A spreadsheet‑based tool for education of chemical process simulation and control fundamentals

CH331 - Project Report
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Content

1. Introduction

2. Problem Statement

3. Features and User Interface

4. Model and Model Design

5. Setting simulation and Output Parameter

6. Simulation and Results

7. Conclusion

8. References

1. Introduction

Understanding the behaviour and properties of processes is essential for engineering research on chemical-technological processes and the design of effective control systems. However, direct measurement in real facilities is often challenging due to safety risks, production disruptions, or limitations in measurement techniques. As a result, dynamic mathematical models serve as invaluable tools for simulating process behaviour, confirming assumptions, and testing control strategies.

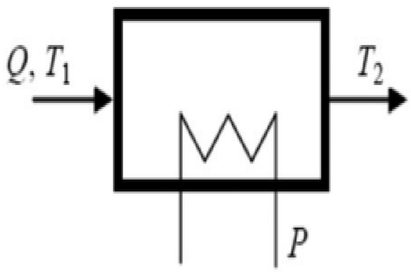
In academic settings, students in fields such as chemical engineering engage in process modelling, simulation, and control using various software tools. These tools range from general-purpose programming languages to specialised simulation environments. While professional simulation systems offer comprehensive features, they often require extensive training to master. To address this challenge, educational institutions develop simpler tools using platforms like Excel. Leveraging students' familiarity with Excel and its widespread availability, these tools provide an intuitive interface for exploring process dynamics and control concepts.

One such tool is the Process Simulation and Control (PSIC) Excel add-in. Unlike traditional approaches, PSIC integrates simulation and control functionalities, allowing students to develop a deeper understanding of chemical processes within a familiar environment. With PSIC, students can build dynamic models of chemical processes and explore various control strategies without the need for advanced programming skills. The add-in facilitates numerical solution of dynamic models, enabling students to perform sensitivity analyses and assess the impact of different parameters on process behaviour.

By using tools like PSIC, students gain practical experience in process simulation and control, bridging the gap between theoretical concepts and real-world applications. Moreover, these tools empower students to explore complex chemical processes in a hands-on manner, fostering critical thinking and problem-solving skills. Overall, software tools like PSIC play a crucial role in enhancing the educational experience in chemical engineering by providing students with the tools they need to succeed in their future careers.

2. Problem Statement

Design a dynamic model of the electrically heated water heater (figure). Using the model, simulate the heater behaviour (i.e. the output temperature T_2 time behaviour) during the estimated simulation period, and study the effect of disturbance variables (i.e. input temperature T_1 water flow Q and power input P) on the output temperature.



Steady-state:

- heater volume $V = 5$ l
- water flow $Q = 0{,}5$ l min^{-1}
- input water temperature $T_1 = 15$ °C
- water density $\rho = 1$ kg l^{-1}
- heat capacity $c_P = 4{,}187$ kJ kg^{-1} K^{-1}
- power input $P = 1$ kW
- heating efficiency $\eta = 90$ %

Assumptions:

- The heater is insulated and the wall accumulation ability is small and can be neglected.
- A spatially constant temperature inside the heater is well mixed and is equal to the output temperature.
- Temperature changes in density and heat capacity are negligible.
- The heater is completely filled with water.

3. Features and User Interface

The PSIC add-in simplifies the process of creating mathematical models, running simulations, and adjusting controller constants. The user interface includes several commands accessible through the PSIC ribbon tab. These commands facilitate tasks such as creating models, configuring feedback loops, running simulations, and tuning controllers.

2.1 Commands

- **New Model:** Generates a new worksheet for inserting input data of a model and setting simulation parameters and outputs.
- **New Loop:** Generates a new worksheet for configuring feedback regulatory control loops and setting simulation parameters and outputs.
- **Mode:** Dropdown list for changing controller mode (direct or reverse) in simulated **feedback** regulatory control loops.
- **Action:** Dropdown list for changing control action (P, PI, PD, or PID) in simulated feedback regulatory control loops.
- **Gain r_0:** Text field for changing controller gain r_0 in simulated feedback regulatory control loops.
- **Integral Time T_i :** Text field for changing controller integral time T_i in simulated feedback regulatory control loops.
- **Derivative Time T_d:** Text field for changing controller derivative time T_d in simulated feedback regulatory control loops.
- **Reset:** Button to restore controller settings used in the last simulation.
- **Run:** Button to generate a new worksheet with simulation results.
- **Rerun**: Button to recalculate simulation results after changing controller settings.
- **Update Add Link:** Button to update the link to the PSIC add-in in a workbook

