Modelling and Initialisation of a Distillation Column for the Separation of Binary Systems

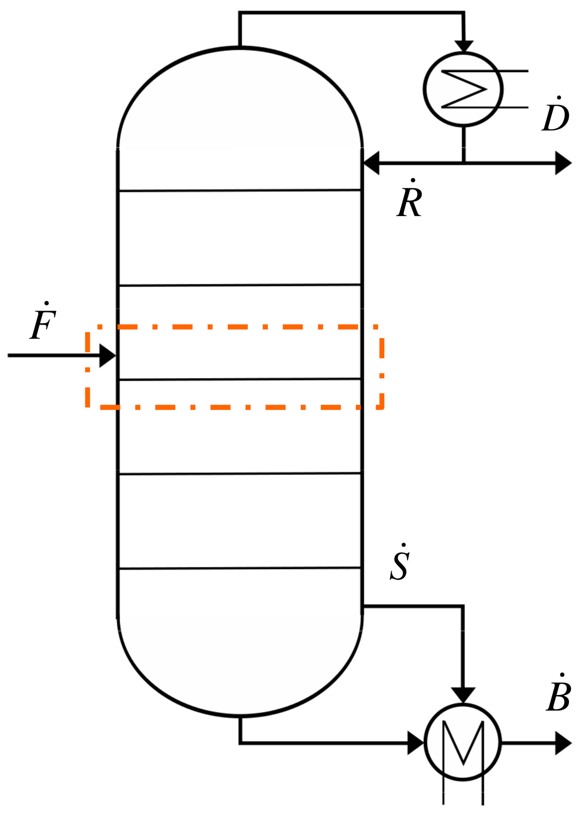
www.thvt.at

Simone Christa, Orestis Almpanis-Lekkas, Walter Wukovits

Institute of Chemical Engineering, Vienna University of Technology, Vienna, Austria Contact: s.christa@gmx.net

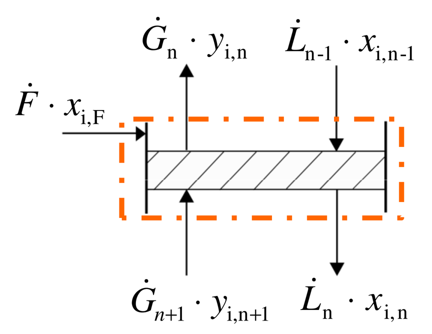
Introduction

Distillation is an important separation process used in different industrial fields. Increasing requirements on yields, product purity and economical feasibility require efficient models to analyse and predict system performances without time consuming and complex investigations on real processes. The target of this work is to develop a mathematical model of a distillation column for binary systems. Due to the flexibility in the programming structure and the flowsheeting capability the implementation of this model took place within the environment of the gPROMS ModelBuilder.



Model Assumptions

- steady state: no material or energy accumulation on the trays
- no reaction terms
- consideration of ideal trays:
  - perfect mixing of the vapour and liquid phase
  - thermal equilibrium for every component on each tray
- no heat loss



Equation	Description
$\varphi_i \cdot y_i \cdot p = \gamma_i \cdot x_i \cdot p_{0,i}$	Equilibrium
$\dot{F} \cdot x_{i,F} + \dot{G}_{n+1} \cdot y_{i,n+1} + \dot{L}_{n-1} \cdot x_{i,n-1} = \dot{G}_n \cdot y_{i,n} + \dot{L}_n \cdot x_{i,n}$	Component mass balance
$\sum_{i=1}^{nc} x_{i,n} = 1 , \sum_{i=1}^{nc} y_{i,n} = 1$	Summation condition
$\dot{F} \cdot h_F + \dot{G}_{n+1} \cdot h^v_{n+1} + \dot{L}_{n-1} \cdot h^l_{n-1} = \dot{G}_n \cdot h^v_n + \dot{L}_n \cdot h^l_n$	Heat balance

Model Description

The steady state column model for the separation of binary mixtures is based on mass and energy balances. It is designed as an n-equilibrium stage model including a total condenser, a splitter and a reboiler. For the calculation of the equilibrium state in each stage, the thermodynamic properties (e.g. enthalpies, activities) of Multiflash are used. For the consideration of the deviation from ideal equilibrium state, the murphree efficiency and pressure drop can be defined.

