CHE 597 Professional M.S. Capstone Project, Summer 2024

Final Report - Dynamically Modeling High Pressure Releases for Complex Fire Suppression Systems

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7/29/24

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Introduction

Fauske & Associates (FAI) has upgraded its DIERS (Design Institute for Emergency Relief Systems) emergency relief sizing tools to FERST (Fauske Emergency Relief System Tool) software powered by CHEMCAD. [1] FERST is a comprehensive solution that combines practical and user-friendly approaches from FAI's PrEVent™ (Practical Emergency Vent Sizing) software with Chemstations™'s knowledge in material properties, thermodynamics, and software development [1].

FERST uses all the latest technologies and appropriate standards to simplify and rigorously evaluate relief systems. [1] Some of the main characteristics of FERST are (a) having abundant options for reactive system type (vapor, gassy, and hybrid), flow regime (homogenous, bubbly, and churn turbulent), and chemicals, (b) designing new relief systems by determining the appropriate dimension of relief device under numerous steady-state scenarios, and (c) evaluating existing relief systems by assessing whether installed relief device adequately protects the vessel from the upset scenario [1].

This project aims to introduce new FERST applications and extend FERST's use beyond runaway chemical reactions by designing and simulating the dynamic release of a CO_2 suppression system. At the beginning of the project, numerous research was requested by the project mentor including emergency relief system (ERS) design, vent sizing and piping technique, and basis of fire suppression system. The research not only helps understand the impacts on vent sizing and piping based on different reaction systems and flow regimes but also gives an overview of fire protection and suppression, such as fire suppression type. During the research, simulation for various chemical reaction problems began, with examples ranging from simple to complicated. First, problems in steady-state conditions were introduced. Next, the same examples were turned into dynamic conditions. After that, the dynamic examples became complex as piping was added. Finally, the suppression system simulation was conducted. The purpose of modeling simulations step by step is to get familiar with the simulator, making achieving the final goal easier.

Review of Relevant Literature

Relief System Sizing for Runaway Chemical Reactions [2], A review on mechanisms and models for the churn-turbulent flow regime [3], The Impact of Two-Phase Flow – Emergency Relief System Design [4]

They briefly summarized the basis of relief device design including vent sizing, each type of reactive system and flow regime, and their impacts on the relief device design. The reactive system can be identified as either gassy, vapor, or hybrid. Gassy reactive systems occur when the reaction generates significant amounts of non-condensable gas. The production of non-condensable gas is the only factor contributing to pressure increases [2], thus, the relief device system must consider the pressure rise rate and be designed to accommodate the peak rate of non-condensable gas generation. [2] Vapor reactive systems occur when the reaction mainly produces vapors and little or no liquid is present. The increase in pressure is due solely to the rise in vapor pressure. [2] In addition, vapor reactive systems have the advantage that the latent heat from boiling prevents the temperature from increasing. [2] As a result, the temperature rise due to the runaway reaction can be controlled by venting, thus, the relief device design must consider the temperature rise rate. [2] Hybrid reactive systems occur when the reaction produces a mixture of gases, vapors, and liquid. In terms of venting, both vapor and non-condensable gas cause the reactive system pressure to rise, therefore, it is crucial to consider both temperature and pressure rise rates for relief design. [2]

When classifying the reactive system for a specific runaway reaction, it can be determined by observing a temperature vs. pressure graph after chemicals heat up and cool down. Vapor reactive systems will have a higher final pressure than their original pressure as shown in **Figure 1** below. The original pressure is 10 psia and the final pressure is approximately 100 psia.

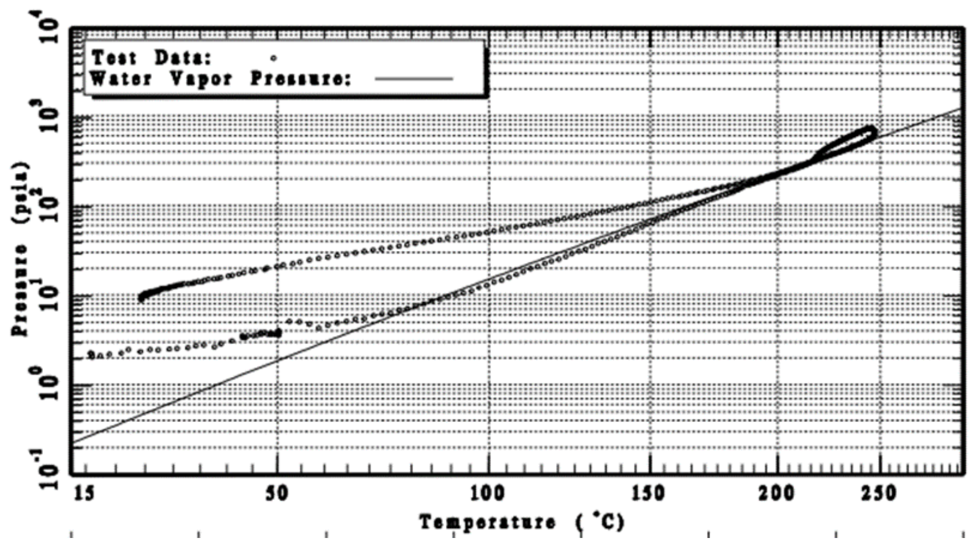

Figure 1. Temperature vs. Pressure graph for vapor reactive system [2]

Hybrid and gassy reactive systems will have almost the same final and original pressure after heating and cooling. For instance, the original pressure is about 100 psia and the final pressure is around 102 psia as shown in **Figure 2**.

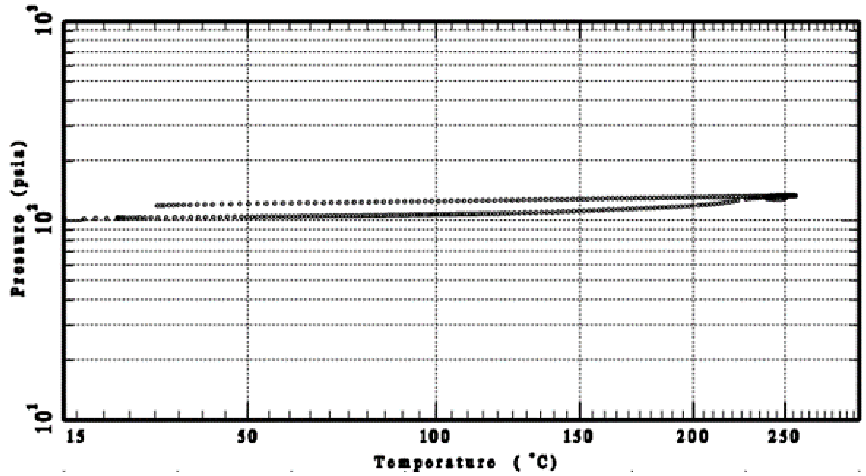

Figure 2. Temperature vs. Pressure graph for gassy reactive system [2]

However, the vapor pressure of chemical species in a hybrid reactive system will be higher than water vapor pressure at some points. For example, according to **Figure 3**, the pressure for chemical species is higher than water vapor pressure between 160°C and 180°C.

