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ChE485

Flash Drums Simulation and Design

Project 2

Submitted for Credit in ChE485 to Dr. R. Young
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Executive Summary

The objective of this project is to simulate a two-stage flash drum process that separates a mixture of hydrocarbons and to determine design parameters for the flash drums given the that the feed flow rate is 75000 kg/h at 140°C and 3500 kPa with the composition tabulated in Table 1. Important assumptions of this simulation include Peng-Robinson thermodynamics and adiabatic flash drums.

The results of this simulation show that separation of the hydrocarbons does occur. For the base case, the lights components mole fraction in the output liquid, stream 7, is 0.460 and the heavy components mole fraction in the output vapor, stream 8, is 0.219. Better separation can be achieved by adjusting the given specifications. For instance, a light components mole fraction of 0.35 in stream 7 can be achieved by adjusting the pressure drops of valves XV13100 or XV13101 to 2419 kPa and 1126 kPa respectively. A heavy components mole fraction of 0.20 for stream 8 can be achieved by lowering the feed temperature to 130.3°C. Decreasing the pressure drops between the valves will decrease the heavy components mole fraction in stream 8, but a mole fraction of 0.20 is unachievable.

Due to cost and performance, carbon steel and spot double-welded butt joints are chosen for the drums, D1301 and D1302, which are determined to have L:D ratios of 16:1 and 29:1 respectively. They are significantly greater than typical L:D ratios of 3:1 or 4:1, which can help optimize the cost of the flash drums for the given design temperatures and pressures. The large L:D ratios can be attributed to assuming that there is no demister. If the flash drums had demisters, the holdup times will decrease, hence the L:D ratio will be smaller.

In real-world applications, certain assumptions made in this simulation, such as Peng-Robinson thermodynamics, adiabatic flash drums, or a lack of demisters, will not hold true. Hence, it is not recommended to build a flash drum process based on the results in this project, but as a general, preliminary simulation, it serves its purpose well. To improve this simulation so that it can be applied in the real world, it would be better to incorporate real-world concepts and algorithms.

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Flash Drums Simulation and Design

Objective

The objectives of this project are to simulate a two-stage flash process that separates a mixed hydrocarbon feed and to determine design parameters for both of the flash drums [1].

Specifications and Assumptions

For the base case of the process, the feed is specified to have a flow rate of 75000 kg/h at 140°C and 3500 kPa, with the following composition [1]:

Table 1: Feed composition

Composition (Molar)		
Ethane	fraction	0.00
Propane	fraction	0.20
Butane	fraction	0.40
Pentane	fraction	0.25
Hexane	fraction	0.00
Heptane	fraction	0.05
Octane	fraction	0.10

Flash drum D1301 is specified to operate at 1700 kPa, in other words, the upstream valve, XV13100, has an output pressure of 1700 kPa [1]. The second valve, XV13101, is specified to have a pressure drop of 500 kPa [1].

There are a few major assumptions in this simulation. Firstly, the fluids are assumed to follow Peng-Robinson thermodynamics [1]. Secondly, both flash drums are assumed to be well-insulated, which means that their duties are both 0 kW [1]. Lastly, both flash drums are assumed to be operating at a 60% level [1].