4. Model and Model Design

Quantities and equations of a model are entered in the yellow cells of the Model worksheet generated by the New Model button. The Model worksheet is protected so the user cannot enter data of other values or types than requested. If you copy data, insert them as values using the Paste Special command. A Model worksheet consists of the following tables:

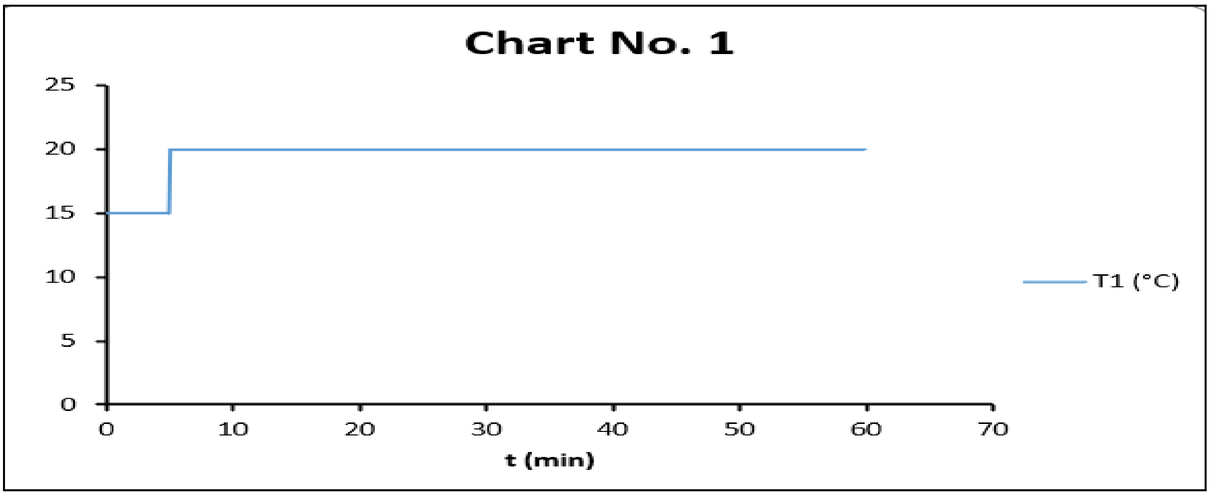
- **Model Variables and Constants:** Enter marks of quantities of the model (Variable column), their values at the beginning of the simulation (Value column), their physical units (Unit column), and their descriptions (Description column).
- **Model First-order ODEs:** Select variables of which the first derivative occurs in the left-hand sides of the 1st ODEs (Derivative column), and insert Excel formulas which calculate derivatives i.e. the right-hand sides of the 1st ODEs (Value column). Arguments of Excel formula must be cell references from the column Value of the table Model Variables and Constants.

5. Setting simulation and Output Parameter

Integration parameters: Enter the final simulation time (Final Time cell) and the simulation step size (Integration Step cell), select the numerical method for solving ODE (Integration Method cell), and select the time unit of a final time and a simulation step (Time Unit cell). The time unit must be the same as in the model.
Output Variable: Select the output variable of the model which you want to observe (Variable column).
Charts Parameters: Select the location of simulation charts (embedded in worksheet or separated chart sheets) in which model variables will be displayed (Location cell).
Model Variables in Charts: In the chosen table row, select the variable of the model which you want to display in the chart (Variable column), chart number (Chart No. column) and if it is needed to check secondary y□axis (Sec Y-axis checkbox).

6. Simulation and Results

For PI controller:



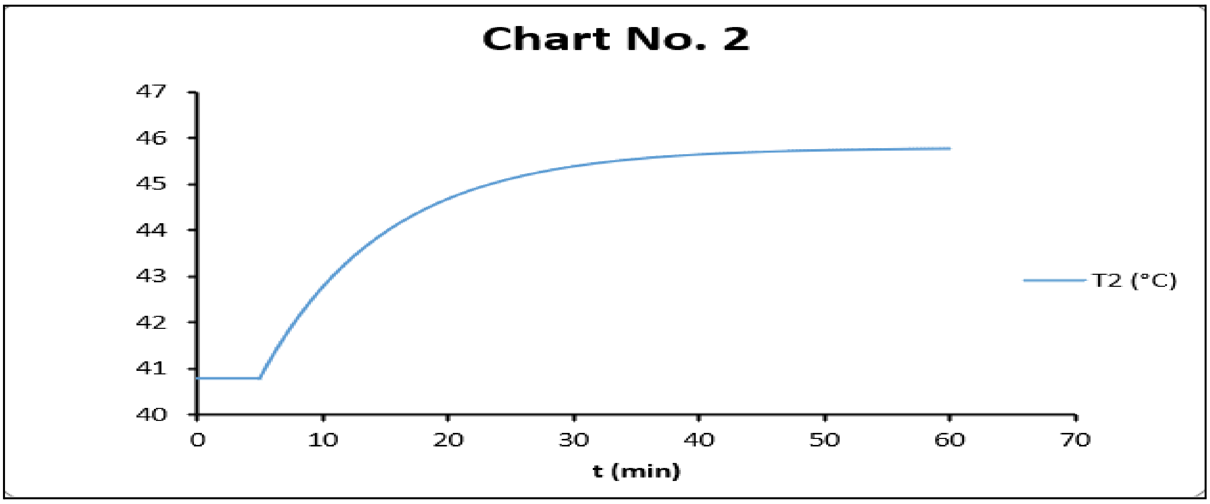


Fig 1. Represents simulation tables and charts of disturbance (No. 1) and model response (No. 2)

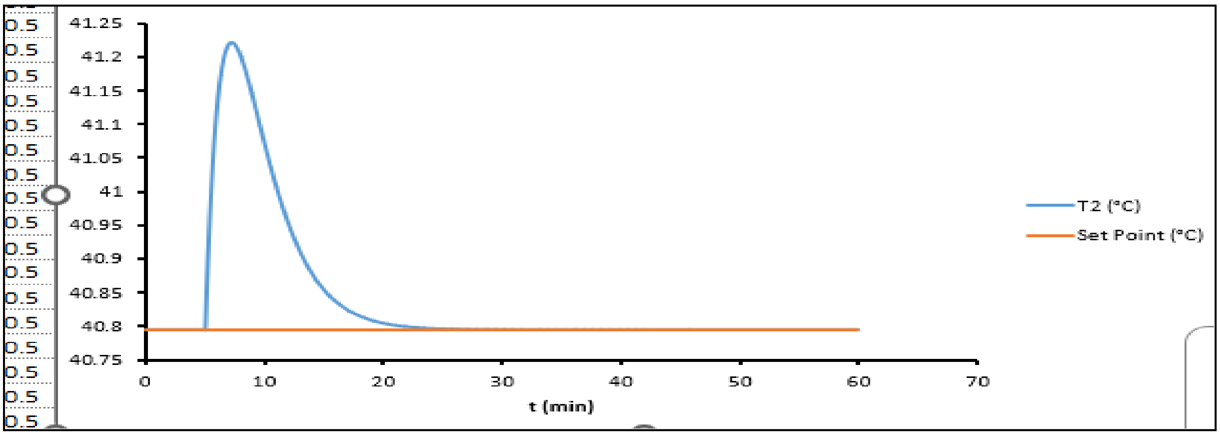


Fig 2 - Represents model response inside feedback loop and setpoint

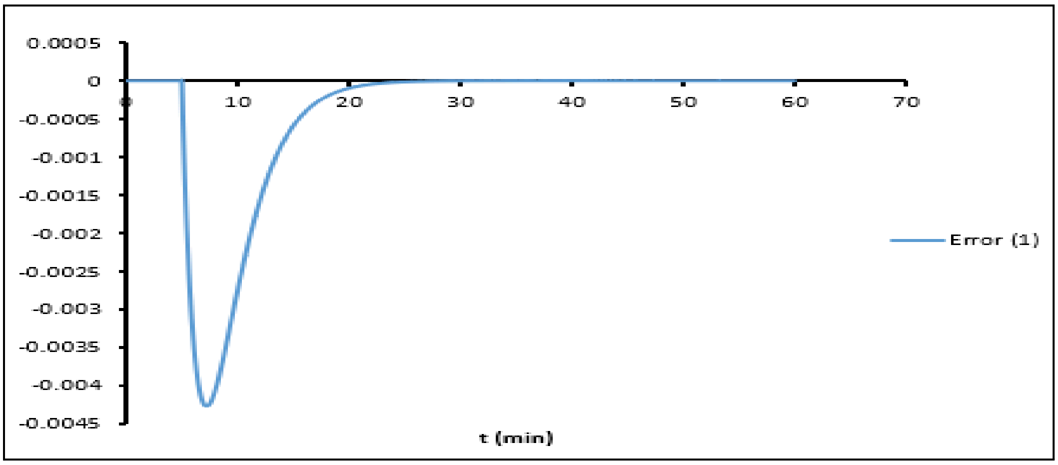


Fig 3 - Graph shows error when plotted against time (min)

