

CHE CALCULATOR®: Empowering Students with Computational Tools for Real-World Engineering Challenges

Dr. Betul Bilgin, The University of Illinois at Chicago

Betul Bilgin is a Clinical Associate Professor of Chemical Engineering at the University of Illinois at Chicago (UIC). With a Ph.D. in Chemical Engineering from Michigan State University, Dr. Bilgin has extensive experience in both biotechnology research and engineering education. Since joining UIC, she has developed and taught various undergraduate courses, integrating innovative teaching methods and industry-relevant content to enhance student learning and engagement.

Dr. Bilgin's research focuses on engineering education, particularly in fostering professional identity among engineering students and integrating data science into the chemical engineering curriculum. She has received multiple awards for her contributions to teaching and mentoring, including the ASEE Ray Fahien Award and the UIC COE Harold Simon Award. Dr. Bilgin is also actively involved in professional service, currently serving as the Director of the Chemical Engineering Division for ASEE and participating in various initiatives to improve engineering education and student success.

CHE CALCULATOR®

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Abstract

Scientific learning involves experimentation, mathematical modeling of physicochemical processes, and rigorous statistical analysis. These methods lead to discoveries in science and engineering, which are often implemented in commercial applications through the effective use of mathematical models. This process enables engineers to predict system performance and design equipment efficiently and economically. However, engineering students frequently find it difficult to apply theoretical principles to real-world problems, particularly those encountered in commercial settings. To address this challenge, we developed an innovative, Excel-based computational tool, CHE CALCULATOR®, at the University of Illinois Chicago (UIC). This tool allows students to apply fundamental concepts from various chemical engineering courses—such as thermodynamics, fluid mechanics, and process control—to solve complex, commercially relevant problems with confidence.

CHE CALCULATOR®, powered by a VBA engine in Microsoft Excel, serves as a state-of-the-art platform that is easily accessible and adaptable for students. It enables them to extend and enhance the software with their own models and calculations, fostering both learning and creativity. The integration of this tool into the curriculum has strengthened students' theoretical understanding while providing them with the practical skills necessary for success in industry.

In this paper, we provide an overview of CHE CALCULATOR®, its applications in areas such as heat and mass transfer and chemical kinetics, and how it engages students in active learning. We also discuss student feedback and engagement, as well as strategies for further enhancing the tool for future cohorts. Our goal is to illustrate how this integrated approach equips students to tackle the complex challenges they will face in their professional careers.

Introduction

The transition from theoretical understanding to practical application remains a persistent challenge in engineering education. While students may grasp fundamental concepts in isolation, they often struggle to apply these principles to real-world scenarios, particularly those encountered in industrial settings. This challenge is especially pronounced in chemical engineering, where complex problems frequently require the simultaneous application of multiple theoretical concepts across different domains such as thermodynamics, fluid mechanics, and process control.

In response to this educational challenge, we developed CHE CALCULATOR®, an Excel-based computational tool designed to bridge the gap between theoretical knowledge and practical application. The tool serves multiple pedagogical objectives:

1. Facilitating the integration of concepts across different chemical engineering courses
2. Providing students with hands-on experience in solving industry-relevant problems
3. Developing students' computational skills within a familiar software environment
4. Encouraging creative problem-solving through customizable modeling capabilities

Literature Review

The integration of computational tools in engineering education has shown significant positive impacts on student learning outcomes [1]. Felder and Brent demonstrated that active learning strategies incorporating computational elements lead to improved student engagement and deeper understanding of engineering concepts. Their research showed that students who regularly used computational tools were more likely to retain complex engineering concepts compared to those using traditional learning methods [2]. Web-based applications, such as those using MATLAB Webserver, enable remote simulations and interactive learning experiences [3]. Despite their potential, the effective implementation of these tools requires addressing non-technical barriers, including maintenance costs and shareability [1]. Additionally, educators need adequate theoretical support and improved model perception to effectively integrate these technologies into curricula. Overall, computational tools offer valuable opportunities for enhancing chemical engineering education when implemented thoughtfully.

Spreadsheets, particularly Microsoft Excel, have become a ubiquitous tool in chemical engineering for various calculations and process modeling tasks. Excel has been recognized for its utility in routine engineering calculations and process design. The integration of Visual Basic for Applications (VBA) has further enhanced Excel's capabilities, allowing for complex computations and linkage with other programming languages. Despite the advent of Industry 4.0 and more sophisticated software, Excel remains a crucial tool in chemical engineering, serving as a bridge between different software systems and playing a significant role in process design and development [4]. Its widespread use underscores its importance in both academic and industrial settings.

Excel, coupled with VBA, is widely used in chemical engineering education to teach programming concepts, numerical methods, and statistical analysis. Students are introduced to both basic and advanced features of Excel, including macro programming and statistical functions, which are applied to solve problems in material and energy balances, thermodynamics, transport, kinetics, and data analysis [4]-[6]. The use of Excel VBA as a problem-solving tool is emphasized in core chemical engineering courses, allowing students to convert complex engineering problems into executable programs [7], [8]. This approach not only teaches programming but also enhances problem-solving skills by comparing Excel VBA with other programming languages and software packages. Excel's Solver feature is particularly useful for teaching process design and optimization. It allows students to solve complex chemical engineering problems by embedding numerical optimization procedures within a spreadsheet environment [9]. This method provides a practical approach to teaching optimization and design concepts, which are crucial for chemical engineering students [10].