Data and Results

Base Case Simulation

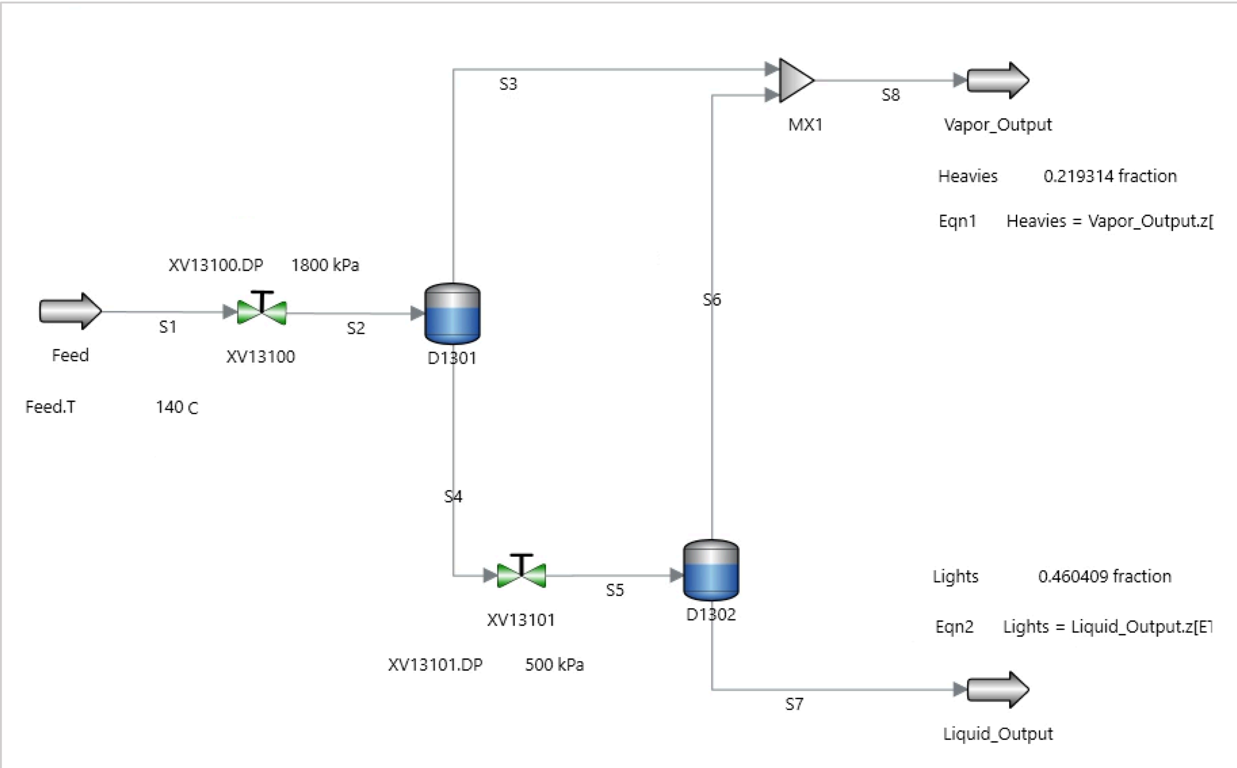

Figure 1: Process flow diagram with base case conditions

The base case simulation shows that with the given specifications and assumptions, separation of the hydrocarbons does occur. The mole fractions for the heavies and the lights of the feed are 0.40 and 0.60 respectively. At the liquid output, the mole fraction of the lights is 0.460 and at the vapor output, the mole fraction of the heavies is 0.219. These results make sense because for a distillation process, it is expected that the vapor output will have more lights due to the lights having lower boiling points and the liquid output will have more heavies due to them having higher boiling points. By adjusting the specifications, better separation can be achieved (see Manipulating "Lights" and "Heavies" Mole Fractions). The following couple of pages are tables containing operating conditions for the streams and the equipment.

Table 2: Base case operating conditions for streams 1 to 4

Parameter/Stream		**S1**	**S2**	**S3**	**S4**
Flow Rate (Mass)	kg/h	75000.0	75000.0	20204.0	54796.0
Flow Rate (Molar)	kmol/h	1127.1	1127.1	350.9	776.3
Volumetric Flow	m^3/s	0.05	0.17	0.14	0.03
Pressure	kPa	3500.0	1700.0	1700.0	1705.8
Temperature	°C	140.0	119.8	119.8	119.8
Vapor Fraction	fraction	0.00	0.31	1.00	0.00
Composition (Molar)					
Ethane	fraction	0.00	0.00	0.00	0.00
Propane	fraction	0.20	0.20	0.33	0.14
Butane	fraction	0.40	0.40	0.45	0.38
Pentane	fraction	0.25	0.25	0.19	0.28
Hexane	fraction	0.00	0.00	0.00	0.00
Heptane	fraction	0.05	0.05	0.01	0.07
Octane	fraction	0.10	0.10	0.02	0.14

Table 3: Base case operating conditions for streams 5 to 8

Parameter/Stream		**S5**	**S6**	**S7**	**S8**
Flow Rate (Mass)	kg/h	54796.0	8153.1	46643.0	28357.0
Flow Rate (Molar)	kmol/h	776.3	140.4	635.9	491.3
Volumetric Flow	m^3/s	0.11	0.08	0.02	0.30
Pressure	kPa	1205.8	1205.8	1211.9	1205.8
Temperature	°C	106.5	106.5	106.5	111.3
Vapor Fraction	fraction	0.18	1.00	0.00	1.00
Composition (Molar)					
Ethane	fraction	0.00	0.00	0.00	0.00
Propane	fraction	0.14	0.30	0.11	0.32
Butane	fraction	0.38	0.47	0.35	0.46
Pentane	fraction	0.28	0.20	0.30	0.19
Hexane	fraction	0.00	0.00	0.00	0.00
Heptane	fraction	0.07	0.01	0.08	0.01
Octane	fraction	0.14	0.01	0.17	0.02

