# Integrated Model Switching and Initialization Procedure for Distillation Columns in Equation-Oriented Simulator EMSO

Breno Henrique Ferreira Batista[a], Felipe Fernando Furlan[a*]

[a]*Chemical Engineering Department (DEQ), Federal University of São Carlos (UFSCar), São Carlos-SP, Brazil*
**furlan@ufscar.br*

## ABSTRACT

Distillation columns are fundamental for separation and purification in the chemical industry, but their simulation remains challenging due to high nonlinearity. Equation-oriented (EO) simulators, while powerful, are highly sensitive to initial guesses, often leading to convergence failure in Newton-type solvers. Although various initialization methods exist, their integrated implementation and the systematic transition to rigorous models within EO environments are poorly documented in the literature. This study proposes an initialization procedure based on linear interpolation of top and bottom conditions, integrated into the EMSO simulator via a 'model switching' framework. The method was validated using an industrial ethanol purification system consisting of two columns with sidestreams. Results indicate that a sequential transition from simplified to rigorous models is critical for stability, as it provides the necessary proximity to the solution for the solver. The proposed methodology enabled the convergence of the rigorous model in cases where standard initialization failed, highlighting its effectiveness for complex process modeling.

**Keywords**: Initialization procedure; Distillation column simulation, MESH model; Hydrous ethanol distillation; Equation-oriented simulators

## 1. Background

Distillation columns play an important role in chemical industry in the feed preparation, product separation and purification and raw material recycling. Due to their complex operation and high energy demand, their design, optimization and control are essential steps to improve process profitability in scenarios with both feedstock composition and market prices changes (Ebrahimpour, 2015). The success of these steps depends on model accuracy, convergence and speed properties (Ivakpour, Kasiri, 2014). To achieve this, MESH models (Material balances, Equilibrium, Summation and Heat balances) are often used for their high accuracy.

Nevertheless, distillation column models are highly nonlinear and interconnected, placing a difficult task for process simulators to find a solution. This is particularly true for equation-oriented ones, which uses general Newton-type locally convergent methods for solving the system of equations. These methods can fail to find the solution if the initial guess is far from the solution, being one of the main drawbacks of equation-oriented technology (Pantelides et al, 2015).

There are several methods for properly initializing the variables in such complex models in order to improve convergence and speed. Traditional methods include the use of linear initial profiles, Inside-Out algorithm, Kremser's group method, Infinite reflux, model initialization procedures, among others (Ivakpour, Kasiri, 2015, Farkas e Rév, 2011, Fletcher, Morton, 2000, Pantelides et al., 2015). These methods consist in solving a simplified version of the rigorous model in order to provide initial guesses for the variables. However, the literature rarely addresses the transition between these simplified methods and the full MESH equations within a single EO simulation environment. While the theoretical foundations of these methods are known, a practical framework for 'model switching', where the simulator automatically moves from an initialization stage to a rigorous one, has not been extensively detailed. This creates a bottleneck in process modeling, as the lack of robust, integrated initialization procedures continues to be a primary cause of convergence failure in Newton-type solvers.

In this context, the present study developed and analysed an initialization procedure based on linear interpolations of top and bottom conditions of distillation columns in order to improve its convergence. The procedure was implemented in the equation oriented simulator EMSO as a single model, in which the user switchs between the simplified equations and the rigorous one in order to achieve convergence, as the former acts as an initialization for the latter. The method was applied to the case study of ethanol purification on a

sugarcane mill, composed of two distillation towers with sidestreams, considering as feed an ethanol-water mixture.

## 2. Methods

### *2.1. Software*

The distillation column and the initialization procedures were modeled and simulated in EMSO (Environment for Modeling, Simulation and Optimization, v 0.10.11). The thermodynamic properties of the components and mixtures were calculated by the VRTherm plugin. Liquid phase fugacity was described by NRTL model and gas phase was considered ideal.

