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Python-based Demonstration for Designing Distillation Columns for Ternary Mixtures

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Python based demonstration for designing distillation columns for ternary mixtures

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Abstract

Chemical engineering undergraduates typically use process simulation software like Aspen Plus or DWSIM to design distillation columns in their capstone design course or in the Separations course. Such software are black boxes and students often are left wondering why certain parameter choices they made resulted in a functioning column, while others did not. We have built a Python code base and Jupyter notebook based demonstrations that will help students understand the fundamentals of ternary (and higher-order) mixture distillation. These notebooks will help students understand under what conditions a column for ternary mixture separation becomes feasible. We have included notebooks that describe the factors that affect extractive distillation performed using a double feed column to separate azeotropic mixtures.

Introduction

Distillation of binary mixtures is standard fare in all chemical engineering programs. Students are introduced to the McCabe Thiele graphical method to design a column in the separations course and are likely to participate in a distillation experimental module in their unit operations / mass transfer lab course. Several interactive Mathematica / Jupyter notebooks can be found online which help students understand the McCabe Thiele graphical method to design distillation columns. Students can use sliders to adjust factors like reflux ratio, feed quality etc and visually observe how this affects the number of stages required for the separation. Such interactive demonstrations allow students to learn at their own pace and allow them to build a deeper understanding of the course material.

To the best of our knowledge we have not found any such demonstrations for ternary (or higher-order) mixtures. Separations involving ternary mixtures are quite common in the industry. In the late eighties and early nineties Doherty and co-workers published a series of papers[1,2,3] where they presented a framework to systematically design distillation columns for non-ideal multicomponent mixtures. In one such paper[4] they present several instructive examples. We have made interactive demonstrations of these as part of our work.

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The paper is structured as follows. First we describe the structure of our Python codebase and explain how new functionality can be added with little effort. Next we present a few concepts that might be useful to describe the examples in Doherty et al's papers which have been turned into Jupyter notebooks. Next we describe the notebooks that we have created. Finally we discuss some future work that we intend to do with this code-base.

Structure of the package

Our Python code-base has four main components and is available for download from Github. It contains code that (i) can estimate vapor-liquid equilibrium data for a c-component mixture based on Raoult's, Van Laar, Wilson and Margules activity coefficient models (ii) estimate saturated vapor pressure using Antoine's equation (iii) predict the rectifying and stripping profiles of a c-component mixture in a single feed distillation column and (iv) predict the rectifying, stripping and middle-section profiles of a c-component mixture in a double-feed distillation column.

VLE Behavior

In all examples we present in our notebooks the gas phase is treated as an ideal gas mixture and the liquid phase as a non-ideal mixture. The following relationship describes the vapor-liquid equilibrium behavior.

$$Py_i = P_i^{sat} \gamma_i x_i \quad \forall \quad i = 1, 2, 3 \ldots c \tag{1}$$

where y_i and x_i are mole fractions of component i in the vapor and liquid phase respectively. P is the pressure and P_i^{sat} is the saturation vapor pressure of component i and c gives the total number of components. γ_i is the activity coefficient. We have defined 4 different classes for (i) Raoult's (ii) Van Laar (iii) Margules and (iii) Wilson's activity coefficient models. All four are defined as child classes of the `VLEModelBaseClass` and therefore share the same structure. Users of our package can easily add other activity coefficient models like NRTL or UNIQUAC by inheriting the `VLEModelBaseClass` and defining a method called `get_activity_coefficient` which accept an array of liquid phase compositions $\{x_i\}$ and a float for temperature and returns a numpy array of activity coefficients $\{\gamma_i\}$. The base class includes methods that accept an array of temperature, pressure and liquid (vapor) phase compositions of a c-component mixture returns the corresponding vapor (liquid) phase compositions at equilibrium.

Rectifying and stripping profiles are difference equations

Our code base contains base classes to estimate rectifying and stripping profiles in a single feed distillation column and a double feed distillation column. The code is built on the equations and methods described in[5,4]. We encourage the reader to refer to chapter 4 in the Conceptual design of distillation systems textbook[5] for a detailed description of the methods involved. Below we will provide minimal a description as required to explain our work.

