

Divided Wall Column Modeling and Simulation in an Open-Source Environment



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The divided wall column (DWC) can achieve sharp separations of three or more components in a single shell, substituting conventional sequences of two or more binary distillation columns, with lower expenses. Despite these advantages, DWC models are not available in commercial chemical process simulators. To simulate DWC, users must employ instances of conventional column model and couple them in different configurations. In this paper, a DWC model was developed in EMSO (Environment for Modeling, Simulation and Optimization). DWC model was then used for simulating the separation of an equimolar mixture of three hydrocarbons. Results show that, depending on the number of trays, DWC presented energy savings compared to two ordinary distillation columns. Better separation was obtained when the number of divided trays was close to half the number of total trays. However, the liquid and vapor flow rates split into the divided section play a key role in the separation.

Keywords:

EMSO environment, divided wall column, modeling, distillation, simulation

Introduction

Proposed in the 1940s by Wright¹, the divided wall column (DWC) is an alternative to multicomponent distillation systems. This separation scheme integrates two conventional columns into one single device, and allows the sharp separation of multicomponent mixtures with a smaller amount of equipment. Since the first equipment implemented by BASF in the 1980s, several papers have been published aiming at the improvement of this distillation system. Schultz *et al.*² introduced a review of the developments in DWC technology in the early 2000s, and presented guidelines for the design of these columns. Navarro *et al.*³ presented a novel strategy for the simulation of thermally coupled dis-

tillation sequences using process simulators, and showed that two side stream connections involved in the thermal coupling can be substituted with a combination of a material and an energy stream connecting the pre-fractionator to a main column. Several researchers have indicated that DWC can save up to 40 % of the reboiler energy consumption⁴, and offers a potential (up to 30 %) reduction in investment. Aspiron and Kaibel⁵ showed how this reduction could be achieved depending on the configuration of the distillation system, and Dejanovic *et al.*⁶ presented relevant patents and provided information on equipment innovations and application areas of industrial interest. In addition to the reduction in equipment construction material, DWC can generate a saving of more than 40 % in the space allotted to the distillation system in industrial sites (plot area)⁷.

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However, even given these advantages, DWC models are generally not available in commercial process simulators such as Aspen Plus®, Aspen HYSYS®, CHEMCAD®, ProSim®, gPROMS®, and PRO/II®⁶. In these simulators, this distillation system is often simulated and represented by the use of instances of conventional distillation column model in different types of couplings. Navarro *et al.*³ presented strategies for robust simulations of thermally coupled distillation sequences. Other works show the possibility of applying optimization models in retrofitting conventional column systems of Fully Thermally Coupled Distillation System (FTCDS)⁸ and process flowsheets, with direct sequence, indirect sequence, and Petlyuk column⁹, to reduce energy consumption and amortized capital expense of the DWC system, when compared to the conventional columns system. Recently, works have extended the intensification provided by DWC. Yang *et al.*¹⁰ combine vapor recompression heat pump (HP) to reactive divided wall columns (RDWC), and evaluate the effects of operating pressure of the stripping section on total annualized costs (TAC) of the system. RDWC are also the focus of another work of the same research group¹¹. In the latter work, Yang *et al.*¹¹ also combine HP to RDWC, but waste heat of the compressed stream is used as heat source in Organic Rankine cycles, to produce clean energy. Research combining DWC-HP coupling to heat integration (HI) can also be found¹². Yang *et al.*¹² explored the proposed combination of HI and DWC-HP techniques to separate an azeotropic mixture with lower TAC, and reduced CO₂ emissions and exergy loss. Navarro *et al.*³, and Premkumar and Rangaiah⁸ used the process simulator Aspen HYSYS®, Pattison *et al.*⁹ used the gPROMS®, and Yang *et al.*^{10–12} employed Aspen Plus.

Navarro *et al.*³ and Rahimi *et al.*¹³ presented some forms of simple column couplings to represent a DWC, such as Thermally Coupled Distillation (TCD), named also Fully Thermally Coupled Distillation Systems (FTCDS). These configurations are presented in Fig. 1.

Fig. 1(a) presents a Petlyuk sequence, which is composed of a pre-fractionator and the main column. In the pre-fractionator, the top product is sent to the top of the main column, while the heavy product of the pre-fractionator is sent to its stripping section. In the main column, the components are distributed through the sections, making it possible to remove another component in the intermediary trays of the main column¹⁴. Most of the energy savings in the Petlyuk distillation column arrangement are attributed to the pre-fractionator, because, unlike the conventional distillation system, this equipment provides no large separation of the

components, which is done in the main distillation column. This way, instead of the pre-fractionator being installed outside the main column, it can be incorporated into the main column employing a wall. Thus, the configuration of the Petlyuk distillation column arrangement, as well as the liquid and vapor streams and their compositions, are maintained, and the system is reduced to a single device. This equivalence between the fully thermally coupled column and the DWC is shown by Seider *et al.*¹⁵ and Amminundin and Smith¹⁶.

Fig. 1(b) shows three columns, presented initially by Becker *et al.*¹⁷, in which liquid and vapor flows cause a similarity to the DWC system. This scheme was used by Rahimi *et al.*¹³ in the modeling and simulation of a DWC for buta-1,3-diene purification from a mixture of eight components containing 98.9 % of buta-1,3-diene in the feed stream. The four-column distillation system presented in Fig. 1(c), where the four sections of the DWC are presented separately⁶, is also an option for representing this system. Fig. 1(d) shows a typical form of the pump-around column configuration, widely used as it has a greater convergence facility when compared with four-column models^{18,19}.

Besides not providing a specific model for DWC, most commercial simulators do not allow users to view or modify the equations that constitute the available models. Users can only set model parameters.

EMSO (Environment for Modeling Simulation and Optimization) is an equation-oriented piece of software with an open-source library of unit operations models and solvers for algebraic and differential-algebraic equations. EMSO also has solvers for optimization problem solution, as presented by Soares and Secchi²⁰, and employed by Rodrigues *et al.*²¹ and Henrique *et al.*²², to reduce the order of models²³ or to interpolate data²⁴. The environment also allows the addition of new plugins to calculate thermodynamic properties or to interface with other software and toolboxes, such as Simulink® toolbox of MATLAB® software²⁵. This dynamic simulator is free of charge for educational and academic research purposes. An interesting feature is the possibility of inspection and modification of all equations the models are comprised of, as well as the creation of entirely new unit operations models. Models are coded in the object-oriented EMSO modeling language, with inheritance and composition properties. Since EMSO is equation-oriented, it assembles all equations that constitute the models of all units and streams of the process flowsheet, and solve them simultaneously. Although the equation-oriented approach avoids unit-by-unit iterations for converging recycle loops in steady-state process simulations, the fact that all equations are solved si-

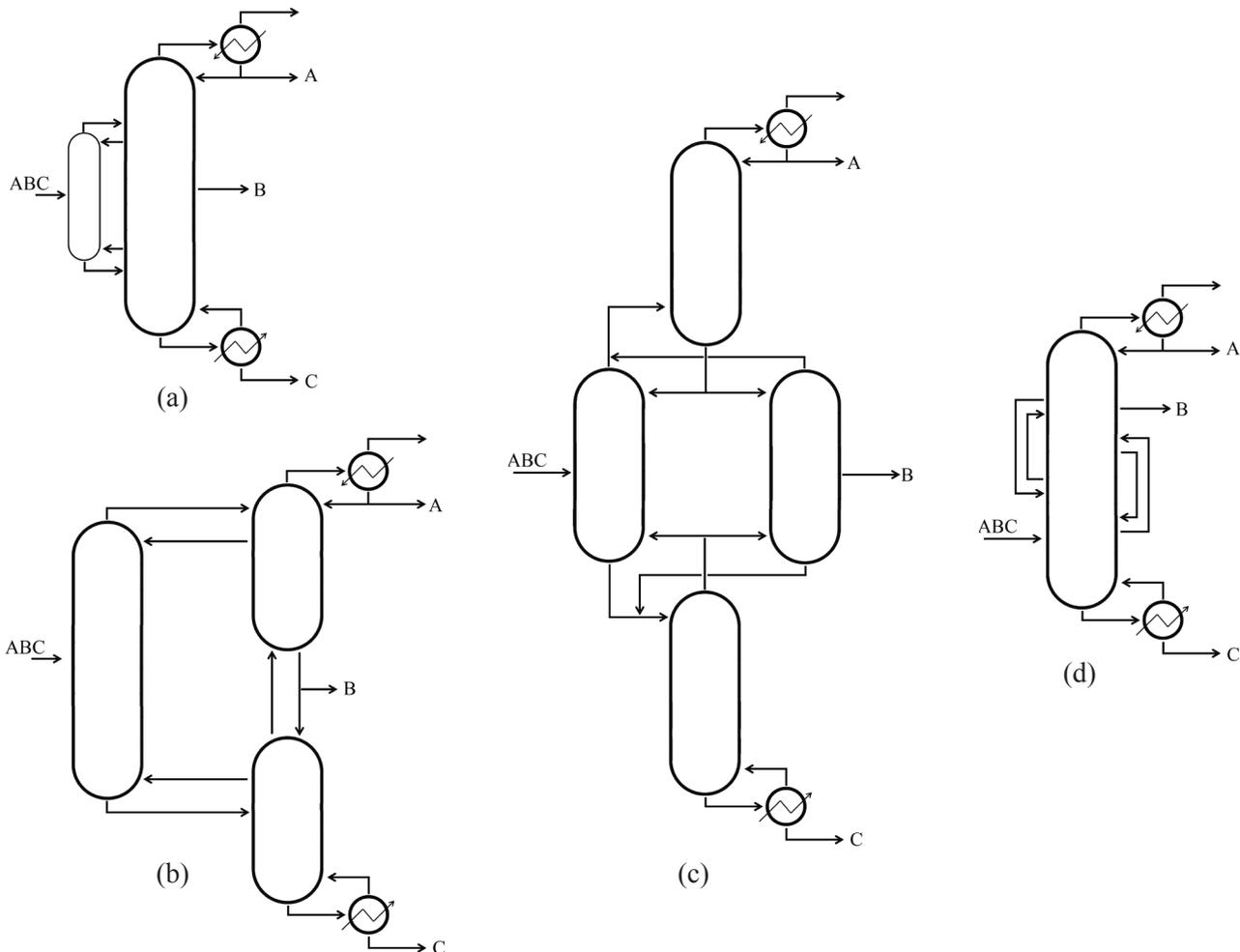


Fig. 1 – Configurations used in commercial software to represent a divided wall column using (a) pre-fractionator system named Petlyuk sequence, (b) three columns sequence, (c) four columns sequence, and (d) pump-around column configuration

multaneously prevents the implementation of strategies for circumventing local convergence problems, so that good initial guess for the model variables is required^{15,24}. One strategy to obtain good initial guess is to run a dynamic simulation of the process for a short period, since the dynamic model can calculate the evolution of all variables during process time. If the dynamic process is simulated for a while, values for all variables by the time the simulation is finished are closer to steady-state values. So, these values can be provided as initial guess for the steady-state calculation, to ease convergence of steady-state simulation.

Since the usual representation of DWC in analysis and simulation reports in the literature is made with the coupling of conventional distillation column models, due to the lack of a model of DWC in process simulators, this paper aimed to develop a DWC model in EMSO. Using EMSO for this purpose, the developed model is open for inspection and extension by any user, and its use is free of charge for teaching and academic research activities. It is important to draw attention to the fact that

previous work has already made an effort to model DWC in a process simulator, but on a commercial program. Pattison *et al.*⁹ implemented a DWC model in commercial simulator gPROMS® to optimally design process flowsheets containing DWCs. This DWC model was implemented as networks of sub-unit models (differential-algebraic equations representing a pseudo-transient model) instead of the traditional MESH equations (mass, equilibrium, mole fraction summation and energy equations), which was suitable for the flowsheet optimization task. In this work, the approach is based on MESH equations. So, this work presents as a novelty, the development of a dedicated DWC model in an open-source environment. Since the environment is free of charge for educational and academic research purposes, and in EMSO it is possible to examine and modify all equations of any process unit model, this model can serve as a basis for teaching activities, future studies on process intensification and optimization, as well as implementation of further improvements by the research community.