The use of Excel and VBA is often compared with other software packages like MATLAB. These comparisons highlight the unique capabilities and ease of use of Excel, especially in educational settings where cost and accessibility are significant considerations. Excel's ability to integrate with other software packages and its user-friendly interface make it a preferred choice for many educational institutions. Excel VBA is particularly effective in solving complex chemical engineering problems due to its flexibility and accessibility. It allows for the development of

custom solutions tailored to specific engineering challenges, such as optimization, process simulation, and numerical analysis. The integration of VBA in chemical engineering curricula not only equips students with programming skills but also enhances their ability to tackle real-world engineering problems efficiently. As a result, many departments incorporate Excel/VBA into their curricula, and numerous spreadsheet-based tools have been developed to support the teaching of various chemical engineering courses. However, existing tools often focus on specific topics or courses, lacking the comprehensive integration necessary for addressing complex, multi-domain problems. CHE CALCULATOR® addresses this gap by providing a unified platform that spans multiple chemical engineering disciplines.

Methods

CHE CALCULATOR® was developed using Microsoft Excel with VBA integration over several years by chemical engineering students under the guidance of their instructor. Initially designed for use in Thermodynamics courses five years ago, it has since evolved to include numerous features, making it applicable across a wide range of chemical engineering courses. Excel/ VBA platform is particularly chosen for its:

- Universal accessibility across academic and professional environments
- Familiar user interface reducing the learning curve
- Robust computational capabilities
- Extensibility through VBA programming
- Built-in visualization and data analysis features

The tool was implemented through a phased approach: Initial deployment in core chemical engineering courses, collection and incorporation of student feedback, iterative refinement of features and user interface and extension to additional course modules.

In Fall 2024, a survey was conducted among senior chemical engineering students (enrolled in Senior Design I course) to gather feedback on the CHE CALCULATOR® tool. Senior Design I class does not incorporate CHE CALCULATOR® directly, but students might use it as a resource. The survey focused on identifying both the strengths and weaknesses of the tool, allowing for a comprehensive understanding of its impact and areas for improvement. Students were presented both open-ended and Likert-scale questions as listed below in Table 1. Out of the total class of 39, 36 students participated in the survey, providing valuable insights.

Table 1: Survey Questions

Survey Questions
<i>Which courses did you use the CHE Calculator in?</i>
<i>How frequently did you use the CHE Calculator during the courses?</i>
<i>How was the CHE Calculator integrated into your coursework? (HW, project, resource)</i>
<i>What challenges, if any, did you face while using the CHE Calculator? (Select all that apply)</i>
<i>How intuitive was the CHE Calculator interface?</i>
<i>How effective was the CHE Calculator in helping you understand complex chemical engineering concepts?</i>

<i>How do you think the CHE Calculator compares to other computational tools you've used in chemical engineering? (Aspen, Python, etc.) (effectiveness, usefulness etc)</i>
<i>Did the CHE Calculator help you develop problem-solving skills relevant to your professional career?</i>
<i>Would you recommend integrating the CHE Calculator earlier in the curriculum?</i>
<i>If the CHE Calculator were to be improved, what feature(s) would you prioritize? (Select all that apply)</i>
<i>What do you perceive as the strengths and weaknesses of the CHE CALCULATOR®?</i>

The survey was distributed via an online platform accessible through the university's learning management system. Participation was voluntary, and no direct incentives were provided for completing the survey.

To analyze the responses, thematic analysis was conducted by identifying recurring themes across student feedback. The project team categorized responses into key themes such as usability, documentation, and problem-solving effectiveness.

This study was reviewed by the institution's Institutional Review Board (IRB) and deemed exempt under educational research guidelines. Ethical considerations, including informed consent and voluntary participation, were followed to protect student confidentiality and ensure compliance with institutional policies.

Implementation

CHE CALCULATOR®'s application is best illustrated through specific examples of its use in chemical engineering courses. In the Thermodynamics course, students used the tool to calculate vapor-liquid equilibrium (VLE) properties for multicomponent systems. It is an innovative, Excel-based computational tool designed to streamline the process of determining thermodynamic properties. It eliminates the need for students to conduct extensive searches across multiple websites or reference materials, offering a user-friendly interface to retrieve critical thermodynamic data with just a few clicks. By integrating property databases and calculation algorithms, the tool enables students to quickly access properties such as enthalpy, entropy, pressure, and temperature for a variety of substances. This functionality not only saves time but also reduces the potential for errors in manual data retrieval and interpretation, enhancing the learning experience by allowing students to focus on applying core chemical engineering principles to solve complex problems. Below is the typical user interface layout (Figure 1).

