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INTEGRATION OF MODERN INFORMATION TECHNOLOGIES INTO MODELLING AND ANALYSIS: COMPARATIVE STUDY OF HEAT-ENERGY DUTY IN BINARY MIXTURE EVAPORATION PROCESS

The article examines the potential of modern information technologies in chemical engineering through a comparative analysis of three software tools – the spreadsheet editor Microsoft Excel, the computer algebra system MathCAD, and the open-source process simulator DWSIM. As a demonstrative case, the evaporation of a binary ethanol-water mixture at atmospheric pressure with varying mole fraction of ethanol was selected. An identical set of calculations was implemented in each environment, including determination of boiling temperature, enthalpy of vaporization, mixture heat capacity, mass flow rate of the evaporated fraction, and the total heat duty composed of sensible and latent components. In Microsoft Excel, a calculation table with fifty rows (sets) of data was prepared, formulas for automatic updating upon parameter changes were embedded, and charts of key dependencies were constructed. MathCAD reproduced the same equations in traditional mathematical notation and enabled the plotting of equivalent relationships between the calculated variables. DWSIM was employed for modeling with the NRTL thermodynamic package and flowsheet elements representing heating to the boiling point and partial evaporation, followed by exporting iterative calculations into tabular form. The comparison revealed strong agreement of results: differences between Microsoft Excel and DWSIM did not exceed a few percent and were explained by the use of simplified correlations in the former and rigorous thermodynamic models in the latter. It was established that Microsoft Excel is convenient for rapid calculations and data visualization, MathCAD – for transparent representation of formulas, particularly in educational contexts, and DWSIM – for more detailed engineering simulations with higher accuracy. The study concludes that a combined use of these programs is most effective: tables and simplified models can serve as a basis for teaching and preliminary assessments, while professional simulators are essential for verification, refinement, and detailed analysis of results. The presented approach has substantial educational value and may serve as a methodological bridge between fundamental professional training in higher education and contemporary engineering practice.

Keywords: information technologies; chemical engineering; Microsoft Excel; MathCAD; DWSIM; process simulation; evaporation; mathematical modelling; simulation modelling; integrated educational technologies.

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ІНТЕГРАЦІЯ СУЧАСНИХ ІНФОРМАЦІЙНИХ ТЕХНОЛОГІЙ У МОДЕЛЮВАННЯ ТА АНАЛІЗ: ПОРІВНЯЛЬНЕ ДОСЛІДЖЕННЯ ТЕПЛОВИКОРИСТАННЯ У ПРОЦЕСІ ВИПАРЮВАННЯ БІНАРНОЇ СУМІШІ

У статті розглянуто можливості сучасних інформаційних технологій у хімічній інженерії шляхом порівняння трьох програмних інструментів – табличного редактора Microsoft Excel, системи комп'ютерної алгебри MathCAD та симулятора хіміко-технологічного обладнання з відкритим кодом DWSIM. У якості демонстраційного прикладу використано задачу випаровування бінарної суміші етанол-вода при атмосферному тиску з варіюванням мольної частки етанолу. Для кожного інструменту реалізовано однаковий набір розрахунків, що включав визначення температури кипіння, ентальпії пароутворення, теплоємності суміші, масової витрати випаруваної частини та повного теплового навантаження, яке складається з чутливої та прихованої складових. У Microsoft Excel сформовано розрахункову таблицю з п'ятдесятьма рядками (наборами) даних, закладено формули для автоматичного оновлення при зміні констант та побудовано графіки ключових залежностей. MathCAD дозволив відтворити ті самі рівняння у традиційній математичній нотації та забезпечив побудову аналогічних залежностей між розрахованими характеристиками. DWSIM використано для моделювання за допомогою термодинамічного пакета NRTL та схемних елементів, які відтворюють процеси нагрівання до точки кипіння та часткового випаровування, з подальшим зведенням ітераційних розрахунків до табличного виду. Порівняння показало високу збіжність результатів: відмінності між Microsoft Excel і DWSIM не перевищували кількох відсотків і пояснювалися використанням спрощених кореляцій у першому випадку та точних моделей у другому. Встановлено, що Microsoft Excel зручний для швидких розрахунків та візуалізації даних, MathCAD – для прозорого подання формул, особливо у навчальних цілях, а DWSIM – для більш детальних інженерних симуляцій з підвищеною точністю. Зроблено висновок про доцільність комбінованого застосування цих програм: таблиці та прості моделі можуть служити основою для навчання й надання попередніх оцінок, а професійні симулятори – для перевірки, уточнення та деталізації результатів. Представлений підхід має значну освітню цінність та може використовуватися як методологічний міст між базовим професійним навчанням при отриманні вищої освіти та сучасною інженерною практикою.