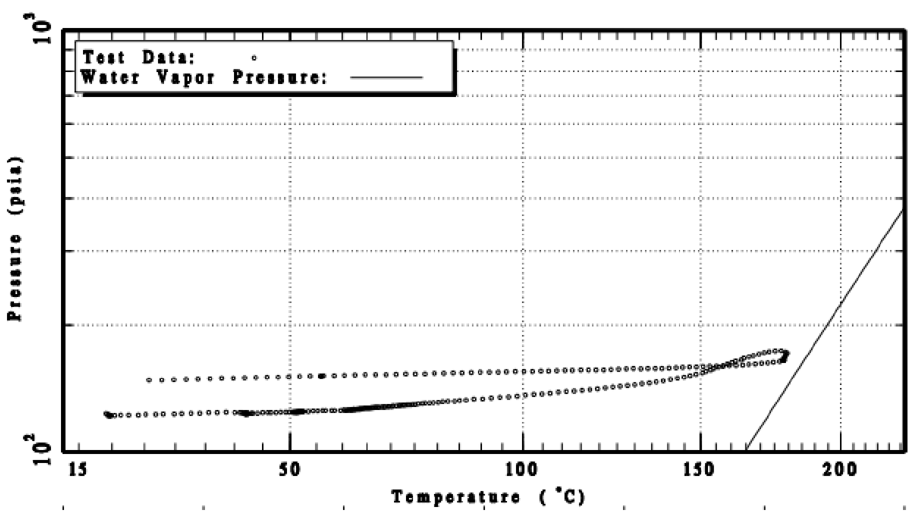

Figure 3. Temperature vs. Pressure graph for hybrid reactive system [2]

Next, each reactive system requires different types of experimental data for relief device design. As mentioned above, the vapor reactive system will focus on the temperature rise factor while the gassy reactive system will focus on the pressure rise factor. The hybrid reactive system will consider both temperature and pressure rise rates for relief device design.

The vessel flow regime should be taken into consideration after the system classification has been determined. The flow regime decides the amount of two-phase flow during venting [4], and this will have an impact on the dimensions that the emergency relief device requires. The presence of a two-phase flow can increase the required size of a relief device [4]. The flow regime can be classified as homogeneous, bubbly, and churn turbulent flow. Homogeneous flow indicates there is no vapor-liquid disengagement [4], and the pressure within the vessel is much greater than the pressure outside, forcing the fluid to discharge rapidly through the relief system. Bubbly flow indicates minimal vapor-liquid disengagement [4] since the discharged fluid comprises dispersed gas bubbles within a continuous liquid phase. Finally, churn turbulent flow results in significant vapor-liquid disengagement [4] since it is a more chaotic flow regime defined by high mixing and agitation of the fluid phases. In terms of relief device design, the vapor-liquid disengagement has a strong relationship with the presence of a two-phase flow. No vapor-liquid disengagement means that the two-phase flow remains well-mixed, thereby the combined flow rate will be large, and the size of the relief device needs to be large enough. On the other hand, the significant vapor-liquid disengagement indicates that vapor and liquid phases have separated flow, thus the single flow rate will be small, and the size of the relief device will be relatively small compared to the case of no vapor-liquid disengagement. As a result, the homogeneous flow should require the biggest relief device, then the bubbly flow, and the churn turbulent flow theoretically. However, the type of flow regime is a parameter set up by prediction. It can’t be determined by any data.

Flow of Fluids THROUGH VALVES, FITTINGS AND PIPE [5]

It introduces piping, such as pipe type and equations related to pipe, and explains how the design of piping will influence the design and performance of relief devices. Although numerous factors show the impact of piping on relief device design, the pressure drop is the most important one that needs to be considered in this project. The length, diameter, and configuration of piping can cause pressure drop. In theory, as the length, diameter, and configuration of piping increase, the pressure drop increases. In terms of relief device design in simulation, the entire relief device must be maintained at a certain flow rate, thereby the outlet pipe will always be set to fix atmospheric pressure to prevent excessive flow rate and the inlet pipe's pressure is variable and will be determined by the simulation. Hence, the larger the pressure drop will cause the pressure of the inlet pipe to increase and easily exceed the maximum allowable working pressure (MAWP). As a result, it is crucial to control the dimensions of the pipe to prevent excessive pressure in the pipe.

6 Main Types of Fire Suppression Systems: Which to Choose for Your Application? [6]**, WHAT ARE THE DIFFERENT TYPES OF SPECIAL HAZARD SUPPRESSION SYSTEMS?** [7]

They provide information about the main types of fire suppression systems, especially CO_2 suppression systems. There are six main types of fire suppression systems, including (1) Water Sprinkler Suppression Systems, (2) Pneumatic Heat Detection Systems, (3) Chemical Foam Suppression Systems, (4) Pressurized Gas Systems, (5) Foam Deluge Systems, and (6) Water Mist Systems. This project is focused on pressurized gas systems since the CO_2 suppression system is one of the types of this system. Pressurized gas systems are a practical and efficient option to prevent fire in large buildings and facilities. [6] They extinguish the fire by using inert gas to displace oxygen while cooling the fire's fuel source. [6] Moreover, the systems have several advantages: (a) they can be automated and remote-controlled, (b) they are easy to install, and (c) they require minimal maintenance. [6]

CO_2 suppression systems can be classified as high-pressure and low-pressure versions. They are able to extinguish fires ranging in size from 50 pounds to 60 tons and protect anything from large rooms to a single item. [7] In addition, there is little to no clean-up after activation and no residue that might damage the sensitive item since CO_2 is a colorless, odorless, and electrically non-conductive gas. [7] Last, CO_2 suppression systems are only installed in areas that are typically unoccupied. [7]

Data and Results

Example problem 1: Fire exposure of Styrene Monomer Tank in steady state

The first example problem in the project was to use FERST to calculate the ideal vent area and diameter of the styrene tank under three different flow regime assumptions: homogenous, churn turbulent, and bubbly flow. A screenshot of the FERST model in the steady-state condition is shown in **Figure A1**. Based on the temperature vs. pressure graph offered by the company as shown in **Figure 4**, the reactive system for styrene was identified as a vapor reactive system since the final pressure, 190 psia, was not the same as the original pressure, 0.1 psia. [2]

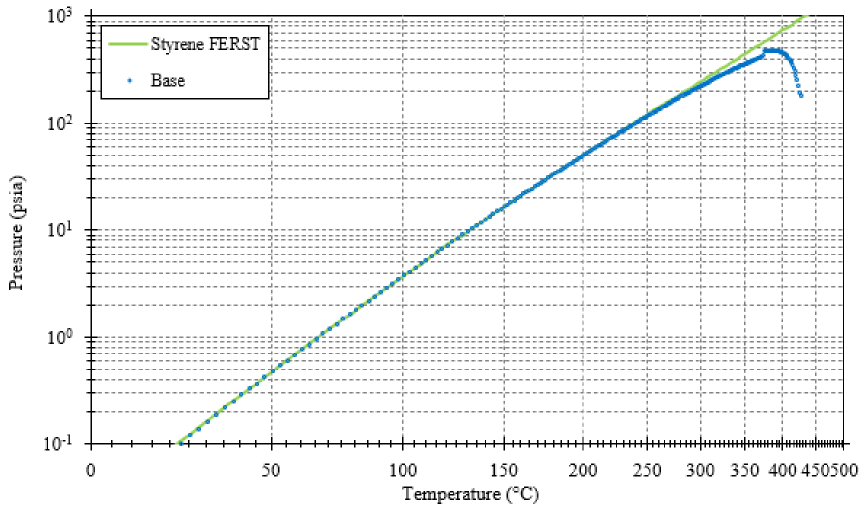

Figure 4. Temperature vs. Pressure graph for styrene

After identifying the reactive system, the temperature rise factors were found in **Figure 5**. FERST required two temperature-temperature rise factor pairs. (140°C, 2.645°C/min) and (159.5°C, 5.68°C/min) were the observed pairs for this example.