Properties of Fluids		Ideal Gas									
Property Name	Units										
Molecular Weight	kg/kmol										
Critical Temperature	C										
Critical Pressure	atm										
Critical Volume	cm ³ /mol										
Compressibility Factor											
Acentric Factor											
Normal Boiling Point	C										
Freezing Point	C										
Liquid Molar Volume	cm ³ /mol										
Enthalpy of Formation	kcal/mol										
Gibbs Energy of Formation	kcal/mol										
Heat of Vaporization	kcal/mol										
Molar Heat Capacity	kcal/(kmol C)										
A1											
A2 x 1.0E3											
A3 x 1.0E6											
A4 x 1.0E9											
A5 x 1.0E12											
A6 x 1.0E15											
Low Temperature Limit	C										
Upper Temperature Limit	C										
Liquid Vapor Pressure	Pa										
V1											
V2											
V3											
V4											
V5											
V6											
V7											
Low Temperature Limit	C										
Upper Temperature Limit	C										
Miscellaneous Parameters											
EOS Parameter P1											
EOS Parameter P2											
Rackett Equation Z Factor											
Binary Interaction Parameters											
KAIj											
KBij											
KCIj											
AIj											
AJi											
BIj											
BJi											
C											

Figure 1. User interface of CHE CALCULATOR.

The drop-down menu at the top of the CHE CALCULATOR® interface provides users with the flexibility to select from a variety of Equations of State (EOS), tailored to different engineering needs and levels of accuracy (Figure 2). This feature allows students and professionals to choose the most appropriate thermodynamic model for their specific application, ensuring both versatility and precision in calculations.

Properties of Fluids		Ideal Gas									
Property Name	Units	Ideal Gas									
Molecular Weight	kg/kmol										
Critical Temperature	C										
Critical Pressure	atm										
Critical Volume	cm ³ /mol										
Compressibility Factor											
Acentric Factor											
Normal Boiling Point	C										
Freezing Point	C										
Liquid Molar Volume	cm ³ /mol										
Enthalpy of Formation	kcal/mol										
Gibbs Energy of Formation	kcal/mol										
Heat of Vaporization	kcal/mol										
Molar Heat Capacity	kcal/(kmol C)										
A1											
A2 x 1.0E3											

Figure 2. Equation of States

This user-friendly interface and streamlined process make the CHE CALCULATOR® an indispensable resource for students, reducing time spent on data gathering and enabling them to focus on problem-solving and application of concepts.

To demonstrate the practical capabilities of the CHE CALCULATOR®, let's transition from discussing its user-friendly interface to exploring a specific application. One of the many

engineering problems the tool simplifies is multistage compression, a common process in chemical engineering. By utilizing the CHE CALCULATOR®'s intuitive input fields, dropdown menus, and built-in calculation algorithms, we can seamlessly analyze the compression of ethylene, illustrating the tool's ability to handle complex thermodynamic scenarios with ease and precision.

Example 1: Single-stage compression of ethylene

Ethylene is compressed from 20 bar, 25°C to 100 bar. The isentropic efficiency of the compressors is 0.75. The flow rate through the compressor is 3600kmol/hr.

Solution 1: From macroscopic energy balance, $\Delta H = W$

Step1: Analysis of reversible process.

For the reversible process, $\Delta S = 0$. Using the calculator, we can easily obtain values for the enthalpy and entropy of inlet stream (S_1).

$$H_1 (P_1 = 20 \text{ bar}, T_1 = 25^\circ\text{C}) = 52335 \text{ kJ/kmol}$$

$$S_1 (P_1 = 20 \text{ bar}, T_1 = 25^\circ\text{C}) = -77.879 \text{ kJ/(kmol}\cdot\text{K)}$$

Since we are analyzing the ideal (reversible-adiabatic) process, we introduce an ideal stream ($S_{2,\text{ideal}}$) whose pressure is 100 bar and temperature has a value that makes the entropy equal to that of stream S_1 . To calculate this temperature, we start with an initial guess, let's say $T_{2,\text{ideal}} = 100^\circ\text{C}$. We then calculate the enthalpy and entropy by dragging the formulas we wrote for getting stream 1 properties in CHE CALCULATOR®. Next, we use the Extended Secant algorithm button on CHE CALCULATOR® to calculate the temperature that makes the entropies of streams S_1 and $S_{2,\text{ideal}}$ equal. The output from the CALCULATOR® is $T_{2,\text{ideal}}$ is 119.96°C .

We can now calculate the ideal work from the macroscopic energy balance.

$$W_s^{\text{ideal}} = m * \Delta H = n(H_{2,\text{ideal}} - H_1)$$

$$W_s^{\text{ideal}} = 4.62\text{MW where } m = 1\text{kmol/s}$$

Step 2: Analysis of the real process

For the real process, the temperature of the stream S_2 (output stream of compressor) is going to be higher than the ideal temperature of 119.96°C because the entropy increases. To start, we guess a temperature, let's say 150°C and then drag the formula for the enthalpy and entropy calculations. Now that we have the enthalpy values, we can calculate the power requirement and efficiency. Using Goal Seek and Secant algorithms in CHE CALCULATOR®, we will set the calculated efficiency equal to 0.75 by varying the temperature. Results are shown below in Figure 3.