Ключові слова: інформаційні технології; хімічна інженерія; Microsoft Excel; MathCAD; DWSIM; симуляція процесів; випаровування; математичне моделювання; імітаційне моделювання; інтегровані навчальні технології.

Introduction.

Recent years computational tools that enable precise modelling, simulation, and data analysis have increasingly shaped a chemical engineering profession. Modern information technologies such as spreadsheets (e.g. Microsoft Excel), symbolic/numeric calculation software (e.g. MathCAD), and process simulators (e.g. DWSIM) allow engineers to handle larger datasets, validate mathematical models, and simulate realistic process conditions – which all contribute to improved design, optimization and operational efficiency. Excel remains ubiquitous for rapid prototyping, what-if studies, and handling data; MathCAD provides clarity and correctness by keeping equations visible alongside calculations; DWSIM adds value by enabling rigorous thermodynamics, equilibrium, mass and energy balances, non-ideal mixtures, and more complex unit operations.

Evaporation of binary mixtures is a prototypical operation in chemical engineering: it requires estimation of boiling behavior, latent heat, sensible heat, and overall

heat duty. In many situations, decisions about process design – such as sizing evaporators, energy requirements, or optimization of feed composition – depend critically on understanding how heat duty varies with composition, temperature, latent heat, and other properties. Yet students, engineers, or researchers often work with incomplete tools or adopt simplified correlations, which may miss non-linearities or interaction effects.

The purpose of this article is to illustrate how Excel, MathCAD and DWSIM each can be used to model, analyze and compare results for the same evaporation problem, and to show what trade-offs exist: in terms of ease of implementation, transparency of formulae, handling large data, realism of thermodynamic behavior, and fidelity of results. Specifically, a demonstrative example will be constructed (with a binary mixture under varying mole fraction) and implemented in all three tools; results will then be compared.

This approach has educational value – helping students understand the full chain from physical modelling through numerical implementation and simulation – and practical value for practicing engineers: enabling them to choose tools appropriately depending on context (e.g. early design vs detailed simulation). Prior works have shown that spreadsheets are widely used in process design education and integration for optimization tasks [1] and that MathCAD can enhance understanding in reactor design via educational case studies [2] besides, DWSIM has been compared to commercial simulators and validated for various steady-state flow-sheet applications in literature, showing good agreement [3].

Literature Review.

The adoption and comparison of Excel, MathCAD, and process simulators (especially open-source ones such as DWSIM) has been steadily increasing in chemical engineering. This review surveys key studies on each tool's strengths, limitations, educational and industrial applications, and how they have been applied to problems similar to heat and energy duty estimations.

1. Excel has been used widely for problem solving, "what-if" analyses, optimization, and data fitting in chemical engineering curricula and in smaller industrial tasks. Authors of the [1] demonstrate multiple chemical engineering applications – reactor network design, mass-exchange networks, pollution prevention – using Excel's Solver for both linear and nonlinear problems. In 2019 there were a chapter "Excel for Chemical Engineering" which shows using Excel to address a variety of unit operations, material balances, data fitting, and integration of Excel in undergraduate problem sets [4]. In the [5], author provides specific cases of heat transfer and heat exchanger problems solved in Excel – replacing some chart (tabular) lookup tasks with formula-based and spreadsheet-based methods, and also examples of thermal-fluid problems using Goal Seek and other built-in tools. These works underscore Excel's accessibility, low cost, broad availability, and good for initial design or educational tasks.