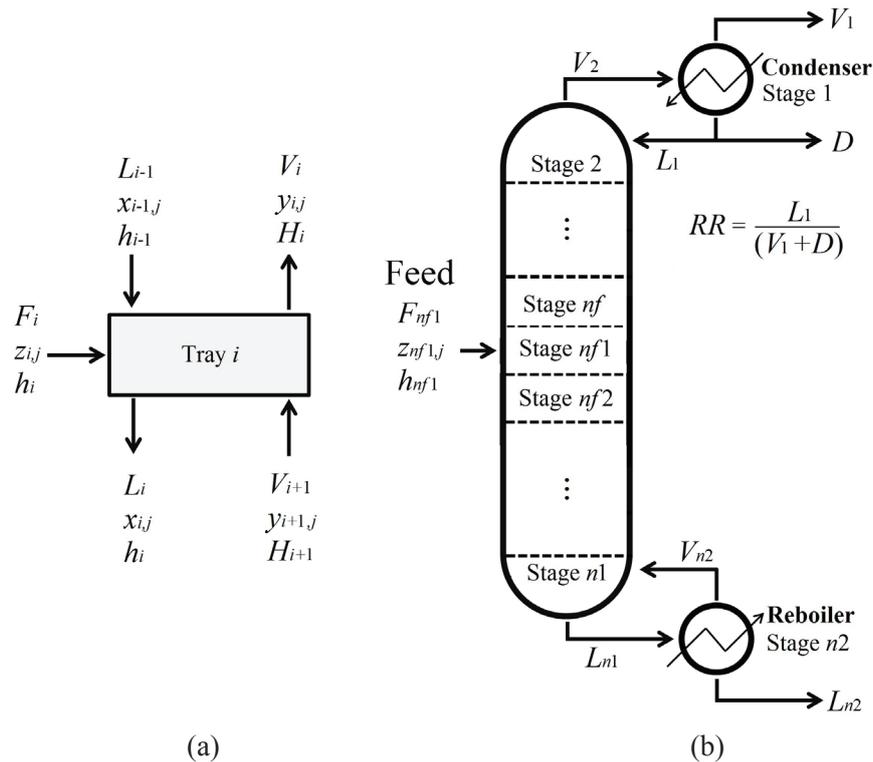


Fig. 2 – Schematic diagram of an ordinary distillation column with (a) generic tray i , and (b) feed stream and withdrawals

With the developed model, a sensitivity analysis of stream composition and heat duties was then performed concerning design (total number of trays and number of divided trays), and operating parameters (reflux ratio and liquid and vapor splitters). Results were also compared to those obtained for a model of a conventional 2-column distillation system in the same environment.

Methodology

DWC model development

The development of the DWC model was based on ordinary distillation column model, which considers the MESH equations (mass, equilibrium, mole fraction summation and energy equations) in each stage²⁶, and on quasi-steady-state assumption with dynamics only for the component molar balances to provide better initial estimates for steady-state simulations.

The schematic diagram of an ordinary distillation column is presented in Fig. 2. Equations 1–13 represent the molar balances (overall and for the j -th component), energy balance, and physical constraints at each stage i . The equilibrium relations and thermodynamic properties are obtained according to Equations 14–26 for a generic stage i of the distillation column with $i \in \{1, 2, \dots, n2\}$ (where the

condenser is represented by $i = 1$ and the reboiler by $i = n2$) and $j \in \{1, 2, \dots, n_{components}\}$. Equations 17–19 use the values that the user defines for condenser and reboiler vapor holdup and internal trays of the columns. Condenser and reboiler holdups are usually two orders of magnitude greater than tray holdups. Equation 20 uses the operating pressure, which must also be set by the user (as a constant value or a given pressure profile).

Condenser (stage 1)

$$RR \cdot (V_1 + D) - L_1 = 0 \quad (1)$$

$$V_2 - L_1 - D - V_1 = 0 \quad (2)$$

$$m_1 \cdot \frac{dx_{1,j}}{dt} = V_2 \cdot y_{2,j} - (L_1 + D) \cdot x_{1,j} - V_1 \cdot y_{1,j} \quad (3)$$

$$Q_c = V_2 \cdot H_2 - (L_1 + D) \cdot h_1 - V_1 \cdot H_1 \quad (4)$$

where RR is the reflux ratio, V is the vapor molar flow rate, D is the top product molar flow rate, L is the liquid molar flow rate, m is the molar liquid holdup, x is the molar fraction in the liquid stream, y is the molar fraction in the vapor stream, t is the time, Q_c is the heat duty of the condenser, H is the vapor molar enthalpy, and h is the liquid molar enthalpy.

Trays of rectifying and stripping sections (from stage 2 to stage nf , and from stage $nf2$ to stage $n1$)

$$L_{i-1} + V_{i+1} - L_i - V_i = 0 \quad (5)$$

$$L_{i-1} \cdot h_{i-1} + V_{i+1} \cdot H_{i+1} - L_i \cdot h_i - V_i \cdot H_i = 0 \quad (6)$$

$$m_i \cdot \frac{dx_{i,j}}{dt} = L_{i-1} \cdot x_{i-1,j} + V_{i+1} \cdot y_{i+1,j} - L_i \cdot x_{i,j} - V_i \cdot y_{i,j} \quad (7)$$

Feed tray (stage $nf1$)

$$F_{nf1} + L_{nf} + V_{nf2} - L_{nf1} - V_{nf1} = 0 \quad (8)$$

$$F_{nf1} \cdot h_{nf1} + L_{nf} \cdot h_{nf} + V_{nf2} \cdot H_{nf2} - L_{nf1} \cdot h_{nf1} - V_{nf1} \cdot H_{nf1} = 0 \quad (9)$$

$$m_{nf1} \cdot \frac{dx_{nf1,j}}{dt} = F_{nf1} \cdot z_{nf1,j} + L_{nf} \cdot x_{nf,j} + V_{nf2} \cdot y_{nf2,j} - L_{nf1} \cdot x_{nf1,j} - V_{nf1} \cdot y_{nf1,j} \quad (10)$$

where $nf1$ is the feed tray, F is the feed molar flow rate, and z is the molar fraction in the feed stream.

Reboiler (stage $n2$)

$$L_{n2} - L_{n1} + V_{n2} = 0 \quad (11)$$

$$m_{n2} \cdot \frac{dx_{n2,j}}{dt} = L_{n1} \cdot x_{n1,j} - L_{n2} \cdot x_{n2,j} - V_{n2} \cdot y_{n2,j} \quad (12)$$

$$Q_r = L_{n2} \cdot h_{n2} + V_{n2} \cdot H_{n2} - L_{n1} \cdot h_{n1} \quad (13)$$

where $n2$ is the last stage of the column (reboiler) and Q_r is the heat duty of the reboiler.

All trays (from stage 1 to stage $n2$)

$$m_{i,j} = M_{i,j} \cdot x_{i,j} \quad (14)$$

$$y_{i,j} = K_{i,j} \cdot x_{i,j} \quad (15)$$

$$\sum_{j=1}^{n_{components}} x_{i,j} = \sum_{j=1}^{n_{components}} y_{i,j}, \quad x_{i,j}, y_{i,j} \geq 0 \quad (16)$$

$$M_{1,j} = M_{cond} \quad (17)$$

$$M_{i,j} = M_{trays} \quad (18)$$

$$M_{n2,j} = M_{reb} \quad (19)$$

$$p_i = p_{op} \quad (20)$$

$$T_i = f(p_i, x_{i,j}) \quad (21)$$

$$K_{i,j} \cdot f_{i,j}^V(T_i, p_i, y_{i,j}) = f_{i,j}^L(T_i, p_i, x_{i,j}) \quad (22)$$

$$H_{i,j} = f(T_i, p_i, y_{i,j}) \quad (23)$$

$$H_i = \sum_{j=1}^{n_{components}} y_{i,j} \cdot H_{i,j} \quad (24)$$

$$h_{i,j} = f(T_i, p_i, x_{i,j}) \quad (25)$$

$$h_i = \sum_{j=1}^{n_{components}} x_{i,j} \cdot h_{i,j} \quad (26)$$

where M is the molar vapor holdup, K is the equilibrium constant, M_{cond} is the condenser molar vapor holdup, M_{trays} is the tray molar vapor holdup, M_{reb} is the reboiler molar vapor holdup, p is the pressure, p_{op} is the operating pressure (parameter set by the user), T is the temperature, f^V is the vapor fugacity, and f^L is the liquid fugacity.

Taking this ordinary column model as a starting point, the DWC model was derived, which uses the nomenclature presented in Fig. 3. In this column, it is possible to choose the position of the wall, define the feed tray (stage $nf1$) and the number of divided trays. The model assumes that the feed and the side draw product streams are located at the central tray of the divided section of the DWC, on opposite sides of the dividing wall, as depicted by $nf1$ and $nsd1$ in Fig. 3. Therefore, the user needs only to define the number of stages, divided trays, and the position of the feed tray. For example, in a column with 27 stages, 13 divided trays and $nf1 = 15$, there are eight trays above and four below the wall.

The liquid that comes down from tray it is split, and sit represents the fraction of this liquid stream that comes down to $n0m$ tray (feed side). Consequently, $(1 - sit)$ is the fraction of the liquid stream that comes down from tray it into the side draw side (into tray $n0sd$). Analogously, sib represents the fraction of the vapor stream that comes up from tray ib into the feed side (into tray $n3m$) and $(1 - sib)$ comes up into the side draw side (into tray $n3sd$). Details of these separations can be observed in Fig. 3. For example, if the intern wall is positioned in the middle of the cross-section of the DWC, the downward liquid flow is equally divided ($sit = 0.5$), and the same happens to the upward vapor ($sib = 0.5$). Due to numerical issues (avoiding indetermination and, consequently, failure in model solution), parameters that define liquid and vapor splits (sit and sib) are supposed to vary between 0.15 and 0.85. These values were found empirically to prevent model solution failure due to numerical issues on the equation-oriented process simulator, which solves simultaneously all equations related to the process flowsheet.

