Distillation process shortcut modeling based on vapour-liquid equilibria (VLE) fitting

Csaba Dezső ANDRÁS[1], László MÁTYÁS[2],
Rozália Veronika SALAMON[1], Éva MOLNOS[1], Alexandru SZÉP[1]

Sapientia Hungarian University of Transylvania

Faculty of Economics Socio-Human Sciences and Engineering, Miercurea Ciuc, Romania

[1]Department of Food Sciences, [2]Department of Bioengineering

6th International Conference on Biosystems and Food Engineering

INTRODUCTION

The distillation is one of most important concentration method of multicomponent liquid mixtures. In food industry for obtaining alcoholic beverages with high alcoholic concentrations different variants are chosen, as follows: repeated simple batch distillation for traditional spirits (kisüsti pálinka, whisk(e)y, cognac, rum), continuous multiple column rectification for vodka, and batch rectification are used to produce modern fruit spirits. For design of the distillation process and columns the VLE data are mandatory. When a mixtures are near ideal, the VLE curves are well described by constant relative volatility models. The water-ethanol equilibria (regarded for distillation in the food industry) is complicated, as the mixture is azeotropic, with inflexion point, with broad change of relative volatility range (figure 1.). An intresting coincidence is, that this highly non-ideal mixture was included on first study on column design based on engineering method, by Warren Kendall Lewis (figure 2.).
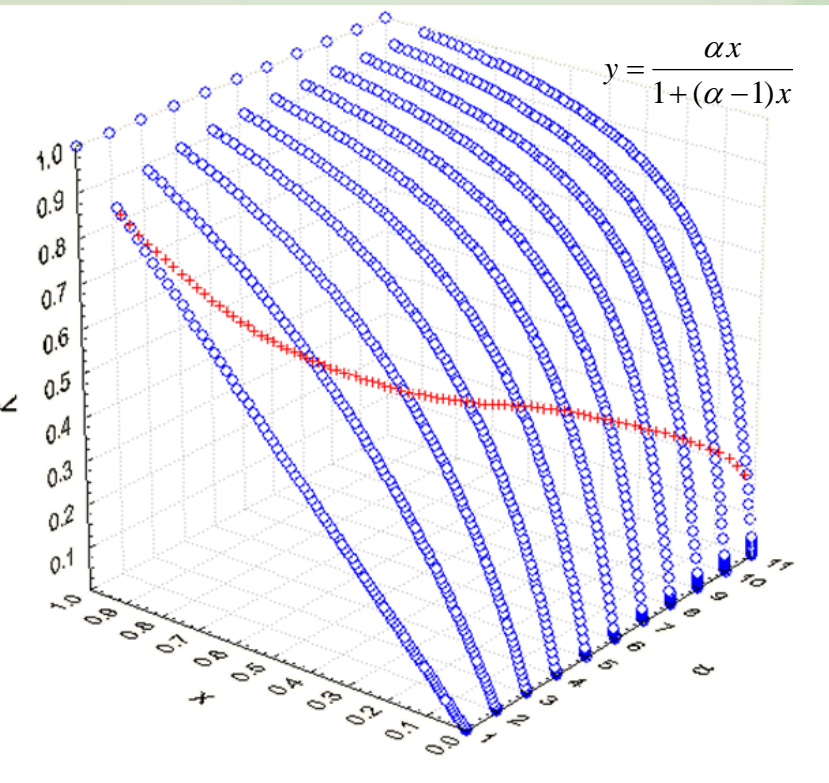

