



Optimising Pressurised Gas Cylinder Filling Rates: A Computational Study of Temperature Variations

Joshua U'Dell

Robert Goodson

School of Engineering

BEng (Hons) Mechanical Engineering

Introduction

Compressed gas cylinders are widely used across various industries, enabling engineers to deliver specific gases or gas mixtures to processes at controlled flow rates using valves and regulators.

Compressed gas cylinders are generally filled using a simple buffer process. This involves storing a set amount of gas in buffer cylinders, usually from a liquid source, then releasing the stored gas into the required cylinders during a filling cycle.

Governing Mathematical Principles

The script created utilises the following mathematical and scientific principles to determine the gas and cylinder wall temperatures, as well as the gas pressure within the cylinder.

- The ideal gas equation

$$pV = nRT$$

- Joule-Thomson Effect

$$\mu_{JT} = \left(\frac{\partial T}{\partial p}\right)_h$$

- Energy Balance Equation

$$E_{total} = (m_{existing} \cdot T_{existing}) + (m_{in} \cdot T_{in})$$

- Adiabatic Compression Heating

$$T_{compressed} = T_{mixed} \cdot \left(\frac{P_{new}}{P_{old}}\right)^{\frac{\gamma-1}{\gamma}}$$

- Convective Heat Transfer

$$Q_{gas \rightarrow wall} = h \cdot A \cdot T_{gas} - T_{wall}$$

- Conductive Heat Transfer

$$Q = -kA \left(\frac{dT}{dx}\right)$$

- Time Discretization in Simulations (Explicit Euler Method)

$$\frac{dT_{gas}}{dt} = -\frac{h \cdot A}{m_{gas} \cdot c_p} \cdot (T_{gas} - T_{wall})$$

(Incropera et al., 2007).

Acknowledgements

- Robert Dean – Senior Mechanical Engineer at BOC

Project Goal

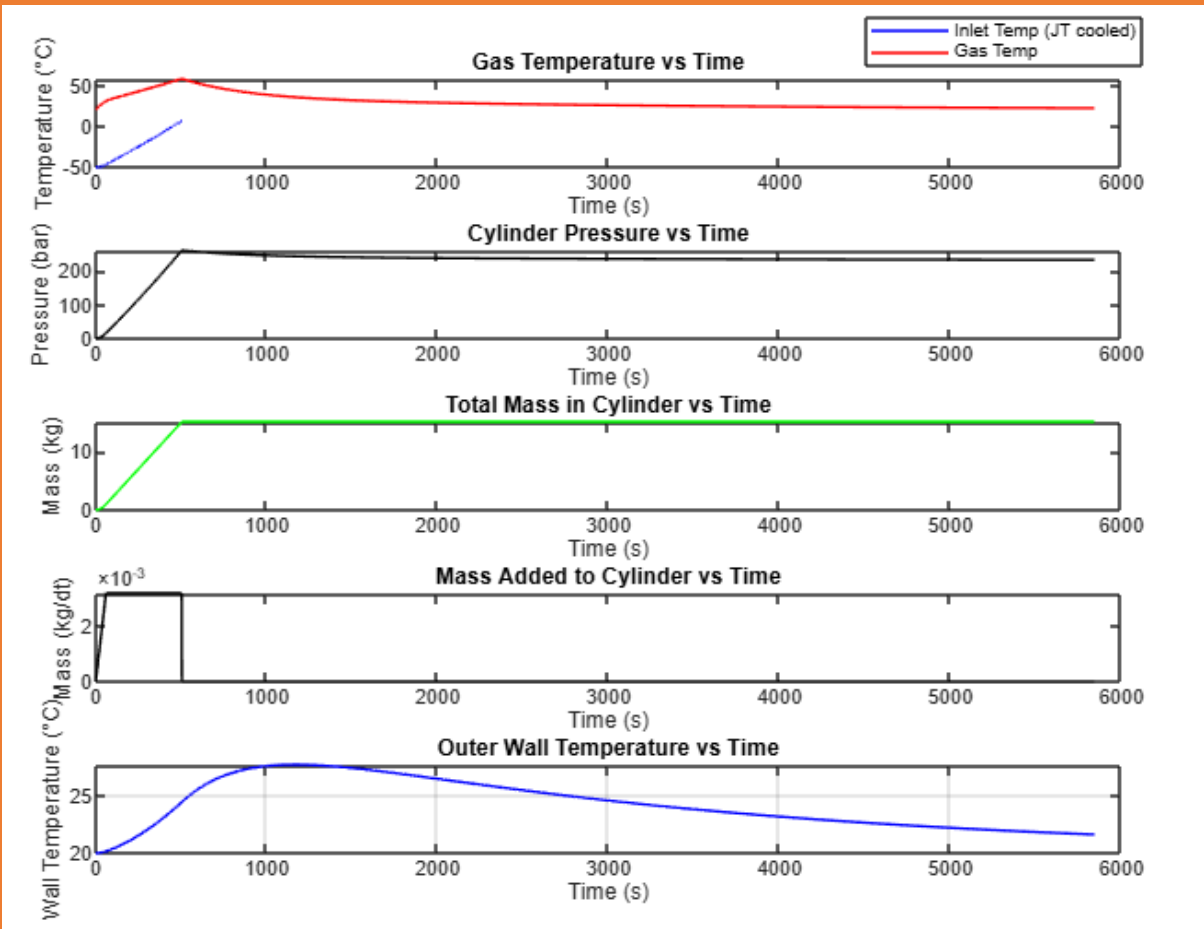
To create a MATLAB script to simulate the cylinder filling of Nitrogen, Oxygen and Argon gas using a pumped buffer system. Track gas pressure, temperature, and cylinder wall temperature.



