

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

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Joshua U'Dell
BOC A LINDE COMPANY
UNIVERSITY OF WALES TRINITY SAINT DAVID

This thesis is the result of the author's original research. It has been composed by the author and has not been previously submitted for examination which has led to the award of a degree.

1.0 Abstract

The safe and efficient filling of high-pressure gas cylinders is critical within the chemical industry. During filling, significant thermal effects arise due to the Joule-Thomson effect, gas compression, and transient heat transfer to the cylinder wall and surrounding environment (Woolley et al., 2014; Lemmon et al., 2018). This study presents a MATLAB-based simulation that models the transient thermal and pressure dynamics of a 50-liter chrome molybdenum steel cylinder filled with either oxygen, nitrogen, or argon. The model incorporates real-time calculations of gas temperature and pressure, including Joule-Thomson cooling through a 4 mm orifice, mixing of inlet and existing gas, adiabatic compression heating, and conductive heat transfer to the cylinder wall with convective loss to ambient air (Timmerhaus and Flynn, 1989; Incropera et al., 2007).

The simulation accounts for valve control logic to prevent overpressure, dynamically pausing filling above the pump feed pressure and resuming below. Heat conduction through the 6 mm cylinder wall is modelled using a numerical approach enabling prediction of outer wall temperature evolution (Patankar, 1980). Key results include time-resolved plots of gas pressure, internal temperature, wall temperature, and inlet flow status, offering detailed insight into the thermodynamic behaviour of each gas type during the filling process.

Findings indicate that gas type significantly influences thermal behaviour, with argon exhibiting the strongest Joule-Thomson cooling and fastest temperature rise due to compression (Baek et al., 2011). The simulation supports improved safety analysis and design of filling protocols, offering a cost-effective alternative to experimental testing. The model can be extended to incorporate real gas equations and validated with experimental data in future work.

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5.0 Introduction

Compressed gas cylinders are essential components in the storage and transportation of gases across a broad spectrum of industrial and domestic applications. These cylinders range in size and specification, small thin-walled cylinders are seen in medical injectors and culinary tools. Medium-sized containers are commonly found in domestic settings such as barbecue grills as seen in figure 1. Larger cylinders are prevalent in fabrication environments like welding shops as seen in figure 2, while high-capacity solutions such as hydrogen tube trailers (figure 3) serve more demanding industrial applications (Smith, 2016; ISO, 2019). The design and material selection of these pressure vessels are governed by stringent engineering standards to ensure safety and reliability under varying operational conditions (Jones and Thomas, 2018).



Figure 1 BOC Propane Cylinder (BOC, n.d.)



Figure 2 BOC Argoshield Universal Cylinder (BOC, n.d.)



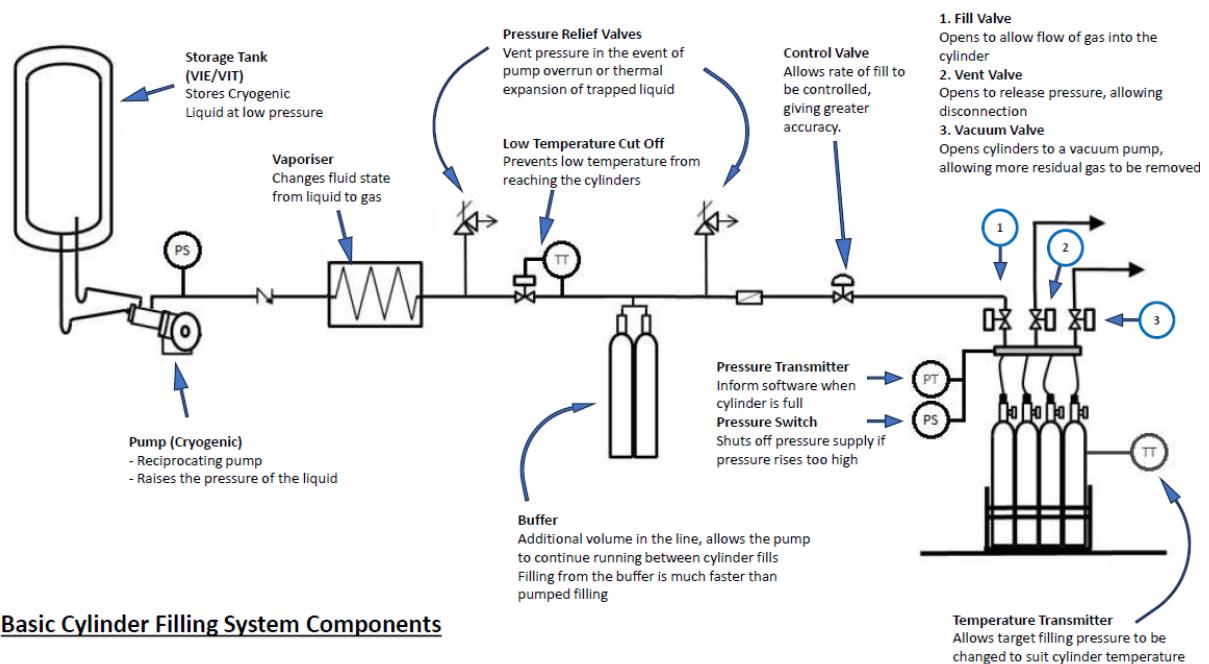
Figure 3 BOC Hydrogen Tube Trailer (BOC, n.d.)

Compressed gas cylinders are commonly filled using a pumped transfer process from a liquid storage source. Typically, this source is a large, low-pressure vessel that stores the product in its liquid phase. The liquid is extracted from the vessel and passed through a vaporiser, a form of heat exchanger designed to convert the liquid into a gaseous state. This transformation is achieved through thermal exchange, often facilitated by finned arrays that increase surface area and enhance heat transfer efficiency (Smith, 2010). Once vaporised, the gas flows through a control valve system that dynamically regulates flow rate during the filling process.

These valves are managed by process control systems to ensure accurate and safe delivery of gas into the receiving cylinders.

Cylinders can be filled either by monitoring internal pressure or by calculating the mass of gas delivered. In pressure-based filling, the process concludes when the gas within the cylinder reaches a specified temperature and pressure. The target pressure can be dynamically recalculated for varying temperature conditions, due to pressure and temperature being proportionally related whilst at a constant volume (as described by the ideal gas law). This form of control typically employs closed-loop feedback systems involving Programmable Logic Controllers (PLCs) and industrial sensors to maintain process reliability and safety (Jones & Patel, 2015).

Alternatively, mass-based filling methods determine the quantity of gas added by calculating the product of mass flow rate and filling time. This method is commonly validated by weigh scales integrated into the production line to ensure accuracy and compliance with quality standards (Brown et al., 2013).



Basic Cylinder Filling System Components

Figure 4 Basic Cylinder Filling System Components (Dean. R, 2024)

During the cylinder filling process, several thermodynamic phenomena occur, leading to an increase in the temperature of the cylinder walls. To safeguard both the cylinder components and the valve assembly, the European Industrial Gases Association (EIGA) has established guidelines for safe filling practices in EIGA Doc 50/11, "Filling of Cylinders with Gases." This document specifies that the temperature of the cylinder wall should not exceed 60°C (140°F)

during filling operations. The temperature limit is designed to protect against over pressurisation and to prevent potential damage to the cylinder and its components (EIGA, 2011). As noted earlier, increases in gas temperature result in corresponding increases in gas pressure, which can present safety risks.

To prevent the cylinder wall temperature from exceeding this critical threshold, cylinder filling systems commonly incorporate surface thermometers to continuously monitor the outer wall temperature. In addition, PLC are employed to regulate the flow of gas. If the cylinder temperature approaches the established limit the PLC-controlled system will adjust the flow rate, thereby ensuring that the temperature remains within safe limits (Jones & Patel, 2015).

This report presents the development and implementation of a MATLAB-based simulation that models the transient filling process of a single high-pressure gas cylinder. To ensure computational efficiency and tractability, the simulation incorporates several simplifying assumptions while retaining the critical physical phenomena that govern the process.

At each time step of the simulation, the temperature of the incoming gas is first determined by accounting for the Joule-Thomson effect, which describes the temperature change of a real gas when it undergoes an isenthalpic expansion from high to low pressure. This effect is commonly observed in everyday applications, such as the cooling sensation experienced when aerosol sprays are released into the atmosphere (Çengel and Boles, 2015).

Following expansion, the cooled incoming gas is assumed to mix homogeneously with the gas already present in the cylinder. A basic energy balance is then applied to determine the new average gas temperature inside the cylinder (Moran et al., 2020). This updated temperature, combined with the known gas mass and volume, is used in conjunction with the ideal gas law to estimate the updated internal pressure.

Subsequently, the adiabatic compression of the gas, due to increasing pressure, is considered, and the resulting temperature rise is calculated assuming no heat loss during the compression phase (Yunus and Michael, 2015). The simulation then evaluates heat losses from the gas to the environment. Heat transfer is modelled via convection and conduction from the internal gas to the cylinder wall and subsequently to the ambient air. Using calculated heat transfer coefficients and wall geometry, the rate of thermal energy loss is estimated. This heat loss is used to update the gas temperature, reflecting the energy transferred to the surrounding material and environment.

Figure 5 displays a simple pictogram that has been created to show the overall process at each time step.

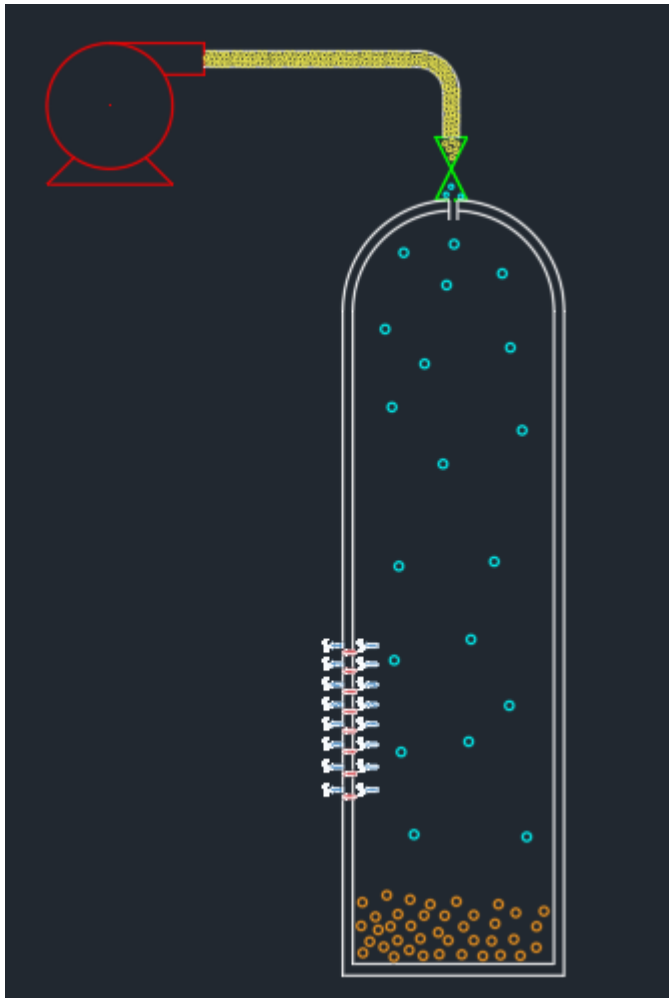


Figure 5 Cylinder Filling Pictogram (U'Dell, J, 2025)

6.0 Physical and Mathematical Principles

This section presents the underlying mathematical models and physical principles that govern the simulation framework.

6.1 Ideal Gas Equation

The ideal gas law defines the relationship between pressure and temperature of a gas at constant volume, while also accounting for the number of moles present in the system. It provides a simplified model that links the macroscopic properties of gases; pressure, volume, temperature, and quantity, under the assumption of ideal behaviour (Hannah and Hillier, 1999).

$$pV = nRT$$

Where:

p = the pressure of the gas [N/m^2]

V = the volume of the gas [m^3]

n = the number of moles of gas [mol]

R = the universal molar gas constant = $8.31 J K^{-1} mol^{-1}$

T = the temperature of the gas [K]

(Muncaster, 1985, P. 204).

6.2 Joule-Thomson Effect

The Joule-Thomson effect describes the change in temperature that occurs when a real gas undergoes a pressure drop at constant enthalpy, such as during throttling through a valve or orifice. This temperature change arises due to intermolecular forces within the gas and is quantified by the Joule-Thomson coefficient (μ_{JT}), which is defined as the partial derivative of temperature with respect to pressure at constant enthalpy:

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

Where:

μ_{JT} = Joule – Thomson coefficient [$Kelvin/Pa$]

T = Temperature of the gas [$Kelvin$]

p = Pressure of the gas [Pa]

h = enthalpy [$Joules$]

(Rogers & Mayhew, 1992, P.99)

The sign and magnitude of μ_{JT} depend on the specific gas and its thermodynamic state. A positive coefficient indicates that the gas cools upon expansion, which is typical for most gases at room temperature and high pressure. Conversely, a negative coefficient implies heating during expansion, as observed in light gases like hydrogen or helium under certain conditions (Rogers and Mayhew, 1992).