The conditions at it and ib trays are described by Equations 27–32. Equations 33–44 represent the conditions of liquid and vapor in the feed side, and

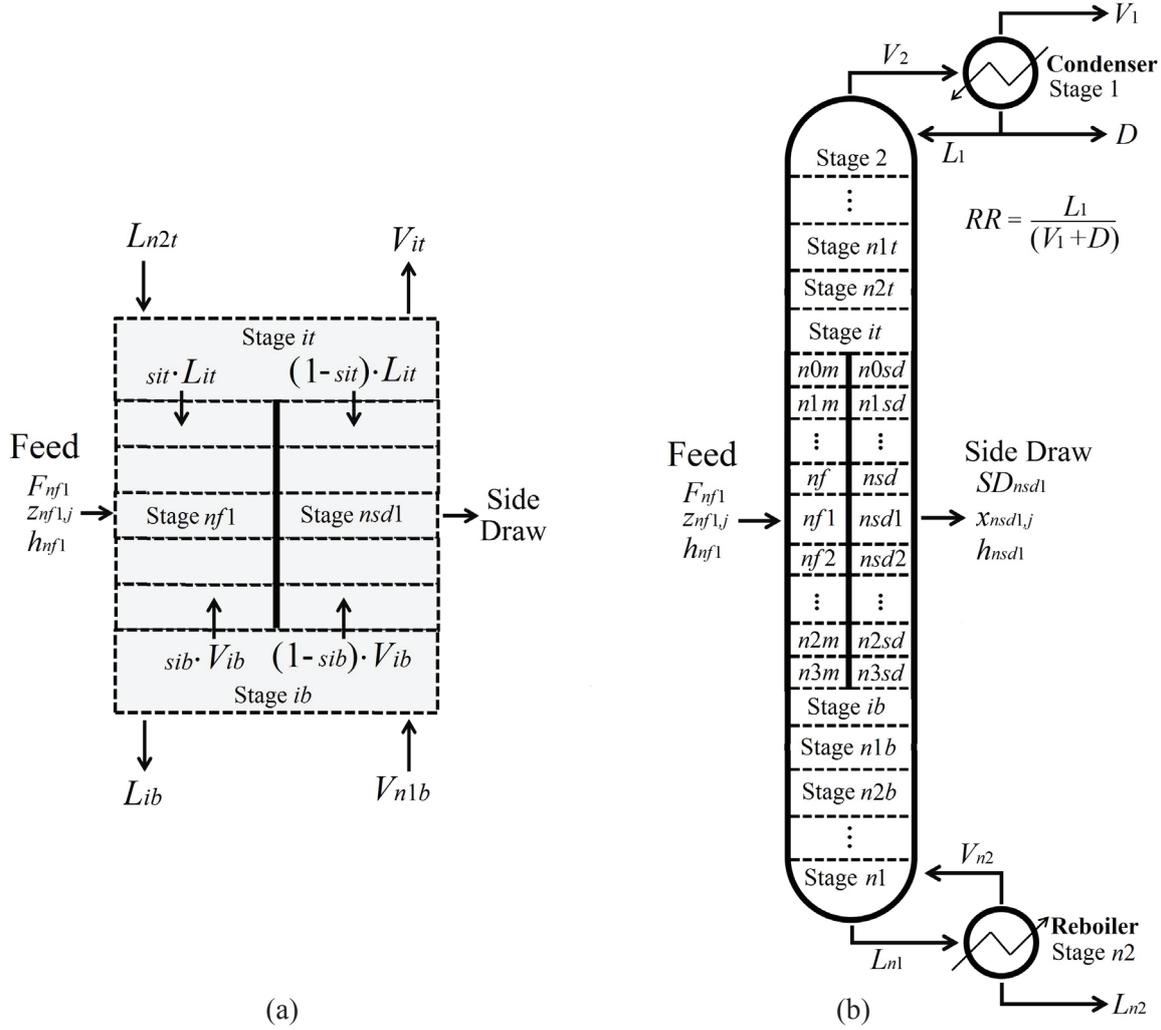


Fig. 3 – Schematic diagram of the DWC with (a) trays in the neighborhood of the wall, and (b) feed stream and withdrawals

Equations 45–56 describe conditions on the other side of the wall. The equations of the rectifying and stripping section, above and below the divided trays (from stage 1 to $n2t$, and from stage $n1b$ to $n2$), are

similar to those of the ordinary column model. Also, the calculation of the thermodynamic properties is analogous to the one performed in the ordinary column model.

Stage it (upper thermal coupling stage)

$$L_{n2t} + V_{n0m} + V_{n0sd}^{sd} - L_{it} - V_{it} = 0 \quad (27)$$

$$L_{n2t} \cdot h_{n2t} + V_{n0m} \cdot H_{n0m} + V_{n0sd}^{sd} \cdot H_{n0sd}^{sd} - L_{it} \cdot h_{it} - V_{it} \cdot H_{it} = 0 \quad (28)$$

$$m_{it} \cdot \frac{dx_{it,j}}{dt} = L_{n2t} \cdot x_{n2t,j} + V_{n0m} \cdot y_{n0m,j} + V_{n0sd}^{sd} \cdot y_{n0sd,j}^{sd} - L_{it} \cdot x_{it,j} - V_{it} \cdot y_{it,j} \quad (29)$$

Stage ib (lower thermal coupling stage)

$$V_{n1b} + L_{n3m} + L_{n3sd}^{sd} - L_{ib} - V_{ib} = 0 \quad (30)$$

$$V_{n1b} \cdot H_{n1b} + L_{n3m} \cdot h_{n3m} + L_{n3sd}^{sd} \cdot h_{n3sd}^{sd} - L_{ib} \cdot h_{ib} - V_{ib} \cdot H_{ib} = 0 \quad (31)$$

$$m_{ib} \cdot \frac{dx_{ib,j}}{dt} = V_{n1b} \cdot y_{n1b,j} + L_{n3m} \cdot x_{n3m,j} + L_{n3sd}^{sd} \cdot x_{n3sd,j}^{sd} - L_{ib} \cdot x_{ib,j} - V_{ib} \cdot y_{ib,j} \quad (32)$$

where sd is the side draw tray.

Feed side, Stage $n0m$

$$sit \cdot L_{it} + V_{n1m} - L_{n0m} - V_{n0m} = 0 \quad (33)$$

$$sit \cdot L_{it} \cdot h_{it} + V_{n1m} \cdot H_{n1m} - L_{n0m} \cdot h_{n0m} - V_{n0m} \cdot H_{n0m} = 0 \quad (34)$$

$$m_{n0m} \cdot \frac{dx_{n0m,j}}{dt} = sit \cdot L_{it} \cdot x_{it,j} + V_{n1m} \cdot y_{n1m,j} - L_{n0m} \cdot x_{n0m,j} - V_{n0m} \cdot y_{n0m,j} \quad (35)$$

where *sit* is the parameter that defines liquid split at tray *it* and *sib* is the parameter that defines vapor split at tray *ib*.

Feed side, Divided trays (from stage $n1m$ to stage nf , and from stage $nf2$ to stage $n2m$)

$$L_{i-1} + V_{i+1} - L_i - V_i = 0 \quad (36)$$

$$L_{i-1} \cdot h_{i-1} + V_{i+1} \cdot H_{i+1} - L_i \cdot h_i - V_i \cdot H_i = 0 \quad (37)$$

$$m_i \cdot \frac{dx_{i,j}}{dt} = L_{i-1} \cdot x_{i-1,j} + V_{i+1} \cdot y_{i+1,j} - L_i \cdot x_{i,j} - V_i \cdot y_{i,j} \quad (38)$$

Feed side, Feed tray (stage $nf1$)

$$F_{nf1} + L_{nf} + V_{nf2} - L_{nf1} - V_{nf1} = 0 \quad (39)$$

$$F_{nf1} \cdot h_{nf1} + L_{nf} \cdot h_{nf} + V_{nf2} \cdot H_{nf2} - L_{nf1} \cdot h_{nf1} - V_{nf1} \cdot H_{nf1} = 0 \quad (40)$$

$$m_{nf1} \cdot \frac{dx_{nf1,j}}{dt} = F_{nf1} \cdot z_{nf1,j} + L_{nf} \cdot x_{nf,j} + V_{nf2} \cdot y_{nf2,j} - L_{nf1} \cdot x_{nf1,j} - V_{nf1} \cdot y_{nf1,j} \quad (41)$$

Feed side, Stage $n3m$

$$sib \cdot V_{ib} + L_{n2m} - L_{n3m} - V_{n3m} = 0 \quad (42)$$

$$sib \cdot V_{ib} \cdot H_{ib} + L_{n2m} \cdot h_{n2m} - L_{n3m} \cdot h_{n3m} - V_{n3m} \cdot H_{n3m} = 0 \quad (43)$$

$$m_{n3m} \cdot \frac{dx_{n3m,j}}{dt} = sib \cdot V_{ib} \cdot y_{ib,j} + L_{n2m} \cdot x_{n2m,j} - L_{n3m} \cdot x_{n3m,j} - V_{n3m} \cdot y_{n3m,j} \quad (44)$$

Side draw side, Stage $n0sd$

$$(1 - sit) \cdot L_{it} + V_{n1sd}^{sd} - L_{n0sd}^{sd} - V_{n0sd}^{sd} = 0 \quad (45)$$

$$(1 - sit) \cdot L_{it} \cdot h_{it} + V_{n1sd}^{sd} \cdot H_{n1sd}^{sd} - L_{n0sd}^{sd} \cdot h_{n0sd}^{sd} - V_{n0sd}^{sd} \cdot H_{n0sd}^{sd} = 0 \quad (46)$$

$$m_{n0sd}^{sd} \cdot \frac{dx_{n0sd,j}^{sd}}{dt} = (1 - sit) \cdot L_{it} \cdot x_{it,j} + V_{n1sd}^{sd} \cdot y_{n1sd,j}^{sd} - L_{n0sd}^{sd} \cdot x_{n0sd,j}^{sd} - V_{n0sd}^{sd} \cdot y_{n0sd,j}^{sd} \quad (47)$$

Side draw side, Divided trays (from stage $n1sd$ to stage nsd , and from stage $nsd2$ to stage $n2sd$)

$$L_{i-1}^{sd} + V_{i+1}^{sd} - L_i^{sd} - V_i^{sd} = 0 \quad (48)$$

$$L_{i-1}^{sd} \cdot h_{i-1}^{sd} + V_{i+1}^{sd} \cdot H_{i+1}^{sd} - L_i^{sd} \cdot h_i^{sd} - V_i^{sd} \cdot H_i^{sd} = 0 \quad (49)$$

$$m_{i,j}^{sd} \cdot \frac{dx_{i,j}^{sd}}{dt} = L_{i-1,j}^{sd} \cdot x_{i-1,j}^{sd} + V_{i+1,j}^{sd} \cdot y_{i+1,j}^{sd} - L_{i,j}^{sd} \cdot x_{i,j}^{sd} - V_{i,j}^{sd} \cdot y_{i,j}^{sd} \quad (50)$$

Side draw side, Side draw tray (stage $nsd1$)

$$L_{nsd}^{sd} + V_{nsd2}^{sd} - L_{nsd1}^{sd} - V_{nsd1}^{sd} - SD_{nsd1} = 0 \quad (51)$$

$$L_{nsd}^{sd} \cdot h_{nsd}^{sd} + V_{nsd2}^{sd} \cdot H_{nsd2}^{sd} - L_{nsd1}^{sd} \cdot h_{nsd1}^{sd} - V_{nsd1}^{sd} \cdot H_{nsd1}^{sd} - SD_{nsd1} \cdot h_{nsd1}^{sd} = 0 \quad (52)$$

$$m_{nsd1,j}^{sd} \cdot \frac{dx_{nsd1,j}^{sd}}{dt} = L_{nsd}^{sd} \cdot x_{nsd,j}^{sd} + V_{nsd2}^{sd} \cdot y_{nsd2,j}^{sd} - L_{nsd1}^{sd} \cdot x_{nsd1,j}^{sd} - V_{nsd1}^{sd} \cdot y_{nsd1,j}^{sd} - SD_{nsd1} \cdot x_{nsd1,j}^{sd} \quad (53)$$

where SD is the side draw product molar flow rate.