For PD controller:

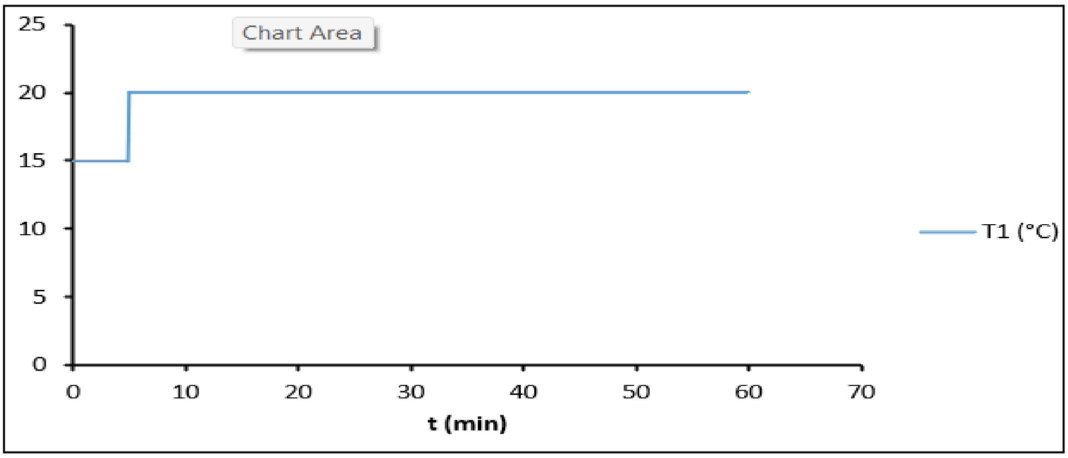


Fig 4 - Simulation Results T_1 vs t

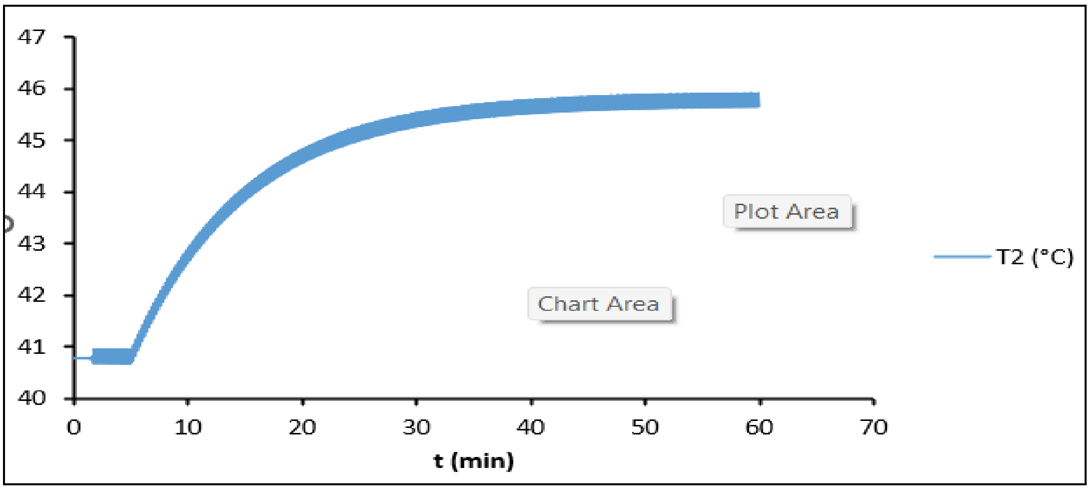
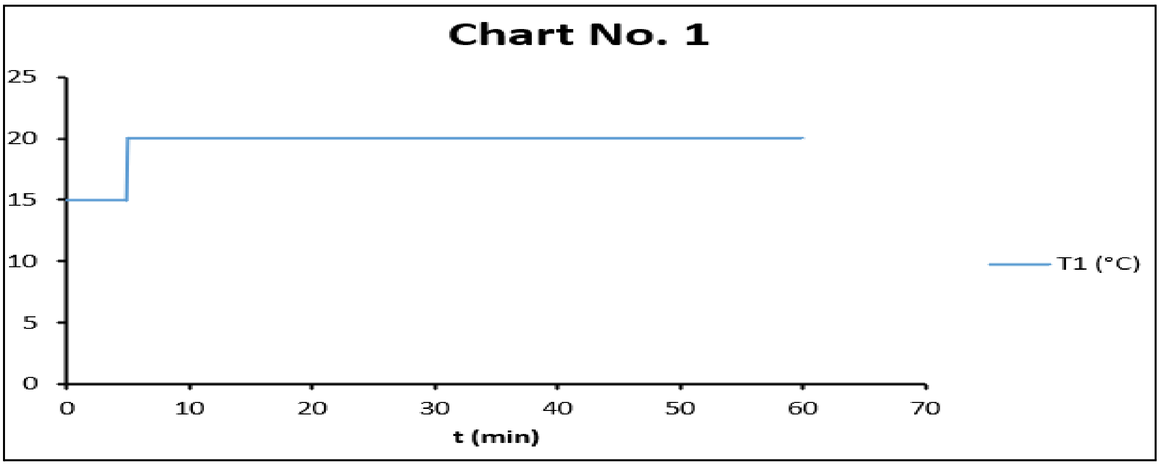