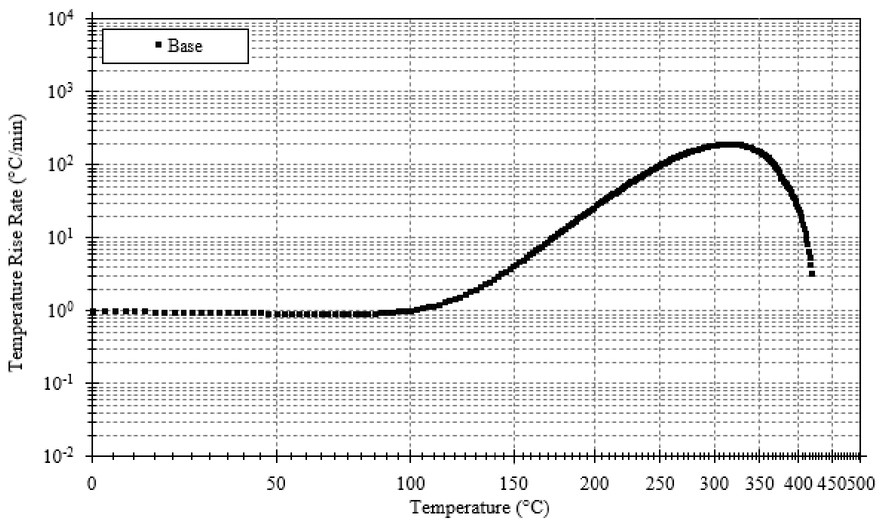

Figure 5. Temperature vs. Temperature Rise Rate graph for styrene

Next, entering the rest of the given parameters, such as set pressure, MAWP, vessel dimensions, and charge mass, into FERST, the results under three different scenarios are shown in **Table 1**.

Table 1. Results for Styrene example problem

Flow Regime	Ideal Vent Area [m^2]	Ideal Vent Diameter [m]
Homogeneous	0.0367	0.2161
Bubbly	0.0339	0.2076
Churn Turbulent	0.0145	0.1358

Example problem 2: Mixture of $TiCl_4$ and H_2O in steady state

The second example problem was to use FERST to calculate the ideal vent area and diameter of the vessel that contains the mixture of $TiCl_4$ and H_2O. According to **Figure 6**, the reactive system was first determined as either a hybrid or gassy system since the final pressure, 120 psia, is close to the original pressure, 98 psia. [2] Then, it was identified as a gassy system because the pressure of the mixture can't compare with water vapor pressure. [2]

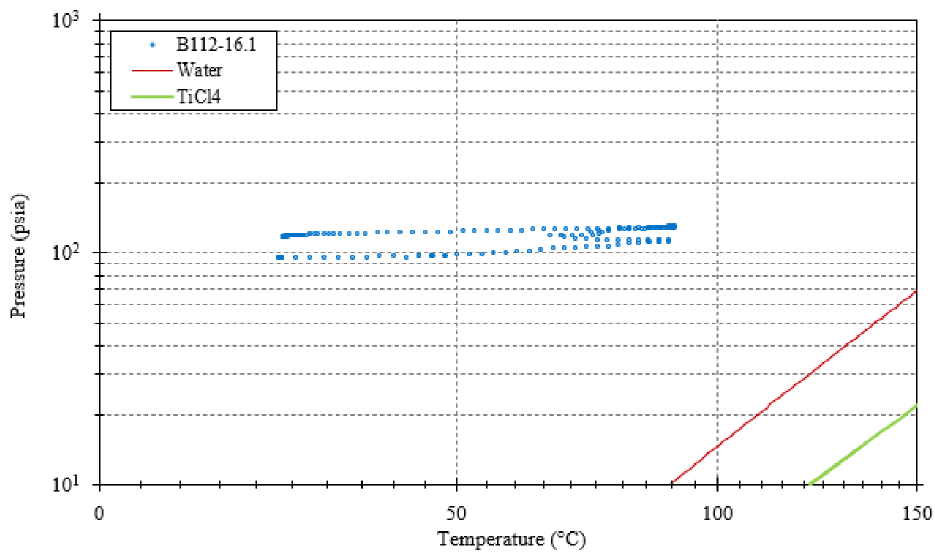

Figure 6. Temperature vs. Pressure graph for the mixture of $TiCl_4$ and H_2O

Next, the pressure rise factor is found in **Figure 7**. FESRT required the data point where the pressure rise factor was at maximum. Thus, (75.1°C, 41.8 psi/min) was observed.

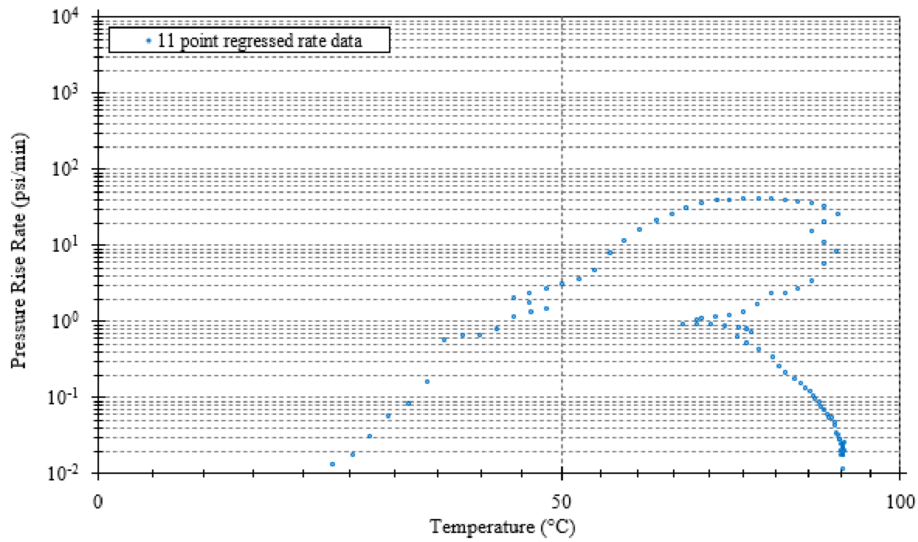

Figure 7. Temperature vs. Pressure Rise Rate graph for the mixture of $TiCl_4$ and H_2O

After the same procedure, the results of the rest of the given parameters are entered into FERST, as shown in **Table 2**.

Table 2. Results for $TiCl_4$ example problem

Ideal Vent Area [m^2]	Ideal Vent Diameter [m]
0.0029	0.0609

Example problem 3: Mixture of $TiCl_4$ and H_2O in dynamic

The third example problem was to practice the example in dynamic conditions. All parameters were carried over from the example problem of $TiCl_4$ and H_2O mixture. However, unlike determining the ideal vent area and pipe diameter in the steady-state condition, FERST created a graph to record customized parameter changes in the vessel and product stream as time passed in the dynamic condition. In this project, the vessel would be focused on calculated temperature, pressure, and liquid level change, and the product stream would be prioritized for the temperature, pressure, and chemical flow rate change. A screenshot of the FERST model in dynamic condition is shown in **Figure A2**. The only new parameter that has to be figured out is the appropriate simulation Run time. It could be determined by first running the simulation at a random time and observing the point where the relief event happened. Then, adjust the total run time to when the relief event was just done and increase the step size to make the data more precise. In this example, the resulting graphs for the vessel and the product stream are shown in **Figure 8** and **Figure 9** respectively.