Molar Composition	S1	S2ideal	S2
C2H4			
Stream Properties	S1	S2ideal	S2
Molar Flow, kmol/s	1.0000	1.0000	1.0000
Mass Flow, kg/s			
Volume Flow, m ³ /s			
Temperature, C	25.0000	119.9571	147.9947
Pressure, bar	20.0000	100.0000	100.0000
Vapor Fraction			
Molecular Weight, kg/kmol			
Molar Enthalpy, kJ/kmol	52335.000	56952.677	58491.904
Vapor Phase			
Liquid Phase			
Molar Entropy, kJ/(kmol K)	-77.879	-77.879	
Vapor Phase			
Liquid Phase			
Molar Density, kmol/m ³			
Heat Capacity, kJ/(kmol K)			
Enthalpy Flow, kJ/s	52335.00	56952.68	58491.90
Entropy Flow, kJ/(s K)			
Duty [Power], kJ/s [kW]		4617.68	6156.90
Efficiency			0.75
Compressibility Factor			
Data and Calculations			

Figure 3. Screenshot of CHE CALCULATOR® for single stage stream properties

Example 2: Multi-Stage Compression of Ethylene

When the compression ratio is high, it is better to use two or more compressors (stages). That results in lower power consumption as well as lower discharge temperatures. In our case, the compression ratio $P_f / P_{in} = 100 / 20 = 5$ is high, so we will use the two stages. Remember that the total power requirement for a single stage is $\dot{W}_s = 13.68 \text{ MW}$. A schematic of a two-stage compressor is given below.

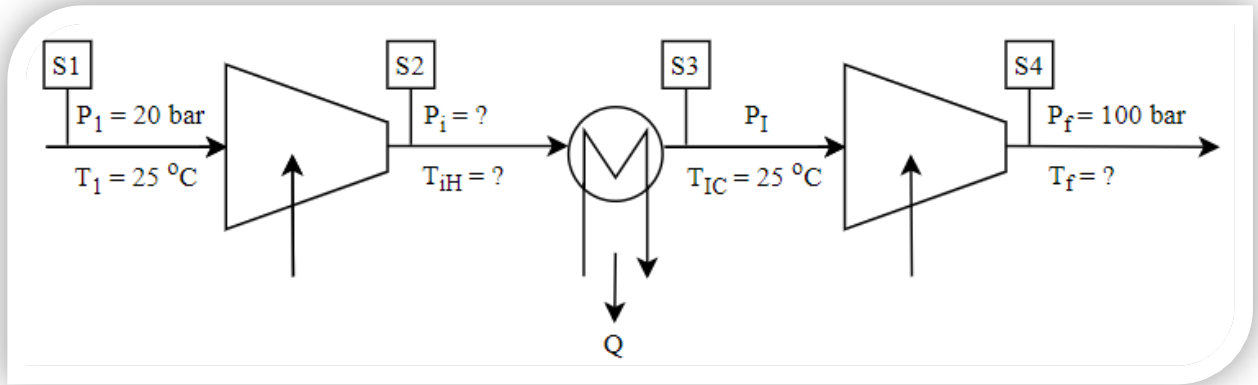


Figure 4: Multi-Stage Compression of Ethylene

The intermediate pressure P_i is usually calculated from the equation:

$$P_i = \sqrt{P_1 P_f} \Rightarrow P_i = 44.72 \text{ bar}$$

To avoid using the analysis of the reversible (ideal) process we can use an advanced function in the **CHE Calculator** that performs the modeling tasks of both the ideal (reversible) and the actual process. The function is described below: The advanced function **GasCompTemp** simulates the compression process of a gas. It combines both the reversible(ideal) and the actual process to calculate the discharge (outlet) temperature of the compressor. The units of this function as well as the corresponding function arguments are given in the table 2 below:

Table 2: CHE Calculator Function information

Process Variable	Function	Units
Compressor Discharge Temperature	GasCompTemp $\left(\begin{array}{l} \boxed{\text{moleFrac}}, \boxed{T_{in}}, \boxed{P_{in}}, \boxed{P_{out}}, \\ \boxed{\eta}, \boxed{Dt}, \boxed{\text{Maxite}}, \boxed{\text{Tol}} \end{array} \right)$	$^{\circ}\text{C}$

In the description of the function above $\boxed{\text{moleFrac}}$ stands either for the component column for a pure fluid or for the molar composition of a mixture, $\boxed{T_{in}}$ is the suction (inlet) temperature, $\boxed{P_{in}}$ is the suction pressure, $\boxed{P_{out}}$ is the discharge pressure, $\boxed{\eta}$ is the compressor isentropic efficiency.

The optional augment \boxed{Dt} is the perturbation step size for derivative calculation and $\boxed{\text{Maxite}}$ and $\boxed{\text{Tol}}$ are optional arguments in the calculation of the discharge temperature. The former is the maximum number iterations for the iterative algorithm used to solve the required equations for the discharge temperature and $\boxed{\text{Tol}}$ is the requested accuracy for convergence.

Here is a description of how the discharge temperature of the first stage as well as the power requirement is calculated. The second stage analysis is similar to the first stage.