Side draw side, Stage $n3sd$

$$(1 - sib) \cdot V_{ib} + L_{n2sd}^{sd} - L_{n3sd}^{sd} - V_{n3sd}^{sd} = 0 \quad (54)$$

$$(1 - sib) \cdot V_{ib} \cdot H_{ib} + L_{n2sd}^{sd} \cdot h_{n2sd}^{sd} - L_{n3sd}^{sd} \cdot h_{n3sd}^{sd} - V_{n3sd}^{sd} \cdot H_{n3sd}^{sd} = 0 \quad (55)$$

$$m_{n3sd,j}^{sd} \cdot \frac{dx_{n3sd,j}^{sd}}{dt} = (1 - sib) \cdot V_{ib} \cdot y_{ib,j} + L_{n2sd}^{sd} \cdot x_{n2sd,j}^{sd} - L_{n3sd}^{sd} \cdot x_{n3sd,j}^{sd} - V_{n3sd}^{sd} \cdot y_{n3sd,j}^{sd} \quad (56)$$

Case study

In this work, in order to validate the ordinary distillation column model and to evaluate the DWC system compared to a series of ordinary distillation columns, the steady-state sharp separation of 100 kmol h⁻¹ of a ternary equimolar mixture of n-pentane, n-hexane, and n-heptane at 27 °C and 510 kPa is proposed as a case study. Such a case study was previously presented by Premkumar and Rangiah⁸.

All steps followed in the methodology of model evaluation and DWC analysis are presented in Fig. 4 as an outline of the employed procedure.

In the model validation task, the separation of this mixture was simulated in both Aspen HYSYS® and EMSO environments, with a scheme named conventional 2-columns (C2C). The first column possessed 38 total stages, while the second column possessed 21 stages. Peng-Robinson equation of state was used to predict the thermodynamic properties; total condensers were used in both columns, and were specified to be operating at 500 kPa ($p_{op} = 500$ kPa). Feeding was performed on the 19th stage of the first column and the 12th stage of the second. The remaining specifications for the simulation were 1.75 and 1.94 for the reflux ratio of the first and second columns, respectively, and distillate rate was 33.4 kmol h⁻¹ for the first column and 33.3 for the second column. In EMSO, vapor holdup parameters were defined as $M_{cond} = 20$ kmol, $M_{reb} = 25$ kmol, and $M_{trays} = 0.4$ kmol. In the model validation task, the profiles of the calculated molar fractions in the liquid phase along the stages of the two conventional columns in the two simulators, as well as temperature profiles were compared. In addition, reboiler and condenser duties calculated by the two programs were also compared.

Subsequently, the separation of the same mixture was simulated in EMSO, considering one single DWC and two ordinary distillation columns (all columns with total condensers). The separation of

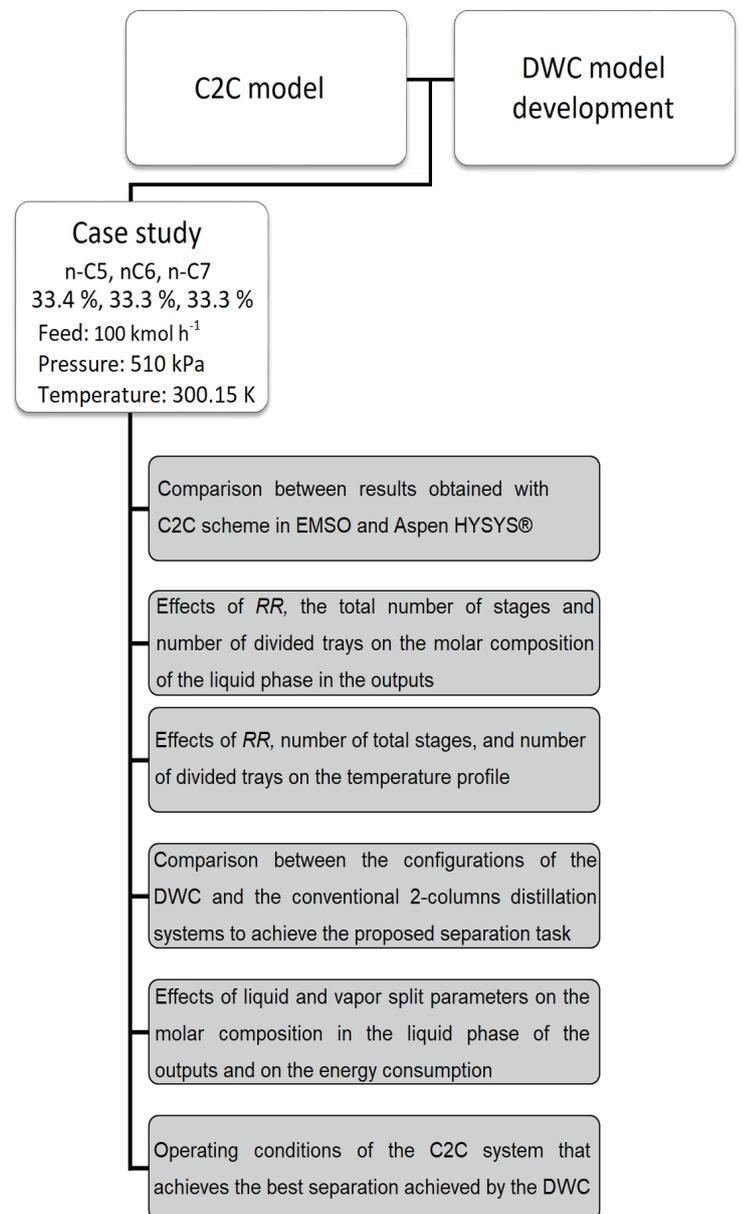


Fig. 4 – Development of the DWC model and steps of the methodology for comparison between the C2C and DWC evaluated models

this mixture was selected because it was among the 6, 18, and 3 mixtures studied by Premkumar and Rangaiah⁸, Rangaiah *et al.*²⁷, and Bek-Pedersen and Gani²⁸, respectively. In both schemes of distillation columns, each output stream had a flow rate between 33.3 and 33.4 kmol h⁻¹. The separation task was defined so that the molar fraction of n-pentane in the top outlet stream of the DWC or of Col 1 (Column 1) of the C2C scheme should be 0.995; the molar fraction of n-hexane in the side draw of the DWC or top outlet stream of Col 2 (Column 2) of the C2C scheme should be 0.875; the molar fraction of n-heptane in the bottom of the DWC or the bottom of Col 2 in the C2C scheme should be 0.880. It is important to note that this separation task may be classified as slightly poor, since molar fractions of key components were not close to unity in their corresponding streams. However, the separation task was specified as such in order to enable the comparison of the results with those reported in the literature, such as in Premkumar and Rangaiah⁸ and Rangaiah *et al.*²⁷ Besides establishing this separation task, this work presents a broader analysis, evaluating parameters related to separation quality. The thermodynamic model, pressure, and holdup parameters were the same as used in the ordinary distillation column model validation task. Different evaluations were made when comparing the separation achieved in both schemes (solely DWC and C2C), as described further herein.

Initially, in the DWC, the effect of the total number of stages (25, 50, and 75), number of divided trays, and the effect of specified reflux ratio (*RR*) on the molar composition of the liquid phase in the outlet streams and on the temperature profile were evaluated considering that the *sib* and *sit* parameters equaled 0.5 (*i.e.*, liquid and vapor stream are equally split into the divided zone). In this study, the feed and the side draw product streams were located at the central tray of the DWC. Furthermore, it was assumed that the symmetrical design of the column concerning the number of trays above and below the divided zone, *e.g.*, in a column with 27 stages and 13 divided trays, there are seven stages above and seven below the wall.

After this first evaluation of the DWC system, the total number of stages in DWC was varied between 25 and 82, considering preliminary tests, and the works of Premkumar and Rangaiah⁸, Bek-Pedersen and Gani²⁸ and Rangaiah *et al.*²⁷ In the simu-

lations and optimizations performed for the separation of these hydrocarbons, Premkumar and Rangaiah⁸ considered columns in sequence with 38 and 21 stages, in addition to DWC with 48 total stages. Rangaiah *et al.*²⁷ considered C2C columns with 43 and 41 total stages, and Bek-Pedersen and Gani²⁸ considered a driving-force-based approach in columns with 36 total stages. For each evaluated total number of trays, the required reflux ratio (*RR*), and the number of divided trays to achieve the specified separation task (considering a maximum absolute error of $\pm 1.0\%$ in the output molar fractions) were determined, keeping *sib* and *sit* parameters equal to 0.5. In this comparison, the feed and the side draw product were no longer fixed at the central part of the DWC (instead, their position was varied, defined by *nf1*). In the same way, the number of divided trays could also vary, aiming to achieve the specified separation task.

In the C2C scheme, the total number of stages in Col 1 (Column 1) was varied between 17 and 55, and in Col 2 (Column 2) between 8 and 27. In this case, since there were no divided trays, only the feed stage could be varied in Col 1 and Col 2 (position defined by variable *nf1*). Also it was determined the *RR* required to achieve the specified separation task.

In addition, the thermal duties of both schemes (DWC and C2C) were compared.

After the comparison of the energy consumption for different sizes of columns with liquid and vapor split parameters set to 0.5, the number of trays in the DWC (both total and divided) were kept constant (consistent with the number of trays in the C2C system that performs the same separation task with the same energy consumption), and *sit* and *sib* were varied between 0.15 and 0.85. Thus, the effects of liquid and vapor split on the total separation difference and reboiler and condenser duties were evaluated. Total separation difference, defined by Equation 57, is a function used in this study to quantitatively assess the quality of the accomplished separation task. Since perfect separation would be represented by molar fractions equal to 1.0 for n-pentane, n-hexane, and n-heptane in stages 1, *nsd1* and *n2*, respectively, and since outputs and feed are connected by mass balances, the closer the proposed assessment function is to zero, the better is the accomplished separation.

$$\text{Total separation difference} = 100 \cdot \left(|1 - x_{1,1}| + |1 - x_{nsd1,2}| + |1 - x_{n2,3}| \right) \quad (57)$$

To finalize the comparisons between the two distillation systems, the operating conditions of the C2C system were varied to accomplish a separation with quality equivalent (in molar fractions of components in outlet streams) to the best one achieved in the DWC system in the previous evaluation task. In this comparison, only the numbers of total stages in the two systems were kept constant.

For all simulated models in the EMSO environment, dynamic models were simulated for a process operating time equal to 8.3 h (which demanded around 5 s of computer processing time), and the values of the variables at the end of the dynamic model execution were used as an initial estimate in Newton's method to obtain the steady-state results. To compare the steady-state simulation convergence time for the conventional distillation column model in EMSO and Aspen HYSYS® (validation task), the convergence time was considered in both simulators.

In the present work, a microcomputer AMD Phenom™ II X6 1090 Processor (3.20 GHz) with 8 GB RAM and GTX 760 graphics card in Windows 7 (32-bit) environment was used.

Results and discussion

Comparison between results obtained with C2C scheme in EMSO and Aspen HYSYS®

As described previously, the same case study was simulated in both simulators for comparison and validation of the EMSO distillation column model. In the commercial software, the simulation convergence time was less than 1.0 second, while in the EMSO environment, all iterations up to the convergence, demanded approximately 13.55 seconds.

Fig. 5(a)-(b) presents the calculated molar fractions in the liquid phase along the stages of the two conventional columns in the two simulators and, as it can be observed, the composition profiles are practically identical. Besides the molar fraction profiles, the temperature profile along the stages was also very close in both pieces of software, as presented in Fig. 5(c)-(d).