Figure 1. VLE and relative volatility of ethanol-water solution
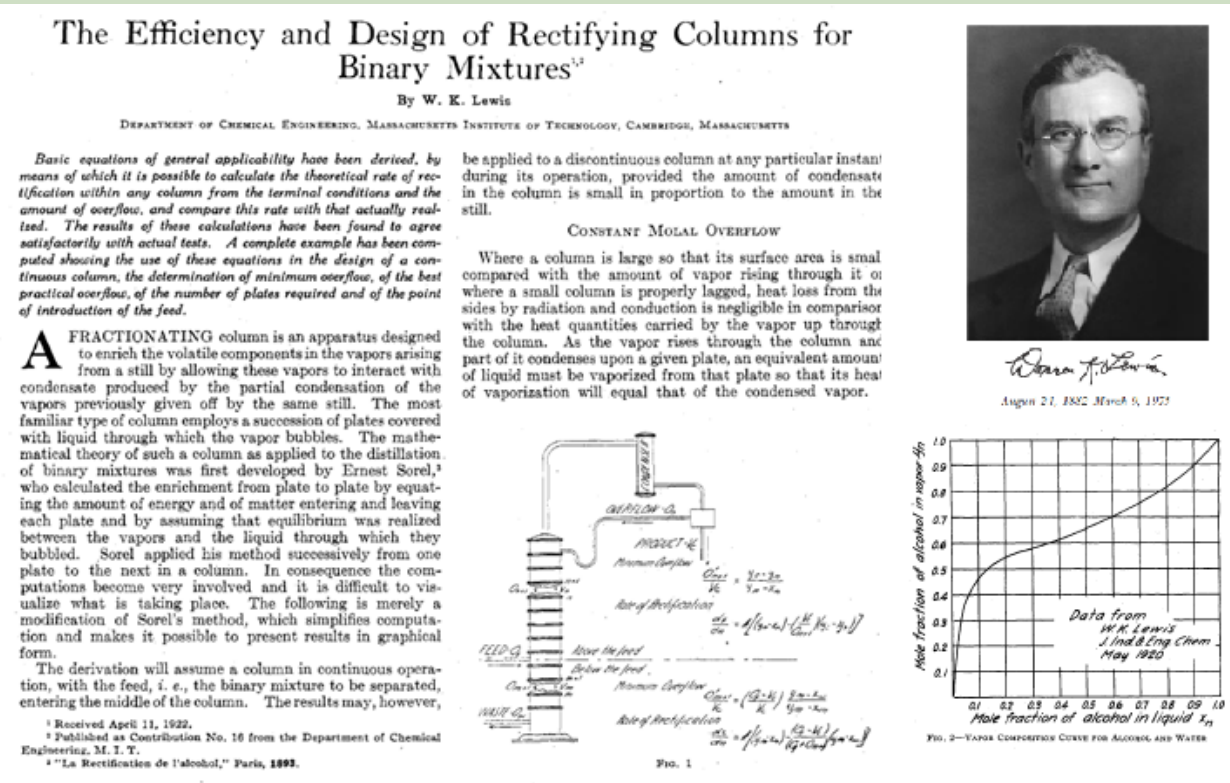

Figure 2. The historical article from 1922 of Warren Kendall Lewis on distillation column design

The most popular, straitforward and efficient graphical design method for tray number estimation is the classical McCabe-Thiele method, developed exactly 100 years ago, based directly on Lewis's method. During decades, has been used widely even for educational purposes in formation of chemical engineers. One of their disadvantages is the difficulty of steps drawing at low reflux ratios, due by closeness of the equilibrium curve and the operation lines. The computer-based variant based on discrete equilibrium data could be complicated and quite inaccurate due to the interpolation constraint. Accurate thermodynamic data (especially VLE) are indispensable for an precise design.

Warren Lee McCabe

The second idea (inspired by Doherty-Malone correction) was to fit firstly a function on relative volatility data, as their behavior is monotonic, with hyperbolic shape, without inflection point. Only after preliminary operation, the VLE function will be determined, as shown on figure 4.

$$y - x = \frac{\alpha x}{1+(\alpha-1)x} - x = \frac{(\alpha-1)x(1-x)}{1+(\alpha-1)x}$$

$$\alpha = 1 + \frac{(x_{az}-x)}{ax^2+bx+c}$$

$$\Rightarrow y = x + \frac{x(1-x)(x_{az}-x)}{ax^2+(b-1)x+(c+x_{az})}$$

Figure. 4. The indirect fitting of VLE curve, using an adequate fitting function for relative volatility

Using Lewis's method, the numerical (or even analytical) determination of the minimal destillation tray number (N_{min}) at total reflux became possible (figure 5.).

$$N_{min} = \int_{x_W}^{x_D} \frac{dx}{y^*-x}$$

Figure 5. Minimal tray number (N_{min}) at different waste (X_W) and distillate (X_D) composition

OBJECTIVES

The research has the objective to obtain continuous fitting functions, usable in computerized McCabe-Thiele method. We focused on ethanol-water VLE, as the main mixture in food industry-related distillations as well as due by the challenging nature of their VLE behavior.

MATERIALS AND METHODS

As the study is basically mathematical modelling, only softwares, Excel (Microsoft, Inc.) and Statistica 8.0 (Statsoft, Inc.) were used.