For the first stage, the temperature of stream **S2** is calculated by using the *GasCompTemp* function. The calculated value is $T_2 = 86.17^\circ\text{C}$. Once the temperature is calculated we can use the functions *HIG* and *SIG* to calculate the enthalpy and entropy of the first stage discharge stream **S2** and then from the energy balance calculate the power requirement. The calculated value for the first stage is $\dot{W}_{s1} = 6.37 \text{ MW}$. A detailed summary of results for this example is shown in the figure below. Lost work calculations and [Second Law] thermodynamic efficiency are also shown in the results.

Process Variable	S1	S2	S3	S4
Temperature, C	25	86.17229676	25	86.17229676
Pressure, bar	20	44.72135955	44.72135955	100
Molar Flow Rate, kmol/s	2.222222222	2.222222222	2.222222222	2.222222222
Phase	Vapor	Vapor	Vapor	Vapor
Vapor Fraction	1	1	1	1
Vapor Molar Enthalpy, kJ/kmol	52335	55201.67289	52335	55201.67289
Vapor Molar Entropy kJ/(kmol K)	-77.87947376	-75.8437654	-84.57027944	-82.53457108
Enthalpy Flow, kW	116300	122670.3842	116300	122670.3842
Entropy Flow, kW/K	-173.0654972	-168.5417009	-187.9339543	-183.410158
Availability Flow, kW	168219.6492	173232.8945	172680.1863	177693.4316
Power Requirement, MW		6.370384202		6.370384202
Total Power Requirement, MW	12.74			
Lost Work, MW	3.27			
Thermodynamic Efficiency	74.4%			

Figure 5: Summary of Results

We can see that the net power requirements for the two-stage compressor are $\dot{W}_{s1} = 6.73 \text{ MW}$ and $\dot{W}_{s2} = 6.73 \text{ MW}$ for total power requirement of $\dot{W}_s = 12.74 \text{ MW}$. We notice that there is a reduction of about 7% in the power requirements, which represents significant savings in operating expenses, but the efficiency of the process has decreased by an increase in the lost work, due to the rejection of heat from the cooler into the infinite environment.

Example 3: Adiabatic Mixing of two Streams of Nitrogen

Consider the mixing of two streams of nitrogen:

☼ Stream 1: $T_1 = -50^\circ\text{C}$, $P_1 = 2\text{ bar}$, $F_1 = 1.5\text{ kmol} / \text{s}$

☼ Stream 2: $T_2 = 35^\circ\text{C}$, $P_2 = 2\text{ bar}$, $F_2 = 3.1\text{ kmol} / \text{s}$

We would like to calculate the temperature of the mixed stream T_3 , the lost work and the entropy change of this process. A schematic of the mixing process is shown in the Figure 6 below.

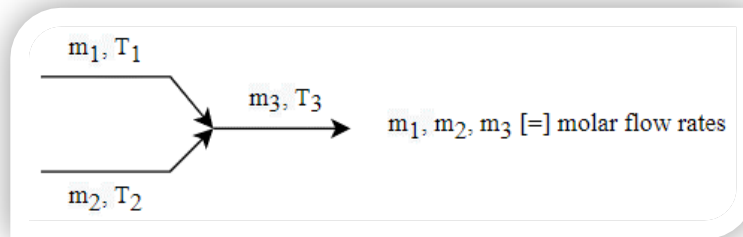


Figure 6: Mixing of Two Ideal Nitrogen Gas Streams

The only equations applicable here is the mass and total energy balance. Since the process is adiabatic and no work is done the mass and energy balance simply become:

$$-\Delta mH = 0 \Rightarrow m_1 H_1 + m_2 H_2 - m_3 H_3 \quad \text{and} \quad m_3 = m_1 + m_2$$

Our approach is now well known. We need to guess a temperature for the mixed stream say $T_3 = 30^\circ\text{C}$ formulate the energy balance by calculating the enthalpies of all streams and then GoalSeek it to zero by varying the mixed stream temperature. Using the CHE Calculator, we obtain the following enthalpy values of all streams:

Stream S1 Enthalpy

$$H_1(T_1 = -50^\circ\text{C}, P_1 = 2\text{ bar}) = \text{HIG}\left(\text{moleFrac}, T_1, \square\right)$$

$$H_1(T_1 = -50^\circ\text{C}, P_1 = 2\text{ bar}) = \underline{\underline{-2192.69\text{ kJ} / \text{kmol}}}$$

Stream S1 Entropy

$$S_1(T_1 = -50^\circ\text{C}, P_1 = 2\text{ bar}) = \text{SIG}\left(\text{moleFrac}, T_1, P_1, \square\right)$$

$$S_1(T_1 = -50^\circ\text{C}, P_1 = 2\text{ bar}) = \underline{\underline{-14.126\text{ kJ} / (\text{kmol} \cdot \text{K})}}$$

Stream S2 Enthalpy

$$H_2(T_2 = 35^\circ\text{C}, P_2 = 2 \text{ bar}) = \text{HIG}(\text{moleFrac}, T_1, \square)$$

$$H_2(T_2 = 35^\circ\text{C}, P_2 = 2 \text{ bar}) = \underline{\underline{291.75 \text{ kJ} / \text{kmol}}}$$