Table 4: Mole fraction of heavies and lights for specific output streams

S8 Heavies	mole fraction	0.219
S7 Lights	mole fraction	0.460

Table 5: Operating conditions for equipment

Equipment	**Variable**	**Units**	**Value**
XV13100	Pressure Drop	kPa	1800.0
D1301	Duty	kW	0.0
	Vapor Fraction	fraction	0.31
	Level	fraction	0.60
	T	°C	119.81
	Operating Pressure	kPa	1700.00
XV13101	Pressure Drop	kPa	500.0
D1302	Duty	kW	0.0
	Vapor Fraction	fraction	0.18
	Level	fraction	0.60
	T	°C	106.48
	Operating Pressure	kPa	1205.78

Base Case Vessel Design

The vessel parameters were calculated based on avoiding carryover with 80 μm droplets of liquid or larger without a demister pad, having no corrosion allowance, and having a holdup time of 5 minutes [2]. Carbon steel was chosen as the material for the vessel due to its ability to withstand the design pressures and temperatures of both flash drums as well as its cheap price [2]. Spot double-welded butt joints were chosen due to its efficiency relative to price [2].

Table 6: Base case vessel design parameters

Parameter/Equipment		**D1301**	**D1302**
Design Pressure	kPa	1878	1384
Design Temperature	°C	130	116
Shell Diameter	m	1.65	1.05
Shell Length	m	26	30
L/D	fraction	16	29
Shell Thickness	m	0.0222	0.0127
	in	0.875	0.500

The L:D ratio based on the base case is 16:1 and 29:1 for flash drums D1301 and D1302 respectively. As a rule of thumb, L:D ratios are at least 2:1, but ideally no greater than 5:1, with the most common L:D ratios being 3:1 and 4:1 [2]. Given the above operating pressures for each flash drum, the L:D ratios for D1301 and D1302 should be 4:1 and 3:1 respectively [2]. A greater length and plot area will require more cost, hence it is most ideal to reduce the L:D ratio.

To decrease the L:D ratio for the base case, perhaps the use of a demister pad will help reduce holdup time, which in turn will reduce the length required for the flash drum. The same can be accomplished by reducing the feed flow rate significantly, but it is not desired for industrial purposes.

Manipulating "Lights" and "Heavies" Mole Fractions

Case 1: "lights" mole fraction of 0.35 in stream 7 by adjusting pressure drop in D1301

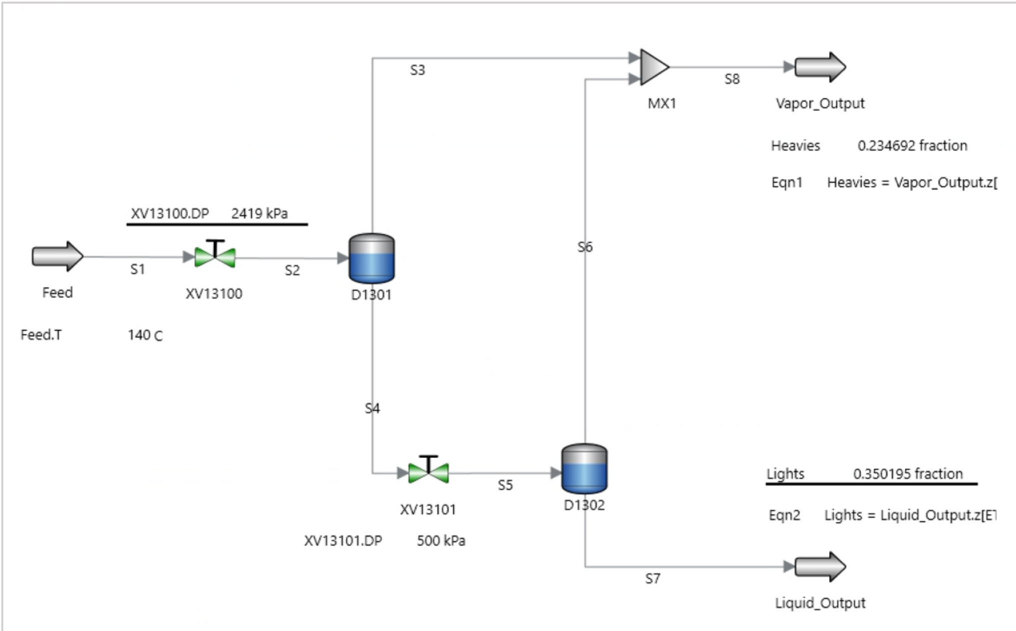

Figure 2: Process flow diagram with new D1301 pressure drop

Case 2: "lights" mole fraction of 0.35 in stream 7 by adjusting pressure drop in D1302