Other parameters evaluated in this validation task were condenser and reboiler duties required to perform the separation task determined by the pro-

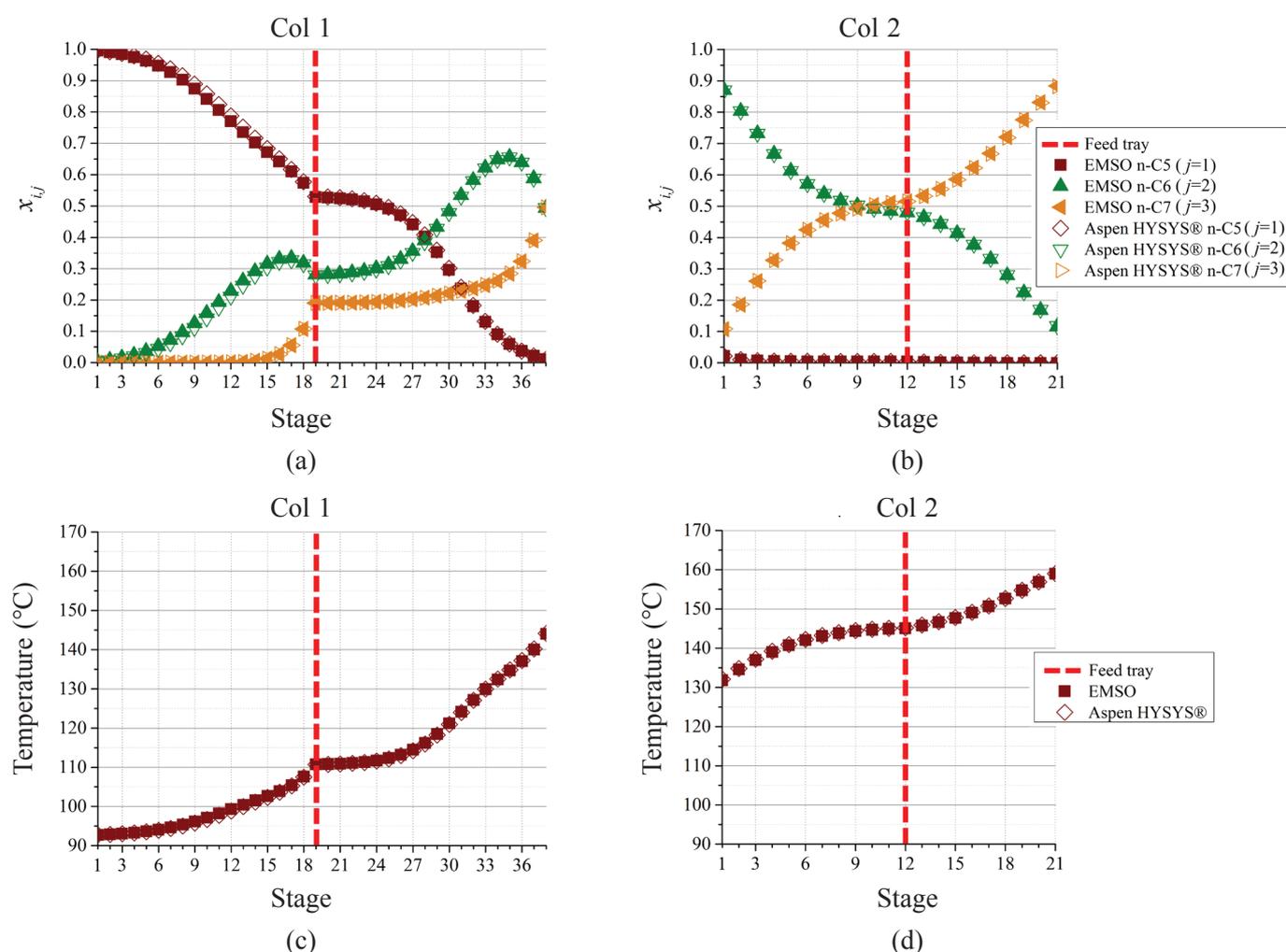


Fig. 5 – Comparison of conventional distillation column model in EMSO and Aspen HYSYS® of (a) profiles of the molar fractions in the liquid phase, and (b) temperature profiles

Table 1 – Condenser and reboiler duties calculated in Aspen HYSYS® and EMSO in the model validation task

Simulator	Col 1 (Column 1)		Col 2 (Column 2)		Total condenser duty (MW)	Total reboiler duty (MW)
	Condenser duty (MW)	Reboiler duty (MW)	Condenser duty (MW)	Reboiler duty (MW)		
Aspen HYSYS®	0.569	1.182	0.691	0.702	1.261	1.884
EMSO	0.568	1.180	0.690	0.701	1.258	1.880
Difference (%)	0.18	0.17	0.14	0.14	0.23	0.21

vided specifications. The model in EMSO presented 0.23 % lower total condenser duty than the one in Aspen HYSYS®. Regarding the total reboiler duty, this difference was about 0.21 % lower in EMSO. Further details can be checked in Table 1 and Fig. 5.

Considering the notable similarity among the presented results, it can be stated that the model for the conventional distillation column in EMSO was validated, reproducing results of the analogous model in the commercial simulator Aspen HYSYS®. Thus, this validated model was considered for the development of the DWC model in EMSO.

Development of the divided wall column (DWC) model

A divided wall column model based on the conventional distillation column model was developed as described previously. The results of the effect of RR , the total number of stages (25, 50 and 75) and the number of divided trays on the molar composition of the liquid in the outlet streams and on the temperature profile are detailed further herein. As described in the case study, the position of the feed stream (n_f1) was not modified in this study, so that feeding was performed on the central tray of the columns.

Effects of RR , the total number of stages, and number of divided trays on the molar composition of the liquid phase in the outputs

If an analysis is performed on the influence of RR in DWC considering sib and sit parameters equal to 0.5 (*i.e.*, liquid and vapor stream are equally split into the divided zone), and feed at the central tray of the columns, one can find that, for a column with 25 stages, there is approximately the same molar composition in liquid phase in the withdrawal trays for the various evaluated values of RR if the DWC has 9 or 12 divided trays. However, with 17 divided trays, it is possible to observe that the bottom and side draw products are not so rich in the desired components (n-heptane and n-hexane, respectively) as with 9 or 12 divided trays. Analogous behavior was observed when the DWC was designed with more than 25 stages: with a large number of divided trays the separation was poorer, since

the achieved fractions of n-hexane and n-heptane in their target streams were smaller than in a column with about half the total number of trays being divided by a wall, although the fraction of n-pentane in its target stream was not so affected.

It could also be observed that RR had a great influence on the molar composition of the outputs, and this effect was more pronounced on columns with the number of divided trays equal to approximately half the number of total trays. For example, if 37 of the 75 total trays were divided, the variation of RR from 2 to 10 would result in a variation of the molar percentage of the n-pentane component in the top product from 76.1 to 94.7 %. For the n-hexane component, the variation would be from 51.9 to 92.0 % in the side draw tray, while the molar percentage of n-heptane in the bottom product would vary from 76.6 to 97.6 %.

As a generally observed trend, when the number of divided trays is approximately half the number of total trays, larger molar fractions of the component of interest in the output streams are noticed. Also with this equipment configuration, a better separation can be observed with RR equal to 10. However, comparing the achieved separation with the proposed separation task, a worse separation is observed in all cases. The molar fraction of n-pentane in the top product of the DWC is between 0.910 and 0.960, and the molar fraction of n-hexane and n-heptane components in liquid output streams of side draw and bottom products of the DWC, respectively, are between 0.673 and 0.976.

Effects of RR , number of total stages, and number of divided trays on the temperature profile

Higher RR values cause an increase in trays temperature located above the wall and a decrease in temperature of inferior trays. Also, increasing the number of trays for low values of RR does not provide good separation, since in these situations, it can be noted that several subsequent trays are at the same temperature. It can be observed that the tendency of equal temperatures in the trays occurs with greater evidence in the divided trays, and the greater the number of divided trays, the lower the temperature variation among them.

Comparison between the configurations of the DWC and the conventional 2-columns distillation systems to achieve the proposed separation task

Considering the case study used in this paper, it was verified that the same separation task accomplished by two conventional columns in series can be achieved by a single DWC with different numbers of total stages (varying from 25 to 82) when *sib* and *sit* parameters are equal to 0.5 (*i.e.*, liquid and vapor stream are equally split into the divided zone), but with location of feed stream (*nf1*) different for each configuration.

Table 2 presents the design (number of stages and divided trays, and location of the feed and the divided trays), and operating parameters (*RR*, and condenser and reboiler thermal duties) of a DWC capable of performing the same separation task detailed in the case study section. To accomplish the separation task, it can be verified that *RR* varies from 12.612 (with 82 stages) to 37.00 (with 25 stages). From 35 to 82 stages in this system, little difference is observed for the minimum *RR* (it changes from 12.900 in the former to 12.612 in the latter), and for required condenser and reboiler duties. This suggests an asymptotic behavior. Concerning the divided trays, from 30 total trays on, its required number falls to around 17 trays, being necessary only to modify the position of the feed tray to perform the necessary task.

To compare the values of condenser and reboiler duties found in this study to those reported by Premkumar and Rangaiah⁸, who considered, for the same separation task, a DWC with 48 stages and 24 divided trays, the duties found here for 45 stages and 17 divided trays (the configuration evaluated in this work that is closer to the cited one) were selected. The mentioned authors reported a process more efficient than the results here found (values of approximately 69.7 and 72.4 % lower in condenser and reboiler duties, respectively). However, the mentioned researchers used thermal couplings of instances of conventional distillation column model to represent the DWC, and the *RR* values adopted in those columns were not reported.

Table 3 shows the necessary configurations of the system of two conventional columns in series to obtain the required separation. The number of stages in Col 1 and Col 2 varied between 17 and 55, and between 8 and 27, respectively. In these same columns, *RR* varied between 1.65 and 6.50 (Col 1), and between 1.85 and 47.00 (Col 2), resulting in duties variation from 1.215 to 12.824 MW for condensers (Col 1 + Col 2), and from 1.838 to 13.446 MW for reboilers (Col 1 + Col 2), respectively. As in the DWC system, asymptotic behavior was observed in the C2C system for total condensers and

Table 2 – Number of divided trays, location of the feed, and the divided trays, *RR*, condenser and reboiler duties required to perform the separation task of the case study in DWC with different number of stages (*sib* = *sit* = 0.5)

Total stages	Divided trays	<i>nf1</i>	<i>it</i>	<i>ib</i>	<i>RR</i>	Condenser duty (MW)	Reboiler duty (MW)
25	13	14	7	21	37.000	7.851	7.880
27	15	15	7	23	32.000	6.819	6.943
30	17	16	7	25	18.000	3.938	4.338
35	17	20	11	29	12.900	2.882	3.428
37	17	22	13	31	12.800	2.861	3.406
40	17	25	16	34	12.700	2.840	3.386
45	17	30	21	39	12.680	2.836	3.383
52	17	36	27	45	12.620	2.824	3.372
55	17	40	31	49	12.615	2.823	3.371
59	17	44	35	53	12.612	2.823	3.370
60	17	45	36	54	12.612	2.823	3.370
67	17	52	43	61	12.612	2.823	3.370
75	17	60	51	69	12.612	2.823	3.370
82	17	67	58	76	12.612	2.823	3.370

reboilers duties from 55 to 82 stages (sum of the number of stages of Col 1 and Col 2).

When comparing the results with those reported by Premkumar and Rangaiah⁸, which considered 59 stages for the conventional distillation system, with 38 stages in Col 1 and 21 stages in Col 2, a considerable difference is also observed. Using commercial Aspen HYSYS® simulator, the authors obtained values of around 1.419 and 1.489 MW for the condenser and reboiler duties, respectively. In the present study, the energy consumption is 11.3 % lower in the condenser, and 26.3 % higher in the reboiler (Table 3). Nonetheless, it is worth stressing that the *RR* values adopted in the work of Premkumar and Rangaiah⁸ were not reported.

Considering the results presented in Tables 2 and 3, Fig. 6 compares the total thermal duties of reboilers (Fig. 6(a)), and condensers (Fig. 6(b)) of the DWC and conventional 2-columns distillation system, varying the number of total stages. The asymptotic behavior is clear. It is possible to determine that, with 25 stages the DWC system had condenser and reboiler duties lower than the C2C system, even with *RR* of 37.00 (in C2C system *RR* was 6.50 in Col 1, and 47.00 in Col 2). From this point onwards, up to 82 stages, the C2C system had a lower total condenser thermal duty, and the smaller difference between the thermal duties of the condensers of the two systems occurs with 35 stages.