In practical engineering applications, interest typically lies in evaluating finite changes in gas properties rather than infinitesimal differentials. As such, the partial derivative in the Joule-Thomson coefficient expression can be reasonably approximated using discrete values over a finite pressure range, yielding:

$$\Delta T \approx \mu_{JT} \cdot (P_1 - P_2)$$

Where:

ΔT = Change in temperature [Kelvin]

μ_{JT} = Joule – Thomson coefficient [Kelvin/Pa]

$P_1 - P_2$ = Pressure difference [Pa]

This simplified relationship enables engineers to estimate the temperature change of a gas during throttling or expansion processes, provided the Joule-Thomson coefficient is known for the gas under the given conditions (Rogers and Mayhew, 1992).

6.3 Energy Balance

When a new mass of gas enters the cylinder at a known temperature, it undergoes mixing with the gas already present within the vessel. Assuming no heat loss during the mixing process and treating the gases as a uniform mixture, the resulting temperature can be determined using a straightforward energy balance based on the principle of conservation of energy. The following equation is used to calculate the mixed gas temperature:

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

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

Where:

E_{total} = Total energy in the cylinder [kg · K]

T_{mixed} = Temperature of the gas in the cylinder once new gas has been added [K]

$m_{existing}$ = Mass in the cylinder before new gas is added [kg]

$T_{existing}$ = Temperature of the gas in the cylinder before new gas is added [K]

m_{in} = Mass being added to the cylinder [kg]

T_{in} = Temperature of the gas being added to the cylinder [K]

6.4 Adiabatic Compression Heating

During the cylinder filling, as pressure increases within the container, the gas undergoes compression, and if the process occurs too rapidly for heat exchange with the environment, it can be assumed to be adiabatic. In an adiabatic process, no heat is transferred to or from the surroundings, meaning that all the work done on the gas increases its internal energy, thereby raising its temperature (Rogers and Mayhew, 1992).

For an ideal gas, the relationship between temperature and pressure during adiabatic compression is given by the following thermodynamic expression:

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

Where:

$T_{compressed}$ = Temperature of the gas due to compression with no heat loss [K]

T_{mixed} = Temperature of the gas in the cylinder once new gas has been added [K]

P_{new} = New pressure of the gas in the cylinder, using the ideal gas law [Pa]

P_{old} = Original pressure in the cylinder at the start of the current time step [Pa]

γ = Adiabatic index for the gas (C_p/C_v)

(Rogers & Mayhew, 1992, P.180)

This equation highlights that compressing a gas adiabatically results in a significant temperature rise, especially when the pressure increase is substantial and rapid, as is typical during high-pressure cylinder fills. Such thermal effects must be accounted for in system design to prevent overheating or exceeding material limits (Roger Muncaster, 1985).

6.5 Heat Transfer through cylinder wall

This section explores the mechanisms governing heat transfer from the compressed gas inside the cylinder to the ambient air through the cylinder wall. The process involves convection between the gas and the cylinder wall, conduction through the cylinder wall, and convection from the outer wall surface to the surrounding air. The governing equations and principles are discussed for each mechanism.

6.5.1 Convective Heat Transfer from Gas to Cylinder Wall

As the gas is compressed within the cylinder, it undergoes adiabatic heating, creating a temperature difference between the gas and the inner surface of the cylinder wall. This gradient drives convective heat transfer, where the hot gas molecules move rapidly, colliding with the cooler surface of the metal. This process, known as convection, transfers heat through the movement of the gas. The faster-moving (higher temperature) gas molecules transfer some of their energy to the metal atoms upon collision. The heat transfer rate, $Q_{gas \rightarrow wall}$, in Watts, can be calculated by dividing the temperature difference between the gas and the wall by the thermal resistance of the cylinder, using the formula:

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

Where:

$Q_{gas \rightarrow wall}$ = Heat transfer rate [W]

h = convective heat transfer coefficient between gas and wall [$W/m^2 \cdot K$]

A = Surface area for heat transfer to occur [m^2]

T_{gas} = Temperature of the gas inside the cylinder [K]

T_{wall} = Temperature of the cylinder wall [K]

The convective heat transfer coefficient depends on factors such as the gas properties (thermal conductivity, viscosity), flow regime (laminar or turbulent), and the geometry of the cylinder (Rogers and Mayhew, 1992; Bejan, 2013).

6.5.2 Conduction Through the Cylinder Wall

Once heat is transferred from the gas to the cylinder wall, it moves through the wall via thermal conduction. The rate of heat transfer by conduction is governed by Fourier's Law of Heat Conduction:

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

$$\therefore Q = -kA \frac{T_2 - T_1}{x_{12}}$$

Where:

Q = heat transfer rate [W]

k = thermal conductivity of the material [W/mK]

A = area for heat transfer to occur [m^2]

$T_2 - T_1 = \text{Temperature difference [K]}$

$x_{12} = \text{spacial limits (Cylinder wall thickness)[m]}$

(Rogers & Mayhew, 1992, P.502)

In practice, the thermal conductivity of materials typically varies with temperature. However, for the sake of simplicity and to reduce computational complexity, a constant value for thermal conductivity will be assumed in this simulation.

6.5.3 Temperature change in the gas

When a hot gas comes into contact with a cooler cylinder wall, convective heat transfer takes place. This mechanism is described by Newton's Law of Cooling, which quantifies the rate of thermal energy transfer based on the temperature difference between the gas and the wall, as outlined earlier.

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

To calculate the temperature drop of the gas, the First Law of Thermodynamics is applied to a closed system, under the assumption that heat is transferred away primarily through convective mechanisms.

$$Q = m \cdot c_p \cdot \Delta T_{gas}$$

Combining the two equations results in:

$$h \cdot A \cdot (T_{gas} - T_{wall}) = m \cdot c_p \cdot \Delta T_{gas}$$

Solving for ΔT_{gas} :

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

Where:

$\Delta T_{gas} = \text{Change in gas temprature [K]}$

$h = \text{convective heat transfer coefficient between gas and wall [W/m}^2 \cdot \text{K]}$

$A = \text{Surface area for heat transter to occur [m}^2\text{]}$

$m_{gas} = \text{Mass of the gas in the cylinder [kg]}$

$c_p = \text{Specific heat capacity } \left[\frac{J}{kg \cdot K} \right]$

$T_{gas} = \text{Temperature of the gas inside the cylinder [K]}$

$T_{wall} = \text{Temperature of the cylinder wall [K]}$

(Incropera et al., 2007).

6.5.4 Time Discretization in Simulations (Explicit Euler Method)

To simulate the transient behavior of gas cooling accurately, it is essential to account for the progression of time. The core objective is to compute the change in gas temperature over discrete, known time intervals (Δt). This requires transforming the energy balance into a time-dependent differential equation. For convective heat transfer between the gas and the wall, the temperature evolution is governed by:

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

The change in temperature of the gas is approximated numerically using the explicit Euler method:

$$T_{gas}(t + \Delta t) = T_{gas}(t) - \frac{h \cdot A}{m_{gas} \cdot c_p} \cdot (T_{gas}(t) - T_{wall}) \cdot \Delta t$$

Where:

$T_{gas}(t)$ = gas temperature at the current time step [K]

$T_{gas}(t + \Delta t)$ = gas temperature at the next time step [K]

Δt = time step [Seconds]

h = convective heat transfer coefficient between gas and wall [$W/m^2 \cdot K$]

A = Surface area for heat transfer to occur [m^2]

m_{gas} = Mass of the gas in the cylinder [kg]

c_p = Specific heat capacity [$\frac{J}{kg \cdot K}$]

T_{wall} = Temperature of the cylinder wall [K]

(Chapra & Canale, 2015)

This allows the simulation to calculate the change in gas temperature due to convection to the cylinder wall over a given time step.

6.5.5 Temperature change in the cylinder wall

The MATLAB script shown in its entirety in appendix A calculates heat transfer due to conduction from the gas to the inner cylinder wall and the corresponding temperature change

in the wall using the first law of thermodynamics and Fourier's law of conduction simplified for lumped-parameter transient modelling.

The rate of heat conducted from the gas to the wall is calculated as:

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

The change in wall temperature is then calculated assuming the wall is a lumped thermal mass:

$$\Delta T_{wall} = \frac{Q_{gas \rightarrow wall} - Q_{wall \rightarrow ambient}}{m_{wall} \cdot c_{p,wall}}$$

(Chapra & Canale, 2015)

6.5.6 Heat loss to ambient air (convection)

The cylinder wall will lose heat via convection to the ambient air.

$$Q_{wall \rightarrow ambient} = \frac{T_{wall} - T_{ambient}}{R_{conv}}$$

Where:

Q = Heat transfer rate [W]

R_{conv} = Thermal resistance for convection $\left[\frac{W}{K}\right]$

$T_{ambient}$ = Temperature of the ambient air [K]

T_{wall} = Temperature of the cylinder wall [K]

(Chapra & Canale, 2015)

6.5.7 Wall temperature drop (convection to ambient)

The cylinder wall temperature will need to be calculated due to convective heat loss to ambient.

$$\Delta T_{wall} = \frac{Q_{wall \rightarrow ambient} \cdot \Delta t}{m_{wall} \cdot c_p}$$

Where:

ΔT_{wall} = Change in cylinder wall temprature [K]

$Q = \text{Heat transfer rate [W]}$

$\Delta t = \text{Change in time [Secomds]}$

$m_{\text{wall}} = \text{Mass of the cylinder wall [kg]}$

$c_p = \text{Specific heat capacity } \left[\frac{\text{J}}{\text{kg} \cdot \text{K}} \right]$

(Chapra & Canale, 2015)

7.0 Simulation Assumptions

This section will outline any assumptions made within the calculations that may affect the results and cause variations to real world outcomes.

7.1 Ideal gas behaviour

The ideal gas law is a fundamental equation used by scientists and engineers to relate pressure (P), volume (V) and temperature (T) of a gas with the amount of moles (n) along with the universal gas constant (R). The ideal gas law is expressed as $PV = nRT$. The ideal gas law is an amalgamation of 4 previously discovered relationships. Firstly Boyles Law (1662), describes an inverse relation between pressure and volume of a gas, meaning at a constant temperature if the gas pressure was to increase, the volume the molecules take up would decrease and vis versa.

Secondly Charles's Law (1787), relates volume and temperature of a gas at a constant pressure, meaning at a fixed pressure if the volume decreases, the temperature will decrease proportionally with the volume.

The third law is Gay-Lussac's Law (1808), describes the relation between pressure and temperature at a constant volume. The law states that pressure and temperature of a gas are directly proportional when the volume remains the same.

Lastly Avogadro's Law (1811) proposes that equal volumes of gases at equal temperature and pressures will contain the same number of molecules. Between the 1830s – 1850s $PV = nRT$ started appearing in scientific literature although it is not attributed to a single person.

Real gases deviate from ideal behaviour under high pressure and low temperature due to the presence of attractive and repulsive forces (Atkins & de Paula, 2014). At high pressures, the gas molecules are compressed closer together. At these close distances intermolecular forces become significant. Similarly, at low temperatures the gas molecules are moving very slowly, at these slow speeds the intermolecular forces are once again more prominent.

Another limitation of the ideal gas law is that it assumes the gas molecules have no volume and therefore occupy no space, in reality the molecules occupy a finite but measurable volume and again as the pressure increases and there are more and more molecules their volume becomes more significant (Atkins & de Paula, 2014).

7.2 No spatial variation in gas or wall temperature (lumped model)

This simulation uses a lumped parameter model to represent the thermal behaviour of the gas and cylinder wall during filling. In this approach, both the gas and the wall are assumed to have uniform temperature at each time step, and no spatial temperature gradients are modelled within either domain. This simplification allows the system to be represented using Ordinary Differential Equations (ODEs) rather than partial differential equations.

The simulation advances in discrete time steps using explicit time integration, where each variable is updated using its value from the previous time step. Although this model does not capture local temperature gradients, it provides a computationally efficient way to estimate thermal behaviour during gas filling and cooldown events. Such models are widely used in practical engineering applications where real-time predictions or system-level understanding is needed (Cengel and Boles, 2015; Moran and Shapiro, 2008).