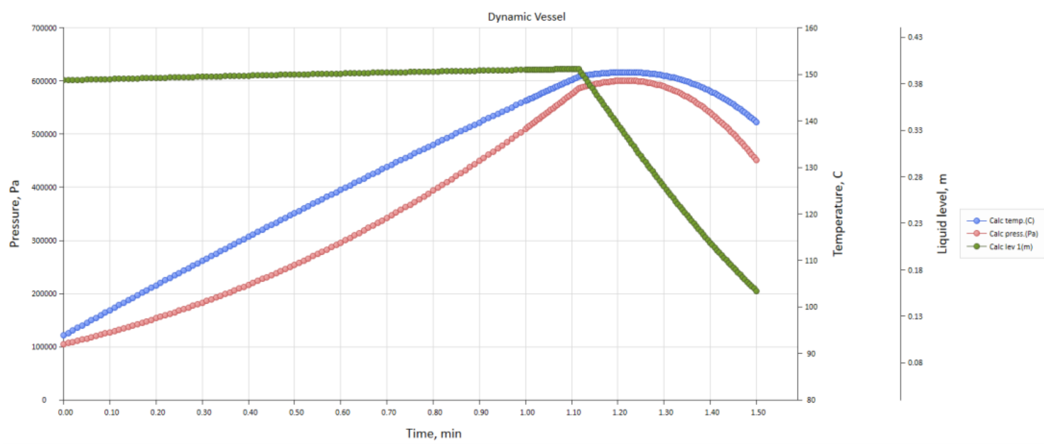

Figure 8. Graph for the Vessel in Dynamic $TiCl_4$ example

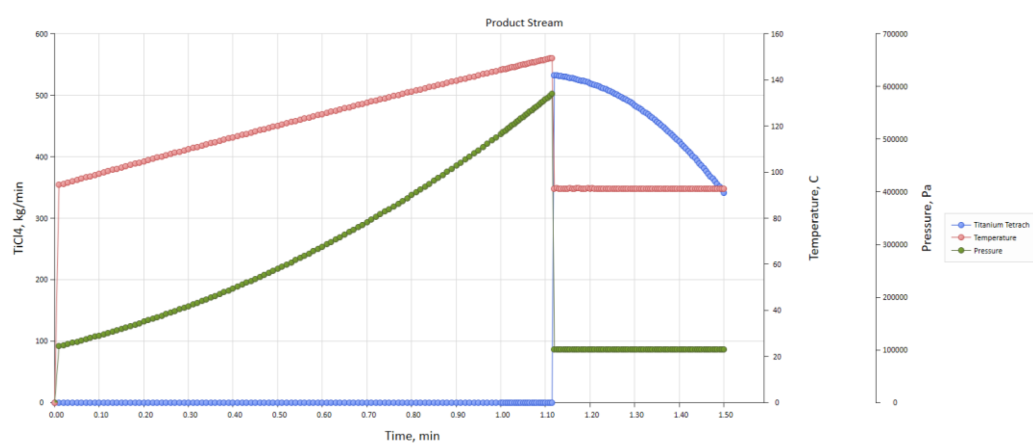

Figure 9. Graph for the Product Stream in Dynamic $TiCl_4$ example

Example problem 4: Piping

The fourth example problem was to explore the impacts of piping on the vessel and product stream. All parameters were still carried over from the dynamic $TiCl_4$ example problem A screenshot of the FERST model after adding pipe and nodes was shown in **Figure A3**. A total of two nodes and one pipe were added to the model. The purpose of the node was to control the pressure and flow rate of the stream since all the streams had to be maintained at a certain flow rate [4]. The only parameter that will be adjusted is the length of the pipe since this project will focus on the effect of pipe length. The resulting graphs for the vessel and product stream after adding piping are shown in **Figure 10** and **Figure 11** respectively.

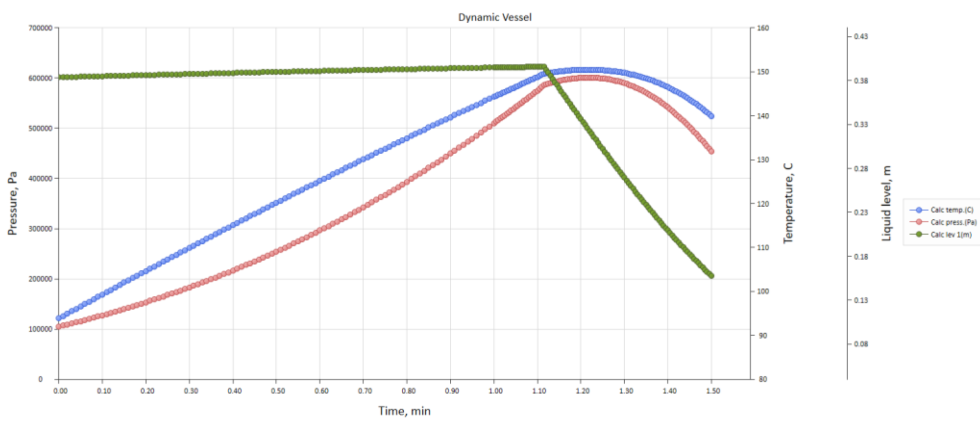

Figure 10. Graph for the Vessel in Dynamic piping $TiCl_4$ example

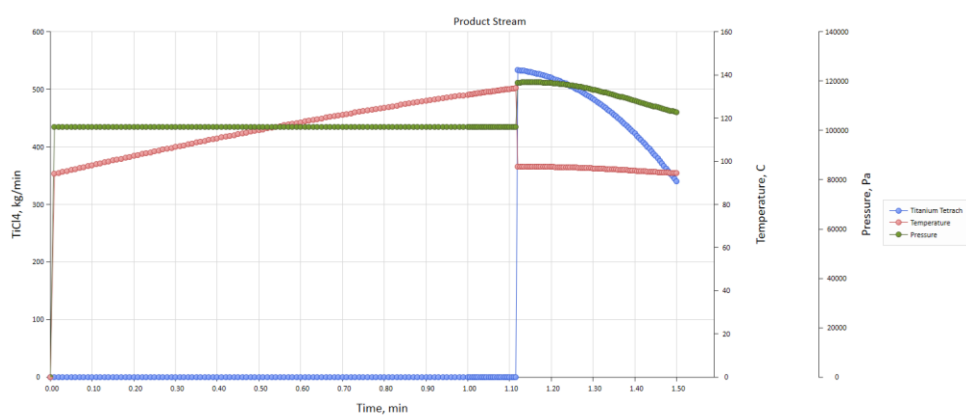

Figure 11. Graph for the Product Stream in Dynamic piping $TiCl_4$ example

Final problem: CO_2 suppression system design

After getting familiar with FERST and understanding the impacts of some parameters on vent sizing, it was time to model the CO_2 suppression system. This suppression system consisted of multiple vessels, pipes, and nodes. The FERST model was set up as shown in **Figure A4.** The original specifications for the vessels and pipes were given, and the nodes' pressure and pipe diameters were allowed to adjust. The goal was to investigate the amount of time that the suppression system will need to spread all the liquid CO_2 out and to observe the change in the calculated CO_2 flow rate at the product stream. However, the simulation could not converge no matter what parameters were set up, thus, the FERST model was simplified as shown in **Figure A5**. The simulation then ran successfully, and the resulting graph was shown in **Figure 12**.