Under the assumptions that the (i) entire column is maintained at constant pressure (ii) the liquid and vapor streams leaving a stage are in equilibrium and (ii) there is constant molal overflow in the rectifying and stripping sections of the column, the material balance equations for the rectifying profile can be written as,

$$\mathbf{y}_{j+1} = \left[\frac{r}{r+1}\right]\mathbf{x}_j + \frac{\mathbf{x}_D}{r+1} \tag{2}$$

Here $\mathbf{y}_j$ and $\mathbf{x}_j$ refer to the array of compositions in the vapor and liquid streams leaving stage j, r is the reflux ratio and $\mathbf{x}_D$ gives the composition of the distillate. Note that the compositions are related to each other via VLE equations as $\mathbf{x}_j = f_{eq}^{-1}(\mathbf{y}_j)$. Equation 2 that helps us estimate the rectifying profile is a difference equation.

Maps or difference equations are discrete versions of differential equations. Consider a differential equation of the form $\frac{dy}{dt} = f(y)$. The variable y evolves with respect to a continuous variable t and its evolution is described by the function $f(y)$. The value y^* such that $f(y^*) = 0$ gives the fixed-point or steady state for variable y. For situations where the variable can only change in discrete steps we have difference equations of the form $y_{n+1} = f(y_n)$. The value y^* such that $y^* = f(y^*)$ gives the fixed-point y^*.

In the context of a rectifying profile equation, a fixed point corresponds to a situation where compositions of the liquid streams that enter and leave a stage are identical suggesting, no separation occurs in the stage and adding more stages does not change composition of streams that exit the stage. In our notebooks we show rectifying composition profiles, describe the role played by the fixed points of these profiles, and how they are influenced by parameters like reflux ratio. In order for a separation to be feasible the rectifying and stripping profiles need to cross each other. This indicates that there is a path to obtaining the target distillate composition starting from the bottoms composition using a finite number of stages. Note that the equation for the stripping operating line together with the VLE relationship is also a difference equation.

List of available Jupyter Notebooks

Example I: Ideal Binary Mixture

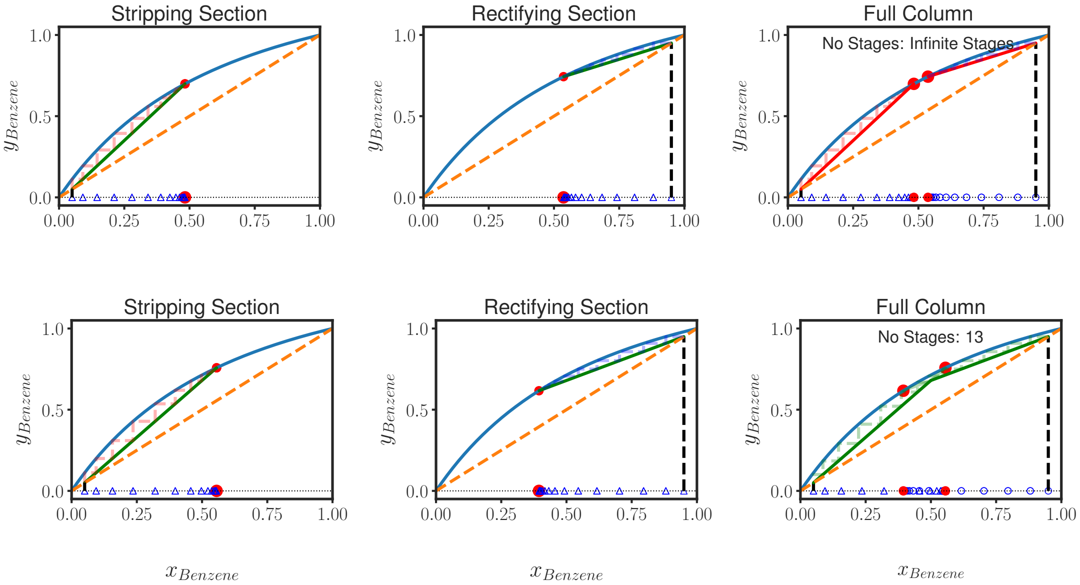


Figure 1: These are two sets of plots from example I where a student can use a slider to adjust the reflux ratio. In the top the reflux ratio is lower than the minimum reflux ratio and therefore the fixed points (red circles) of the rectifying and stripping profiles(blue symbols on the x-axis) are far from each other and the profiles do not overlap. The bottoms plots show a case where the two profiles overlap indicating that the separation is feasible.