7.3 Constant thermal properties (C_p , JT coefficient)

In the present simulation, the specific heat capacity at constant pressure (C_p) and the Joule-Thomson (JT) coefficient are assumed to be constant throughout the filling process. These properties are assigned fixed values based on typical conditions for the chosen gas at room temperature and moderate pressure, which is reasonable for engineering estimations in the absence of real gas property tables or full thermophysical libraries.

Although C_p and JT values vary with temperature and pressure, assuming them constant significantly simplifies the implementation and still provides useful insight into the thermal behaviour of the system. This approach is common in lumped thermal models and early-stage design simulations where computational speed and clarity are prioritized over detailed accuracy (Çengel and Boles, 2015; Moran and Shapiro, 2008).

7.4 Instant mixing of incoming and existing gas

The simulation assumes instantaneous and uniform mixing of the incoming argon with the existing gas in the cylinder at each time step. This simplifies the thermodynamic modelling by

treating the gas within the cylinder as a well-mixed control volume with a single, spatially uniform temperature and pressure at any point in time.

In reality, the filling process may involve jet penetration, entrainment, and temperature stratification, particularly in large or fast-filling cylinders (Timmerhaus and Flynn, 1989; Van Sciver, 2012). However, modelling these effects requires computational fluid dynamics (CFD) or multi-zone models, which are significantly more complex and computationally expensive.

The instantaneous mixing assumption is common in early design simulations and control models, where it provides a practical balance between physical fidelity and computational efficiency (Turns, 2006; Moran and Shapiro, 2008). It is especially reasonable when the filling process occurs over a moderate time scale and the flow is turbulent enough to ensure effective mixing within the cylinder.

7.5 1D heat transfer from gas → wall → ambient

The simulation assumes one-dimensional (1D) radial heat transfer from the internal gas to the cylinder wall and then to the ambient air. This assumption simplifies the transient thermal model while still capturing the essential physics of internal conduction and external convection.

These convective boundaries allow the simulation to capture cooling of the cylinder over time as it loses heat to the environment. Although real systems may experience multi-dimensional effects or radiative heat transfer at high temperatures, the 1D approximation is widely accepted for pressurised gas cylinders due to their high aspect ratio and radial temperature gradients dominating over axial or circumferential variations (Incropera et al., 2007; Çengel and Ghajar, 2015).

This approach offers a practical compromise between accuracy and computational cost, especially suitable for transient simulations involving gas compression and thermal response of thick-walled metal cylinders.

8.0 Code technical explanation

This section offers a comprehensive walkthrough and explanation of how the previously discussed mathematical and scientific principles are applied within the MATLAB script. Its purpose is to provide a step-by-step overview of the script's functionality while justifying the design choices made during its development.

For simplicity the script is displayed in its entirety in appendix A and is also attached as a separate file within the submission of this paper. This script line numbers are used within this section when referring to appendix A.

8.1 Script Details

Lines 1-9 of the MATLAB script shown in appendix A detail the following information using the MATLAB comment feature, this feature allows text to be added that is not execute in the code but is simply there to be read by the users or creator of the script.

- Title
- Details
- Author
- Last edited date

8.2 Clean the existing MATLAB workspace

The first executed commands are lines 10-12, these are 3 commands that are used to tidy the MATLAB workspace and prepare it for a new instance of the script to be executed. The semi colon after any executed code means that it will not show on within the command window, this is used to create a neater environment, only text and values designed to be displayed in the command window are shown.

- `clc`
 - This command removes any text left from previous scripts or user inputs left in the command window
- `clear`
 - Erases all variables and values from the workspace, essentially clearing the stored data within MATLAB
- `Close all`
 - Closes any figures left over from previous scripts

(MathWorks, 2025)

8.3 User defined variables

This section specifies the simulation parameters that are configurable by the user to tailor the model to different scenarios. These parameters are defined directly within the script rather than as interactive command window inputs. This design choice mitigates the risk of user input errors and streamlines the workflow, as typical simulation variations generally involve modifying only a limited subset of variables, such as inlet temperature or pressure. By embedding the parameters in the script, consistency and ease of use are enhanced without compromising flexibility.

Lines 14-38 set the values for the following parameters in the following units:

Table 1 User defined variables (U'Dell, 2025)

Variable Name	Description	Unit
dt	Time step	Seconds
V	Cylinder volume	Litres
P1	Pressure inside the cylinder at simulation start	Bar
T1	Gas temperature inside the cylinder at simulation start	°C
T_p	Gas temperature from pump supply	°C
P_i	Pressure of pump supply	Bar
P_t	Target pressure of the gas inside the cylinder at end of simulation	Bar
T_t	Target temperature of the gas inside the cylinder at end of simulation	°C
T_t_p	Factor of target temperature	NA
t_flow	Time to full pump flow	Seconds
time_max	Maximum simulated time, used in case inputs do not allow target mass to be reached.	Seconds
T_amb_c	Ambient temperature	°C
T_wall	Initial cylinder wall temperature	°C
Cyl_count	Cylinders per pump flow rate	NA
d_outer	Outer diameter of the cylinder	m
thickness	Thickness of the cylinder	m
rho_wall	Density of cylinder material	kg/m^3
cp_wall	Specific heat capacity of the cylinder material	$J/kg \cdot K$
h_conv	Convection coefficient (pre set for free convection)	$W/m^2 \cdot K$

The cylinder and cylinder valve used for the default code is provided in appendix D.

The user can adjust any of these values to set the simulation to the desired scenario, the default values are for the following scenario.

A cylinder with 1 bar of the chosen gas stored within it at 20°C, the ambient temperature is 20°C and the incoming gas from the pump is 20°C. The target pressure of the cylinder is 230 bar at 20°C. The flow from the pump has a back pressure of 320 bar and a temperature of 20°C. The cylinder also has an initial wall temperature of 20°C.

The cylinder properties are set to chromium-molybdenum alloy steel and the convection coefficient is set to $10 \text{ W/m}^2 \cdot \text{K}$, this is the respective value for free convection inside a cylinder or pipe. The cylinder has an internal volume of 50 litres.

The default time step is 0.1 seconds with a maximum simulated time of 36000 seconds (10 hours). Lastly the pump supply is divided between 15 cylinders.

8.4 User prompts

Lines 41–79 prompt the user to select from various buttons. The selections made determine whether the simulation includes a gas cooldown after filling, as well as which gas, oxygen, argon, or nitrogen, is used in the simulation.

The menu function is used to display a window within MATLAB that has buttons as responses. The menu function stores a numerical response to a variable when a button is selected.

The first user prompts asks the user to “Confirm all variable have been checked” or “cancel simulation”. A simple if statement is used in line 45–48 to check the response and if cancel simulation is selected then the simulation ends by executing the return function that simply returns control of the MATLAB environment back to the user and ends any running functions (MathWorks, 2025).

The next choice for the user is if they would like to simulate the post fill cooldown, the logic for this is explained in a later section.

Lastly the gas type is selected by the user. The switch and case functions are used to store the variable for each gas type. Using these functions frees up memory space and make the script more efficient instead of storing eh variable values for each gas type on every run on the selected gas values are stored in memory (MathWorks, 2025).

The cooldown option simply continues the simulation until the desired target temperature is reach (target temperature is multiplied by the factor selected in the user inputs).

The following variables are stored for each gas type;

Table 2 User prompts (U'Dell, 2025)

Variable Name	Description	Unit
Gas_Name	Name of the gas	NA
JT	Joule-Thomson coefficient	$^{\circ}\text{C}/\text{MPa}$
Gamma	Adiabatic index for the gas	NA
m_mass	Molar mass of the gas	kg/mol
M	Mass flow rate from the pump	kg/hr

The properties of the gases are provided in Appendix B, while the corresponding mass flow rates for each gas are detailed in Appendix C.

8.5 Conversions to SI units and constants

The calculations performed by the script necessitate that all parameter values be expressed in SI units. However, engineers often work with a variety of unit systems depending on regional or industry-specific conventions. Consequently, some user inputs may need to be converted to SI units to ensure consistency and accuracy in computation.

The following variables are converted to SI units in lines 81-90.

Table 3 SI Conversion calculations (U'Dell, 2025)

Variable Name	Description	Conversion calculation
V	Volume of the cylinder is converted from Litres to cubic metres	$V/1000$
P1	Pressure in the cylinder is converted from bar to Pascals	$P1 * 100,000$
T1	Temperature of the gas is converted from degrees Celsius to Kelvin	$T1 + 273.15$
M	Mass flow rate is converted to kg per second and divided for 1 cylinder.	$M/3600$ $/\text{Cyl_count}$

P_i, P_t, T_t, T_p and T_amb are also converted to the appropriate SI units.

The universal gas constant is stored within a usable variable at this stage on line 93.

Table 4 Universal gas constant

Variable Name	Description	Unit
R	Universal gas constant = 8.314	$J/mol/K$

8.6 Cylinder calculations

This section of the script performs various calculations on the cylinder properties stored earlier in the script. This section calculates the following variables using the following equations (MathWorks, 2025).

Table 5 Cylinder calculations (U'Dell, 2025)

Variable Name	Description/ Calculation	Unit
d_inner	Inner diameter of the cylinder $= d_{outer} - (2 \cdot thickness)$	m
L_cyl	Approximate length of the cylinder $= V / (\pi \cdot (d_{inner}/2)^2)$	Meters
V_wall	Volume of the cylinder wall $= \pi \cdot (d_{outer}^2 - d_{inner}^2) / 4 \cdot L_{cyl}$	m^3
m_wall	Mass of the cylinder wall $= \rho_{wall} \cdot V_{wall}$	Kg
T_wall	Temperature of the wall is converted to Kelvin by adding 273.15	Kelvin
A_outer	Outer surface area of the wall $= \pi \cdot d_{outer} \cdot L_{cyl}$	m^2
R_conv	The convective thermal resistance $= \frac{1}{h_{conv} \cdot A_{outer}}$	K/W

8.7 Target and initial values

Lines 107–111 initialize several key variables prior to the execution of any loops. This ensures that the code consistently begins with the necessary predefined values, providing a reliable starting point for subsequent computations.

Table 6 Target and Initial values (U'Dell, 2025)

Variable Name	Description	Value	Unit
m_total	Initial mass of gas inside the cylinder	$= \frac{P1 \cdot V \cdot m_{mass}}{R \cdot T1}$	Kg
time	Simulated time	0	Seconds
t_mass_filled	Simulated time of mass being filled, used to differentiate between filling time and cooldown time.	0	seconds

8.8 Log generation

Lines 112–119 establish the data logs used to record variable values at each time step. These logs are later utilized for plotting the results at the end of the script. Since the number of time steps is not predetermined, the logs are initialized as dynamically sized matrices without fixed dimensions.

Table 7 Log generation (U'Dell, 2025)

Log Name	Description
Time_log	Used to log the simulated time
T_in_JT_log	Captures the inlet gas temperature due to the Joule-Thomson effect
T_log	Captures the compressed mixed gas temperature
P_log	Stores the cylinder pressure at the end of the time step
m_total_log	Stores the total mass in the cylinder at the end of each time step
m_added_log	Stores the mass being added to the cylinder at each time step
T_wall_log	Stored the temperature of the cylinder wall at the end of each time step

8.9 Simulation while loop

The core logic of the program is encapsulated within a while loop, which repeatedly executes its block of code as long as the loop's condition evaluates to True. The loop condition is evaluated at the beginning of each iteration. Execution continues until the condition becomes False or a break statement is encountered, which immediately terminates the loop regardless of the condition (MathWorks, 2025).

The while loop is contained in lines 122-208.

8.9.1 While loop condition

The while loop condition is defined as $\text{time} < \text{time_max}$, which ensures that the loop continues to execute as long as the simulated time remains below the maximum time specified by the user-defined variable time_max (MathWorks, 2025).

8.9.2 Initial while variable updates (time & m_added)

The initial lines of execution (lines 123 and 124) update the simulation time and accumulated mass. The current time is incremented by adding the time step dt to the previous time value, while the incremental mass is calculated by multiplying the time step dt by the mass flow rate M .

8.9.3 End condition checks

There are three conditions that can terminate the simulation (i.e., exit the while loop). The first is when the loop condition ($\text{time} < \text{time_max}$) is no longer satisfied. The second and third termination criteria depend on whether the cooldown effect is enabled.

If cooldown is not enabled, the simulation ends when the total mass of gas in the cylinder reaches the target mass, defined as the mass corresponding to the target pressure and temperature.

If cooldown is enabled, the simulation continues beyond the target mass condition and only terminates once both the target mass is reached and the internal gas temperature falls within the specified tolerance range defined by the user.

These conditions are encased within if statements in lines 125-136.

8.9.4 Mass flow rate linear ramp up

Lines 138–141 compute the mass increment added to the cylinder during the current time step. As previously noted, the mass flow rate increases linearly to simulate the gradual

opening of the fill valve. This ramp-up behaviour is implemented to reflect more realistic valve dynamics during the initial filling phase.