Strengths identified include familiarity (students often already know Excel), immediacy of visualization (charts, pivot tables), and ability to handle moderate datasets without steep learning curves. Weaknesses include limited symbolic manipulation, more manual work for error checking, potential for formula errors, and less suitability for large or highly non-linear systems. Nevertheless, it's a valuable tool with fairly low threshold of entry, which is currently platform-independent.

2. MathCAD has been used in undergraduate and postgraduate engineering education for thermodynamics, heat transfer, reactor design, and property evaluation. Authors of the [6] discuss a MathCAD-based educational experience for non-isothermal plug flow reactors, showing how having visible formulas and symbolic manipulation helps students understand the theory and avoid treating process simulation as a black box. Author of the [7] constructed a set of MathCAD functions for thermodynamics (for steam, refrigerants, ideal gases) to avoid tedious interpolation and to facilitate transparent property computations in education settings. Similarly, his [8] shows robust capabilities for property sets and cycle analyses. Authors of the [9] more recently describe implementing residual property evaluations in MathCAD grounded in first principles for generalized thermodynamics, which shows: this software still advancing for research-level tasks.

From these sources, MathCAD's strengths are clarity (formulas shown in familiar mathematical notation), ease of units/handling, good for educational and research tasks, ability to combine symbolic and numeric computations. Limitations include lower capability for large, fully dynamic process simulation (fewer built-in unit operations compared to simulators), sometimes slower for very large datasets than pure numeric tools, and dependence on manual formulation of property correlations or functions.

3. An increasingly large body of literature has evaluated DWSIM, especially in open source vs proprietary software comparisons, to verify whether its results are close enough for engineering applications. Author of the [10] presents an evaluation of DWSIM using a plant-wide oil & gas separation plant flowsheet, including many unit operations (flash vessels, mixers, heat exchangers, pumps, etc.). The results are within about 1% deviation for many variables under steady-state conditions so the paper concludes that DWSIM is credible for professional environments for many settings. Similarly, in the [11] modelled a vapor absorption refrigeration system (NH_3-H_2O) in DWSIM, and compared results to Aspen HYSYS or Honeywell UniSim Design. Educational usage demonstrates that DWSIM's results are comparable to commercial simulators under many conditions. Next, in the [12] authors compared DWSIM with Aspen HYSYS for three case studies: mixer & separator, shortcut distillation, and shell & tube heat exchanger. Deviation in key outputs was <5% in most cases; DWSIM was found easier to use & report. Also, authors of the [13] similarly shows strong agreement for heat and mass flows between Aspen Plus and DWSIM.

These studies commonly find that under steady-state, moderate complexity, and with well-chosen thermodynamic models, DWSIM gives results close to expensive licensed (commercial) tools. Weaknesses show up when high non-ideality, dynamic behaviour, transient effects, many recycle loops, or very precise property data are needed – then discrepancies widen, computational effort increases, user must carefully choose correlations and settings.

Integration, Interfaces and Pedagogical Issues.

There is literature exploring how to integrate these tools in teaching so that students benefit from both conceptual clarity and realistic simulation. Authors of the [14] investigate using MathCAD Prime plus a commercial simulator (Aspen One) in parallel in undergraduate courses, to reduce the "black box" effect – letting students derive or verify model behavior via MathCAD while understanding simulator results. The integrative approach [15] describes simulation-based exercises that use open-source process simulators plus MathCAD in chemical engineering education. Such approaches help students understand not just "what" results come out, but why (how assumptions, correlations, and models matter).

While many studies focus more on reactor networks, heat exchangers, distillation or absorption, fewer focus directly on evaporation, latent heat, energy duty variation over composition. Some works use spreadsheets or MathCAD functions for thermodynamics or property tables [7], which implicitly involve latent heat. Others, comparisons of simulators [10] and [12] include unit operations with latent heat flows (flash vessels, evaporators, etc.). The work [11] explicitly models a vapor absorption system where latent heat and heat duty are central. But there is still a gap: few studies present the same problem implemented identically in Excel, MathCAD and DWSIM and compare all three side by side, especially focusing on how heat duty depends on mixture composition.

Problem Statement.