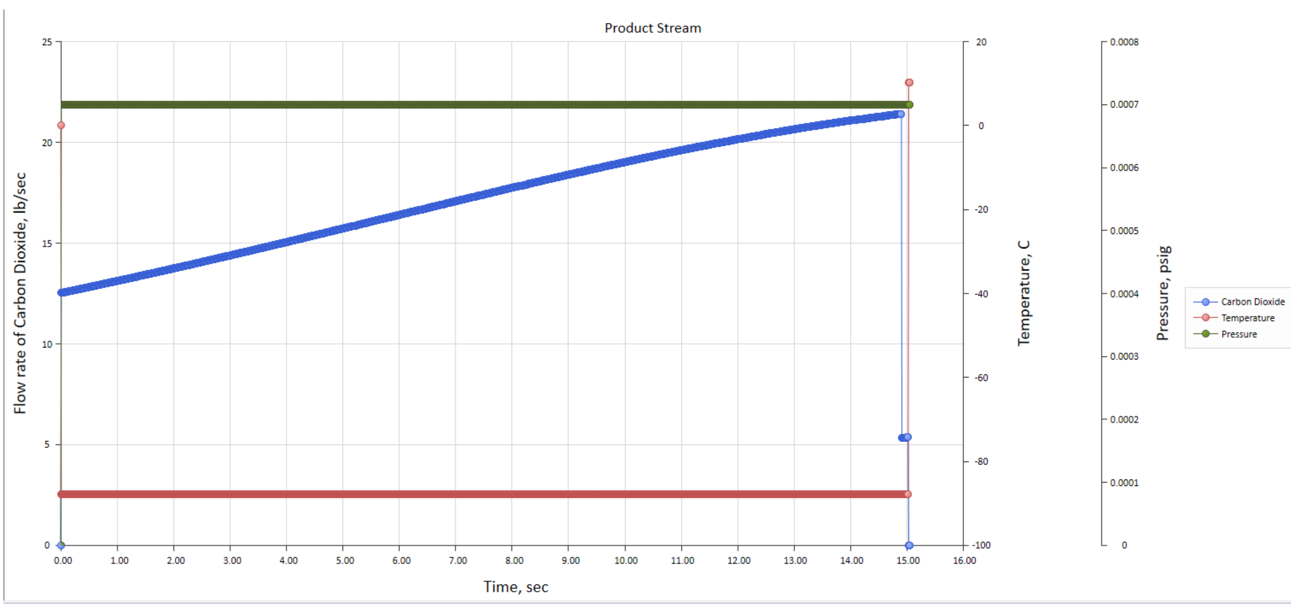

Figure 12. Graph for the Product Stream in CO_2 suppression system simulation

Discussion

Effect of Flow Regime

Refer to **Literature [4]**, the ideal vent area and diameter of the relief device will be smaller and smaller as the flow regime becomes more chaotic, i.e., homogeneous, then bubbly, and churn turbulent, because the homogeneous flow has no vapor-liquid disengagement. In contrast, the churn turbulent has significant vapor-liquid disengagement. No vapor-liquid disengagement means that the two-phase flow is well-mixed, thereby the combined flow rate will be large, and the size of the relief device needs to be large enough. On the other hand, the significant vapor-liquid disengagement indicates that vapor and liquid phases have separated flow, thus the single flow rate will be small, and the size of the relief device will be relatively small compared to the case of no vapor-liquid disengagement. In **Figure 13**, the comparison shows that the one in churn turbulent flow has the smallest ideal vent area and diameter. Bubbly flow and homogeneous flow have the second largest and largest respectively. Therefore, the result predicted by FERST in the steady state is accurate and can be supported by theory.

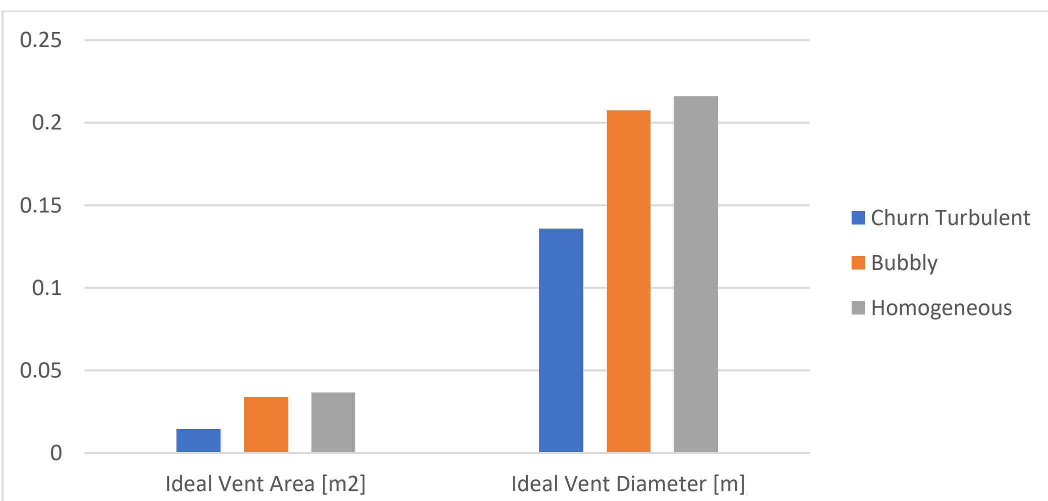

Figure 13. Comparison of Ideal Vent Area and Diameter

Graphs in Dynamic condition

In the steady-state example problem, FERST will only determine the ideal vent area and diameter of the relief device. However, in dynamic mode, FERST can provide the exact time when the relief event happened and how the temperature, pressure, and flow rate will change with time. According to **Figure 8** and **Figure 9**, the relief event occurred approximately 1.1 minutes after the simulation started since all the variables had a significant change and the pressure reached the MAWP. **Figure 8** indicates that the temperature and pressure rise gradually, and the liquid level remains almost the same in the vessel until the relief event happens. After that, the temperature and pressure drop gradually, and the liquid level decreases quickly. These patterns are reasonable since the $TiCl_4$ reaction is highly exothermic. As the reaction occurs, the reaction temperature and pressure will increase rapidly so will the vessel, and the liquid level won't change since it is in a dynamic condition that the reaction won't stop. **Figure 9** explains that the temperature and pressure increase and the flow rate of $TiCl_4$ remains zero at the product stream until the relief event happens. Then, the temperature and pressure immediately have a drastic decline while the flow rate increases rapidly and decreases gradually. These patterns are also reasonable. The product stream is connected to the vessel so as the vessel temperature and pressure increase, the product stream will also have the same pattern. The flow rate remains zero because the product stream will be used only when the relief event occurs. As a result, FERST's evaluation of the relief device in dynamic is reasonable and accurate.

Effect of Pipe Length

In the pipe exercise, experiments were conducted on pipes of different lengths. The result on the product stream is the focus point and the variables are 2m, 5m, and 8m. According to **Figure 14**, different pipe lengths won't influence the flow rate of chemicals.