RESULTS AND DISCUSSIONS

First result was a fitting function with a 5th degree polynomial in denominator, with higher accuracy, than the Doherty-Malone fitting, but it was not really esthetic, nor generally applicable for VLE of other mixtures (figure 3.).
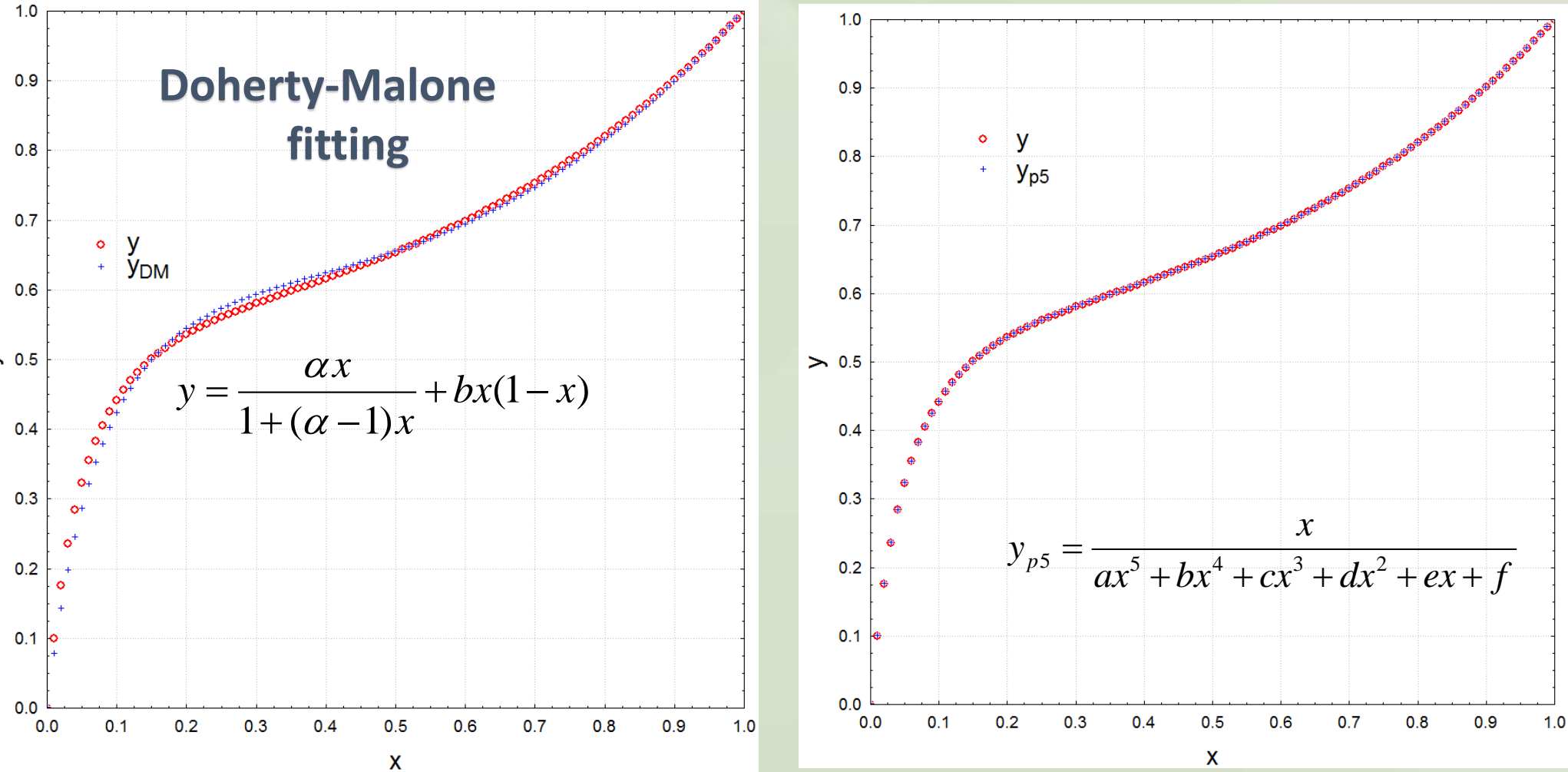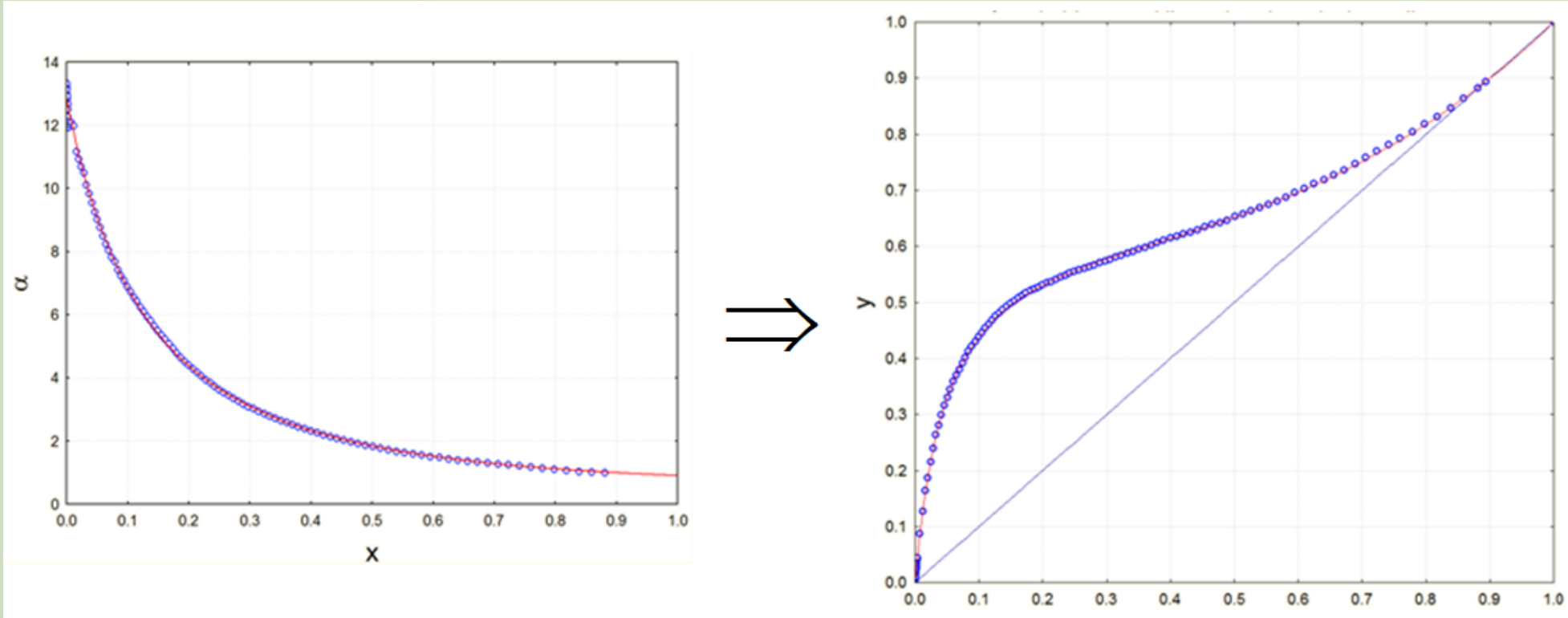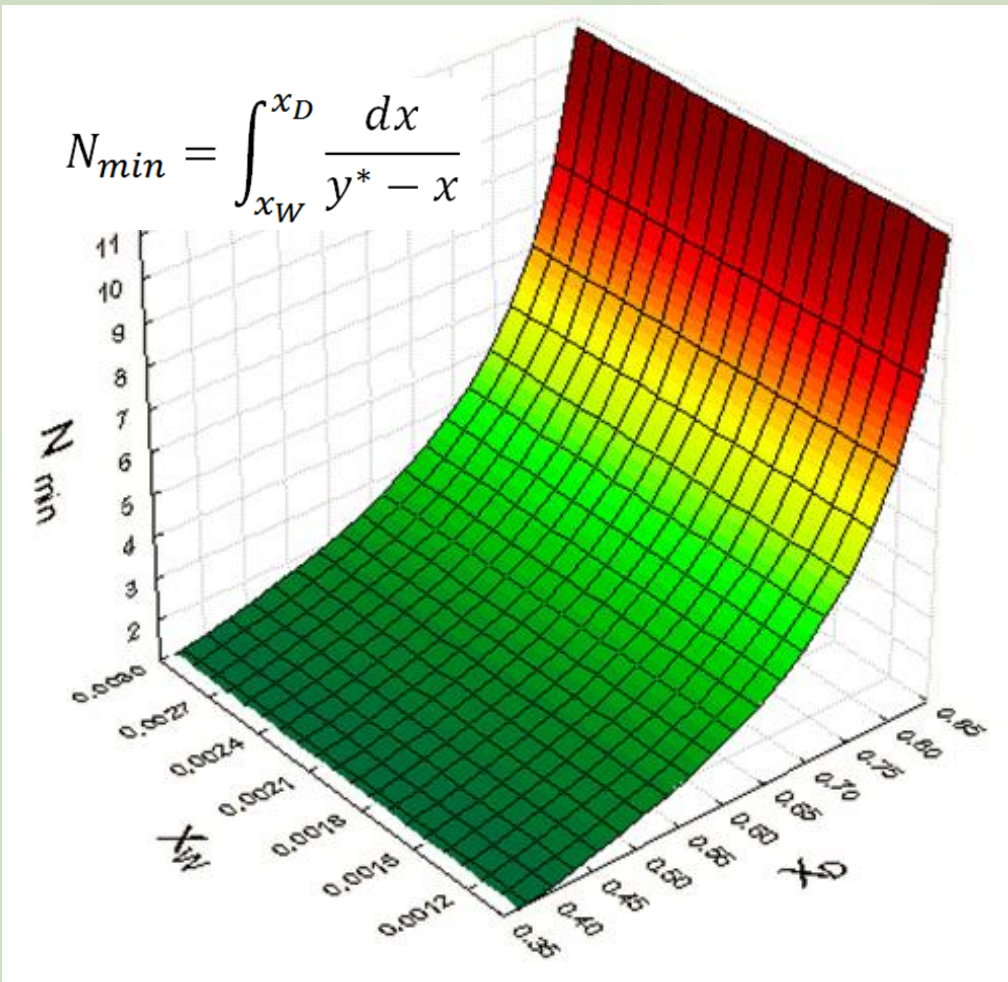
CONCLUSIONS