Stream S2 Entropy

$$S_2(T_2 = -50^\circ\text{C}, P_2 = 2 \text{ bar}) = \text{SIG}(\text{moleFrac}, T_2, P_2, \square)$$

$$S_2(T_2 = -50^\circ\text{C}, P_2 = 2 \text{ bar}) = \underline{\underline{-4.691 \text{ kJ} / (\text{kmol} \cdot \text{K})}}$$

We now calculate the enthalpy and entropy of the mixed stream S3 by guessing a temperature $T_3 = 30^\circ\text{C}$. The results are

Stream S3 Enthalpy

$$H_3(T_3^{(0)} = 30^\circ\text{C}, P_3 = 2 \text{ bar}) = \text{HIG}(\text{moleFrac}, T_3^{(0)}, \square)$$

$$H_3(T_3^{(0)} = 30^\circ\text{C}, P_3 = 2 \text{ bar}) = \underline{\underline{145.88 \text{ kJ} / \text{kmol}}}$$

Stream S3 Entropy

$$S_3(T_3 = 30^\circ\text{C}, P_3 = 2 \text{ bar}) = \text{SIG}(\text{moleFrac}, T_3, P_3, \square)$$

$$S_3(T_3 = 30^\circ\text{C}, P_3 = 2 \text{ bar}) = \underline{\underline{-4.691 \text{ kJ} / (\text{kmol} \cdot \text{K})}}$$

We now formulate the total energy balance and GoalSeek it to zero by manipulating the mixed stream temperature. This results in a temperature $T_3 = 7.24^\circ\text{C}$. We can now calculate the entropy of stream S3 to be equal to $-7.446 \text{ kJ} / (\text{kmol} \cdot \text{K})$.

From the entropy balance we have

$$\begin{aligned} -\Delta mS + \dot{S}_{gen} &= 0 \Rightarrow \dot{S}_{gen} = m_3 S_3 - m_1 S_1 - m_2 S_2 \Rightarrow \\ \dot{S}_{gen} &= 1.48 \text{ kW} / \text{K} > 0 \end{aligned}$$

The lost work can be calculated from the equation

$$\begin{aligned} LW &= -\Delta mB \Rightarrow LW = m_3 B_3 - m_1 B_1 - m_2 B_2 \Rightarrow \\ LW &= \underline{\underline{443.53 \text{ kW}}} \end{aligned}$$

A detailed summary of results is shown in **Figure 7** below:

Process Variable	S1	S2	S3
Temperature, C	-50	35	7.237979757
Pressure, bar	2	2	2
Molar Flow Rate, kmol/s	1.5	3.1	4.6
Phase	Vapor	Vapor	Vapor
Vapor Fraction	1	1	1
Vapor Molar Enthalpy, kJ/kmol	-2192.691487	291.7470174	-518.3959731
Vapor Molar Entropy kJ/(kmol K)	-14.12592986	-4.691230375	-7.4463618
Enthalpy Flow, kW	-3289.03723	904.4157538	-2384.621476
Entropy Flow, kW/K	-21.18889479	-14.54281416	-34.25326428
Availability Flow, kW	3067.631206	5267.260003	7891.357808
Energy Balance, kW	-4.54747E-11		
Lost Work, kW	443.53		
Entropy Change, kW/K	1.48		

Figure 7: Summary of Results for Example 3

Results and Discussion

The survey results provided valuable insights into the effectiveness and challenges associated with integrating CHE CALCULATOR® into the curriculum.

CHE CALCULATOR® was primarily used in Thermodynamics, and process control courses.

Over 50% of respondents reported extensive or regular use in assignments and projects.

However, students noted inconsistency in its integration across courses, highlighting the need for a standardized curriculum approach to maximize its benefits. Figure 8 illustrates the frequency of usage among students.