### *2.2. Distillation column model*

Distillation column models included total condensers, reboilers and the column stages section. In order to implement the initialization procedure inside the stages section model, the molar balance, energy balance and equilibrium equations had to be rewriten as show in equations (1) to (3), respectively.

$$F_j z_{i,j} + V_{j+1} y_{i,j+1} + L_{j-1} x_{i,j-1} - V_j y_{i,j} - L_j x_{i,j} = G1_{i,j}, i = 1 - m, j = 1 - n \quad (1)$$

$$F_j H_j^F + V_{j+1} H_{j+1}^V + L_{j-1} H_{j-1}^L - V_j H_j^V - L_j H_j^L = G2_j, j = 1 - n \quad (2)$$

$$y_i - K_i x_i = G3_{i,j} \quad (3)$$

In these equations, F, V and L represent the molar flow rates of the feed, vapor and liquid streams, respectively. Z, x and y represent the molar fractions of lhe feed, liquid and vapour streams, respectively. H represents the enthalpy of the streams. K represents the equilibrium constant. I and j represent the component and stage indexes, respectively. Each equation was rewritten in order to include a residual variable: G1 for the molar balance, G2 for the energy balance and G3 for the equilibrium equation. Total condenser and reboiler were implemented directly, without an initialization procedure.

### *2.3. Initialization procedure*

Residual equations allowed the use of simplified equations to initialize the molar flows, compositions and temperature of vapor and liquid streams of each plate. Although resulting in non-zero residuals, the procedure brings the model variables closer to the final solution than the standard initial values provided by the simulator, improving both convergence and simulation speed.

The initialization procedure was based on user-supplied initial guesses for top and bottom compositions, as well as usual column specifications. Top and bottom temperatures were estimated by bubble point calculation. With composition and temperature estimates for top and bottom, linear equations were used to calculate plate temperature and compositions (Eq. 4-6).

$$x_{i,j} = x_i^{Top} + \left( x_i^{Bottom} - x_i^{Top} \right) \frac{j}{n_{plates}}, i = 1,2, ..., m, j = 1,2,.., n \quad (4)$$

$$y_{i,j} = y_i^{Top} + \left( y_i^{Bottom} - y_i^{Top} \right) \frac{j}{n_{plates}}, i = 1,2, ..., m, j = 1,2,.., n \quad (5)$$

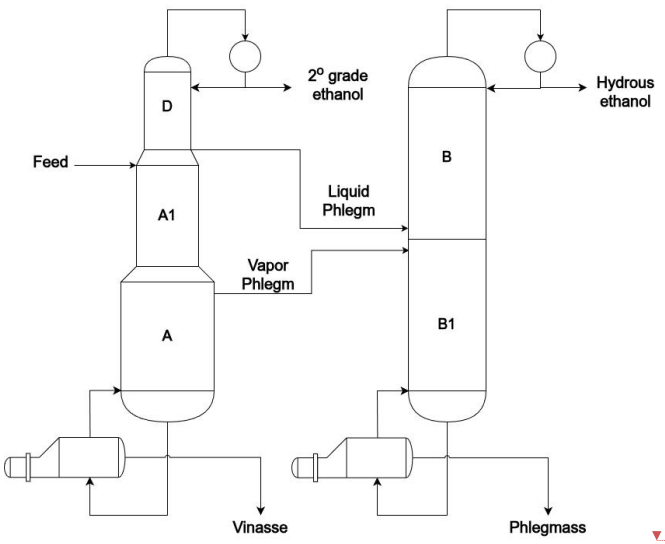
$$T_j = T^{Top} + \left( T^{Bottom} - T^{Top} \right) \frac{j}{n_{plates}} j = 1,2,.., n \quad (6)$$

Once the initialization model converged, Equations 4-6 were replaced, by the specification that the residual variables were equal to zero, using EMSO's switch parameter. Through this switch, initial and rigorous models could be alternated. When more than one column is present, the procedure consisted in simulating all columns in the initialization model, than changing each column to the rigorous one, sequentially. At each change, a new initial guess is generated and used in the subsequent simulation.

*2.4. Case study*

The case study consisted of the sequence of distillation columns used for ethanol purification in a sugarcane mill. In this sequence (Figure 1), a mixture of etanol (7,3% m/m) and water is fed, at a molar flowrate of 20203.5 kmol/h, to the first column sequence consisting of columns A, A1 and D (30 stages). This sequence yields two streams, a liquid stream leaving the bottom of column D and a vapour stream leaving the top of column A. These two streams are fed to the second sequence (columns B and B1) at stages 20 and 21, respectively. Columns A, A1 and D were simulated as a single column section (named column AA1D), with total condenser and reboiler. Columns B and B1 were simulated as separated columns with 20 and 21 stages, respectively. The former contains a total condenser and no reboiler, the latter a reboiler and no condenser. Columns AA1D reflux ratio was set at 99 and heat duty at the reboiler of column B1 at 7086 kW. Previous information, as well as pressure profiles were based on the information reported by Dias (2008).