From the reviewed literature, the following emerge:

1) tool overlap and trade-offs – Microsoft Excel is great for teaching, rapid prototyping, data analysis; MathCAD adds clarity and correctness; DWSIM adds realism and capacity for process-scale simulation;

2) accuracy and validation – for many steady-state, moderate non-ideal systems, DWSIM yields results within ~1-5% compared to commercial tools;

3) educational value – combining tools helps mitigate the black-box problem, improves student understanding;

4) lack of direct comparative studies for evaporation composition and heat duty relationships – although latent heat and boiling point variation are part of many works, an explicit study across Excel, MathCAD, and DWSIM for evaporation over full composition sweep appears rare.

Thus, this article does address a need: to provide a clean, directly comparable demonstration of how the dependence of heat duty on composition (evaporation) plays out in the three tools, with discussion of implementation effort, sources of discrepancy, and trade-offs in practice.

Research Design.

The research question addressed in this study is how different computational environments – Microsoft Excel, MathCAD, and DWSIM – can be used to implement the same chemical engineering problem and what strengths and weaknesses emerge from each implementation. The selected case study focuses on the evaporation of an ethanol-water binary mixture at atmospheric pressure. The system was chosen for several reasons: it's widely used in chemical engineering education and industry; it involves both sensible and latent heat contributions; it allows for continuous variation of mole fraction and thus generates a dataset suitable for analysis.

The design of the research involves three steps. First, a dataset covering fifty composition points of ethanol in water was prepared, including mole fraction, mass fraction, boiling temperature, enthalpy of vaporization, mixture heat capacity, evaporated mass flow, and calculated heat duties. Second, the same dataset and formulas were implemented in three software tools – Excel, MathCAD, and DWSIM – with consistent assumptions and thermodynamic simplifications. Third, results were compared in terms of numerical values, ease of calculation, visualization, transparency of formulas, and suitability for educational and professional contexts.

I. Implementation in Microsoft Excel.

Excel was selected as the first environment because of its ubiquity and ease of use. In this implementation, the dataset was structured into a spreadsheet with columns for mole fraction of ethanol, mass fraction, boiling temperature, enthalpy of vaporization, mixture heat capacity, evaporated mass flow, sensible heat duty, latent heat duty, and total heat duty. All formulas written using native Excel functions without macros or external add-ins.

The advantages of Excel in this task include rapid handling of large tables, clear structure for tabular data, immediate recalculation when changing assumptions or constants, and straightforward visualization via built-in chart tools. By plotting the total heat duty as a function of ethanol mole fraction, Excel allows the user to quickly recognize nonlinear trends and composition regions of higher or lower energy requirements. Moreover, error tracing is simple since each formula is visible in the spreadsheet.

Limitations were also observed. Microsoft Excel lacks symbolic capabilities, so formulas are hidden in cell expressions rather than being displayed in conventional mathematical notation. This may obscure the underlying theoretical model for students. Furthermore, accuracy depends on careful manual entry of formulas; mistakes can propagate without clear warnings. Nevertheless, Excel provides an accessible baseline solution that is useful both in introductory education and for preliminary industrial assessments.

The implementation of the evaporation case study in Microsoft Excel followed a structured sequence of steps to ensure transparency and reproducibility. A spreadsheet

was created with columns corresponding to the main thermodynamic variables and calculated results. Each column was linked by formulas, so that modifying constants or assumptions would automatically update the entire dataset. This approach highlights the advantage of Excel as a flexible environment for data analysis and visualization.

The core of the Microsoft Excel model was a set of eight equations that link composition, thermodynamic properties, and heat duties of the ethanol–water system. Below, each equation is presented along with definitions of the variables involved.

1. Mass fraction of ethanol:

$$w_{eth} = \frac{x \cdot M_{eth}}{x \cdot M_{eth} + (1-x) \cdot M_w}, \quad (1)$$

where w_{eth} – mass fraction of ethanol;

x – mole fraction of ethanol;

M_{eth}, M_w – molar mass of ethanol and water, respectively (g+/mol).