This is achieved by using the following calculation and if statement.

if $T_{wall} \geq 65 + 273.15$

then

$$m_{added} = \left(\frac{time}{t_{flow}} \right) \cdot m_{added}$$

8.9.5 Other filling rate checks

Once the filling rate is determined, either through the linear ramp-up calculation or the initial mass addition, several safety and operational checks are performed. First, if the outer cylinder wall temperature exceeds the safety threshold of 65 °C, filling must be halted. Second, if the internal cylinder pressure exceeds the supply pressure, flow would either cease or potentially reverse, so filling is also stopped in this case. Finally, if the mass of gas within the cylinder reaches or exceeds the target mass, filling is terminated.

It is important to note that no gradual ramp-down of the flow rate is implemented; instead, the flow rate is instantaneously set to zero when any of these stopping conditions are met. These conditions are enforced through a series of if statements spanning lines 143–159 (MathWorks, 2025).

8.9.6 Step 1: Inlet gas cooling via Joule-Thomson effect

Lines 161–169 compute the temperature of the incoming gas due to the Joule-Thomson (JT) cooling effect, as described in Section 5.2 of this paper. The JT effect occurs when a gas undergoes a rapid expansion from a high-pressure region to a lower-pressure region, resulting in a temperature drop.

The temperature change is calculated using the equation provided in Section 5.2, with the resulting values stored in both degrees Celsius and Kelvin in separate variables. This calculation is enclosed within an if statement that ensures it is only executed when there is active flow into the cylinder. If no flow is occurring, the temperature variables are assigned NaN (Not a Number), a MATLAB placeholder used to represent undefined or unrepresentable values, which also prevents them from appearing in visual plots (MathWorks, 2025).

8.9.7 Step 2: Energy balance (mixing of gas)

Lines 171–174 implement the energy balance equation outlined in Section 5.3 to compute the temperature of the mixed gas, storing the result in the variable T_{mixed} . This temperature is determined by dividing the total energy of the system by the total mass of the gas mixture.

8.9.8 Step 3: Pressure update from ideal gas rule

Once the temperature of the mixed gas has been determined, a corresponding change in pressure occurs. According to the ideal gas law, if the volume remains constant—as is the case with a rigid cylinder—a change in temperature results in a proportional change in pressure (Cengel and Boles, 2015). The updated pressure is calculated using the ideal gas equation, with the result stored in $P2$ (in Pascals) and $P2_b$ (in bar).

$$P2 = \frac{m_{total} \cdot R \cdot T_{mixed}}{m_{mass} \cdot V}$$

$$P2_b = \frac{P2}{100000}$$

8.9.9 Step 4: Compression heating

Following the calculation of the new pressure from the mixed gas temperature, the next step is to determine the temperature rise due to adiabatic compression. Adiabatic compression occurs when a gas is compressed rapidly enough that no heat is exchanged with the surroundings, causing the internal energy, and thus the temperature, of the gas to increase (Cengel and Boles, 2015). Lines 180–184 perform this calculation, storing the resulting temperature in both Celsius and Kelvin. This section also updates the pressure and temperature variables in preparation for the next iteration of the while loop.

$$T2 = T_{mixed} \cdot \left(\frac{P2}{P1} \right)^{\frac{\gamma-1}{\gamma}}$$

$$T1 = T2$$

$$T1_c = T1 - 273.15$$

$$P1 = P2$$

8.9.10 Step 5: Heat loss from gas to wall

The heat transfer equation outlined in Section 5.5 is employed to determine the rate of convective heat loss from the internal gas to the cylinder wall. Subsequently, the corresponding change in gas temperature resulting from this convective heat transfer is

calculated (Incropera et al., 2007). The equations used within the script are presented below. Lines 186-189 in the MATLAB script execute these calculations using a basic variable value update command.

$$Q_{loss} = \frac{T1 - T_{wall}}{R_{conv}}$$

$$dt_{gas\ loss} = \frac{Q_{loss} \cdot dt}{m_{total} \cdot cp_{wall}}$$

$$T1 = T1 - dt_{gas\ loss}$$

8.9.11 Step 6: Wall temperature update

Once the convective heat loss from the internal gas to the cylinder wall has been determined, the resulting change in wall temperature can be evaluated using the equations provided below.

$$dT_{wall\ gain} = \frac{Q_{loss} \cdot dt}{m_{wall} \cdot cp_{wall}}$$

$$T_{wall} = T_{wall} + dT_{wall\ gain}$$

8.9.12 Step 7: Heat loss from wall to ambient

The final component of the heat transfer analysis involves calculating the rate of heat loss from the cylinder wall to the ambient air, followed by the evaluation of the resulting change in wall temperature.

$$Q_{wall\ loss} = \frac{T_{wall} - T_{amb}}{R_{conv}}$$

$$dT_{wall\ loss} = \frac{Q_{wall\ loss} \cdot dt}{m_{wall} \cdot cp_{wall}}$$

$$T_{wall} = T_{wall} - dt_{wall\ loss}$$

8.9.13 Logging the data

After computing all the necessary variables for the current time step in the thermodynamic simulation, the results are stored in the previously defined log matrices. This is achieved by indexing the next available position in each matrix, specifically by referencing the last element in the first row and incrementing its column index by one. The MATLAB end keyword is used to identify the final column index, allowing data to be appended sequentially.

Table 8 Log data input (U'Dell, 2025)

Log Name	Description/ Calculation	Unit
Time_log	Log for current time step	Seconds

T_in_JT	Log for incoming gas temperature due to JT effect	°C
T_log	Log for compressed gas temperature	°C
P_log	Log for pressure of mixed gas in the cylinder	Bar
m_total_log	Log for total mass in the cylinder, including added gas	Kg
m_added_log	Log for mass of the gas being added to the cylinder	Kg
T_wall_log	Log for cylinder wall temperature	°C

8.10 Results plot

Once the condition for the while loop is no longer satisfied, or the break command has been triggered during execution, the data stored in the log matrices is visualised in a single MATLAB figure. In MATLAB, a figure serves as a graphical interface for presenting data through plots, charts, and other visual representations. The subplot function is utilised to display five individual plots within a single figure window, allowing the user to observe all relevant data simultaneously and draw correlations without the need to toggle between multiple windows. The following graphs are created (MathWorks, 2025).

- Simulated time (s) Vs Inlet gas temperature (JT effect) (°C)
- Simulated time (s) Vs Compressed gas temperature (°C)
- Simulated time (s) Vs Compressed gas pressure (bar)
- Simulated time (s) Vs Compressed gas mass (kg)
- Simulated time (s) Vs Mass added per time step (kg)
- Simulated time (s) Vs Cylinder wall temperature (°C)

In addition to the graphical outputs shown in Figure 1, the simulation code also displays key summary data in the MATLAB Command Window using the fprintf function. This function enables the formatted display of text combined with variable values, providing a clear summary of results. The data output includes the selected gas type, fill rate per cylinder, time to reach the target mass, cooldown time to the desired temperature (if cooldown is enabled), total simulation duration, maximum and minimum compressed gas temperatures, maximum and minimum cylinder wall temperatures, maximum compressed gas pressure, and the final gas pressure and temperature at the conclusion of the simulation (MathWorks, 2024).

9.0 Simulation results

This section presents the results obtained from a series of simulations conducted using the developed code. It begins by outlining the input parameters used in each case, followed by a detailed presentation of the corresponding graphical and numerical outcomes.

9.1 Simulations 1 – 6

Simulations 1 through 6 utilize a standard set of input parameters, with all initial temperature values set to 20 °C. Each simulation models the filling of a 230 bar cylinder from a supply line at 320 bar. The inlet flow ramps up to its maximum over 60 seconds. For simulations involving cooldown, the target temperature is defined as 1.1 times the baseline, corresponding to 22 °C. All remaining parameters are summarized in Figure 6 below.

```
% --- Update variables in this section ---
% --- User Variables ---
dt = 0.1;           % Time step in seconds
V = 50;             % Volume of cylinder in liters
P1 = 1;             % Pressure in cylinder at start of fill in bar
T1 = 20;            % Gas temperature in cylinder in Celsius
T_p = 20;           % Gas temperature from the pump in Celsius
P_i = 320;          % Pressure of pump flow in bar
P_t = 230;          % Target pressure of the gas in cylinder in bar
T_t = 20;           % Target temperature of the gas in cylinder in Celsius
T_t_p = 1.1;        % Target temperature percentage (1.5 = 50% over target, eg 20 deg c target would = 30 deg c)
t_flow = 60;        % Time to full pump flow in seconds
time_max = 36000;   % Max simulation time in seconds
T_amb_c = 20;       % Ambient temperature in Celcius
T_wall = 20;        % Initial cylinder wall temprature Celcius
Cyl_count = 15;     % Cylinders per pump flow rate

% --- Cylinder properties chromium-molybdenum alloy steel ---
d_outer = 0.228;     % Outer diameter in meters
thickness = 0.006;   % Wall thickness in meters
rho_wall = 7850;     % Density of chrome moly steel (kg/m³)
cp_wall = 460;       % Specific heat (J/kg·K)
h_conv = 10;         % Convection coefficient (W/m²·K)
```

Figure 6 Simulation 1 Input parameters (U'Dell, 2025)

9.1.1 Simulation 1 – Oxygen no cooldown

In this simulation, the cooldown effect was disabled, and oxygen was selected as the filling gas.

```
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)
Total simulated time 504.30 seconds (8.41 minutes, 0.14 hours)
Maximum gas temperature: 57.97 deg C
Minimum gas temperature: 20.00 deg C
Maximum cylinder wall temperature: 24.48 deg C
Minimum cylinder wall temperature: 20.00 deg C
Maximum Gas Pressure: 259.82 bar
Final Gas Pressure: 259.82 bar
Final Gas Temperature: 57.97 deg C
```

Figure 7 Simulation 1 Outputted command window results (U'Dell, 2025)

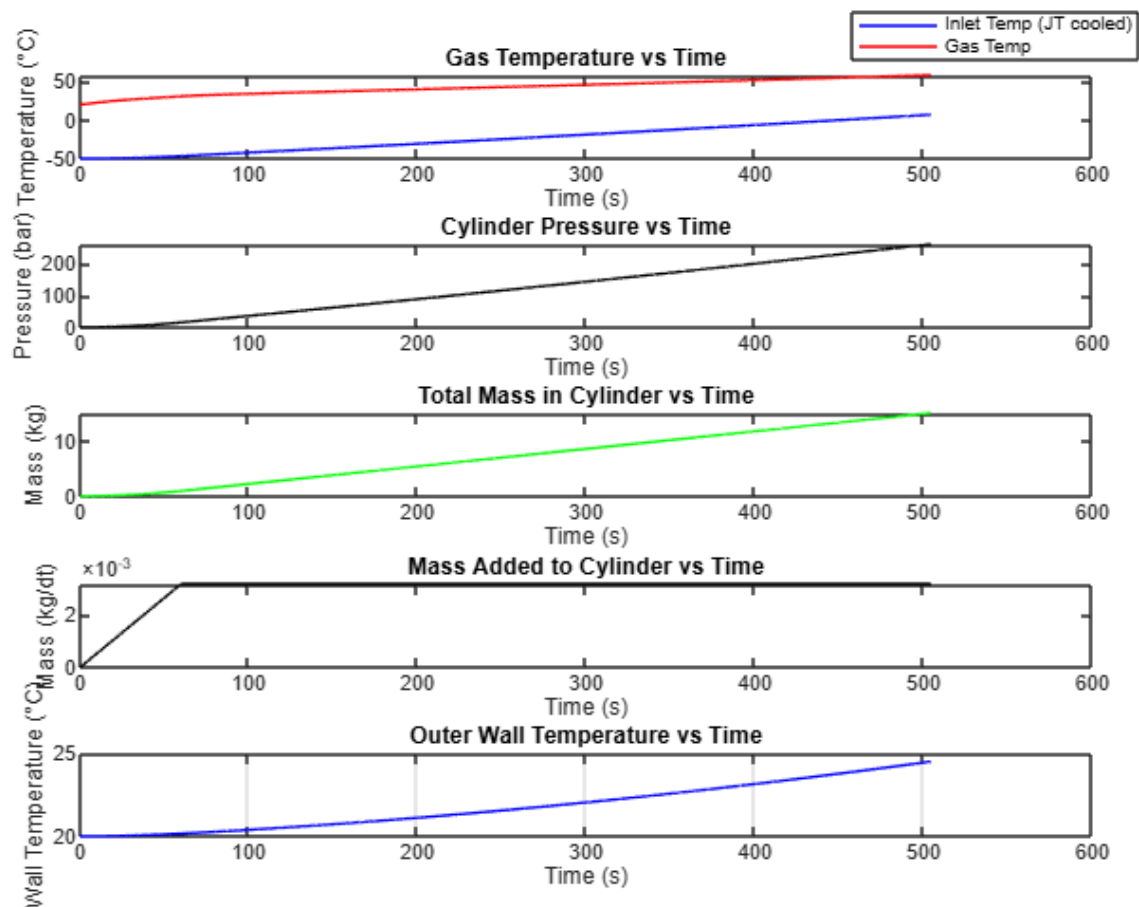


Figure 8 Simulation 1 Graphical results (U'Dell, 2025)