*Figure 1: Simplified diagram of the industrial distillation system configuration for hydrous ethanol purification, adapted from Dias (2008).*




Deleted[felipe]: To explore different aspects of optimization, the system explores two different objective functions: maximize the titer (final product concentration) and maximize the productivity (titer divided by the total culture time).

## *3.* Results

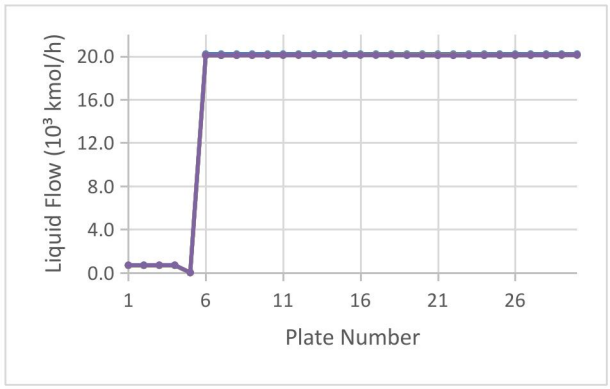
Model initialization was based on estimates of composition in specific sections of the column. Ethanol mole fractions used as initial guess for the three columns are shown in Table 1.

Table 1: Top and bottom ethanol molar fraction used for the initialization of columns AA1D, B and B1.

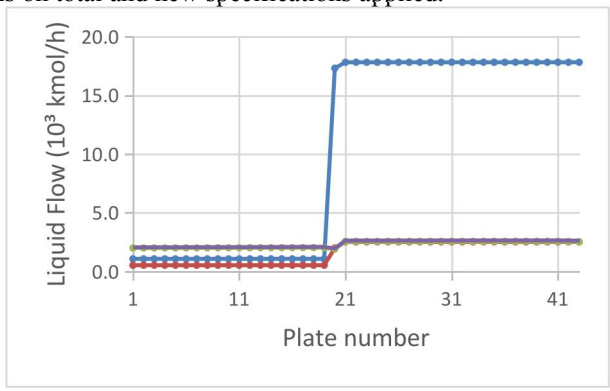
| | Column AA1D | Column B | Column B1 |
|---|---|---|---|
| Top | 0.81 | 0.84 | 0.14 |
| Bottom | 0.00007 | 0.16 | 0.03 |

The initialization procedure consisted in simulating all columns using the simplified equations. After that, rigorous calculation of column AA1D was applied and finally all three columns were simulated in the rigorous mode. In each step, the previous conveged values were used to initialize the next one. On a final step, two process specifications (column AA1D distillate molar flow rate, of 6.7 kmol/h, and column B distillate flow rate, of 630 kmol/h) were exchanged by two project ones: ethanol molar fraction at the bottom of column AA1D, equal to 0.00007, and at the top of column B, equal to 0.846. Figure 2 shows liquid and vapor molar flows and stage temperatures while Figure 3 shows stage liquid and vapor compositions in each column. Data from columns B and B1 were condensed in single figures, with column B1 starting at stage 21.

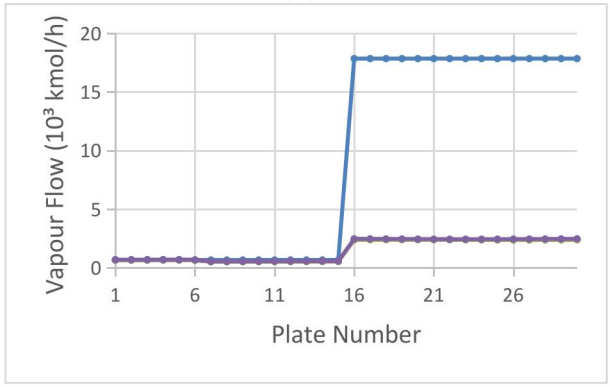
Figure 2: Liquid and vapour molar flows and temperature profiles for columns AA1D and BB1: a) liquid flowrate of column AA1D, b) vapor flowrate of column AA1D, c) liquid flowrate of column BB1, d) vapor flowrate of column BB1, e) temperature of column AA1D, f) temperature of column BB1. The colors represent the initialization procedure stages: Blue - both columns on initial, red - column AA1D on total, column BB1 on initial, violet - both columns on total, green - both columns on total and new specifications applied.