Process Initialisation Procedure

The mass/energy balances and equilibrium conditions form a complex system of non-linear coupled equations. For the handling of this numerical challenge, an initialisation procedure is developed in regard to both, model robustness and flexibility in user defined specification. The following sequence of initialisation steps proved to be effective:

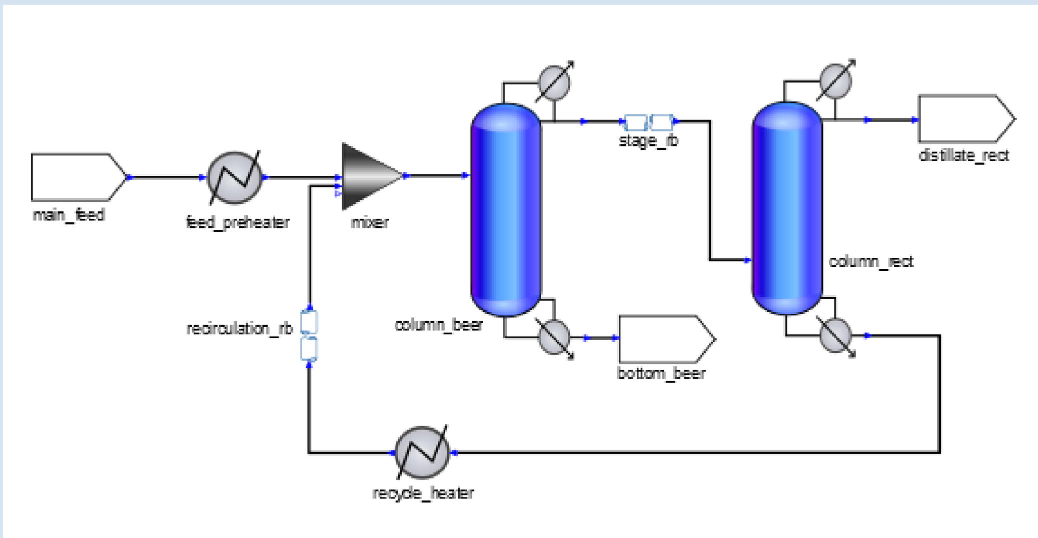
Initial state → Condenser equilibrium → Condenser enthalpy balance → Reboiler equilibrium → Stage equilibrium → Stage enthalpy balance → Reboiler enthalpy balance → Reflux ratio → Pressure drop → Murphree efficiency

Simulation Results

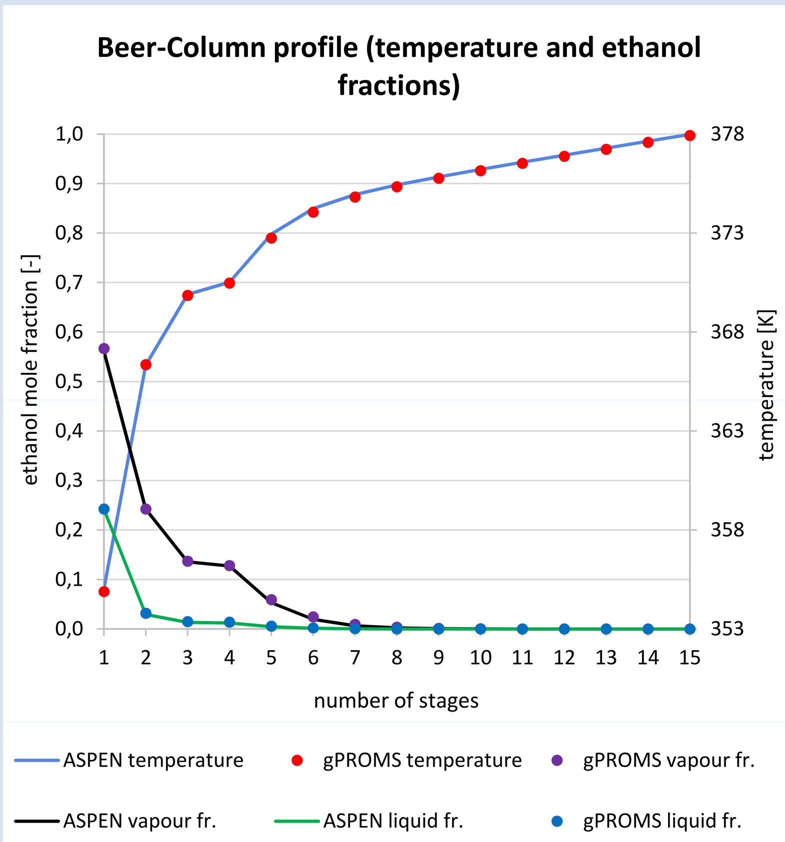
To validate the model, simulation results of two different binary systems are cross-referenced with Aspen Plus. The reboiler and condenser data are added as stages in the graphics.