Fig 5 - Simulation Results T_2 vs t

For PID controller:



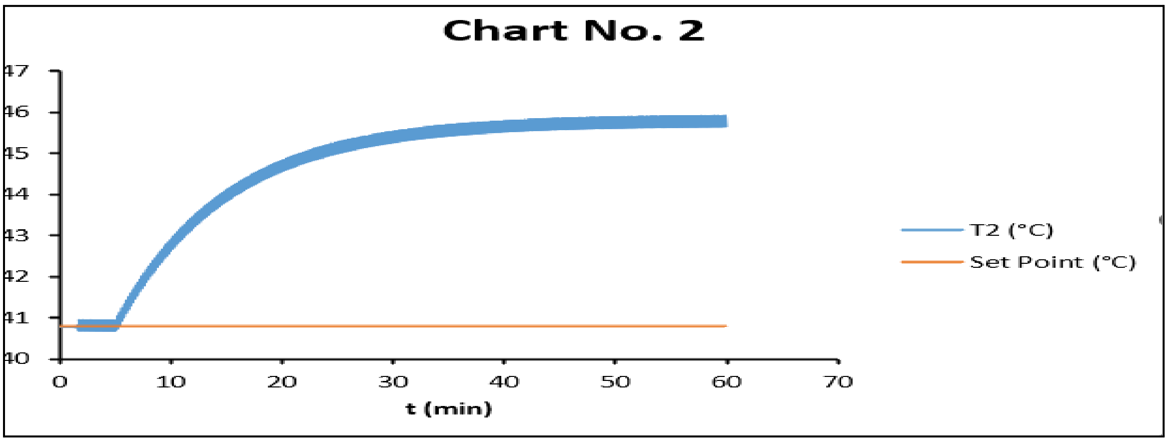


Fig 6 - Represents simulation tables and charts of disturbance (No. 1) and model response (No. 2)