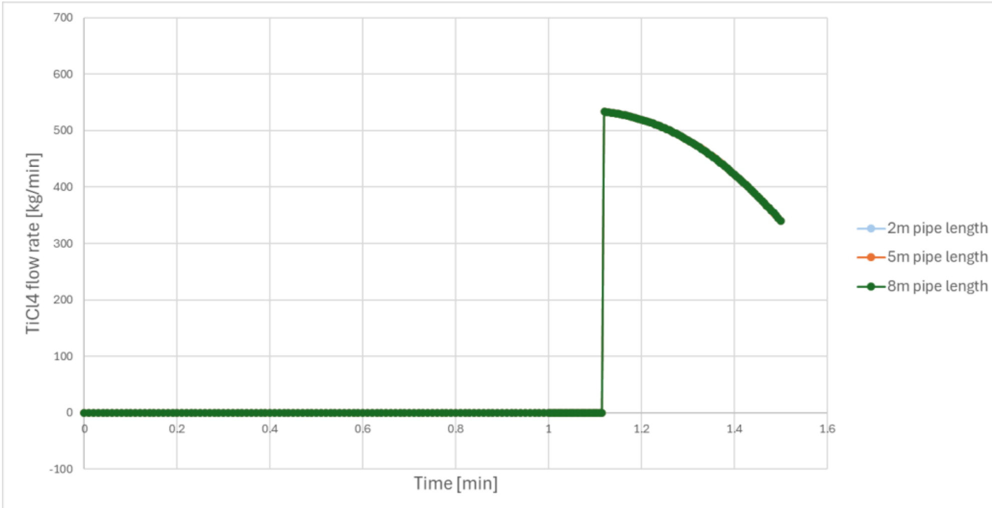

Figure 14. Time vs. Flow rate of chemicals in different pipe lengths

However, as the length of the pipe increased, the overall temperature and pressure after the relief event also increased as shown in **Figures 15** and **16**.

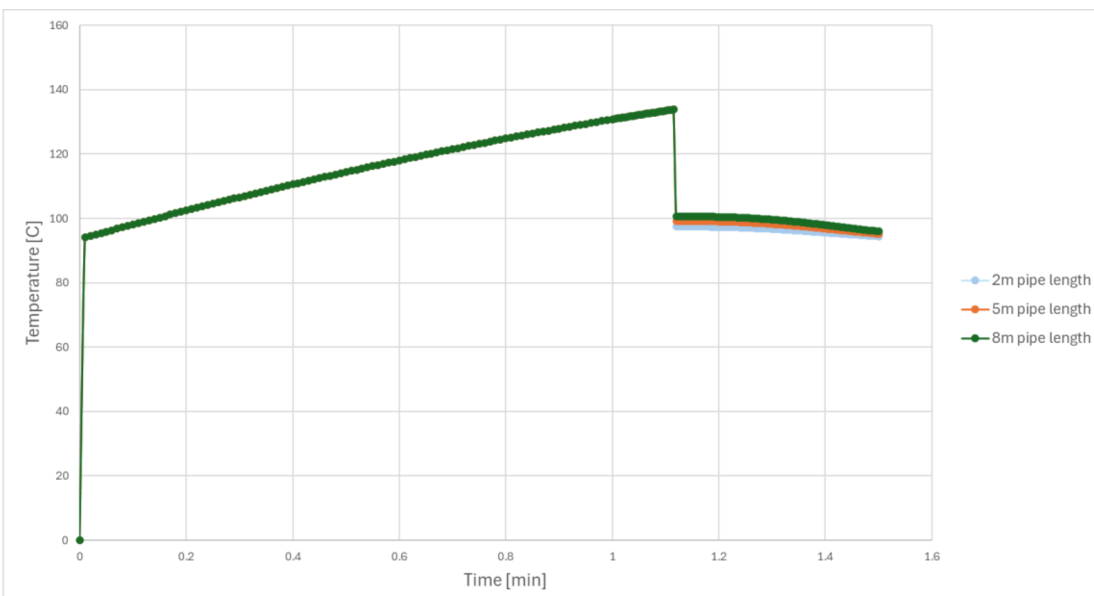

Figure 15. Time vs. Temperature in different pipe lengths

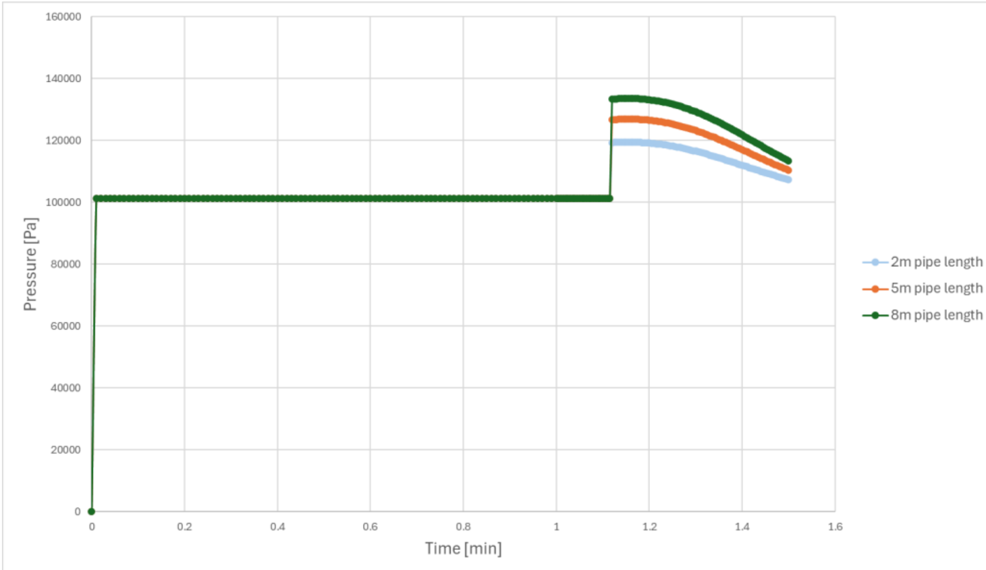

Figure 16. Time vs. Pressure in different pipe lengths

This result is reasonable because as the pipe length increases, it will cause the pressure of the inlet pipe to rise [5] which is at the point connected with the product stream. The temperature will have the same pattern as the pressure. As a result, FERST proves its accuracy in modeling the relief device under more complex conditions.

Results of CO_2 Suppression System

According to **Figure 12,** the total time for the suppression system to spread all the liquid CO_2 out was approximately 15 seconds. The product stream's pressure and temperature are maintained at 0.0007 psig and -87.9°C respectively. This pressure is equivalent to 1 atm and is the same as the setup while the temperature is calculated by FERST. The flow rate rapidly increases to 12.53 lb/sec within 0.01 seconds. Then, it gradually increases to 21.42 lb/sec within 14.9 seconds. After that, it immediately drops to 5.35 lb/sec for 0.1 seconds and to 0 at last since the vessels are out of liquid CO_2. Although the result was reasonable, there was no opportunity to explore the impacts of the pipe diameters and lengths on the total spread time and the flow rate of CO_2 since there was no time to continue running this project. As a result, investigating the effects of the pipe dimensions on the CO_2 suppression system will be the main part of the proposed steps forward.

Conclusions

In conclusion, this project shows how powerful FERST is in simulating runaway chemical reactions. On top of that, FERST successfully extends its use by simulating the CO_2 fire suppression system. Moreover, as the simulation's scenario gets more and more complex, it becomes closer to real-world applications. It surprises me how complicated designing a relief device is. One small change can lead to the entire result being different and this can apply to most things. As a result, this project not only teaches me about the basis of relief device design but also reminds me to be more aware of all the details in the future.