2. Boiling temperature of the mixture:

$$T_b = 100 - (100 - 78{,}37) \cdot x - 5 \cdot x \cdot (1-x), \quad (2)$$

where T_b – approximate boiling point of the ethanol-water mixture (°C);

constant values 100°C and 78,37°C represent boiling points of pure water and pure ethanol, respectively;

interaction term $5 \cdot x \cdot (1-x)$ accounts for non-ideal behavior.

3. Enthalpy of vaporization of the mixture:

$$\Delta H_{vap.mix} = w_{eth} \cdot \Delta H_{vap.eth} + (1-w_{eth}) \cdot \Delta H_{vap.w} - 50 \cdot x \cdot (1-x), \quad (3)$$

where $\Delta H_{vap.mix}$, $\Delta H_{vap,eth}$, $\Delta H_{vap.w}$ – mixture latent heat of vaporization latent heats of pure ethanol and pure water, respectively (kJ/kg·K);

last term represents empirical interaction correction.

4. Heat capacity of the liquid mixture:

$$c_{p.mix} = w_{eth} \cdot c_{p.eth} + (1-w_{eth}) \cdot c_{p.w}, \quad (4)$$

where $c_{p.mix}$, $c_{p.eth}$, $c_{p.w}$ – specific heat capacity of the mixture, pure ethanol and water, respectively (kJ/kg·K).

5. Mass flow of evaporated liquid:

$$m_{evap} = m_{feed} \cdot (0{,}05 + 0{,}4 \cdot x), \quad (5)$$

where m_{evap} and m_{feed} – evaporated mass flow and total feed mass flow, respectively (kg/h);

empirical coefficient approximates the fraction of feed undergoing evaporation.

6. Sensible heat duty:

$$Q_{sens} = m_{feed} \cdot c_{p.mix} \cdot (T_b - T_{feed}), \quad (6)$$

where Q_{sens} – sensible heat load (kJ/h);

T_{feed} – feed temperature (°C).

7. Latent heat duty:

$$Q_{lat} = m_{evap} \cdot \Delta H_{vap.mix}, \quad (7)$$

where Q_{lat} – latent heat load (kJ/h).

8. Total heat duty:

$$Q_{total} = (Q_{sens} + Q_{lat}) / 3600, \quad (8)$$

where Q_{total} – total heat load (kW);

the denominator converts energy from kJ/h to kW.

Sets of 50 data lines were used, generated by formulas (1)-(8). The baseline was the change in ethanol mole fraction from 0,02 to 0,99. Once the dataset was completed (fig. 1), built-in Excel chart functions were employed to visualize the relationships, particularly the variation of the total heat duty with ethanol mole fraction (fig. 2) and enthalpy of vaporization with boiling temperature of the mixture (fig. 3). These plots provided an immediate graphical interpretation of the non-linear dependence of energy demand on mixture composition.

	A	B	C	D	E	F	G	H	I	J
1	idx	x_mole_eth	w_mass_eth	T_b_C	Hvap_kJ_per_kg	cp_kJ_per_kgK	mass_evap_kg_h	Sensible_kJ_h	Latent_kJ_h	Total_Q_kW
2	1	0,020	0,050	99,469	2184,834	4,094	58,000	304854,907	126720,376	119,882
3	2	0,040	0,096	98,948	2118,475	4,013	65,920	296771,041	139649,841	121,228
4	3	0,060	0,139	98,431	2055,877	3,937	73,836	289123,644	151797,749	122,478
50	49	0,970	0,988	78,870	856,348	2,461	438,080	132555,289	375148,908	141,029
51	50	0,990	0,996	78,537	846,072	2,447	446,000	130996,289	377348,135	141,207

Fig. 1 – Spreadsheet in Excel with calculated data (shortened):
x_mole_eth – mole fraction of ethanol; w_mass_eth – mass fraction; T_b_C – boiling point; Hvap_kJ_per_kg – enthalpy of vaporization; cp_kJ_per_kgK – heat capacity; mass_evap_kg_h – mass flow rate of evaporated liquid; Sensible_kJ_h, Latent_kJ_h, Total_Q_kW – energy consumption