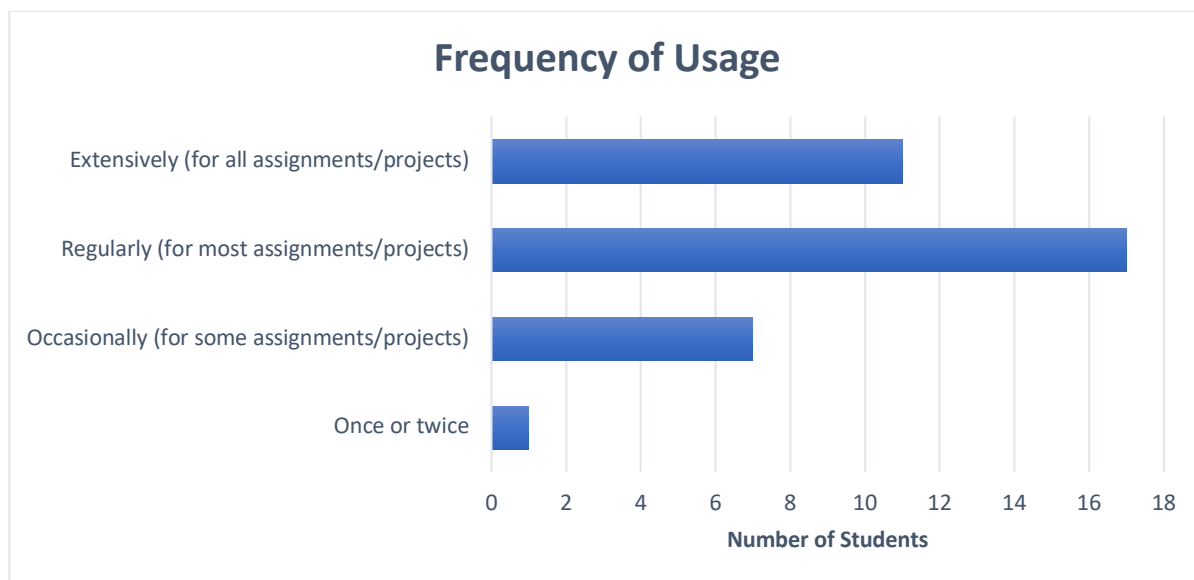


Figure 8: Frequency of usage in listed classes.

A significant challenge identified was the steep learning curve, which was the most commonly cited issue among students. Over 70% of respondents reported difficulties in navigating the tool due to the lack of comprehensive documentation and help resources. Figure 9 presents the percentage of students who experienced various challenges. Additionally, concerns regarding the user interface were raised, with students suggesting that a more modernized design would improve usability.

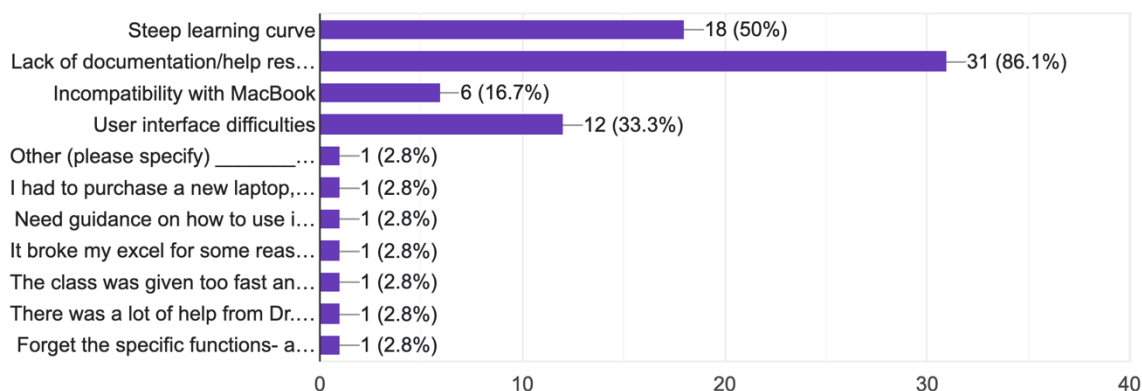


Figure 9: Most common experiences challenges.

Despite these challenges, CHE CALCULATOR® was rated moderately effective in helping students understand complex chemical engineering concepts. The average rating for interface intuitiveness was 3.1 out of 5, while its effectiveness in understanding theoretical concepts received an average rating of 3.3 out of 5. Figure 10 presents the distribution of these ratings.

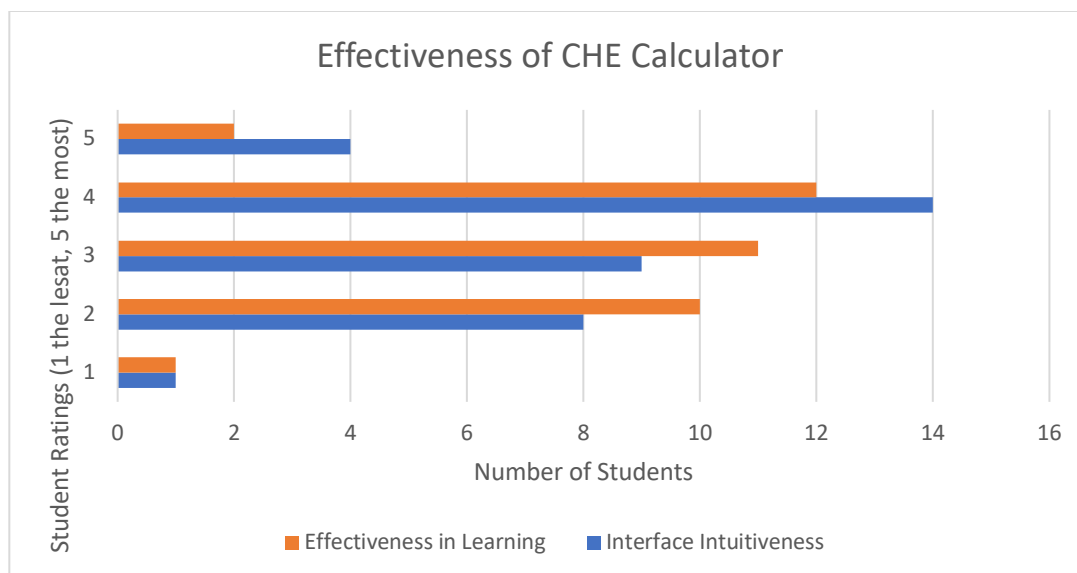


Figure 10: Distribution of Student Responses on effectiveness and intuitiveness.