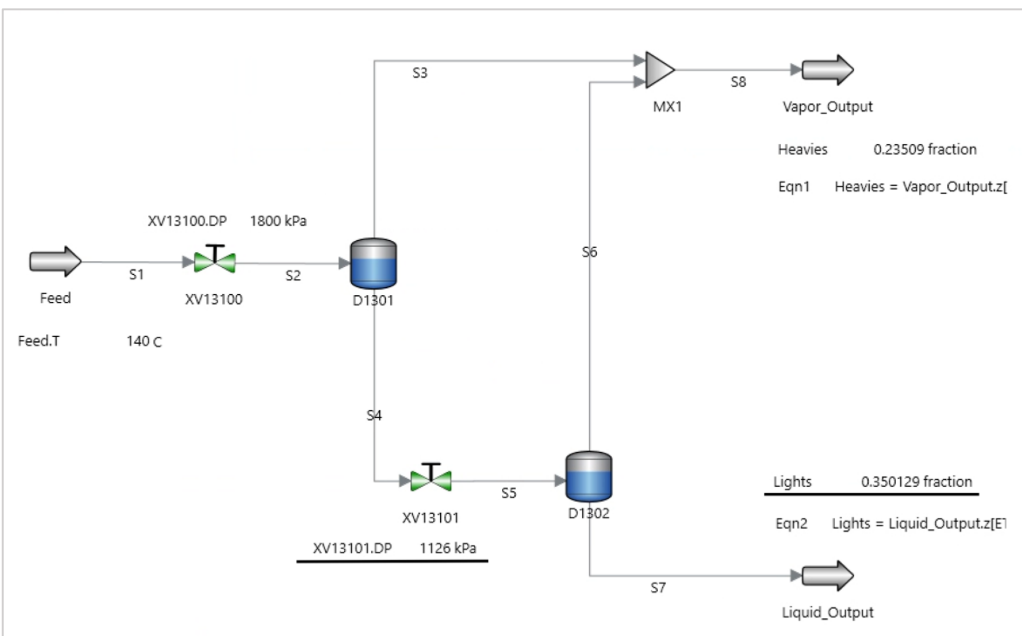

Figure 3: Process flow diagram with new D1302 pressure drop

Case 3: "heavies" mole fraction of 0.20 in stream 8 by adjusting varying parameters