The first notebook is on designing a column for separating a benzene toluene mixture which is described by the Raoult's law model. The interactive plots in the notebook describe how the rectifying and stripping profiles change with reflux ratio. The profiles are plotted as compositions of the liquid stream leaving a stage along the x axis (blue symbols in figure 1). These profiles end at fixed points which are indicated using red dots. Students can use sliders to study how the location of fixed points are affected by reflux ratio. If the fixed points of the stripping and rectifying profiles are such that there is no overlap between the profiles then this implies that the separation is not feasible. This would correspond to the value of reflux ratio set below the minimum reflux ratio. As the reflux ratio increases the profiles overlap indicating that the column is feasible. Note that there are several such demonstrations available online. Ours just introduces students to looking at rectifying and stripping profiles and the associated fixed points as a means to decide if a column design is feasible.

Example II: Tangent pinch

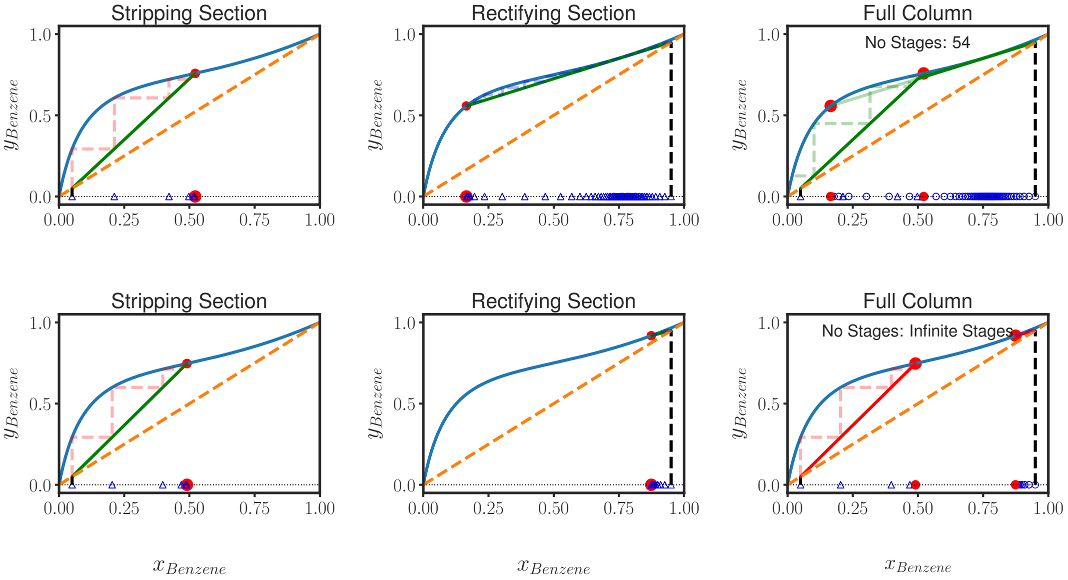
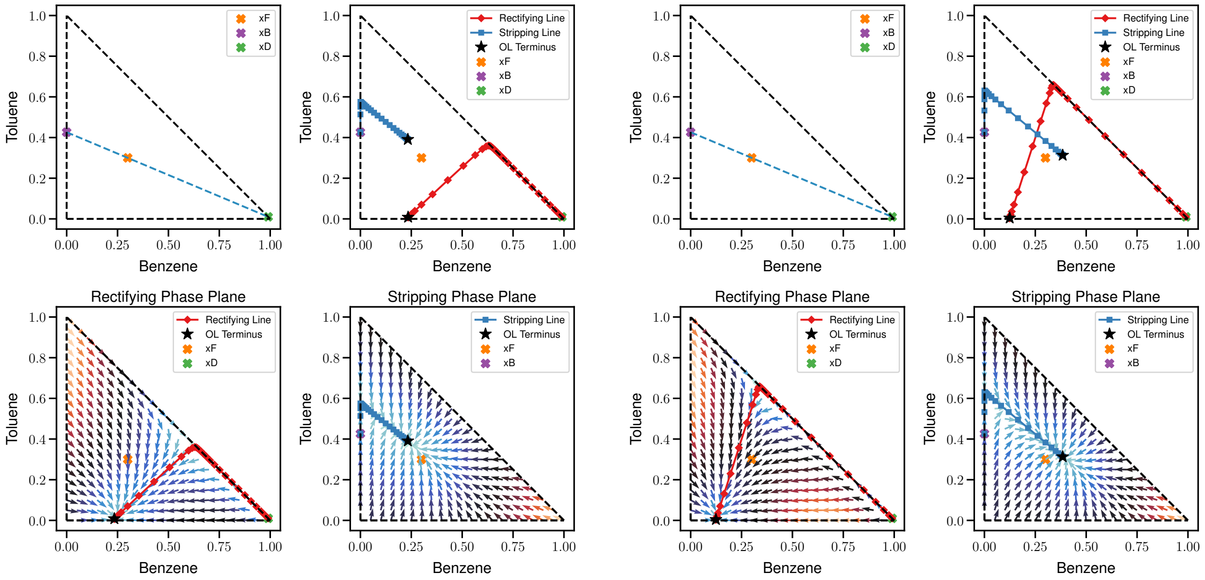