When compared to other computational tools like Aspen and Python, student feedback was mixed. Some respondents found CHE CALCULATOR® more user-friendly and easier to grasp than Aspen, while others preferred industry-standard tools due to their broader applications. Furthermore, ~80% of students acknowledged that the tool contributed to developing problem-solving skills relevant to their professional careers. However, concerns were raised about its long-term applicability given the shift in industry trends toward specialized software solutions.

The last question in the survey highlights both its strengths and areas for improvement. Feedback reveals a range of experiences, particularly among students who have actively engaged with the tool.

Strengths of CHE CALCULATOR®

Students who used CHE CALCULATOR® extensively commended its ability to streamline complex chemical engineering calculations. One student remarked, “*The CHE CALCULATOR is extremely beneficial for calculating numbers quickly and efficiently. It’s packed with data and equations, saving us from manual calculations.*” Another highlighted its versatility, stating, “*It allows for complex problems to be solved easier than if it was done by hand.*” The intuitive layout of the Excel-based interface was a recurring point of praise, enabling users to access multiple values and functionalities simultaneously.

Specific features, such as VLE (vapor-liquid equilibrium) calculations, were particularly appreciated for their practical relevance. A student noted, “*My favorite section is the VLE calculations section; it’s extremely useful in integrating theoretical concepts into real-world applications.*” Another student mentioned, “*The extensive database of chemical properties and the ability to input components across various functions makes it a valuable tool.*”

CHE CALCULATOR®’s foundation in Excel was also highlighted as a strength. As one student explained, “*The fact that it’s in Excel—a universally recognized and accessible platform—makes it convenient and cost-effective compared to proprietary software like Aspen.*” This accessibility

ensures that students gain valuable experience in Excel, a skill often demanded in professional environments.

Weaknesses and Challenges

Despite its strengths, CHE CALCULATOR® faced criticism for its steep learning curve. Several students indicated that without proper guidance, the tool can be challenging to navigate. One student commented, *“It’s a hassle to use without a comprehensive user manual or structured tutorials.”*

The dependency on Excel posed additional challenges. Compatibility issues, particularly for MacBook users, were a common complaint. *“I couldn’t download it on my MacBook,”* noted one student, while another stated, *“It would be helpful if it were made into a standalone app rather than being tied to Excel.”* The transition of Excel from VBA to Python was also flagged as a potential issue, with one student expressing curiosity about how the tool will adapt to this change.

Another common critique was the lack of documentation and support resources. As one student explained, *“There needs to be a detailed list of functions and what they calculate. Searching through the VBA code for answers is inefficient.”* The absence of error-handling mechanisms and clear guidance for troubleshooting further compounded these challenges.

Observations on Usage and Adoption

Students who had prior exposure to CHE CALCULATOR® in multiple courses reported a better understanding and appreciation of its capabilities. One student observed, *“If this tool was introduced earlier in foundational courses like 201 or 210, students would have a stronger grasp by the time they reach advanced classes.”* Others suggested expanding its use across more chemical engineering courses to reinforce familiarity and proficiency over time. Addressing these concerns through better integration and support mechanisms could significantly enhance the overall learning experience.

To maximize its impact, students suggested several enhancements to CHE CALCULATOR®. These included:

- Developing a centralized help resource, such as an interactive guide or searchable database of functions, to improve usability.
- Introducing structured training modules, including video tutorials and example problems, to facilitate learning.
- Expanding the tool’s capabilities to include predictive methods and additional chemical property databases.
- Creating a standalone version of the tool to eliminate compatibility issues and improve accessibility.
- Implementing error-handling features and providing clear explanations for common issues encountered during usage.

The feedback on CHE CALCULATOR® underscores its potential as a transformative educational tool for chemical engineering students. While its ability to facilitate quick, accurate calculations and integrate multiple engineering concepts is well-recognized, addressing its challenges related

to usability, accessibility, and support will be critical. By implementing the proposed improvements, CHE CALCULATOR® can become an indispensable resource for chemical engineering education, equipping students with the computational skills needed for academic and professional success.

Conclusions

CHE CALCULATOR® exemplifies the potential of computational tools in enhancing chemical engineering education by bridging the gap between theoretical concepts and practical applications. It empowers students to perform complex calculations efficiently, facilitates integration across multiple engineering domains, and provides hands-on experience with industry-relevant problem-solving.

Despite its strengths, feedback from students has highlighted the need for enhancements, particularly in user support and accessibility. Addressing the steep learning curve through comprehensive documentation, tutorials, and in-class training will ensure broader adoption and effective utilization. To further support students, we plan to prepare detailed video tutorials and written instructions for the CHE CALCULATOR®, making it more accessible and user-friendly for diverse learning styles. Additionally, improving compatibility and expanding functionality will position CHE CALCULATOR® as a versatile tool capable of adapting to evolving technological trends and educational needs.

By embracing these improvements, CHE CALCULATOR® has the potential to become a cornerstone of chemical engineering education, fostering both technical proficiency and confidence among students. Its continued evolution will not only enhance learning outcomes but also prepare students to meet the challenges of an increasingly data-driven engineering landscape.

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