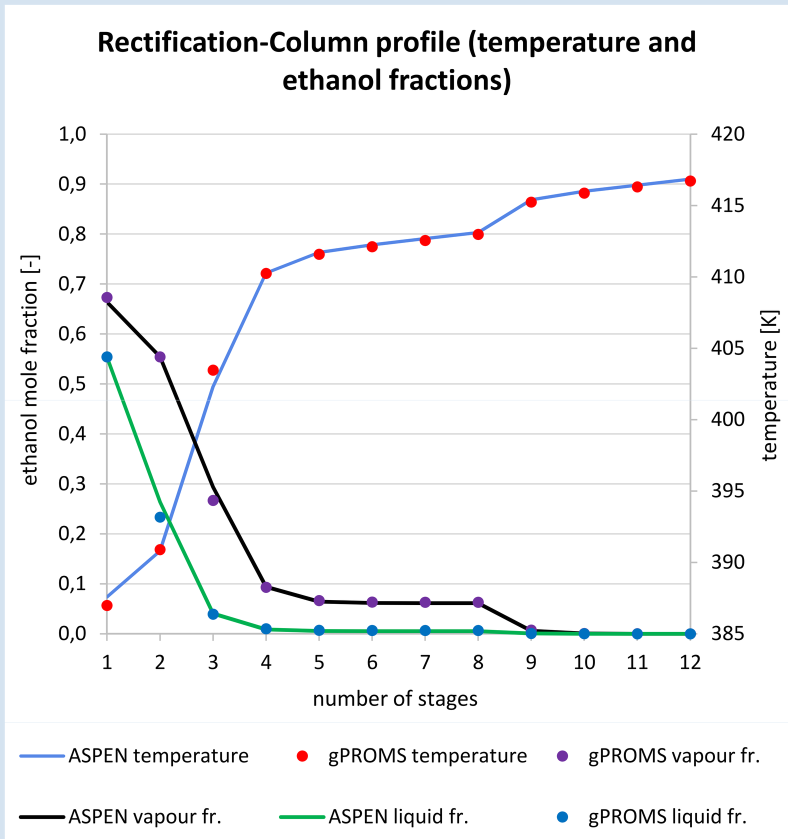
a) C_2H_5OH / H_2O mixture

Specifications		
Feed	Feedflow [kg/h]	89000
	Concentration ethanol in feed [wt %]	0.08
	Temperature feed [K]	308
	Pressure feed [mbar]	1000
Feed preheater	Temperature [K]	368
	Pressure [mbar]	2000
Mixer	Pressure [mbar]	2000
Recycle heater	Temperature [K]	308
	Pressure [mbar]	1000



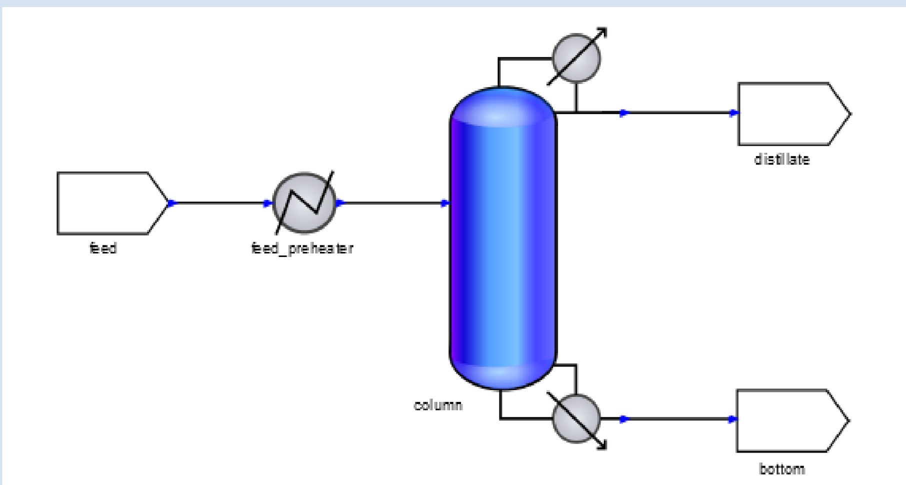
Column specifications	Number of trays [-]	Feed tray location [-]	Reflux ratio (mole based) [-]	Distillate rate [kg/h]	Condenser pressure [mbar]	Pressure drop [mbar]	Murphree efficiency [-]	Activity coefficient model
Beer-Column	13	3	1	19822	1000	200	1	NRTL
Rectification-Column	10	7	9	9360	3500	500	1	NRTL