9.1.2 Simulation 2 – Oxygen with cooldown

In this simulation, the cooldown effect was enabled, and oxygen was selected as the filling gas.

```

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
    
```

Figure 9 Simulation 2 Outputted command window results (U'Dell, 2025)

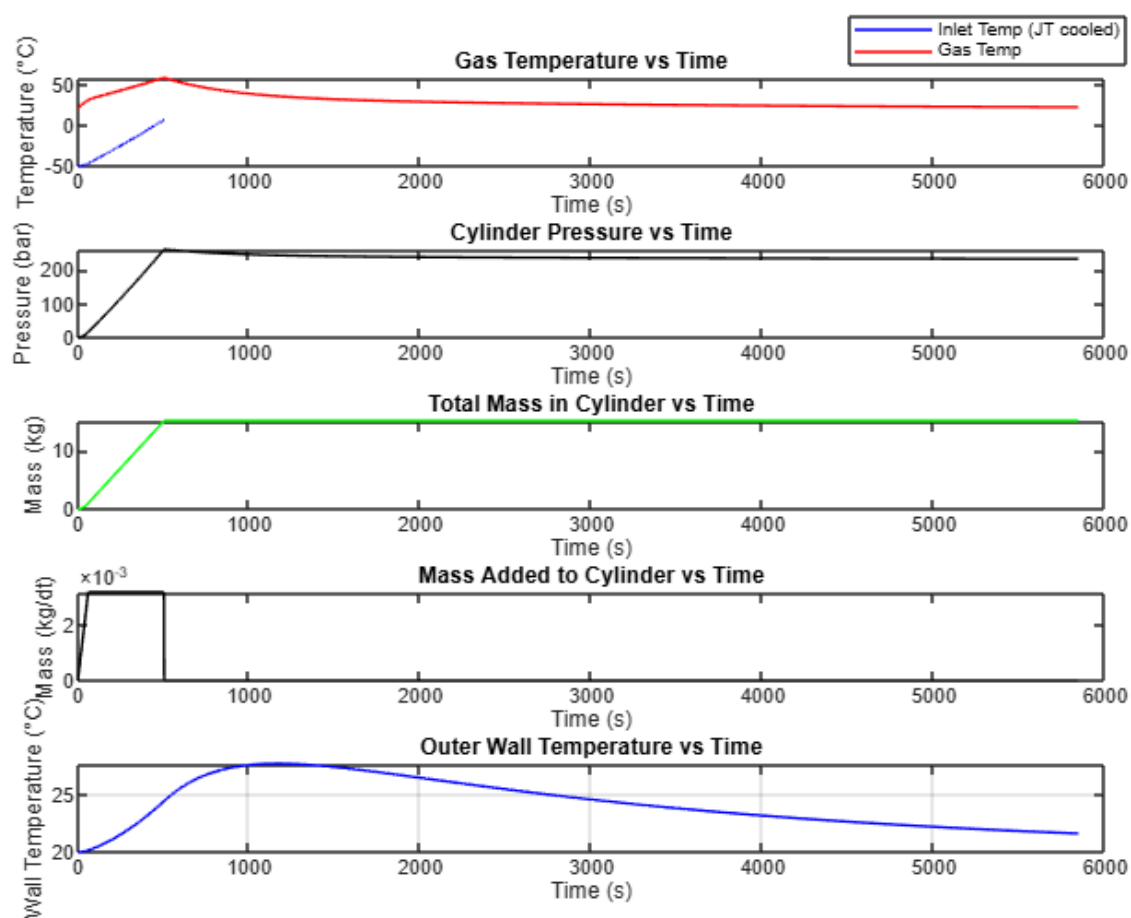


Figure 10 Simulation 2 Graphical results (U'Dell, 2025)

9.1.3 Simulation 3 – nitrogen no cooldown

In this simulation, the cooldown effect was disabled, and nitrogen was selected as the filling gas.

```

Gas selected: Nitrogen
Fill rate per cylinder: 0.0224 kg/s
Time to reach required mass of 13.22 kg: 617.90 seconds (10.30 minutes, 0.17 hours)
Total simulated time 617.90 seconds (10.30 minutes, 0.17 hours)
Maximum gas temperature: 47.21 deg C
Minimum gas temperature: 19.47 deg C
Maximum cylinder wall temperature: 22.93 deg C
Minimum cylinder wall temperature: 19.99 deg C
Maximum Gas Pressure: 251.35 bar
Final Gas Pressure: 251.35 bar
Final Gas Temperature: 47.21 deg C
    
```

Figure 11 Simulation 3 Outputted command window results (U'Dell, 2025)

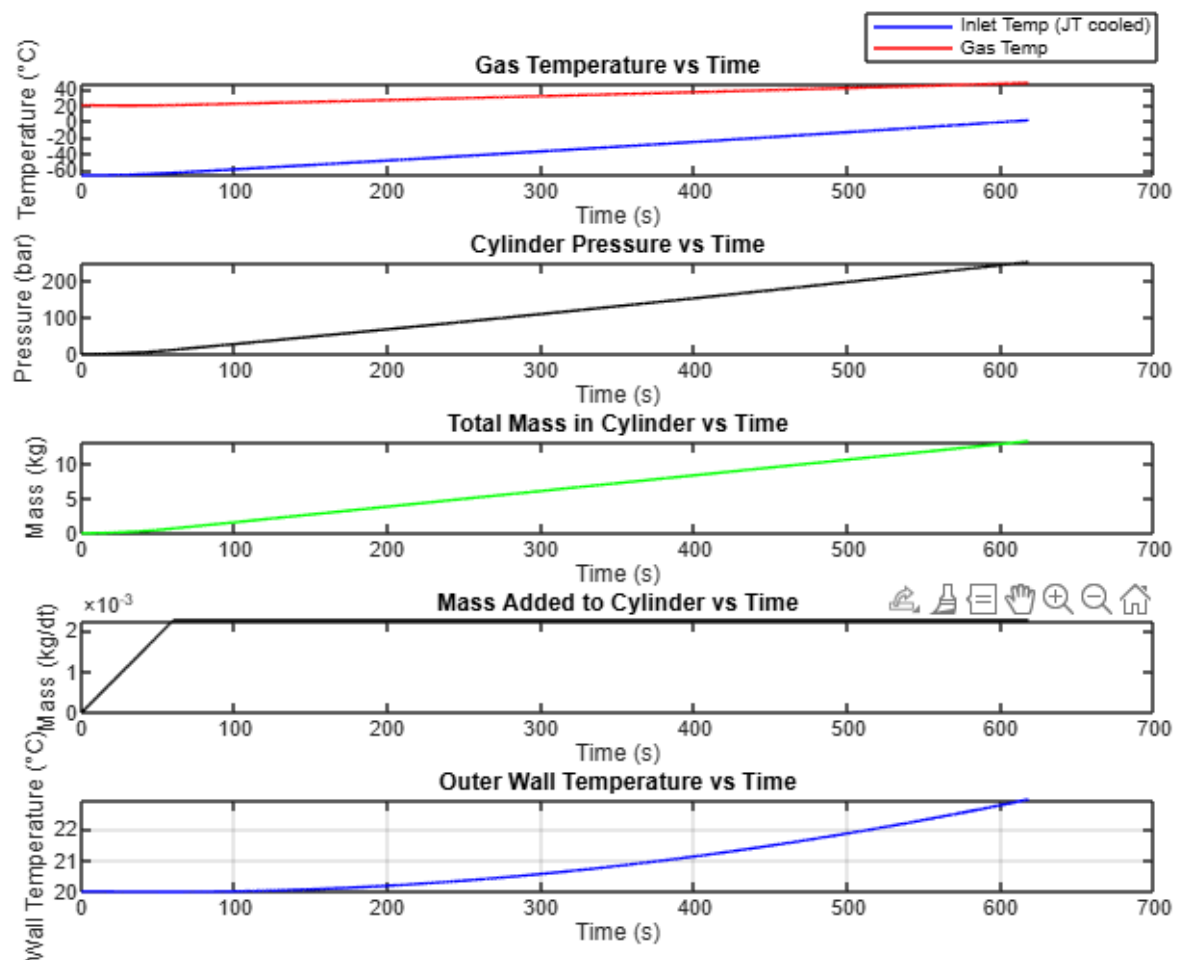


Figure 12 Simulation 3 Graphical results (U'Dell, 2025)

9.1.4 Simulation 4 – nitrogen with cooldown

Figure 13 Simulation 4 Input parameters (U'Dell, 2025)

In this simulation, the cooldown effect was enabled, and nitrogen was selected as the filling gas.

```

Gas selected: Nitrogen
Fill rate per cylinder: 0.0224 kg/s
Time to reach required mass of 13.22 kg: 617.90 seconds (10.30 minutes, 0.17 hours)
Time to cool down to 22 deg C: 3991.70 seconds (66.53 minutes, 1.11 hours)
Total simulated time 4609.60 seconds (76.83 minutes, 1.28 hours)
Maximum gas temperature: 47.21 deg C
Minimum gas temperature: 19.47 deg C
Maximum cylinder wall temperature: 25.16 deg C
Minimum cylinder wall temperature: 19.99 deg C
Maximum Gas Pressure: 251.36 bar
Final Gas Pressure: 231.58 bar
Final Gas Temperature: 22.00 deg C
    
```

Figure 14 Simulation 4 Outputted command window results (U'Dell, 2025)

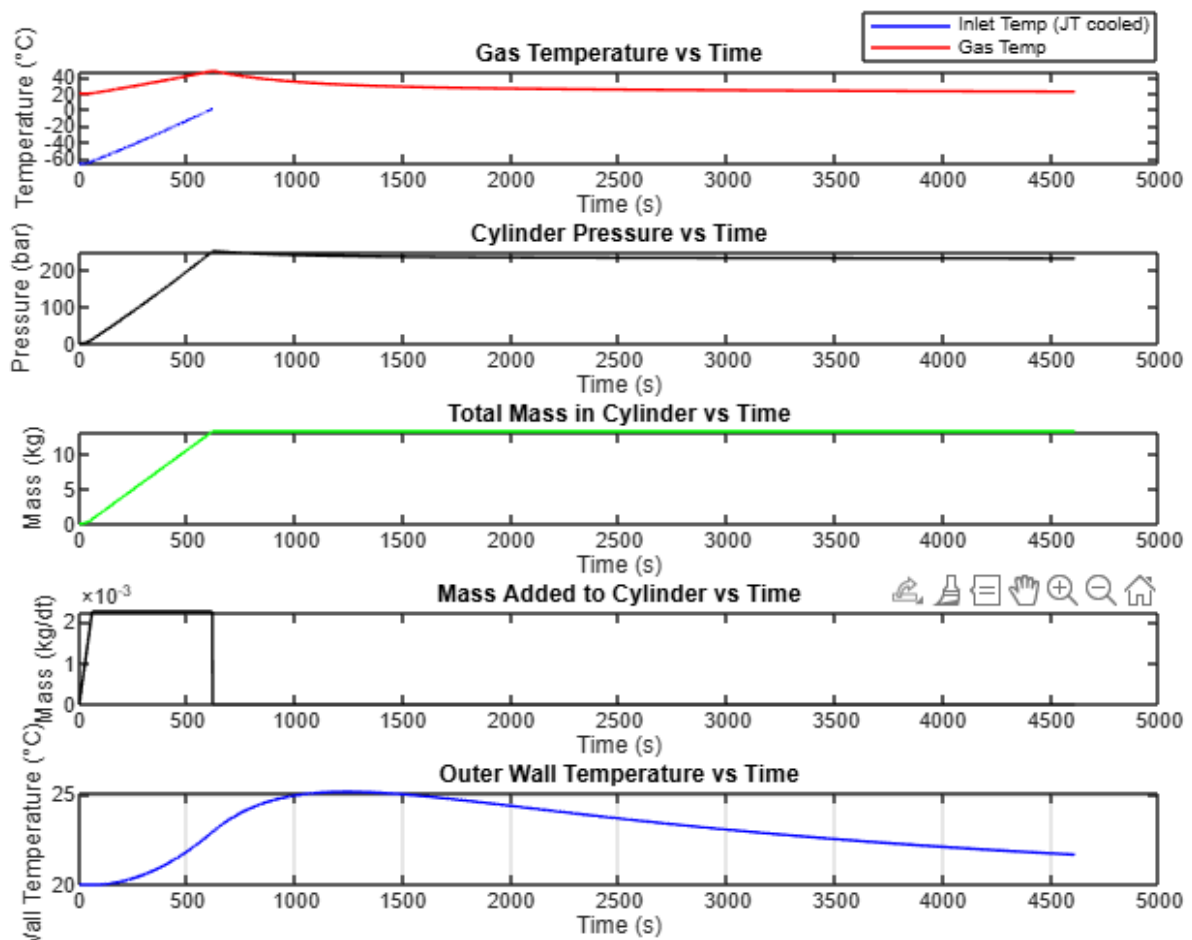


Figure 15 Simulation 4 Graphical results (U'Dell, 2025)