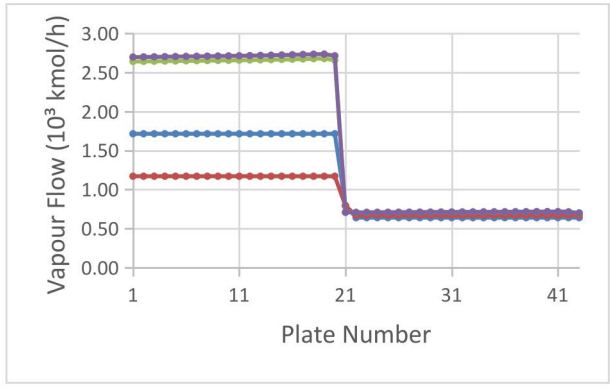

(a)



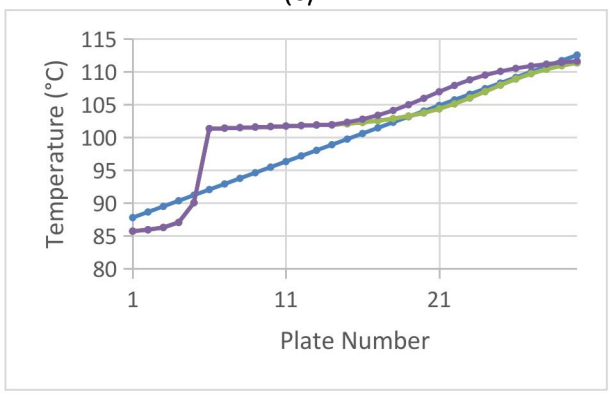

(b)



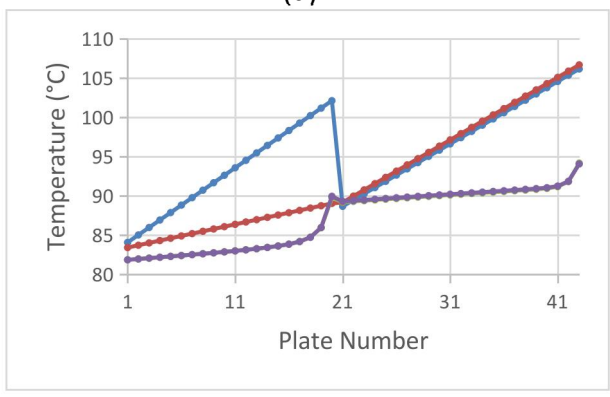

(c)




(d)



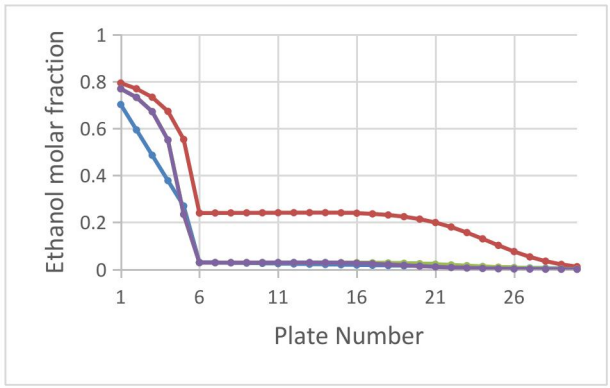

(e)



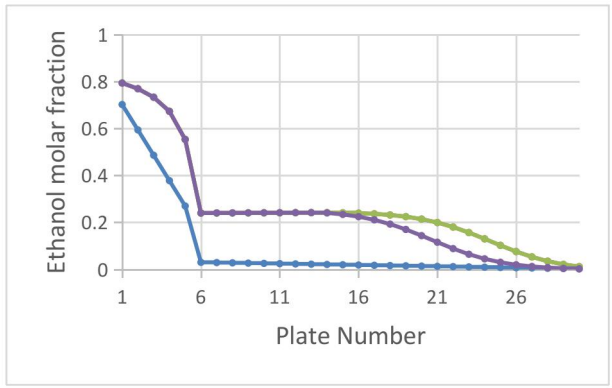

(f)

There is a great difference between initial guess and final value for the internal vapor flow in column AA1D at stages 15 to 30 (Figure 2c). This results from the specification that 76% of ethanol is recovered in the vapor phlegm stream, as considered in Dias (2008). Since the initial guess underestimates ethanol fraction in the vapor stream in initial guess (blue line in Figure 3b), this is compensated by a greater sidestream and, consequently a greater vapor stream in this section of the column. This flowrate difference also influences column B1 (Figure 2b), increasing liquid flow rate since most of the vapor phlegm condenses at its feed stage (20). Nevertheless, this difference in streams did not prevent the convergence of the rigorous simulation.