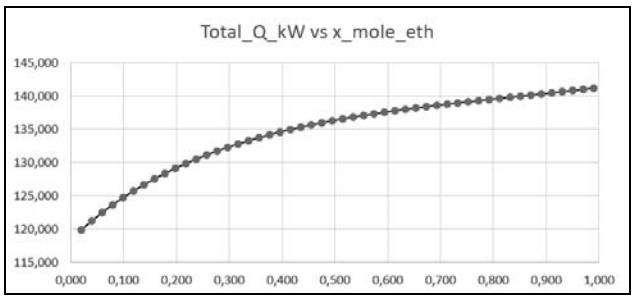

Fig. 2 – Relationships between the variations of total heat duty with ethanol mole fraction (in Excel)

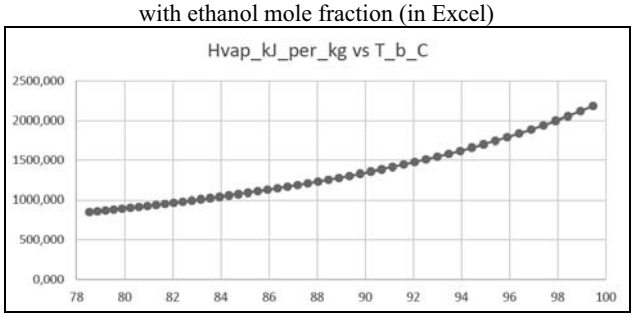

Fig. 3 – Relationships between the enthalpy of vaporization with boiling temperature of the mixture (in Excel)

II. Implementation in MathCAD.

MathCAD provides a complex symbolic-numerical environment where equations are written in conventional mathematical notation, displayed directly in the worksheet. This feature makes it particularly well suited for educational purposes: the theoretical background is not hidden inside spreadsheet cells but explicitly visible. For this reason, the evaporation case study was reproduced in MathCAD using the same dataset and assumptions as in Excel.

Same equations (1)-(8) were entered into MathCAD worksheet – fig. 4.

$M_{eth} := 46.07$ g/mol $\quad \Delta H_{vap.eth} := 846$ kJ/kg

$M_w := 18.015$ g/mol $\quad \Delta H_{vap.w} := 2257$ kJ/kg

$c_{p.eth} := 2.44$ kJ/kg*K $\quad m_{feed} := 1000$ kg/h

$c_{p.w} := 4.18$ kJ/kg*K $\quad T_{feed} := 25$ °C

$x := 0, 0.02 .. 1$

$$w_{eth}(x) := \frac{x \cdot M_{eth}}{x \cdot M_{eth} + (1-x) \cdot M_w}$$

$$T_b(x) := 100 - (100 - 78.37) \cdot x - 5 \cdot x \cdot (1-x)$$

$$\Delta H_{vap.mix}(x) := w_{eth}(x) \cdot \Delta H_{vap.eth} + (1 - w_{eth}(x)) \cdot \Delta H_{vap.w} - 50 \cdot x \cdot (1-x)$$

$$c_{p.mix}(x) := w_{eth}(x) \cdot c_{p.eth} + (1 - w_{eth}(x)) \cdot c_{p.w}$$

$$m_{evap}(x) := m_{feed} \cdot (0.05 + 0.4 \cdot x)$$

$$Q_{sens}(x) := m_{feed} \cdot c_{p.mix}(x) \cdot (T_b(x) - T_{feed})$$

$$Q_{lat}(x) := m_{evap}(x) \cdot \Delta H_{vap.mix}(x)$$

$$Q_{total}(x) := \frac{Q_{sens}(x) + Q_{lat}(x)}{3600}$$

Fig. 4 – Spreadsheet in MathCAD PRIME

Implementation in MathCAD PRIME emphasizes transparency: all equations are written in symbolic form, and variables are defined in sequence. This makes the workflow more intuitive for students and researchers, who can verify each step, adjust constants, or explore alternative assumptions. Moreover, MathCAD manages units automatically, reducing the risk of dimensional inconsistencies – an advantage over Excel. Graphical outputs, such as plots of Q_{total} versus mole fraction or enthalpy of vaporization versus boiling temperature of the mixture, can be generated directly within same worksheet, providing immediate visual feedback – figs. 5, 6.