9.1.5 Simulation 5 – argon no cooldown

In this simulation, the cooldown effect was disabled, and argon was selected as the filling gas.

```
Gas selected: Argon
Fill rate per cylinder: 0.0388 kg/s
Time to reach required mass of 18.85 kg: 514.30 seconds (8.57 minutes, 0.14 hours)
Total simulated time 514.30 seconds (8.57 minutes, 0.14 hours)
Maximum gas temperature: 62.49 deg C
Minimum gas temperature: 5.47 deg C
Maximum cylinder wall temperature: 22.18 deg C
Minimum cylinder wall temperature: 19.25 deg C
Maximum Gas Pressure: 263.34 bar
Final Gas Pressure: 263.34 bar
Final Gas Temperature: 62.49 deg C
```

Figure 16 Simulation 5 Outputted command window results (U'Dell, 2025)

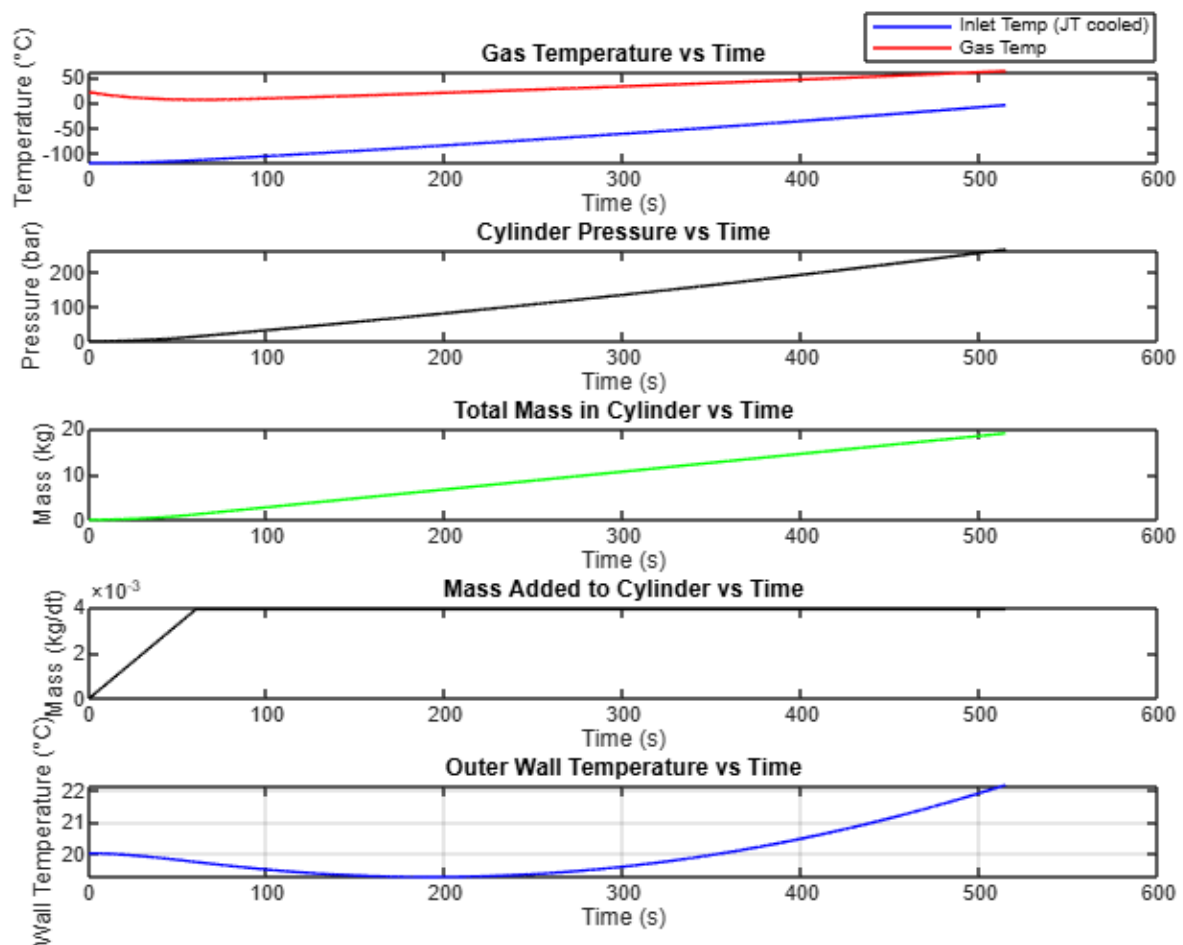


Figure 17 Simulation 5 Graphical results (U'Dell, 2025)

9.1.6 Simulation 6 – argon with cooldown

```
Gas selected: Argon
Fill rate per cylinder: 0.0388 kg/s
Time to reach required mass of 18.85 kg: 514.30 seconds (8.57 minutes, 0.14 hours)
Time to cool down to 22 deg C: 5346.60 seconds (89.11 minutes, 1.49 hours)
Total simulated time 5860.90 seconds (97.68 minutes, 1.63 hours)
Maximum gas temperature: 62.50 deg C
Minimum gas temperature: 5.47 deg C
Maximum cylinder wall temprature: 27.10 deg C
Minimum cylinder wall temprature: 19.25 deg C
Maximum Gas Pressure: 263.37 bar
Final Gas Pressure: 231.59 bar
Final Gas Temperature: 22.00 deg C
```

Figure 18 Simulation 6 Outputted command window results (U'Dell, 2025)

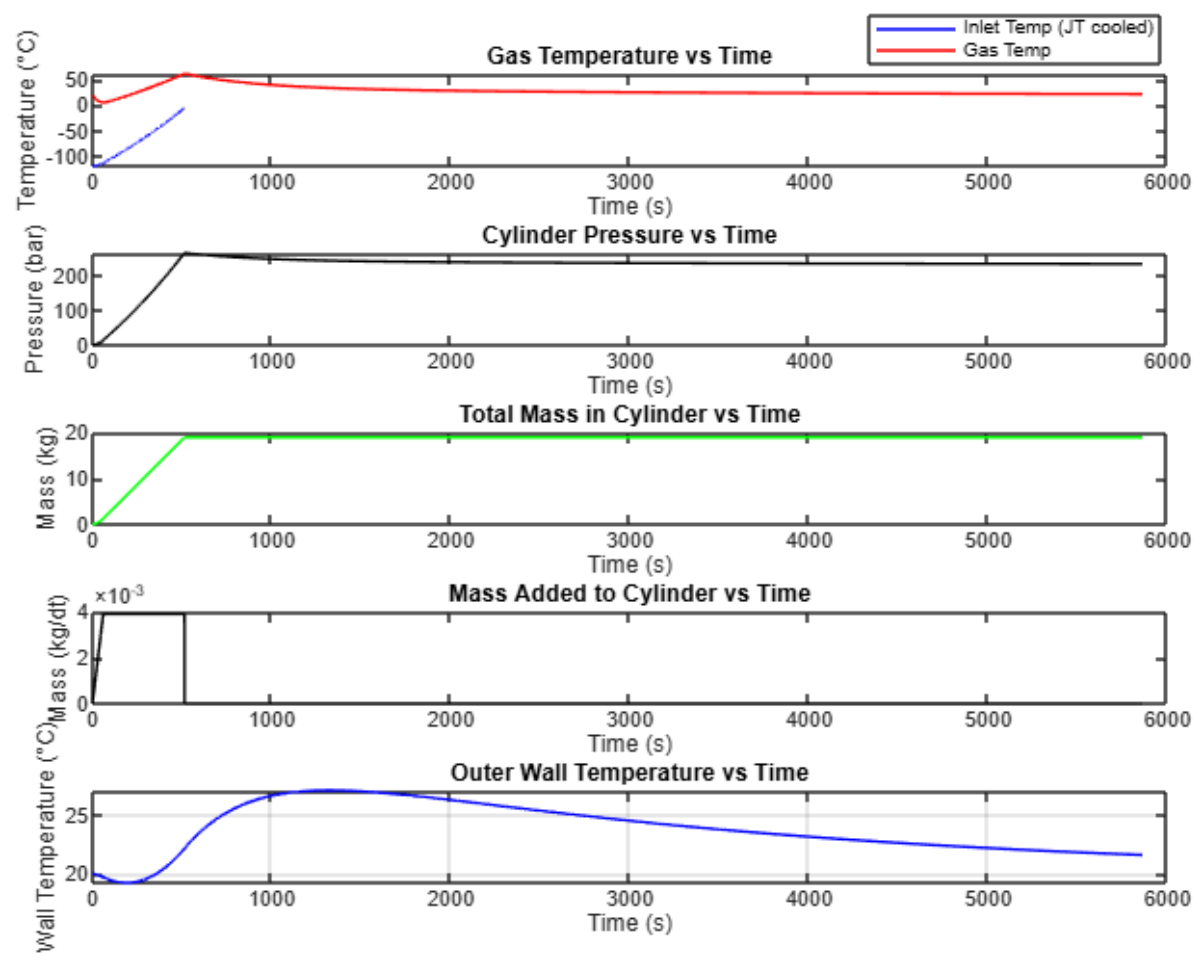


Figure 19 Simulation 6 Graphical results (U'Dell, 2025)

9.2 Simulations 1 – 6 results discussion.

The results from simulations 1-6 have been summarised in the below table.

Simulation number	Gas	cooldown	Fillingtime (S)	Cooldown time (S)	Max gas temp (deg C)	Min gas temp (deg C)	Max cyl temp (deg C)	Min cyl temp (deg C)	Max gas pressure (bar)	Final gas pressure (bar)	Final gas temp (deg C)		
1	O2	N	504.30		57.97	20.00	24.48	20.00	259.82	259.82	57.97		
2	O2	Y	504.30	5338.60	57.97	20.00	27.73	20.00	259.83	231.61	22.00		
3	N2	N	617.90		47.21	19.47	22.93	19.99	251.35	251.35	47.21		
4	N2	Y	617.90	3991.70	47.21	19.47	25.16	19.99	251.36	231.58	22.00		
5	Ar	N	514.30		62.49	5.47	22.18	19.25	263.34	263.34	62.49		
6	Ar	Y	514.30	5346.60	62.50	5.47	27.10	19.25	263.37	231.59	22.00		

Figure 20 Simulations 1-6 Results summary (U'Dell, 2025)

As shown in Figure 20, the cooldown phase accounts for the majority of the total cylinder filling time, particularly for argon and oxygen, where it exceeds 5,000 seconds (approximately 1.4 hours). During this period, the hot, compressed gas gradually cools through convective heat transfer to the inner cylinder wall, which in turn dissipates the heat to the surrounding ambient air via external convection. Among the three gases, nitrogen exhibits the shortest cooldown duration, indicating more efficient thermal equilibration. In contrast, argon and oxygen require significantly longer cooldown times, with argon taking slightly longer than oxygen, likely due to differences in their thermophysical properties such as thermal conductivity and specific heat capacity (Incropera et al., 2007).

Argon exhibits the greatest reduction in final gas temperature, which can be attributed to the Joule-Thomson (JT) cooling effect. As the argon expands through the filling orifice, its temperature drops significantly due to the JT effect. When this colder incoming gas mixes with the existing warmer gas in the cylinder, the resulting temperature of the gas mixture decreases substantially, reaching a minimum of approximately 5.47 °C. This temperature drop reduces the internal temperature, highlighting the strong influence of the JT effect during high-pressure argon filling (Incropera et al., 2007).

10.0 Considerations for future iterations of the script

10.1 Non-Ideal gas behaviour

The current MATLAB script models the thermodynamic behaviour of the gas during cylinder filling using the ideal gas law, which assumes that intermolecular forces and the volume occupied by gas molecules are negligible. While this assumption simplifies calculations and is reasonably accurate at low pressures and moderate temperatures, it becomes increasingly inaccurate under high-pressure conditions, such as those encountered during gas cylinder filling systems, where gas molecules are closely packed, and real gas effects become significant (Çengel and Boles, 2015).