➤ The main advantage of the new method is, that make possible the concomitant determination of the number of stages N and the corresponding reflux ratio R, that is it extremely useful for simplifying the column design, furthermore, would be useful for both pedagogical and modeling purposes.
➤ The developed function is generally applicable on binary azeotropic mixtures, with or without inflexion point.
➤ In food industry, is very important the exact knowledge of distillation column behavior, to obtaining high quality distillate, mainly fruit spirits.

REFERENCES

András, C.D., Molnos, É., Mátyás, L., Szép, A.: New fitting method for Vapour-Liquid Equilibrium data and its application for ethanol-water distillation process modeling, *Revista de Chimie*, 71(7), 114-158 (2020).

Altay, Ö et al.: Principles of distillation process, In: Jafari, S.M., Malekjani, N. (eds.): Mass Transfer Operations in Food Processing, 45-81, Elsevier-Woodhead Publishing, London (2025).

Mathias, P. M: Visualizing the McCabe-Thiele diagram. Chemical Engineering Progress, 105(12), 36-44, (2009).

Lewis, W.K.: The efficiency and design of rectifying columns for binary mixtures, *Industrial & Engineering Chemistry*, 14(6), 492-496, (1922).

McCabe, W.L., Thiele, E.W.: Graphical design of fractionating columns. *Industrial & Engineering Chemistry*, 17(6), 605-611, (1925).

Seader, J.D., Henley, E.J., Roper, K.D.: Separation Process Principles with Applications using Process Simulators, 4th ed., John Wiley & Sons, Hoboken (2015).

Kong, L., Maravelias, C.T.: From graphical to model-based distillation column design: A McCabe-Thiele-inspired mathematical programming approach. *AIChE Journal*, 65(11), e16731(2019).

Doherty, M.F., Malone, M.F.: Conceptual Design of Distillation Systems, McGraw-Hill, Boston (2001).

Sorensen, E.: Principles of binary distillation. In: Gorák, A., Sorensen, E. (eds.): Distillation: Fundamentals and Principles, 145-185, Elsevier Academic Press, Amsterdam (2014).

Doherty-Malone fitting

$$y = \frac{\alpha x}{1+(\alpha-1)x} + bx(1-x)$$

$$y_{p5} = \frac{x}{ax^5+bx^4+cx^3+dx^2+ex+f}$$

Figure. 3. First attempt for function fitting on ethanol-water VLE