Proposed Steps Forward

FAI will continue to design the dimensions of the pipes for numerous scenarios. For instance, completing the original FERST model for the CO_2 suppression system as shown in **Figure A4**. After that, FAI may try to explore the impacts of the pipe diameters and lengths on the total spread time and the flow rate of CO_2 to optimize the entire simulation.

Appendix

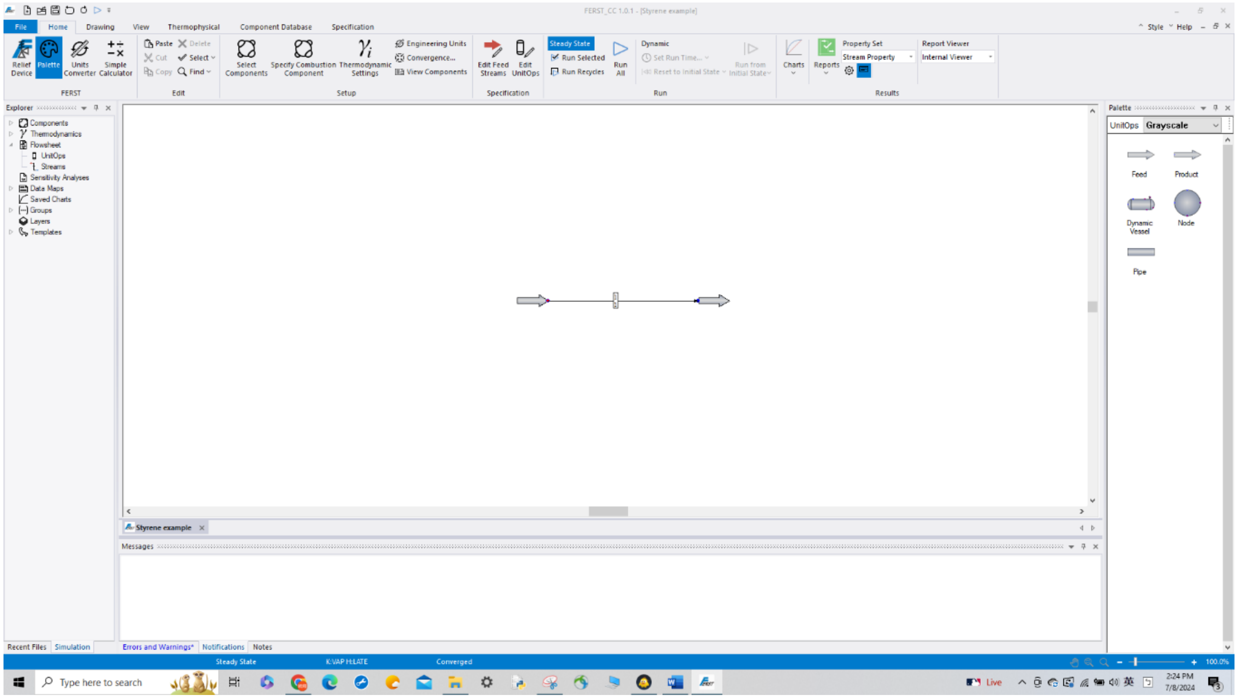

Figure A1. FERST model in steady-state conditions