Neglecting non-ideal behaviour can lead to discrepancies in predicted values of temperature, pressure, and density, particularly in the later stages of filling. For example, the ideal gas law may underestimate the pressure rise or overestimate the gas temperature due to its linear assumptions. In reality, gas compressibility, non-linear heat capacities, and intermolecular interactions affect these parameters, and their exclusion may compromise the fidelity of the simulation (Van Wylen et al., 1994).

To enhance the accuracy of future iterations of the model, the implementation of a real gas Equation Of State (EOS) could be implemented. Common models such as the van der Waals, Redlich-Kwong, or Peng-Robinson EOS could be incorporated to account for non-ideal behaviour. These equations introduce correction factors for molecular volume and attraction forces, offering more realistic predictions, especially at high pressures (Reid, Prausnitz and Poling, 1987). Integration of real gas properties could be achieved by referencing thermodynamic property tables or libraries such as NIST REFPROP or CoolProp (Bell et al., 2014), or by implementing a real gas EOS directly within the MATLAB environment.

Moreover, using temperature- and pressure-dependent values for specific heat capacity (C_p) and enthalpy would further improve the thermodynamic accuracy. This would allow the simulation to capture the non-linear response of the gas to compression and expansion, especially when accounting for the Joule-Thomson effect and heat transfer with the cylinder wall.

Implementing these improvements would inevitably increase the complexity of the code and computational time, but would result in a significantly more accurate and robust tool for simulating gas cylinder filling under real-world conditions.

10.2 Phase change considerations

Another limitation of the current simulation is the assumption that the gas remains in a single-phase gaseous state throughout the filling process. This assumption is generally valid under moderate pressures and temperatures. However, in certain scenarios under rapid pressurisation and cooling conditions—phase change (e.g., gas-to-liquid condensation) can occur. Neglecting phase transitions can introduce inaccuracies in thermodynamic predictions, especially in the calculation of temperature, pressure, and energy balances.

When gases are compressed, their temperature tends to rise due to compression heating. However, depending on the Joule-Thomson coefficient and ambient cooling effects, the temperature may subsequently drop, potentially bringing the gas close to or below its saturation temperature at a given pressure. If the conditions reach or cross the saturation curve, condensation may begin, leading to the formation of a two-phase mixture (Çengel and Boles, 2015). This process involves latent heat exchange, which is not accounted for in the current model, and can significantly alter energy transfer rates and pressure dynamics within the cylinder.

To improve the realism of future simulations, phase change behaviour could be incorporated by implementing a two-phase thermodynamic model. This would require access to accurate saturation data and phase diagrams for the gases of interest, along with numerical methods to handle the coexistence of liquid and gas phases. Tools such as NIST REFPROP (Lemmon et al., 2022) or CoolProp (Bell et al., 2014) can provide necessary property data for these calculations. Additionally, models based on the Gibbs phase rule and enthalpy-concentration methods could be used to simulate dynamic phase behaviour.

Introducing this level of detail would enhance the script's applicability to a wider range of industrial gases and extreme operating conditions. However, it would also increase the computational complexity and require more advanced thermodynamic solvers capable of handling non-linear, multiphase calculations.

10.3 Basic enhancements

The current script is configured to simulate gas filling for oxygen, nitrogen, and argon, as these represent the primary products of air separation units and are commonly handled in high-pressure cylinder filling operations. However, these are not the only gases used in such applications. To enhance the versatility of the script, future users could expand its capability by incorporating additional gases as needed. This could be achieved by extending the existing

switch statement to include relevant thermophysical properties, such as the Joule-Thomson coefficient, molar mass, and specific heat capacity associated with the new gases. This modification would allow the model to accommodate a broader range of industrial gases with minimal structural changes to the code.

10.4 Computational and real-world tests

Computational Fluid Dynamics (CFD) simulations offer a powerful tool for testing and validating the results generated by the MATLAB script. Unlike the script's simplified lumped element model, CFD employs multi-element analysis and incorporates more advanced thermodynamic calculations, providing a higher-fidelity representation of real-world behaviour. By comparing the outputs of both approaches, it becomes possible to identify the strengths, limitations, and accuracy of the script.

Additionally, integrating real-world filling data would further enhance the script's reliability. By aligning the script's input variables with historical filling cycle parameters, its predictive accuracy can be assessed through direct comparison with empirical data. Any discrepancies or consistencies between the simulation and actual results would offer valuable insights for refining the model.

11.0 Conclusion

None of the simulations conducted resulted in cylinder wall temperatures approaching the 65 °C safety threshold outlined in EIGA Document 50/11 (EIGA, 2011). This outcome is likely influenced by the relatively low initial and ambient air temperatures assumed in the simulations. Additionally, both the inlet and target pressures significantly affect the thermal response. A larger pressure drop across the orifice generally results in a greater temperature decrease due to the Joule-Thomson effect. However, higher target pressures and increased flow rates lead to greater adiabatic compression heating, which can elevate the internal gas temperature.

Given these complex interactions, it is recommended that multiple iterations of the simulation be performed with varying parameters. Process and chemical engineers would benefit from using the developed script to explore a wide range of scenarios. Their expertise would allow them to draw meaningful conclusions and apply the tool to inform engineering decisions in future cylinder filling projects or system upgrades.

The simulation script itself is built on sound engineering principles and provides a practical means to analyse gas cylinder filling dynamics. It offers a valuable tool for engineering teams to conduct rapid assessments of proposed changes to real-world equipment. For example, the script could be used to evaluate the effects of different pump flow rates, pre-cooling or heating of the incoming gas, pre-conditioning the cylinder temperature, or implementing active cooling strategies such as forced convection on the cylinder wall.

While there is room for further refinement and expansion, the current version of the script serves as a robust foundation. It addresses a clear gap: the lack of a fast, effective simulation tool for modelling gas cylinder filling. As such, it holds significant potential for continued development and practical application.

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13.0 Appendices

13.1 Appendix A (MATLAB SCRIPT)

```
% --- Script Details ---
% Title: Gas Cylinder Filling Simulation
% Details: This script will simulate a gas cylinder being filled with
%          a chosen gas (O2, N2 or Ar), the script will then output
%          a temperature, pressure and mass graph over time.
% Author: Joshua U'Dell
% Last edited: 01/05/2025
%

clc;
clear;
close all;

% --- Update variables in this section ---
% --- User Variables ---
dt = 0.1;           % Time step in seconds
V = 50;             % Volume of cylinder in liters
P1 = 1;             % Pressure in cylinder at start of fill in bar
T1 = 30;            % Gas temperature in cylinder in Celsius
T_p = 30;           % Gas temperature from the pump in Celsius
P_i = 411;          % Pressure of pump flow in bar
P_t = 320;          % Target pressure of the gas in cylinder in bar
T_t = 20;           % Target temperature of the gas in cylinder in Celsius
T_t_p = 1.6;        % Target temperature percentage (1.5 = 50% over target,
eg 20 deg c target would = 30 deg c)
t_flow = 120;       % Time to full pump flow in seconds
time_max = 36000;   % Max simulation time in seconds
T_amb_c = 30;       % Ambient temperature in Celcius
T_wall = 40;        % Initial cylinder wall temprature Celcius
Cyl_count = 15;     % Cylinders per pump flow rate

% --- Cylinder properties chromium-molybdenum alloy steel ---
d_outer = 0.228;    % Outer diameter in meters
thickness = 0.006;  % Wall thickness in meters
rho_wall = 7850;    % Density of chrome moly steel (kg/m³)
cp_wall = 460;      % Specific heat (J/kg·K)
h_conv = 10;        % Convection coefficient (W/m²·K)

% -----
% -----

% --- User Prompts ---
fprintf('This script will simulate a chosen gas being filled into a compressed gas\n');
fprintf('cylindder\nPlease confirm that you have updated the appropriate variables in the\n');
fprintf('script for the simulation you wish to run.\n');
Confirmation = menu('', 'Confirm all variable have been checked', 'Cancel\nSimulation');

if Confirmation == 2
    fprintf('Simulation Cancelled\n');
    return
end
```

```
% --- Cylinder cooldown option ---
Cooldown_yn = menu('Would you like to simulate cylinder cool down post
fill?', 'Yes', 'No');

% --- Gas selection ---
Gas_Type = menu('Select the gas to simulate', 'Oxygen', 'Nitrogen', 'Argon');

% --- Gas Properties ---
switch Gas_Type
case 1
    % --- Oxygen Properties ---
    Gas_Name = 'Oxygen';
    JT = 0.22;           % Joule-Thomson coefficient (K/bar)
    gamma = 1.4035;      % The adiabatic index
    m_mass = 0.0319988;  % Molar mass in kg/mol
    M = 1712;            % Mass flow rate from pump in kg/hr
case 2
    % --- Nitrogen Properties ---
    Gas_Name = 'Nitrogen';
    JT = 0.27;           % Joule-Thomson coefficient (K/bar)
    gamma = 1.4;         % The adiabatic index
    m_mass = 0.0280134;  % Molar mass in kg/mol
    M = 1209;            % Mass flow rate from pump in kg/hr
case 3
    % --- Argon Properties ---
    Gas_Name = 'Argon';
    JT = 0.44;           % Joule-Thomson coefficient (K/bar)
    gamma = 1.667;       % The adiabatic index
    m_mass = 0.039948;   % Molar mass in kg/mol
    M = 2093;            % Mass flow rate from pump in kg/hr
end

% --- conversions to SI units ---
V = V / 1000;           % Volume in m^3
P1 = P1 * 100000;       % Pressure in Pa
T1 = T1 + 273.15;       % Temperature in Kelvin
M = M / 3600 / Cyl_count; % Mass flow rate in kg/s for 1 cylinder
P_i = P_i * 100000;     % Pressure in Pa
P_t = P_t * 100000;     % Pressure in Pa
T_t = T_t + 273.15;     % Temperature in Kelvin
T_p = T_p + 273.15;     % Temperature in Kelvin
T_amb = T_amb_c + 273.15; % Temperature in Kelvin

% --- Constants ---
R = 8.314;              % Universal gas constant in J/mol.K

% --- Cylinder calculations ---
d_inner = d_outer - 2 * thickness;
L_cyl = V / (pi * (d_inner / 2)^2); % Approximate cylinder length
V_wall = pi * (d_outer^2 - d_inner^2) / 4 * L_cyl;
m_wall = rho_wall * V_wall;
T_wall = T_wall + 273.15; % Temperature in Kelvin
A_outer = pi * d_outer * L_cyl; % Outer surface area
R_conv = 1 / (h_conv * A_outer); % Thermal resistance

% --- Calculate target mass for filling ---
m_target = (P_t * V * m_mass) / (R * T_t); % Target mass in kg
```

```
% --- Initial values ---
m_total = (P1 * V * m_mass) / (R * T1);      % Initial mass in kg
time = 0;
t_mass_filled = 0;

% --- Create logs ---
Time_log = [];
T_in_JT_log = [];
T_log = [];
P_log = [];
m_total_log = [];
m_added_log = [];
T_wall_log = [];

% --- loop until time is at time max or mass contion/ cooldown conditions are met-
--
while time < time_max
    time = time + dt;          % Current time step
    m_added = dt * M;         % Mass added at each time step
    if Cooldown_yn == 1
        if m_target <= m_total & (T1-273.15) <= (T_t-273.15) * T_t_p
            fprintf('Gas cooldown completed.\n',T_t)
            break
        end
    else
        if m_target <= m_total
            fprintf('Target mass pumped into cylinder.\n',T_t)
            t_mass_filled = time;
            break
        end
    end
end

% --- Ramp up filling rate ---
if time <= t_flow
    m_added = (time / t_flow) * m_added;
end

% --- Filling rate checks ---
if T_wall >= 65 + 273.15
    m_added = 0;
    fprintf('CYLINDER WALL TEMPRATURE TOO HIGH, Inlet flow paused\n')
end

if P1 >= P_i
    m_added = 0;
    fprintf('CYLINDER PRESSURE TOO HIGH, Inlet flow paused\n')
end

if m_target <= m_total
    m_added = 0;
    if t_mass_filled == 0
        t_mass_filled = time;
    end
end

% --- Step 1: Inlet gas cooling via Joule-Thomson effect ---
if m_added == 0
    t_in = NaN;
    T_in_c = NaN;
```

```
else
    deltaT_JT = JT * (P_i/100000 - P1/100000);
    T_in = T_p - deltaT_JT;
    T_in_c = T_in - 273.15;
end

% --- Step 2: Energy balance (mixing of gas) ---
E_total = m_total * T1 + m_added * T_in;
m_total = m_total + m_added;
T_mixed = E_total / m_total;

% --- Step 3: Pressure update from ideal gas law ---
P2 = (m_total * R * T_mixed) / (m_mass * V);
P2_b = P2 / 100000;

% --- Step 4: Compression heating ---
T2 = T_mixed * (P2 / P1)^((gamma - 1)/gamma);
T1 = T2;
T1_c = T1 - 273.15;
P1 = P2;

% --- Step 5: Heat loss from gas to wall ---
Q_loss = (T1 - T_wall) / R_conv; % Heat from gas to wall (W)
dT_gas_loss = (Q_loss * dt) / (m_total * cp_wall);
T1 = T1 - dT_gas_loss;

% --- Step 6: Wall temperature update ---
dT_wall_gain = (Q_loss * dt) / (m_wall * cp_wall);
T_wall = T_wall + dT_wall_gain;

% --- Step 7: Heat loss from Q_wall wall to ambient ---
Q_wall_loss = (T_wall - T_amb) / R_conv;
dT_wall_loss = (Q_wall_loss * dt) / (m_wall * cp_wall);
T_wall = T_wall - dT_wall_loss;

% --- Logging the data ---
Time_log(end+1) = time;
T_in_JT_log(end+1) = T_in_c;
T_log(end+1) = T1 - 273.15;
P_log(end+1) = P2_b;
m_total_log(end+1) = m_total;
m_added_log(end+1) = m_added;
T_wall_log(end+1) = T_wall - 273.15;
end

% --- Plot results ---
figure;
subplot(5,1,1);
plot(Time_log, T_in_JT_log, 'b', Time_log, T_log, 'r');
xlabel('Time (s)'); ylabel('Temperature (°C)');
legend('Inlet Temp (JT cooled)', 'Gas Temp');
title('Gas Temperature vs Time');

subplot(5,1,2);
plot(Time_log, P_log, 'k');
xlabel('Time (s)'); ylabel('Pressure (bar)');
title('Cylinder Pressure vs Time');

subplot(5,1,3);
```

```
plot(Time_log, m_total_log, 'g');
xlabel('Time (s)'); ylabel('Mass (kg)');
title('Total Mass in Cylinder vs Time');

subplot(5,1,4);
plot(Time_log, m_added_log, 'k');
xlabel('Time (s)'); ylabel('Mass (kg/dt)');
title('Mass Added to Cylinder vs Time');

subplot(5,1,5);
plot(Time_log, T_wall_log, 'b');
xlabel('Time (s)'); ylabel('Wall Temperature (°C)');
title('Outer Wall Temperature vs Time');
grid on;

% --- Results Output ---
fprintf('\nGas selected: %s\n',Gas_Name)
fprintf('Fill rate per cylinder: %0.4f kg/s \n',M)
fprintf('Time to reach required mass of %0.2f kg: %0.2f seconds (%0.2f minutes, %0.2f hours)\n',m_target, t_mass_filled, t_mass_filled / 60, t_mass_filled / 3600)
if Cooldown_yn == 1
    fprintf('Time to cool down to %0.0f deg C: %0.2f seconds (%0.2f minutes, %0.2f hours)\n',(T_t -273.15) * T_t_p, time - t_mass_filled, (time - t_mass_filled) / 60, (time - t_mass_filled) / 3600)
end
fprintf('Total simulated time %0.2f seconds (%0.2f minutes, %0.2f hours)\n',time,time / 60, time / 3600)
fprintf('Maximum gas temprature: %0.2f deg C\n',max(T_log))
fprintf('Minimum gas temprature: %0.2f deg C\n',min(T_log))
fprintf('Maximum cylinder wall temprature: %0.2f deg C\n',max(T_wall_log))
fprintf('Minimum cylinder wall temprature: %0.2f deg C\n',min(T_wall_log))
fprintf('Maximum Gas Pressure: %0.2f bar\n',max(P_log))
fprintf('Final Gas Pressure: %0.2f bar\nFinal Gas Temprature: %0.2f deg C\n',P_log(end),T_log(end))
```