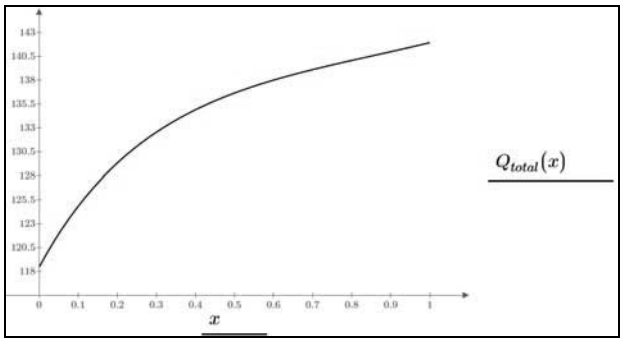

Fig. 5 – Relationships between the variations of total heat duty with ethanol mole fraction (in MathCAD)

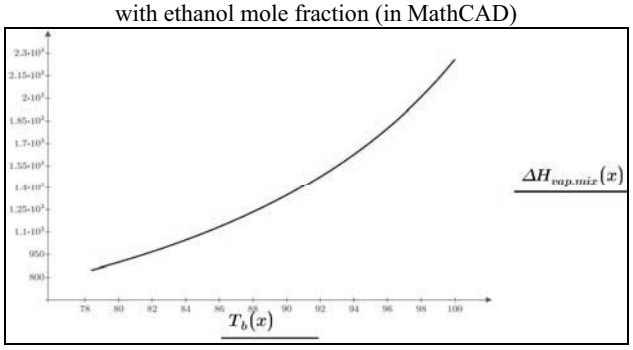

Fig. 6 – Relationships between the enthalpy of vaporization with boiling temperature of the mixture (in MathCAD)

III. Implementation in DWSIM.

DWSIM is an open-source process simulator that provides rigorous thermodynamic models, phase equilibrium calculations, and unit operation modules comparable to those of commercial software. Unlike Excel and MathCAD, which require explicit user-defined equations, DWSIM allows the engineer to represent the process flowsheet graphically, assign thermodynamic packages, and obtain results through built-in property methods. For this study, the ethanol–water evaporation problem was implemented as a steady-state simulation in DWSIM.

The simulation setup involved the following components.

1. Thermodynamic package – the Non-Random Two-Liquid (NRTL) model was selected for handling non-idealities of ethanol-water mixtures;

2. Material streams – a feed stream was defined with mass flow m_{feed} = 1000 kg/h, variable mole fraction of ethanol x and feed temperature T_{feed} = 25°C;

3. Heater unit – a heater block was introduced to raise the stream temperature from the feed value to its boiling point, corresponding to the sensible heat duty;

4. Flash separator – a flash drum operating at atmospheric pressure was connected downstream to represent partial evaporation. The vapor fraction was adjusted according to the empirical function:

$$\phi_{vap} = 0,05 + 0,4 \cdot x, \quad (9)$$

where ϕ_{vap} – fraction of feed undergoing evaporation,

x – ethanol mole fraction.

5. Energy streams – the heater and flash block automatically reported energy duties, which together represent the total heat requirement:

$$Q_{total} = Q_{heater} + Q_{flash}, \quad (10)$$

where Q_{heater} and Q_{flash} – heater and flash block heat loads, respectively (kW).

The advantage of DWSIM is that all thermodynamic properties (T_b, $\Delta H_{vap.mix}$, c_p) are calculated internally based on the chosen property package. This eliminates the need for explicit user-defined correlations, providing higher accuracy and consistency. Furthermore, sensitivity analyses were performed by varying ethanol mole fraction, allowing DWSIM to generate datasets directly comparable to those produced in Excel and MathCAD.

While DWSIM offers greater rigor, it is less transparent to beginners, since equations are not visible as in MathCAD. Nevertheless, for professional design and research purposes, it provides reliable predictions of mixture behavior and energy requirements.