Simulation Results output

Screenshots from Oxygen simulation

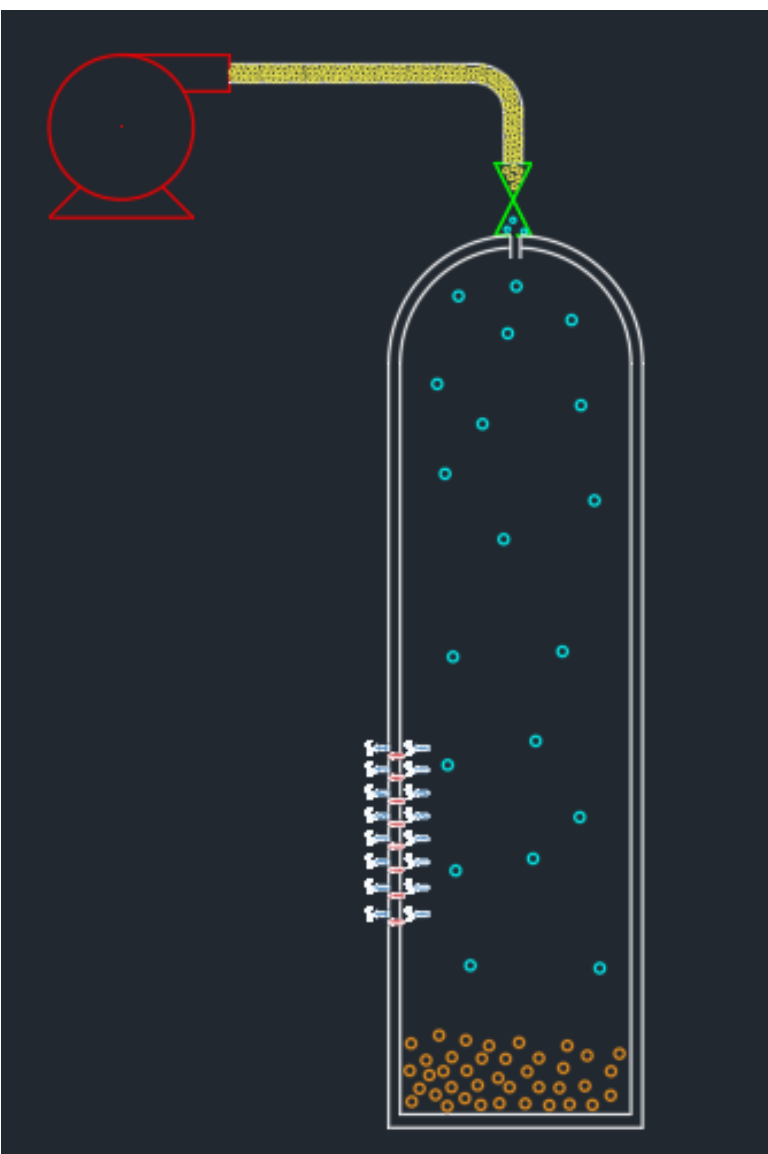
```
Gas selected: Oxygen
Fill rate per cylinder: 0.0317 kg/s
Time to reach required mass of 15.10 kg: 504.30 seconds (8.41 minutes, 0.14 hours)
Time to cool down to 22 deg C: 5338.60 seconds (88.98 minutes, 1.48 hours)
Total simulated time 5842.90 seconds (97.38 minutes, 1.62 hours)
Maximum gas temperature: 57.97 deg C
Minimum gas temperature: 20.00 deg C
Maximum cylinder wall temperature: 27.73 deg C
Minimum cylinder wall temperature: 20.00 deg C
Maximum Gas Pressure: 259.83 bar
Final Gas Pressure: 231.61 bar
Final Gas Temperature: 22.00 deg C
```



Calculation Loop

At each time step, multiple checks are made to determine if the data has achieved an ending condition; if not, the following principles are applied, and outputs are calculated.

- The mass flow rate for incoming gas is ramped up to 100% over time
- Inlet gas temperature is calculated using the Joule-Thomson effect
- Cooled gas is mixed with existing gas using the energy balance equation
- Mixed gas pressure is calculated using the ideal gas law
- Adiabatic heating calculation is used to calculate the mixed gas temperature
- Heat transfer through the cylinder wall and to the ambient is calculated, and new cylinder and gas temperatures are calculated.



Methodology

The fundamental methodology of the MATLAB script is to split the filling cycle into tiny time steps of around 0.1 seconds (the user can adjust this). The script then runs a series of calculations using the governing equations to estimate the change in values from the incoming data when a known amount of gas at known pressure and temperature is added. This cycle is looped until an end condition is met.

Ending conditions

The simulation/ script will end if the while loop condition is no longer true, this is simply a maximum simulated time that is equal to the cosine time step divided by a set amount of time. The simulation will also end if the mass of gas in the cylinder is equal to or greater than the target amount. This corresponds to a constant pressure of product at a constant temperature. The mass is then calculated using the ideal gas law.

Conclusion

The report summarises how the script functions and the assumptions put in place for the governing principles to be used. The report also goes into additional principles that are excluded from this simulation.

The script can be used by engineers to quickly rule out or back up proposed changes to cylinder filling systems without the need to produce prototypes and invest capital where it is not required.

References

Incropera, F.P., DeWitt, D.P., Bergman, T.L. and Lavine, A.S., 2007. Fundamentals of Heat and Mass Transfer. 6th ed. Hoboken, NJ: John Wiley & Sons.

Moran, M.J. and Shapiro, H.N., 2008. Fundamentals of Engineering Thermodynamics. 6th ed. Hoboken, NJ: John Wiley & Sons.