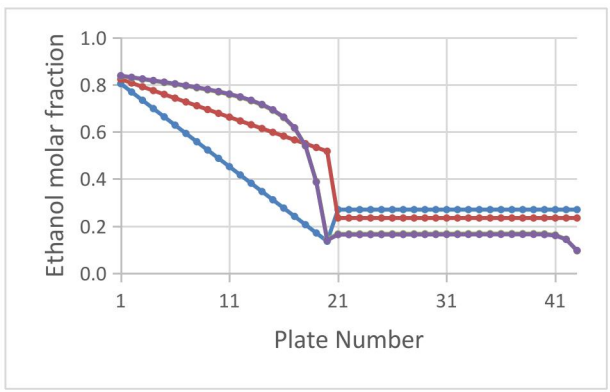
*Figure 3: Molar fraction of ethanol in liquid and vapor phases for columns AA1D and BB1: a) liquid phase of column AA1D, b) vapor phase of column AA1D, c) liquid phase of column BB1, d) vapor phase of column BB1. The colors represent the initialization procedure stages: Blue - both columns on initial, red - column AA1D on total, column BB1 on initial, violet - both columns on total, green - both columns on total and new specifications applied.*



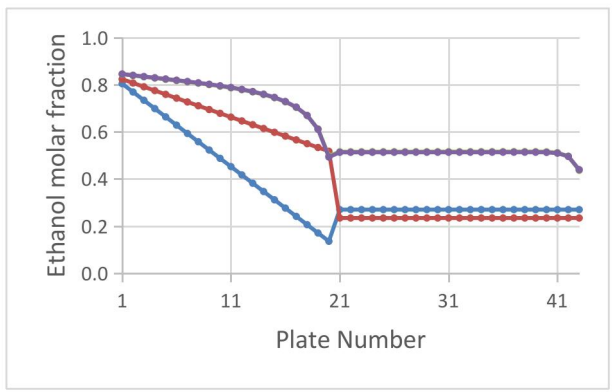

(a)




(b)




(c)




(d)

Figures 2f, 3c, and 3d highlight the critical role of the sequential transition from the initialization model to the rigorous formulation. These results demonstrate that the temperature profiles and ethanol mole fractions (liquid and vapor) in column BB1 closely approach their steady-state values only after column AA1D transitions to the rigorous model. This behavior confirms that the initialization of upstream units is essential to provide the necessary data to properly initialize the downstream model. Although substantial differences exist between the initial profiles and the final converged state, the initialization procedure remains indispensable, as the rigorous model otherwise fails to reach a solution.

## 4. Conclusion

This study presented an initialization procedure for distillation columns in equation-oriented simulators, addressing a critical gap regarding integrated model switching in the literature. By implementing linear profiles as a starting point within the EMSO environment, the inherent sensitivity of Newton-type solvers to initial guesses was successfully mitigated. The application to a hydrous ethanol distillation case study demonstrated that a sequential transition, moving each column from a simplified to a rigorous model, is vital for the convergence of interconnected units. Even when initial profiles differ significantly from final solutions, the procedure was successfull in enabling convergence. This framework proves to be a valuable tool for improving the reliability and speed of complex process simulations in equation-oriented technology.

**Acknowledgements**: This study was financed, in part, by the São Paulo Research Foundation (FAPESP), Brasil. Process Number #2024/05814-0

## References

Dias, M. O. S. Simulação do processo de produção de etanol a partir do açúcar e do bagaço, visando a integração do processo e a maximização da produção de energia e excedentes do bagaço. Master's dissertation, Campinas University, Campinas, 2008.

Ebrahimpour, M. Dynamic and Steady State Modeling of VRD Column in Equation-Oriented Environment. Master's dissertation, São Paulo University, São Paulo, 2015.

Farkas, C. I., Rév, E. Initial column profile with composition-dependente relative volatility. Chemical Engineering Research and Design, 89, 581-585, 2011.

Fletcher, R., Morton, W. Initialising distillation column models. Computers and Chemical Engineering, 23, 1811-1824, 2000.

Ivakpour, J., Kasiri, N. Developing a new initialization procedure for distillation column simulation. Journal of Petroleum Science and Technology, 4(1), 41-46, 2014.

Pantelides, C. C., Nauta, M., Matzopoulos, M. Equation-oriented process modelling technology: recent advances & current perspectives. In: 5th Annual TRC - Idemitsu Workshop, Abu Dhabi, February 2015.

Soares, R. P., & Secchi, A. R. EMSO: A new environment for modelling, simulation and optimisation. Computer Aided Chemical Engineering, 14, 947–952, 2003.