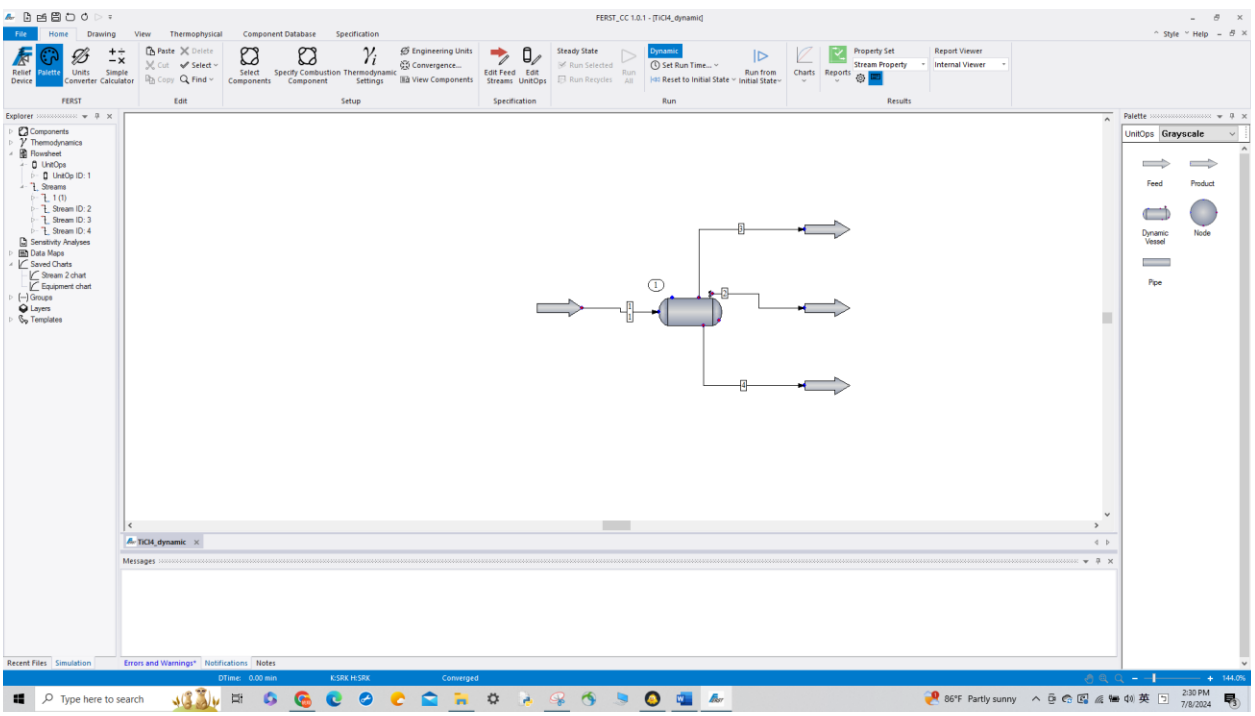

Figure A2. FERST model in dynamic condition

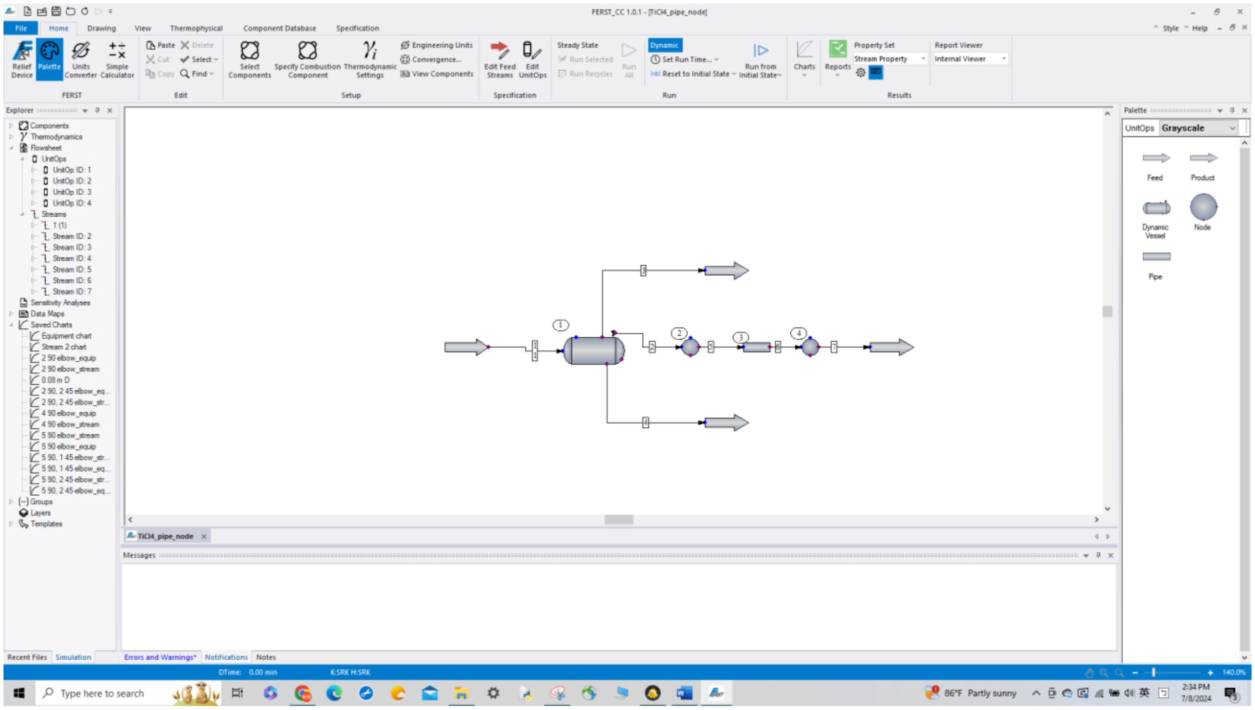

Figure A3. FERST model in dynamic and piping condition

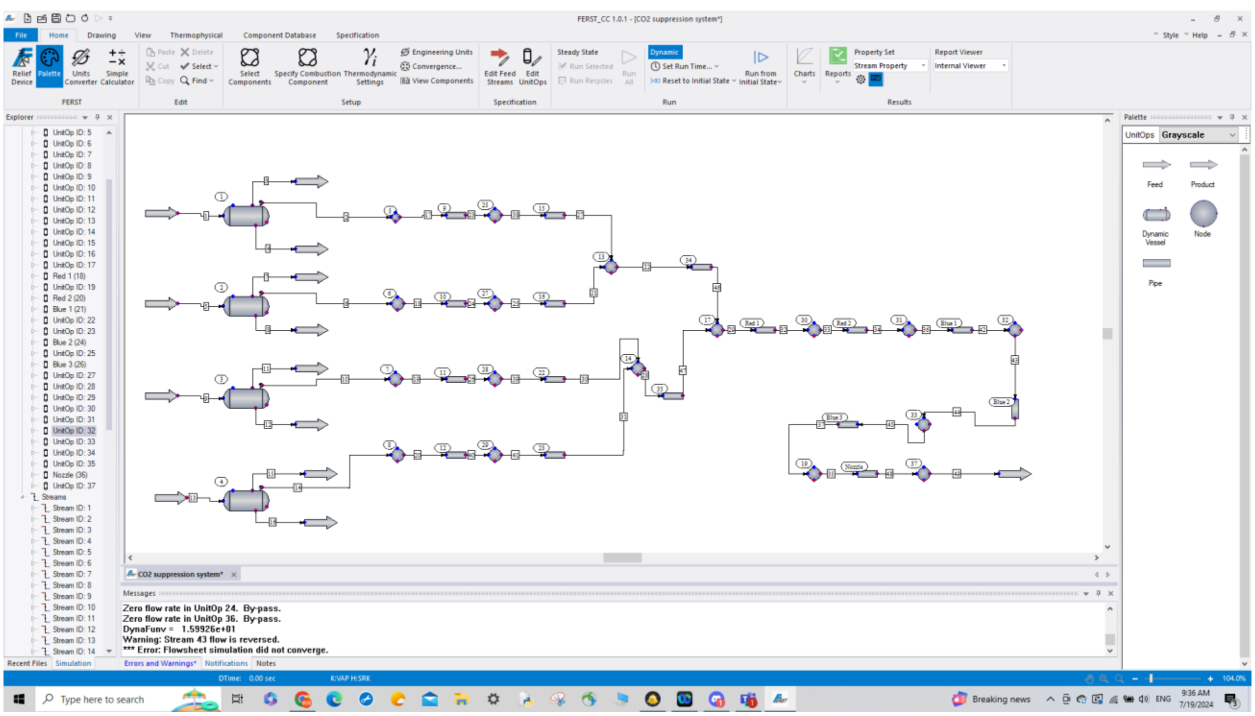

Figure A4. Original FERST model for CO_2 suppression system

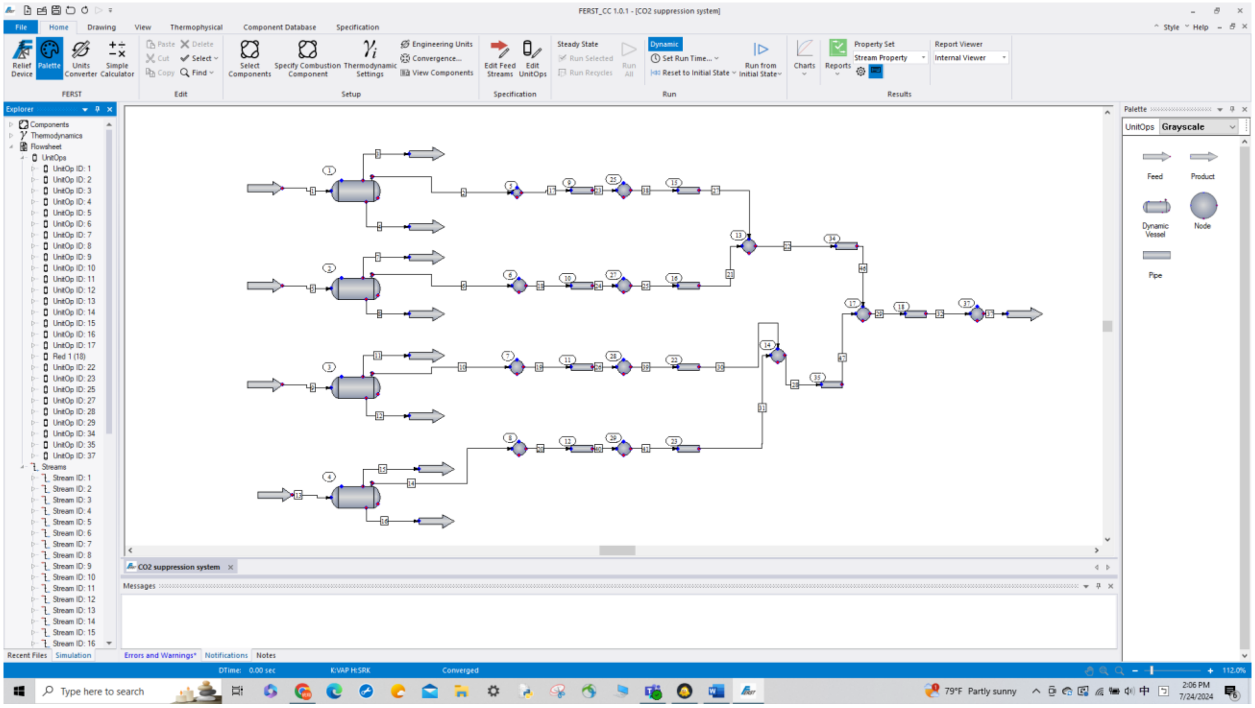

Figure A5. Simplified FERST model for CO_2 suppression system

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