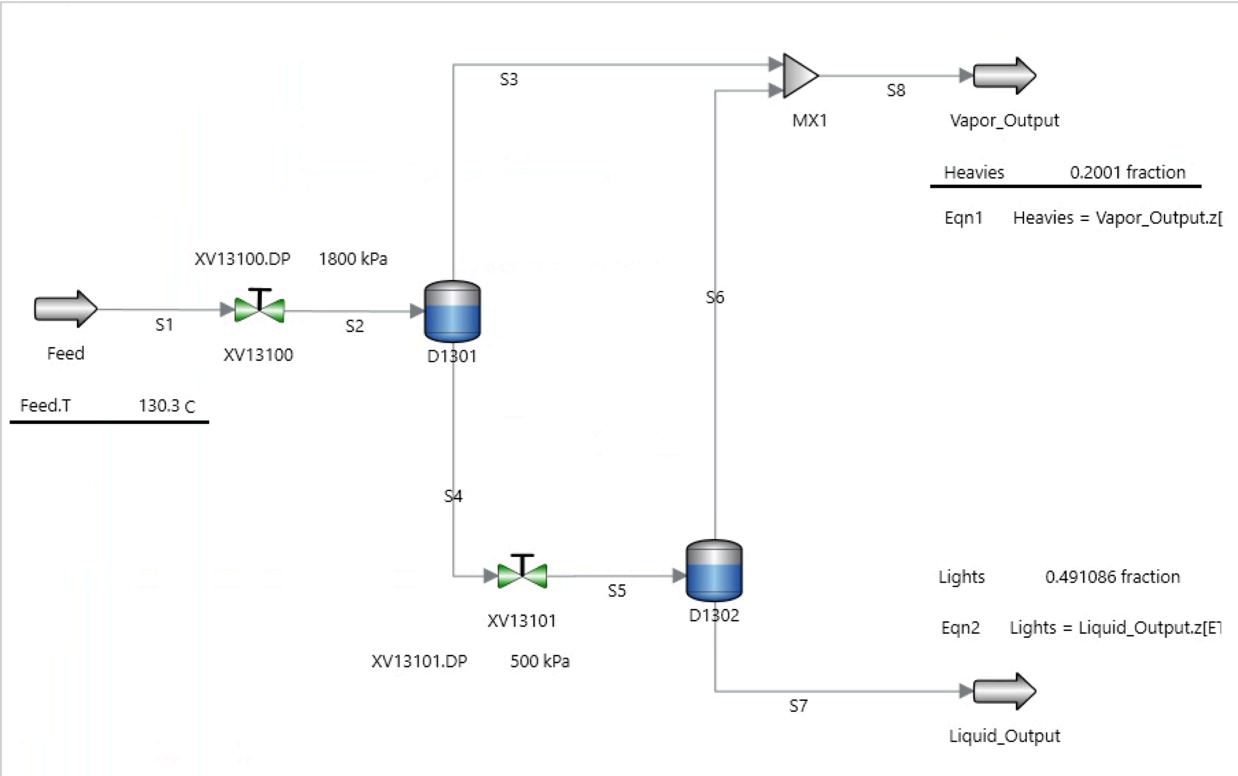

Figure 4: Process flow diagram with new feed temperature

By adjusting values in the simulation, it is determined that a "lights" mole fraction of 0.35 in stream 7, the output liquid, is achievable with a pressure drop of 2419 kPa or 1126 kPa across valves XV13100 and XV13101 respectively, as seen in Figures 2 and 3. A lower mole fraction of the light components indicates a better separation, which is desirable for many purposes. Figure 4 shows that a "heavies" mole fraction of 0.20 in stream 8, the output vapor, is achievable by decreasing the feed temperature to 130.3°C. Adjusting the pressure drops across either valve will not decrease the "heavies" mole fraction in stream 8 to 0.20. This is because if the pressure drop is too small, the fluid entering the flash drums will have too high of a pressure such that no vapor will be formed in the drums and no separation will occur. If the pressure drop is too large, more vapor will be formed, particularly the heavy components, resulting in an increase in the "heavies" mole fraction in stream 8. These two notions limit the degree in which separation can be achieved with two flash drums.

Conclusion

The objectives of this experiment are to simulate a two-stage flash drum process that separates hydrocarbons and to determine the design parameters of the vessels. For the base case, the feed has mole fractions of 0.60 and 0.40 for the light and heavy components respectively. The output liquid has a light component mole fraction of 0.460 whereas the output vapor has a heavy component mole fraction of 0.219. These results show that separation occurs as expected. Due to light components having lower boiling points than heavy components, more light components should be in the vapor output and more heavy components should be in the liquid output.

Table 6 shows the vessel design parameters for the base case. The L:D ratio for flash drums D1301 and D1302 are 16:1 and 29:1 respectively, which are significantly greater than typical L:D ratios of 3:1 or 4:1 for the given design temperatures and pressures. The huge L:D ratios for the simulation can be attributed to the assumptions that no demister pad is used and the process having a holdup time of 5 minutes. By using a demister pad, which is used in realistic flash drums, the holdup time should decrease, which will result in a lower L:D ratio. Another way to decrease the L:D ratio is by decreasing the feed flow rate significantly, which is no desirable for industrial purposes. As for materials and welds, carbon steel and spot double-welded butt joints were chosen due to their cheap prices and effectiveness under the design conditions.

Figures 2 to 4 show that better separation can be achieved by adjusting design specifications. By changing the pressure drop across valves XV13100 and XV13101 to 2419 kPa and 1126 kPa respectively, a lower mole fraction of 0.35 for the light components in stream 7 can be achieved. By changing the feed temperature to 130.3°C, a lower mole fraction of 0.20 for the heavy components in stream 8 can be achieved. Decreasing the pressure drop across the valves can decrease the mole fraction of heavies in stream 8, but it cannot reach a mole fraction of 0.20. This is because if the pressure drop across the valve is too small, the fluid entering the flash drums have high pressures such that no separation can be performed, given the drum specifications. Physically, this means that there will be no vapor flowing out of the drums.

Many assumptions made in this simulation are obsolete in a real-world setting. Perhaps the biggest ideal assumption is that the flash drums are well-insulated with no duties. For such reasons, it is not recommended to build the process simulated in this project for real-world applications as it may lead to dangerous accidents.