13.2 Appendix B (Gas properties)

Table 9 Joule-Thomson index values (NIST, 2025)

Gas	JT index (K/bar)	Adiabatic index	Molar mass kg/mol
Oxygen	0.22	1.4035	0.0319988
Nitrogen	0.27	1.4	0.0280134
Argon	0.44	1.667	0.039948

13.3 Appendix C (Pump flow rates)

CALCULATION		Pump Runaway Case			
		Oxygen	Nitrogen	Argon	
Fluid		32.00	28.01	39.95	REFPROP
Molar Mass	kg/kmol	1141.17	806.08	1395.40	REFPROP
Saturated Liquid Density	kg/m³	25.00	25.00	25.00	REFPROP
Pump Flowrate	L/min	0.03	0.03	0.03	Maximum MRP Pump Flow
	m³/min	1.50	1.50	1.50	Unit Conversion
	m³/hr	1.712	1.209	2093	m= p V
Mass Flowrate	kg/hr	53	43	52	Unit Conversion
Molar Flowrate	kmol/hr	1198	967	1174	Unit Conversion
	Nm³/hr	1265	1021	1239	Unit Conversion
	Sm³/hr				

(BOC, Linde Group, 2025)

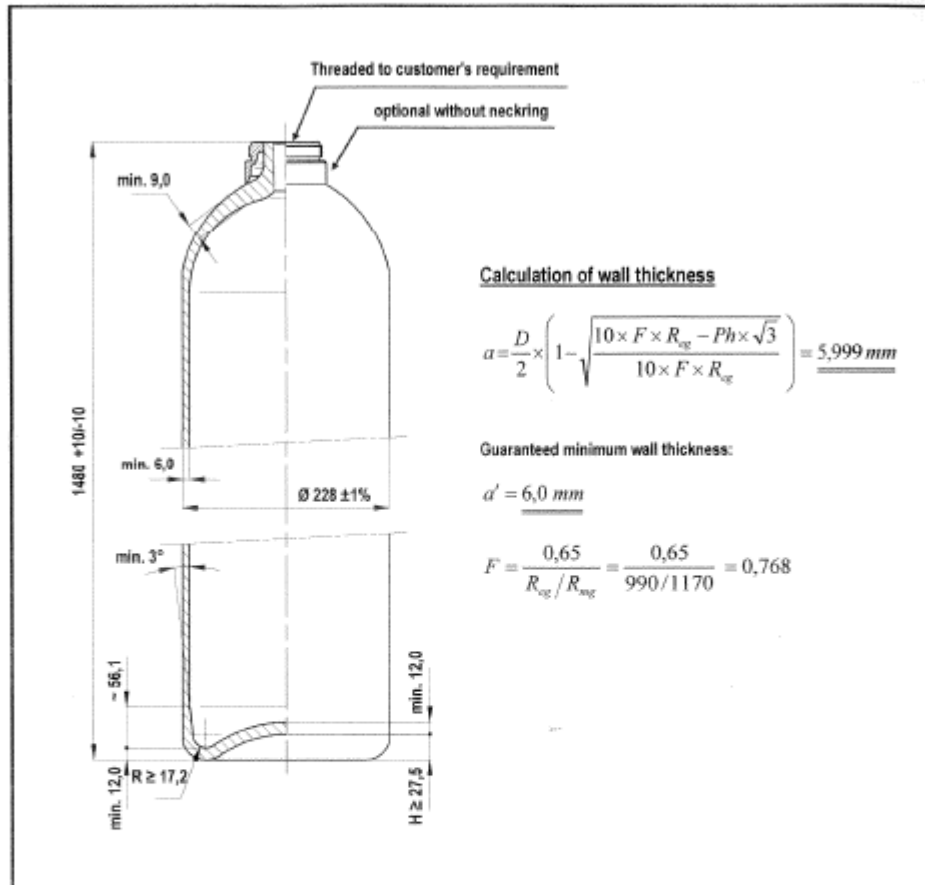
13.4 Appendix D (Cylinder properties)

 TECHNICAL SPECIFICATION	Doc't No:	19313652
	Sheet No:	2 of 3
	Issue No:	4

Material:	Cylinder (Seamless steel)
Water capacity (litre):	50 + 5% / - 0%
Area of use:	Worldwide
Standards/Specification:	ISO 9809-2
Approval:	TPED
Material of construction:	Chrome Molybdenum Steel
Material yield strength (MPa):	990 (min design)
Material tensile strength (MPa):	1170 - 1290
Outside diameter (mm):	228 ± 1%
Length (mm):	1480 ± 10mm
Average weight (kg):	61
Maximum weight (kg):	63
Neck thread:	ISO 11363-1 25E
External collar thread:	W80 x 1/11"
Filling Ratio (kg/litre):	-
Working pressure at 15°C (bar):	300
Test pressure (bar):	450
Shape/type of base:	Concave
Supplier:	Worthington
Vendor drawing reference:	N5000 228 60 11 date: 18.11.14
Stamp marking reference:	Linde specification 50002062
Cleaning code:	Clean Ind "C2" – Linde Specification: PKG 01-06-LG, other codes are possible, have to be specified in the order
Gas(es):	All gases, except Hydrogen and other embrittlement gases.

...

 TECHNICAL SPECIFICATION	Doc't No:	19313652
	Sheet No:	3 of 3
	Issue No:	4



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Austria

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+) Allowable gases to be filled:

- UN1002 Air
- Gases of group 1,4,5,6,7,8,9,10 according to EN ISO 11114-1

Specification	EN 1964-2:2001 ISO 9809-2:2000 EN ISO 9809-2:2010	Material	34CrMo4-Steel	Yield point (R _{eg})	min.	990	MPa
		Heat treatment	quenched and tempered	U.T.S. (R _{mg} / R _{me max})		1170 / 1290	MPa
		Chemical composition		Elongation A _{5-105 vs V}	min.	12	%
Type	EXTRA-5	C	0,32 - 0,36 %	S	≤ 0,005 %	Impact value (cross)	A-value 35 J/cm²
Name of gas	+)	Mn	0,60 - 0,80 %	Cr	0,90 - 1,10 %	(SO-V (-50°C))	B-value 50 J/cm²
Water capacity	50 l	Si	0,15 - 0,30 %	Mo	0,17 - 0,27 %	Drawn	Actual
Working pressure (P _W)	≤ 300 bar	P	≤ 0,015 %	Ni	≤ 0,30 %	PJ	Name
Test pressure (P _t)	450 bar	P+S	≤ 0,020 %			18.11.14	Date
Weight empty	~ 61,0 kg	V+Nb+Ti+B+Zr	≤ 0,15 %				Checked
Title: Seamless Steel Cylinder							Date
Notes: Manufacturer's process: from billet Burst pressure P _b ≥ 720 bar; Yield pressure P _y ≥ 586 bar				Draw no. N5000 228 60 11			

carnegie group

DESCRIPTION		UNIT		SCALE		SHEET	
ITEM	DESCRIPTION	UNIT	SCALE	ITEM	DESCRIPTION	UNIT	SCALE
12	Top assembly lever valve	1	1/2	1071000067			
11	Top assembly lever valve	1	1/2	0170000130			
10	O-Ring D 7.65x1.75	1	1/2	0471100101			
9	Anti-siphon ring	1	1/2	1521101228			
8	Sealing ring D 26	1	1/2	0021104025			
7	Oxygen pressure indicator B 315 bar	1	1/2	3021100219			
6	Pin	2	1/2	0021104071			
5	Front part of cover	1	1/2	3021103405			
4	Rear part of cover	1	1/2	3021103406			
3	Washer	1	1/2	0021100271			
2	Operating mechanism	1	1/2	1321000003			
1	Manufactured body	1	1/2	0171007003			

Markings

- CARNEGIE GROUP SYMBOL
- E3
- ISO V
- ZSE
- ISO (see per drawing 4001102002)
- Year and month of construction
- Production order
- 10355252
- 10355252 (see 2001101756)
- 10355252 (see 2001101756)

Technical information:

- Max. pressure: 3 - 5 bar
- Pin Range: 4 mm
- O-ring: D - 4 mm
- W.P. 200 bar
- CV: 0.35

Active cylinder pressure indicator

Changes in the previous version

ITEM	DESCRIPTION	UNIT	SCALE	ITEM	DESCRIPTION	UNIT	SCALE
12	Top assembly lever valve	1	1/2	1071000067			
11	Top assembly lever valve	1	1/2	0170000130			
10	O-Ring D 7.65x1.75	1	1/2	0471100101			
9	Anti-siphon ring	1	1/2	1521101228			
8	Sealing ring D 26	1	1/2	0021104025			
7	Oxygen pressure indicator B 315 bar	1	1/2	3021100219			
6	Pin	2	1/2	0021104071			
5	Front part of cover	1	1/2	3021103405			
4	Rear part of cover	1	1/2	3021103406			
3	Washer	1	1/2	0021100271			
2	Operating mechanism	1	1/2	1321000003			
1	Manufactured body	1	1/2	0171007003			