Table 3 – Number of stages, location of feed, and RR in each column, condenser and reboiler duties required to perform the separation task of the case study in the system of two conventional columns in series with different number of total stages

Total stages	Col 1 (Column 1)			Col 2 (Column 2)			Condenser duty (MW)	Reboiler duty (MW)
	Stages	n_f	RR	Stages	n_f	RR		
25	17	9	6.50	8	5	47.00	12.824	13.446
27	18	10	5.00	9	5	9.50	3.704	4.326
30	20	11	3.50	10	6	5.50	2.455	3.077
35	24	13	3.45	11	6	3.90	2.067	2.690
37	25	13	2.36	12	7	3.43	1.732	2.355
40	27	14	2.11	13	7	2.70	1.511	2.134
45	30	16	1.90	15	8	2.42	1.401	2.024
52	35	18	1.80	17	9	2.20	1.328	1.951
55	36	19	1.78	19	10	2.00	1.278	1.900
59	38	19	1.75	21	12	1.94	1.258	1.880
60	40	21	1.70	20	11	1.92	1.243	1.866
67	45	23	1.68	22	12	1.88	1.229	1.852
75	50	26	1.66	25	13	1.86	1.220	1.843
82	55	28	1.65	27	14	1.85	1.215	1.838

Given the similarity in energy consumption between the two systems when the total number of stages is 35, this configuration was chosen for a comparison of the profiles of liquid phase components molar fractions (Fig. 7) and temperature (Fig. 8). The number of total stages of the DWC equaled the total number of stages of the conventional 2-column distillation system (35), with 17 divided trays, and RR of 12.90 (according to Table 2). In the case of the conventional 2-column distillation system, Col 1 was composed of 24 stages, and Col 2 of 11 stages, operating with RR of 3.45 and 3.90 (Table 3), respectively.

In Fig. 7 it is possible to verify the difference in molar fraction profiles between the two distillation systems, but in the withdrawal trays the same composition is observed, *i.e.*, in stages 1, 20, and 35 of Fig. 7(c), the same molar fraction values of stage 1 of Col 1, Fig. 7(a), and of stages 1 and 11 of Col 2, Fig. 7(b), respectively, are observed. Furthermore, in Fig. 7(c), it is possible to verify the difference in the liquid phase molar fraction profiles on both sides of the wall.

Fig. 8 shows that the top (stage 1), side draw (stage 20), and bottom (stage 35) of the DWC exhibit fairly close temperatures to the corresponding stages of the conventional 2-column distillation system. For the conventional 2-column distillation system, these temperatures are 92.68 °C, 132.03 °C, and 158.94 °C, while in the DWC distillation system, the corresponding values are 93.05 °C, 130.26 °C, and 159.26 °C, respectively. In Fig. 8(c), it can

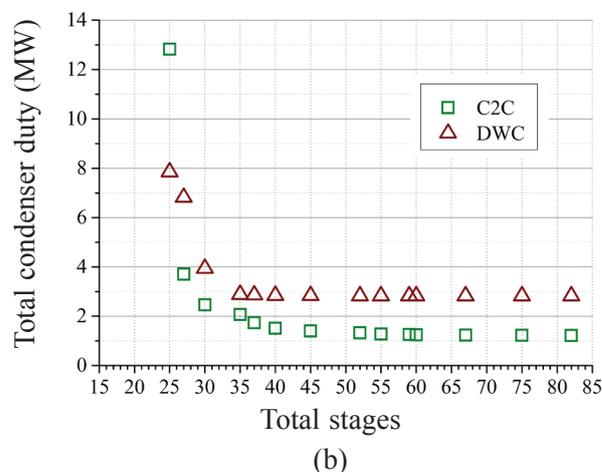
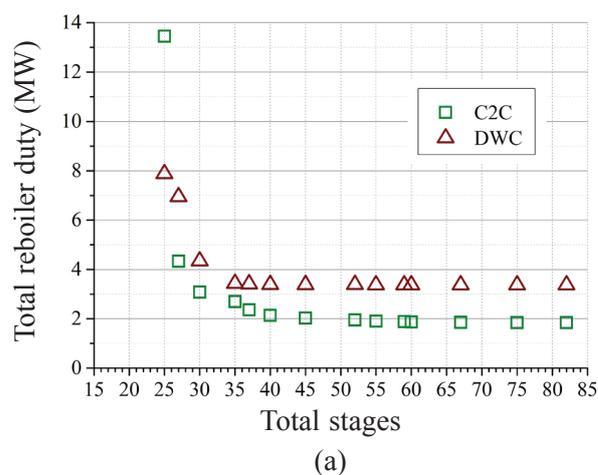


Fig. 6 – Comparison of (a) reboiler and (b) condenser energy consumption by DWC and C2C systems as a function of the total number of stages

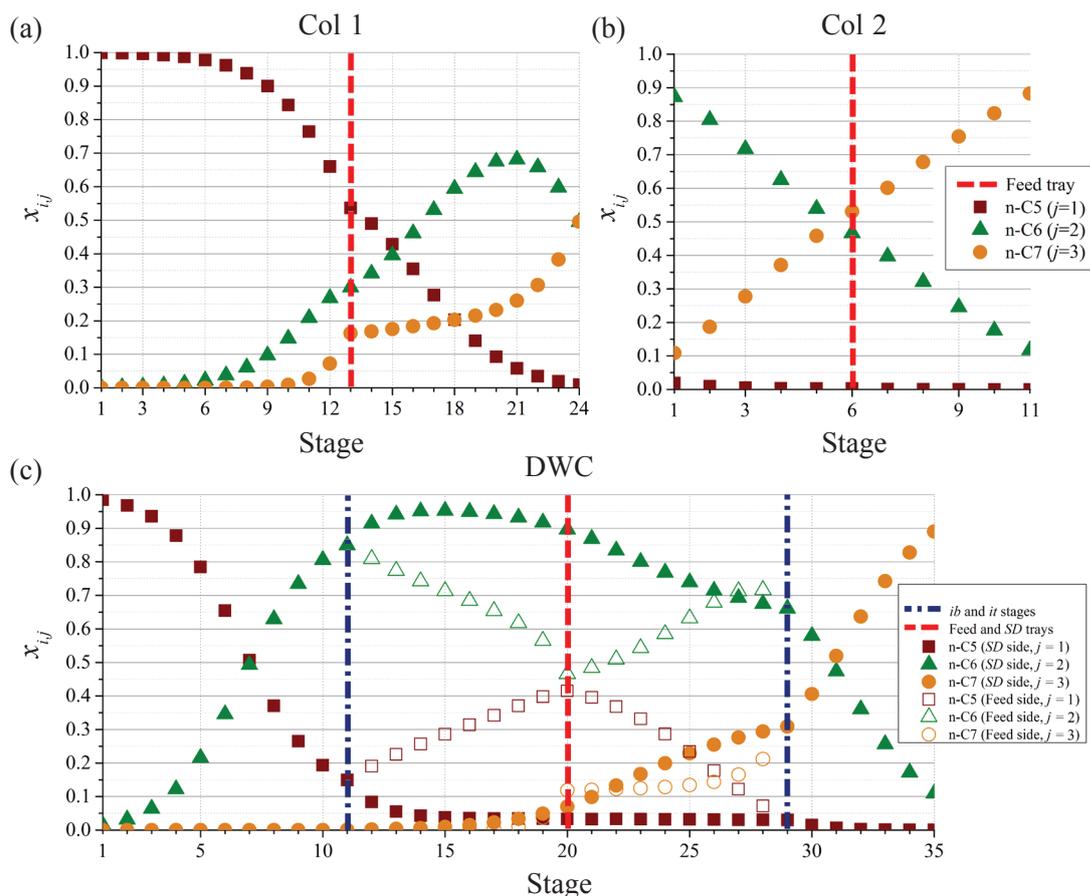


Fig. 7 – Profiles of the molar fractions in the liquid phase along the 35 stages for the separation scheme with (a) two conventional columns in series, and (b) a DWC

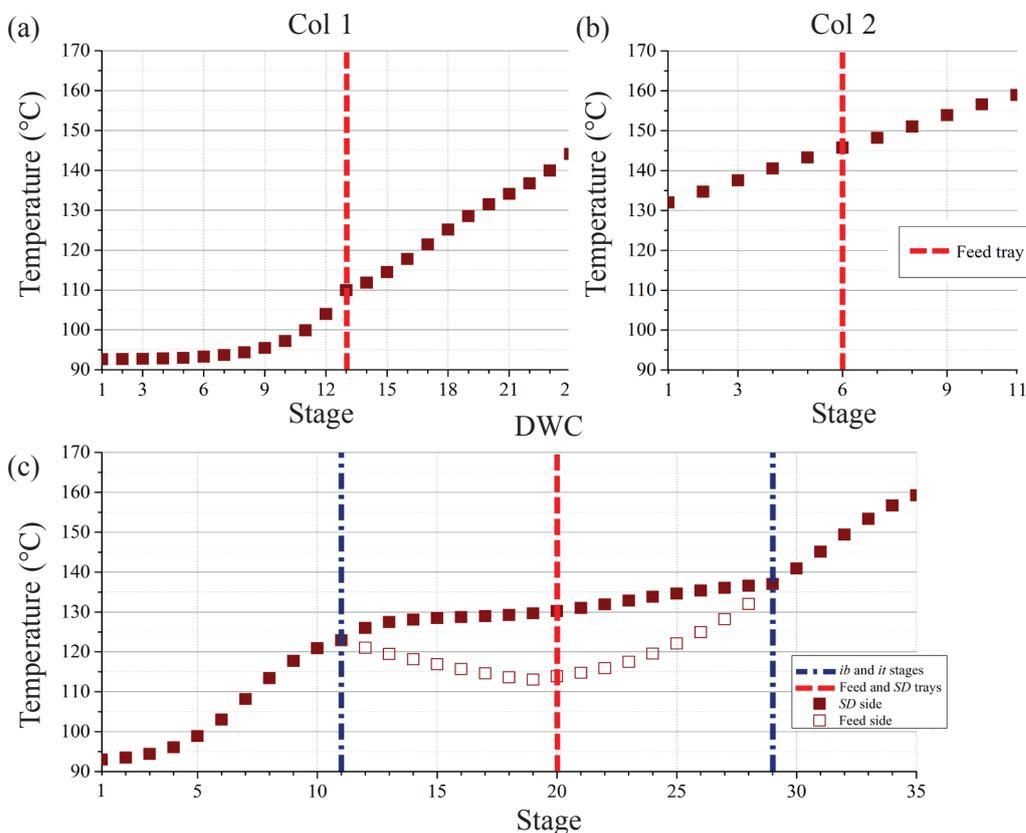


Fig. 8 – Temperature profiles along the 35 stages for the separation scheme with (a) conventional 2-column distillation in series, and (b) a DWC

be further observed that the temperature profiles on the side withdrawal and feed sides differ from each other, reaching a difference of up to 16.66 °C (in stage 19).