The material flow Feed with different mole fractions of ethanol passes through the Heater, where it is heated to the boiling point at a given pressure. After starting the simulation, the energy flow of this block will show Q_{heater} – the heat of heating. Next, the heated Flash enters the Flash Separator, where it is separated into two phases (evaporates), due to which the energy flow of this block will show the flow Q_{flash} – the heat of evaporation. The sum of these components according to (10) will show the total heat duty. For the scheme shown at Fig. 7, a series of simulations were carried out – 50 iterations with a change in the mass fraction of ethanol. Its results summarized in a tabular form for clarity and ease of comparison – Fig. 8.

The comparison of simulation results between Excel and DWSIM revealed an almost identical trend in the calculated heat duties. Minor deviations were observed, which can be attributed to the simplified empirical correlations embedded in the Excel spreadsheet versus the rigorous thermodynamic models applied in DWSIM. Nevertheless, the consistency across both tools confirms the robustness of the approach.

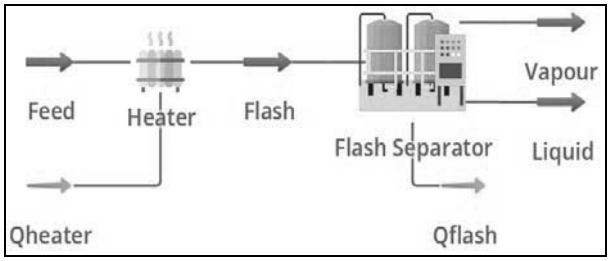

Fig. 7 – Flowsheet for demonstration example (in DWSIM)

	A	B	C	D	E	F	G	H	I	J
1	idx	x_mole_eth	w_mass_eth	T_b_C	Hvap_kJ_per_kg	cp_kJ_per_kgK	mass_evap_kg_h	Sensible_kJ_h	Latent_kJ_h	Total_Q_kW
2	1	0,02	0,04960137	99,4694	2184,834062	4,093693617	58	304854,9074	126720,3756	119,8820231
3	2	0,0398	0,095840758	98,9480462	2118,474529	4,01323708	65,92	296771,041	139649,8409	121,2280228
50	49	0,9702	0,988131771	78,8700142	856,3479458	2,460650718	438,08	132555,2891	375148,9081	141,0289437
51	50	0,99	0,996065688	78,5368	846,072052	2,446845704	446	130996,2891	377348,1352	141,2067845

Fig. 8 – Spreadsheet in DWSIM with calculated data (shortened):
x_mole_eth – mole fraction of ethanol; w_mass_eth – mass fraction; T_b_C – boiling point; Hvap_kJ_per_kg – enthalpy of vaporization; cp_kJ_per_kgK – heat capacity; mass_evap_kg_h – mass flow rate of evaporated liquid; Sensible_kJ_h, Latent_kJ_h, Total_Q_kW – energy consumption

Discussion of Results.

The obtained results demonstrate that the heat duty required for the heating and partial vaporization of ethanol-water mixtures exhibits a non-linear dependence on composition. Both Excel and DWSIM showed that the total energy demand decreases as the ethanol mole fraction increases, reflecting lower boiling temperature and smaller enthalpy of vaporization of ethanol compared to water. The quantitative agreement between the two platforms was remarkably strong. Differences, where present, did not exceed a few percent and followed a consistent direction, with DWSIM generally predicting slightly lower duties due to the use of the NRTL model for phase equilibria. Overall, the high level of concordance indicates that simplified correlations can be trusted for conceptual design, while process simulators are indispensable for detailed and accurate modeling.

Conclusions.

This study confirms the practical value of integrating modern information technologies to chemical engineering workflows. Excel proved to be a transparent and flexible tool for rapid prototyping of calculations, enabling easy data manipulation and visualization. MathCAD ensured symbolic validation and reproducibility of same formulas,

while DWSIM offered a rigorous thermodynamic framework to simulate real process conditions. The strong agreement of results across all three platforms highlights their complementarity: spreadsheets are suitable for quick estimates, equation-based tools for documentation and verification, and process simulators for accurate, industry-ready calculations. The ethanol-water evaporation case demonstrated that the relative error between Excel and DWSIM outputs was negligible, reinforcing confidence in the reliability of simplified models when used with caution. Ultimately, combining these tools provides a balanced methodology that bridges conceptual understanding with professional process simulation, thereby enhancing both the educational and practical aspects of chemical engineering practice.

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