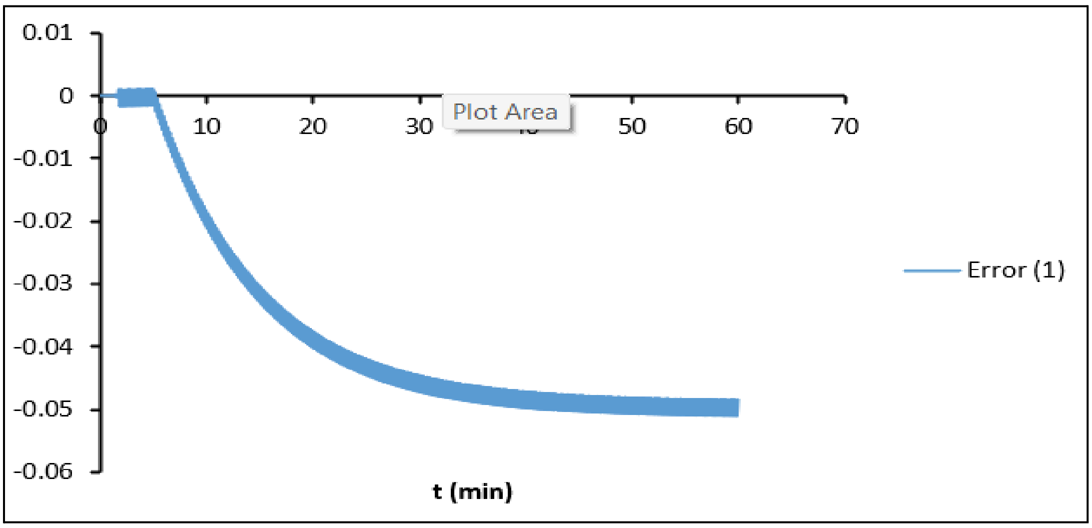


Fig 7 - Error vs time

7. Homework Problem

We've been tasked with designing a dynamic model for an electrically heated water heater and simulating its behaviour over a given period. The model should allow for the study of the effects of disturbance variables (input temperature, water flow, and power input) on the output temperature. Several assumptions are made to simplify the model, including neglecting wall accumulation, assuming spatially constant temperature inside the heater, and negligible changes in density and heat capacity. The heater is considered to be completely filled with water, and the energy balance equation is modified to express the derivative of the output temperature.

Critical Analysis:

The problem statement outlines a comprehensive task involving the design and simulation of a dynamic model for an electrically heated water heater. Let's break down the critical components and provide a brief analysis:

1. Mathematical Model Design: The initial step involves designing a mathematical model based on energy balance equations and system assumptions. Key considerations include neglecting certain factors to simplify the model while ensuring it accurately represents the behaviour of the system.
2. Simulation and Verification: Using the designed mathematical model, simulation is conducted to verify its accuracy. This step involves simulating steady-state conditions and responses to step disturbances in input variables. The verification process ensures that the model accurately reflects the behaviour of the real-world system.
3. Calculation of Time Constant and Gain: The time constant and gain values of the model equation are calculated to understand the dynamics of the system. These values provide insights into the system's response to changes in input variables and help in controller tuning.
4. Analysis of Simulation Results: Simulation charts are generated to analyse the response of the model to step changes in input quantities. The time constant

and gain values obtained from the simulation are compared with those calculated from the model equation to assess the accuracy of the model.

5. Controller Tuning Rules: While not explicitly mentioned in the problem statement, understanding the dynamics of the system through the designed model can inform controller tuning rules. This involves adjusting controller parameters to achieve desired system performance and stability.

Overall, the problem statement presents a structured approach to modelling and simulating the behaviour of an electrically heated water heater. By following the outlined steps, one can gain valuable insights into the system's dynamics and make informed decisions regarding its control and operation.

8. Conclusion

In conclusion, the utilisation of the Process Simulation and Control(PSIC) add-in proved to be instrumental in our understanding of chemical process simulation and control fundamentals. Through our experimentation with PSIC, we were able to:

- Gain practical insights into modelling, simulating, and designing control systems for chemical engineering processes within the familiar environment of Microsoft Excel.
- Successfully validate the simulation and control of an electrically heated water heater, demonstrating the efficacy of PSIC in replicating real-world scenarios.
- Develop a comprehensive homework problem statement, showcasing our ability to apply theoretical knowledge to practical situations.
- Explore and attempt various controller tuning rules, providing us with valuable hands-on experience in fine-tuning control parameters for optimal system performance.

Through the user-friendly interface and extensive functionality of PSIC, we were able to build dynamic simulation models, simulate complex systems, and analyse the behaviour of feedback control loops without the need for advanced programming skills or complex mathematical transformations. This not only enhanced our understanding of process control principles but also equipped us with valuable skills that are highly relevant in the field of chemical engineering. Moving forward, the knowledge and experience gained from this lab exercise will undoubtedly serve as a solid foundation for our future endeavours in process simulation and control. We believe that PSIC has proven to be an invaluable tool for education in chemical engineering, empowering students to bridge the gap between theory and practice in a highly intuitive and accessible manner. We look forward to further exploring the capabilities of PSIC and applying them to tackle more complex challenges in the realm of process control. Overall, this lab experience has been enriching and enlightening, providing us with a deeper understanding of process simulation and control fundamentals while honing our problem-solving skills and analytical abilities. We are confident that the insights gained from this exercise will serve us well in our academic and professional journey in the field of chemical engineering.

8. References

- PSIC Add-on file [https://github.com/nachtigi/PSIC]
- Research Paper