Effects of liquid and vapor split parameters on the molar composition in the liquid phase of the outputs and on the energy consumption

The effect of liquid and vapor split parameters (sit and sib) on components molar fractions in the liquid phase of the outputs, and on condenser and reboiler duties was evaluated in a DWC with 35 stages, 17 divided trays, operating with RR of 12.90, and the 20th stage as the feed tray. In DWC real equipment, the configuration of these split parameters is made in the design stage, in the location of the inner wall (percentage tray area allotted to each side). As the values of split parameters varied between 0.15 and 0.85, molar fractions of each component in the liquid phase of the output tray in which it was the main substance, varied between 0.720 and 0.999, as shown in Fig. 9. The component with the narrower observed range was n-pentane (Fig. 9(a)): its molar fraction varied between 0.929 and 0.999. The highest purity ($x_{1,1} = 0.999$) in this figure was inside the region formed by points A, B, C, and D, which correspond to the fractions $sit = 0.15$ and $sib \approx 0.33$, $sit = 0.15$ and $sib \approx 0.70$, $sit \approx 0.58$ and $sib = 0.85$, $sit = 0.85$ and $sib \approx 0.65$, respectively. On the other hand, n-hexane exhibited a wide range of variation: on the liquid of the side draw tray, its molar fraction can change from 0.728 to 0.973, as may be seen in Fig. 9(b). The region of the highest purity was defined by points $sit \approx 0.15$, $sib = 0.45$ and $sit \approx 0.65$, $sib = 0.85$. Fig. 9(c) shows that the bottom output had a content of n-heptane between 79.1 % and 98.4 %. The region of the highest purity was defined by points of sit between 0.15 and 0.60, and sib between 0.45 and 0.85.

Fig. 10 presents the reboiler and condenser duties, and the total separation difference (defined in Equation 57). This figure demonstrates that, although energy consumption was not affected much (observe that thermal duties vary not more than 14.0 %), there were values for the pair of parameters sib and sit associated with poor separation. For example, when $sib \approx 0.15$ and $sit \approx 0.60$, condenser and reboiler duties were 3.511 and 2.928 MW, respectively, while the total separation difference was almost 54 %. On the other hand, a total separation difference around 9 % was achieved with condenser and reboiler duties of 3.258 and 2.870 MW, respectively (configuring $sib \approx 0.35$ and $sit \approx 0.15$). If the analysis is expanded, *i.e.*, if a separation better than that of the proposed task is sought, very small values of the total separation difference should be pursued. The analysis of Fig. 10(c), along with Fig. 9, indicated that molar compositions of 0.998, 0.973,

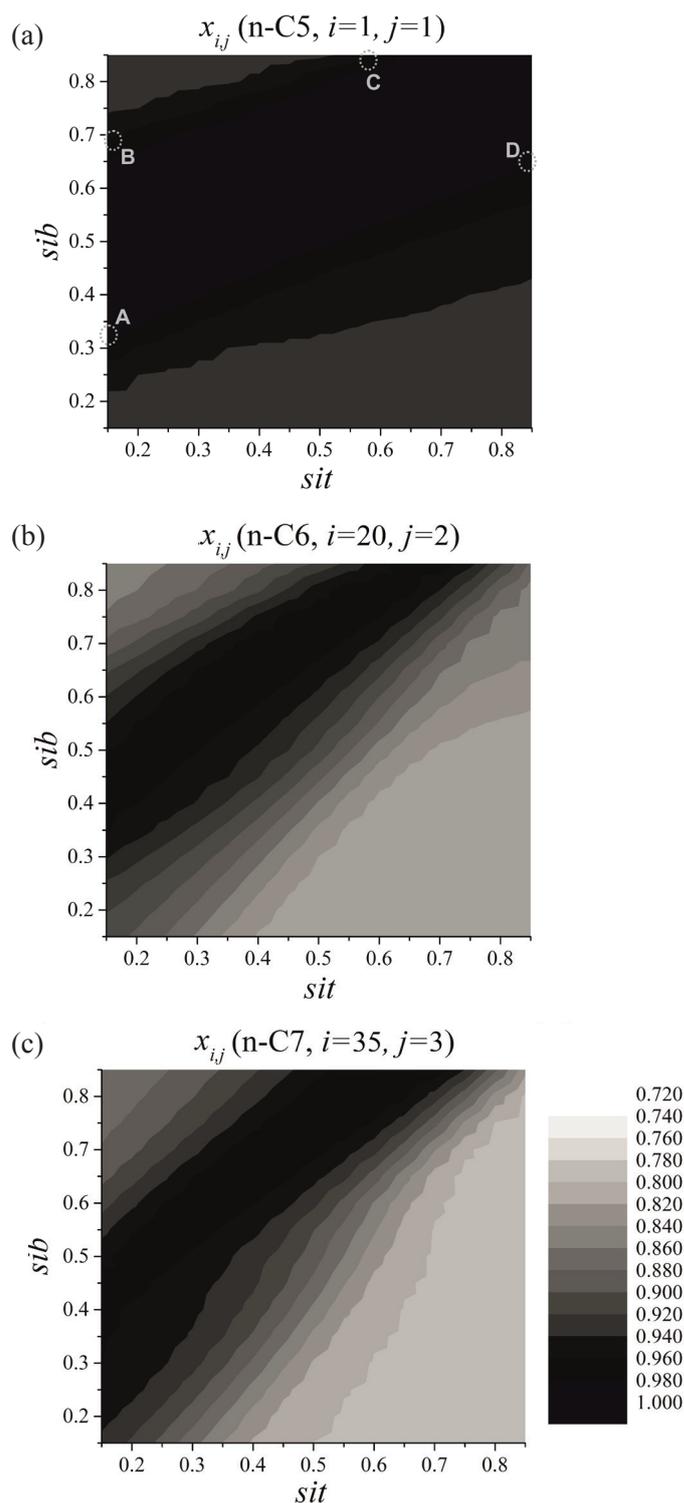


Fig. 9 – Molar fractions of (a) n-pentane, (b) n-hexane, and (c) n-heptane in the liquid phase of the output tray in which each one is the main substance as a function of split parameters

and 0.981 (respectively for n-pentane, n-hexane, and n-heptane in the output tray in which each one is the main substance) can be achieved when sib and sit are around 0.75 and 0.50, respectively. With these values for sib and sit , the total separation difference was slightly lower than 5 %. Aurangzeb and

Jana²⁹ reported values of $sib \approx 0.66$ and $sit \approx 0.42$ as optimal for the separation of other hydrocarbons, such as n-hexane, n-heptane, and n-octane, leading to molar fractions of 0.983, 0.969, and 0.956 for the referred components in the corresponding streams. Considering that configuration ($sib \approx 0.66$ and $sit \approx 0.42$), in the DWC developed, molar separation of 0.999, 0.968, and 0.975 were obtained (respectively for n-pentane, n-hexane, and n-heptane in the output tray in which each one is the main substance).

Operating conditions of the C2C system that achieves the best separation achieved by the DWC

In this last comparison, the C2C system (Col 1 with 24 stages and Col 2 with 11 stages) was submitted to several *RR* conditions, aiming to achieve the best separation obtained in the DWC system, described in the previous section. As shown in Table 4, although the quality of the separation achieved in the C2C system is fairly similar, the energy requirement of the C2C system is much higher. The necessary reflux ratios for the C2C system were 2.93 and 40.00 for Col 1 and Col 2, respectively. This increase in the reflux ratio in Col 2 markedly increased the total reboiler and condenser duties to approximately 10.912 MW and 10.286 MW, respectively. Even with these high values of thermal duty, the total separation difference was 13.18 %. The total separation difference of the DWC system was 8.39 % lower, using 69.24 % and 72.11 % less reboiler and condenser duty.

Conclusions

The development of a divided wall column (DWC) model in the equation-oriented process simulator EMSO has been presented in this paper, and the effects of design and operating parameters were evaluated. The results of conventional distillation column models in EMSO and Aspen HYSYS® were practically the same, which validates the EMSO column model serving as the basis for the development of the DWC model. EMSO software presents great versatility in editing and comparing models, besides being free of charge for educational and academic research purposes. The results of the separation of a ternary equimolar mixture of hydrocarbons with DWC were compared with those of conventional 2-column distillation systems and with literature reports. The results show that DWC can accomplish sharp separations, with quality equivalent to those of the conventional 2-column distillation system, even with a lesser number of trays. Though the capital investment can be lower for the DWC system, due to the lesser number of trays,

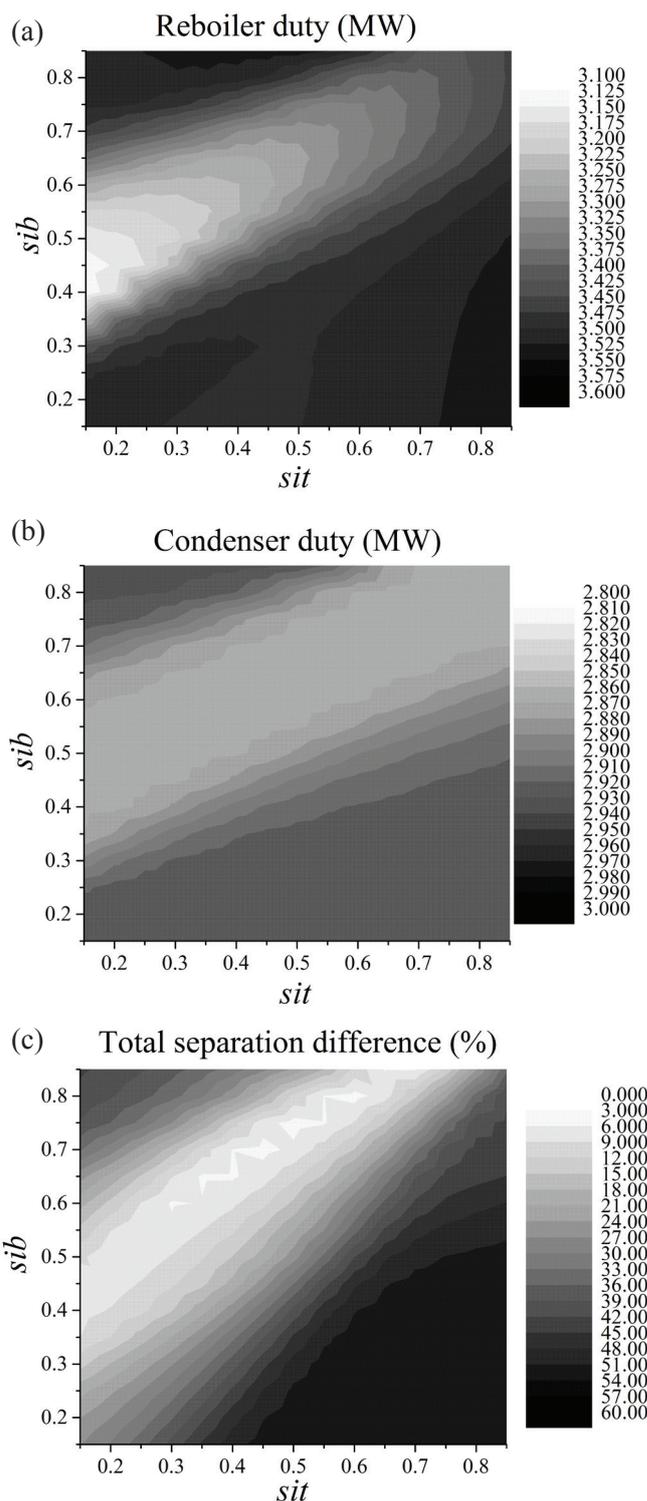


Fig. 10 – (a) Reboiler and (b) condenser duties, and (c) total separation difference as a function of split parameters

with few trays a much larger *RR* is necessary to accomplish the separation task, increasing the operating cost. It was also possible to verify the great influence of the DWC vapor and liquid splitters on the proposed separation task, and how it can be improved, leading the DWC system to surpass the

Table 4 – Comparison between operating parameters and achieved results for C2C and DWC systems to attain the best separation observed in this work

DWC		C2C	
Total stages	35	Total stages	35
Divided trays	17	<i>nf1</i> (Col 1)	13
<i>nf1</i>	20	<i>nf1</i> (Col 2)	6
<i>RR</i>	12.90	<i>RR</i> (Col 1)	2.93
<i>sit</i>	0.50	<i>RR</i> (Col 2)	40.00
<i>sib</i>	0.75		
$x_{1,1}$ (n-C5)	0.998	$x_{1,1}$ (n-C5)	0.998
$x_{20,2}$ (n-C6)	0.973	$x_{1,2}$ (n-C6)	0.930
$x_{35,3}$ (n-C7)	0.981	$x_{11,3}$ (n-C7)	0.941
Total separation difference (%)	4.79	Total separation difference (%)	13.18
Total reboiler duty (MW)	3.357	Total reboiler duty (MW)	10.912
Total condenser duty (MW)	2.869	Total condenser duty (MW)	10.286

C2C system. All these features pave the way for deep exploration of concepts of intensification of separation processes. Furthermore, the developed DWC model aids future studies of this system, so that optimal design and operating parameters can be sought, making the developed model suitable for courses in chemical processes optimization. Future developments on DWC modeling can focus on making it more general, since some simplifying hypotheses were adopted, such as the feed and side draw product streams being located at the same height, one on each side of the wall, with no energy transfer through the wall. The extension of the model can provide wider search spaces in optimization studies of this type of distillation column.