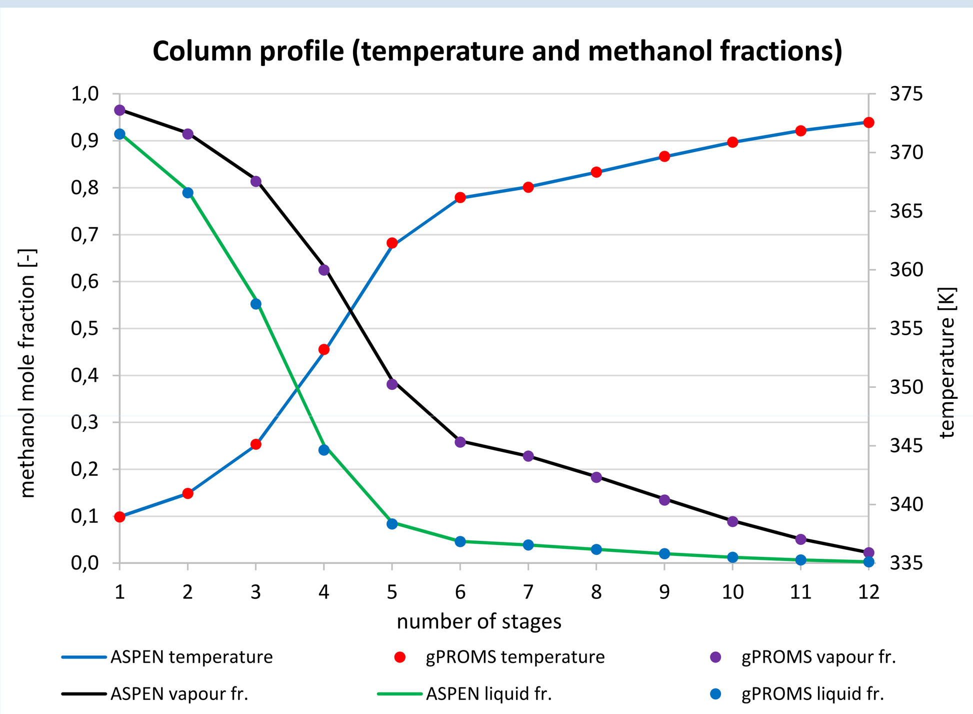




b) CH_3OH / H_2O mixture

Specifications		
Feed	Feedflow [kg/h]	10000
	Concentration methanol in feed [wt %]	0.05
	Temperature feed [K]	293
	Pressure feed [mbar]	1013
Feed preheater	Temperature [K]	313
	Pressure [mbar]	1013





Column specifications	
Number of trays [-]	10
Feed tray location [-]	6
Reflux ratio (mole based) [-]	4.36
Distillate rate [kg/h]	473
Pressure drop [mbar]	0
Activity coefficient model	NRTL

Conclusion & Outlook

- Good accordance between the simulation results of gPROMS and ASPENplus
- The initialisation procedure is robust for different user defined specifications
- Further validation of different binary systems

References

A. Friedl, lecture notes for "Thermische Verfahrenstechnik 1": course 159.731, version 3, Vienna University of Technology, 2000.

R.H. Perry, D.W. Green & J.O. Maloney, Perry's Chemical Engineers' Handbook: 7th ed., New York: VCH, 1997.

K. Sattler, Thermische Trennverfahren: Grundlagen, Auslegung, Apparate, Cambridge: VCH Verlagsgesellschaft mbH, 1988.

A. Schönbucher, Thermische Verfahrenstechnik: Grundlagen und Berechnungsmethoden für Ausrüstungen und Prozesse. Berlin: Springer, 2002.

Advanced Process Modelling Forum 2014 – London, United Kingdom, 2 – 3 April 2014