References

[1] R. Young, "CHE 485 Project 2: Flash Drums Simulation and Design" CHE485, 2019.

[2] R. Young, "Pressure Vessels and Flash Drum Sizing" CHE485, 2019.

[3] R. Young, "08 PV Design Written Notes" CHE 485, 2019.

Sample Calculations

Most of the calculations are carried out by SimCentral. Below are calculations that are not automatically produced by SimCentral.

"Heavies" mole fraction in stream 8:

$$x_{heavies} = \frac{\sum_{i=5}^{8} x_{Ci}}{\sum_{i=2}^{8} x_{Ci}}$$

$$0.219 = \frac{0.19 + 0.00 + 0.01 + 0.02}{0.00 + 0.32 + 0.46 + 0.19 + 0.00 + 0.01 + 0.02}$$

"Lights" mole fraction in stream 7:

$$x_{lights} = \frac{\sum_{i=2}^{4} x_{Ci}}{\sum_{i=2}^{8} x_{Ci}}$$

$$0.460 = \frac{0.00 + 0.11 + 0.35}{0.00 + 0.11 + 0.35 + 0.30 + 0.00 + 0.08 + 0.17}$$

Vessel Diameter [3]:

$$D^* = D_s \left[\frac{\rho_g(\rho_L - \rho_g)g}{\mu_g^2}\right]^{\frac{1}{3}} = 80\times10^{-6}\left[\frac{39.70(491.11 - 39.70)9.8}{(9.82\times10^{-6})^2}\right]^{\frac{1}{3}} = 9.77$$

$$v_t^* = \left[\frac{18}{(D^*)^2} + \frac{0.591}{(D^*)^{0.5}}\right]^{-1} = \left[\frac{18}{(9.77)^2} + \frac{0.591}{(9.77)^{0.5}}\right]^{-1} = 2.65$$

$$v_t = v_t^* \left[\frac{\rho_g^2}{\mu_g(\rho_L - \rho_g)g}\right]^{-\frac{1}{3}} = 2.65\left[\frac{39.70^2}{9.82\times10^{-6}(491.11 - 39.70)9.8}\right]^{-\frac{1}{3}} = 0.080\ m/s$$

$$D_v = \left(\frac{4Q}{\pi v_t}\right)^{\frac{1}{2}} = \left(\frac{4\times0.14}{\pi 0.080}\right)^{\frac{1}{2}} = 1.50\ m \approx 1.65\ m$$

The vessel diameter is rounded up to the nearest 15 cm.

Vessel Length [3]:

$$L_{liq} = \frac{Q_L \times holdup\ time \times v_t}{Q_g} = \frac{0.03 \times 300 \times 0.080}{0.14} = 24.0\ m$$

$$L_v = 0.2 + L_{liq} + L_1 + L_2 = 0.2 + 24.0 + 0.495 + 1.155 = 26\ m$$
$$where\ L_1 = greater\ of\ 0.7D_v\ or\ 0.9\ m$$
$$L_2 = greater\ of\ 0.3D_v\ or\ 0.3\ m$$

L:D ratio [3]:

$$\frac{L}{D} = \frac{26}{1.65} = 16$$

Design Pressure [2]:

$$P_i = P_{max} + greater\ of\ 0.1P_{max}\ or\ 25\ psi\ (172\ kPa) = 1705.8 + 172 = 1878\ kPa$$

Design Temperature [2]:

$$T_i = T_{max} + 50°F\ (10°C) = 119.8 + 10 = 130°C$$

Shell Thickness [3]:

Carbon steel and spot double-welded butt joints were chosen for this simulation, hence S = 88942 kPa and E = 0.85.

$$t_{hoop} = \frac{P_i D_i}{2SE - 1.2P_i} = \frac{1878 \times 1.65}{2 \times 88942 \times 0.85 - 1.2 \times 1878} = 0.0208\ m$$

$$t_{longitudinal} = \frac{P_i D_i}{4SE - 0.8P_i} = \frac{1878 \times 1.65}{4 \times 88942 \times 0.85 - 0.8 \times 1878} = 0.0102\ m$$

$$t = greater\ of\ t_{hoop}\ or\ t_{longitudinal} = 0.0208\ m \approx 0.0222\ m = 0.875\ in$$

The thickness of the sheet metal is rounded up to the nearest 1/8" as it is under 1" thick. If the thickness is greater than 1", then the value should be rounded up to the nears 1/4" [1]. This is because sheet metals are typically sold in these increments of thickness.