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DECLARATION OF INTEREST

There is no conflict of interest to declare.

Nomenclature

A, B, and C	– Components of a generic ternary mixture
C2C	– Conventional 2-columns distillation system
Col 1	– Column 1
Col 2	– Column 2
<i>D</i>	– Top product flow rate (kmol h ⁻¹)
<i>DT</i>	– Divided trays
DWC	– Divided wall column distillation system
<i>F</i>	– Feed flow rate (kmol h ⁻¹)
<i>f</i>	– Fugacity
FTCDS	– Fully thermally coupled distillation systems
<i>h</i>	– Liquid molar enthalpy (kJ kmol ⁻¹)
<i>H</i>	– Vapor molar enthalpy (kJ kmol ⁻¹)
<i>ib</i>	– Lower thermal coupling stage
<i>it</i>	– Upper thermal coupling stage
<i>K</i>	– Equilibrium constant
<i>L</i>	– Liquid flow rate (kmol h ⁻¹)
<i>m</i>	– Liquid holdup (kmol)
<i>M</i>	– Vapor holdup (kmol)
M_{cond}	– Condenser vapor holdup (kmol)
M_{reb}	– Reboiler vapor holdup (kmol)
M_{trays}	– Tray vapor holdup (kmol)
<i>p</i>	– Pressure (MPa)
p_{op}	– Operating pressure (MPa)
<i>Q</i>	– Heat duty (MW)
<i>RR</i>	– Reflux ratio
<i>sib</i>	– Parameter defining vapor split at tray <i>ib</i>
<i>sit</i>	– Parameter defining liquid split at tray <i>it</i>

<i>SD</i>	– Side draw product flow rate (kmol h ⁻¹)
<i>t</i>	– Time (h)
<i>T</i>	– Temperature (°C)
TCD	– Thermally coupled distillation
<i>V</i>	– Vapor flow rate (kmol h ⁻¹)
<i>x</i>	– Molar fraction in the liquid stream
<i>y</i>	– Molar fraction in the vapor stream
<i>z</i>	– Molar fraction in the feed stream

Subscripts

<i>c</i>	– Condenser
<i>i</i>	– Stage of the column, $i \in \{1, 2, \dots, n2\}$, considering the condenser ($i = 1$) and the reboiler ($i = n2$)
<i>j</i>	– Components of the multicomponent mixture, $j \in \{1, 2, \dots, n_{components}\}$
<i>n2</i>	– Last stage of the column (Reboiler)
<i>nf1</i>	– Feed tray
<i>nsd1</i>	– Side draw tray
<i>r</i>	– Reboiler

Superscripts

<i>L</i>	– Liquid
<i>V</i>	– Vapor
<i>sd</i>	– Side draw trays

References

1. *Wright, R. O.* (Standard Oil Development Co.) Patent US2,471,134A, 24 May 1949.
2. *Schultz, M. A., Stewart, D. G., Harris, J. M., Rosenblum, S. P., Shakur, M. S., O'Brien, D. E.*, Reduce costs with dividing-wall columns, *Chem. Eng. Prog.* **98** (2002) 64.
3. *Navarro, M. A., Javaloyes, J., Caballero, J. A., Grossmann, I. E.*, Strategies for the robust simulation of thermally coupled distillation sequences, *Comput. Chem. Eng.* **36** (2012) 149.
doi: <https://doi.org/10.1016/j.compchemeng.2011.06.014>
4. *Sangal, V., Kumar, V., Mishra, M.*, Optimization of a divided wall column for the separation of C4-C6 normal paraffin mixture using Box-Behnken design, *Chem. Ind. Chem. Eng. Q.* **19** (2012) 47.
doi: <https://doi.org/10.2298/CICEQ121019047S>
5. *Asprion, N., Kaibel, G.*, Dividing wall columns: Fundamentals and recent advances, *Chem. Eng. Process.* **49** (2010) 139.
doi: <https://doi.org/10.1016/j.cep.2010.01.013>
6. *Dejanovic, I., Matijasevic, L., Olujić, Z.*, Dividing wall column – A breakthrough towards sustainable distilling, *Chem. Eng. Process.* **49** (2010) 559.
doi: <https://doi.org/10.1016/j.cep.2010.04.001>
7. *Dunneber, G., Pantelides, C. C.*, Optimal design of thermally coupled distillation columns, *Ind. Eng. Chem. Res.* **38** (1999) 162.
doi: <https://doi.org/10.1021/ie9802919>
8. *Premkumar, R., Rangaiah, G. P.*, Retrofitting conventional column systems to dividing-wall columns, *Chem. Eng. Res. Des.* **87** (2009) 47.
doi: <https://doi.org/10.1016/j.cherd.2008.06.013>
9. *Pattison, R. C., Gupta, A. M., Baldea, M.*, Equation-oriented optimization of process flowsheets with dividing-wall columns, *AIChE J.* **62** (2016) 704.
doi: <https://doi.org/10.1002/aic.15060>
10. *Yang, A., Sun, S., Eslamimanesh, A., Wei, S., Shen, W.*, Energy-saving investigation for diethyl carbonate synthesis through the reactive dividing wall column combining the vapor recompression heat pump or different pressure thermally coupled technique, *Energy* **172** (2019) 320.
doi: <https://doi.org/10.1016/j.energy.2019.01.126>
11. *Yang, A., Su, Y., Shen, W., Chien, I.-L., Ren, J.*, Multi-objective optimization of organic Rankine cycle system for the waste heat recovery in the heat pump assisted reactive dividing wall column, *Energ. Convers. Manage.* **199** (2019) 112041.
doi: <https://doi.org/10.1016/j.enconman.2019.112041>
12. *Yang, A., Saimeng, J., Weifeng, S., Peizhe, C., Chien, I.-L., Ren, J.*, Investigation of energy-saving azeotropic dividing wall column to achieve cleaner production via heat exchanger network and heat pump technique, *J. Clean. Prod.* **234** (2019) 410.
doi: <https://doi.org/10.1016/j.jclepro.2019.06.224>
13. *Rahimi, R., Soodmand, M. H., Zivdar, M., Alborzi, A., Rahmanian, M.*, Modeling and simulation of a divided wall column for 1,3 butadiene purification, *Iran. J. Chem. Eng.* **12** (2015) 60.
14. *Ammunudin, K. A., Smith, R., Thong, D. Y.-C., Towler, G. P.*, Design and optimization of fully thermally coupled distillation columns part 1: Preliminary design and optimization methodology, *Chem. Eng. Res. Des.* **79** (2001) 701.
doi: <https://doi.org/10.1205/026387601753192028>
15. *Seider, W. D., Lewin, D. R., Seader, J. D., Widagdo, S., Gani, R., Ng, K. M.*, *Product and Process Design Principles: Synthesis, Analysis and Evaluation*, Wiley, New York, 2017, 4th ed, p. 164–165, 257.
16. *Ammunudin, K. A., Smith, R.*, Design and optimization of fully thermally coupled distillation columns Part 2: Application of dividing wall columns in retrofit, *Chem. Eng. Res. Des.* **79** (2001) 716.
doi: <https://doi.org/10.1205/026387601753192037>
17. *Becker, H., Godorr, S., Kreis, H., Vaughan, J.*, Partitioned distillation columns-why, when and how, *Chem. Eng.* **108** (2001) 68.
18. *Dejanović, I., Matijašević, Lj., Olujić, Z.*, Dividing wall column – A breakthrough towards sustainable distilling, *Chem. Eng. Process.* **49** (2010) 559.
doi: <https://doi.org/10.1016/j.cep.2010.04.001>
19. *Kiss, A. A.*, *Advanced Distillation Technologies: Design, Control and Applications*, John Wiley & Sons, New York, 2013. 1st ed., pp 67–110.
20. *Soares, R. P., Secchi, A. R.*, EMSO: A New environment for modelling, simulation and optimisation, *Comp. Aided Chem. Eng.* **14** (2003) 947.
doi: [https://doi.org/10.1016/S1570-7946\(03\)80239-0](https://doi.org/10.1016/S1570-7946(03)80239-0)
21. *Rodrigues, R., Soares, R. P., Secchi, A. R.*, Teaching chemical reaction engineering using EMSO simulator, *Comp. App. Eng. Educ.* **18** (2010) 607.
doi: <https://doi.org/10.1002/cae.20255>
22. *Henrique, J. P., Sousa Jr., R., Secchi, A. R., Ravagnani, M. A. S. S., Costa, C. B. B.*, Optimization of chemical engineering problems with EMSO software, *Comput. Appl. Eng. Educ.* **26** (2018) 141.
doi: <https://doi.org/10.1002/cae.21867>

23. Ribeiro, L. D., Secchi, A. R., Biscaya, E. C., A new technique of model order reduction based on weighted residuals in discrete domain, *Comp. Aided Chem. Eng.* **28** (2010) 1639.
24. Furlan, F. F., Lino, A. R. A., Matugi, K. A., Cruz, J. G., Secchi, A. R., Giordano, R. C., A simple approach to improve the robustness of equation-oriented simulators: Multilinear look-up table interpolators, *Comput. Chem. Eng.* **86** (2016) 1.
doi: <https://doi.org/10.1016/j.compchemeng.2015.12.014>
25. Ospino, J., Sánchez, M. E., Secchi, A. R., Implementation of a block-oriented model library for undergraduate process control courses in EMSO simulator, *Educ. Chem. Eng.* **18** (2017) 45.
doi: <https://doi.org/10.1016/j.ece.2016.08.002>
26. Seader, J. D., Henley, E. J., Roper, D. K., *Separation Process Principles – Chemical and Biochemical Operations*, Wiley, New York, 2011. 3rd ed., pp 378–412.
27. Rangaiah, G. P., Yue, C. T., Hidajat, K., Optimization of complex distillation columns, *Chem. Eng.* **113** (2006) 60.
28. Bek-Pedersen, E., Gani, R., Design and synthesis of distillation systems using a driving-force-based approach, *Chem. Eng. Process.* **43** (2004) 251.
doi: [https://doi.org/10.1016/S0255-2701\(03\)00120-X](https://doi.org/10.1016/S0255-2701(03)00120-X)
29. Aurangzeb, M., Jana, A. K., Dividing wall column: Improving thermal efficiency, energy savings and economic performance, *Appl. Therm. Eng.* **106** (2016) 1033.
doi: <https://doi.org/10.1016/j.applthermaleng.2016.06.079>