**. *ρ* and *V* are the fluid density and velocity at that point in the pipe.

Subsonic: Vehicle airspeed is below Mach 1 (see Mach number).

Supersonic: Vehicle airspeed is above Mach 1 (see Mach number).

References:

Ref. 1: Dr Bruce P. Dunn, University of British Columbia and Dunn Engineering: Several articles on self-pressurised peroxide rockets and experiments on propane tanks, as well as email communications with the author on the subject of numerical modelling of the tank emptying process; many thanks.

Ref. 2: Engineering Sciences Data Unit (ESDU) sheet 91022, “Thermophysical properties of nitrous oxide.” Available in hardcopy from some U.K. University libraries, or accessible over the Web to students.

Ref. 3: “Space Propulsion Analysis and Design”, Ronald W. Humble, Gary N. Henry and Wiley J. Larson, McGraw Hill Space Technology Series ISBN 0-07-031320-2

Ref. 4: “Rocket Propulsion Elements 7th edition”, Sutton and Biblarz

Ref. 5: “Generalised Isentropic Relations in Thermodynamics”, Pim Nederstigt and Rene Pecnik, Department of Process and Energy, Delft University of Technology, *Energies*, *16*(5), Article 2281. https://doi.org/10.3390/en16052281 2023. See: https://research.tudelft.nl/en/publications/generalised-isentropic-relations-in-thermodynamics

Ref.6: https://www.thermopedia.com/content/1107/