Figure 2: These are two sets of plots from example II where a student can use a slider to adjust the reflux ratio. In the top the reflux ratio is such that the rectifying and stripping profiles (blue symbols on the x-axis) overlap and therefore the separation is feasible. In the bottom case the rectifying operating line is tangential to the VLE curve and therefore a new fixed point (tangent pinch) arises which prevents the profiles from overlapping.

In example II we design a column to separate a Benzene Ethylenediamine mixture. The VLE behavior is described by an empirical model described in chapter 2 of the Conceptual design of distillation systems textbook^5. This notebook focusses on how a tangent pinch affects feasibility of separation. A tangent pinch occurs when the operating curve is tangential to the VLE curve. Figure 2 shows such a case and one can observe how the fixed point of the rectifying section is far from that of the stripping section. Overlap between the sections is made impossible as the tangent pinch (fixed point) controls how far the rectifying section profile extends. Tangent pinches are common in ternary and higher order mixtures. Students can use sliders to study how reflux ratio affects the position of the tangent pinch and how they can avoid it by changing the value of the distillate composition.

Example III: Ideal Ternary Mixture

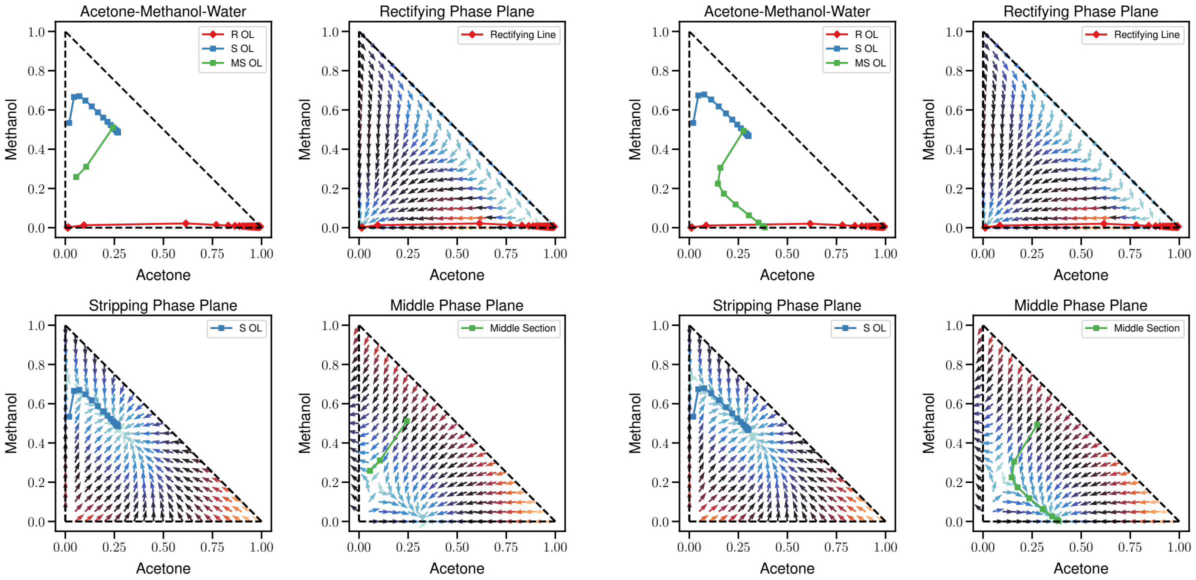


(a) (b)

Figure 3: These are two sets of plots from example III where a student can use a slider to adjust the reflux ratio. In the left the reflux ratio such that the rectifying (red) and stripping (blue) profiles do not cross each and therefore the separation is infeasible. In the right the two profiles cross each other indicating that separation is feasible. The phase planes of the rectifying and stripping difference equations for both cases are also shown. Students can use sliders to observe how modifying reflux ratio changes the landscape of the phase planes.

The third notebook is on designing a column for separating a Benzene Toluene Xylene ternary mixture. The VLE behavior is described by the Raoult's law model. In the two binary mixture cases presented above the rectifying and stripping profiles and their fixed points sit on the x-axis. For ternary mixtures the profiles are curves in 2D and not necessarily linear. The demonstration shows how reflux ratio and the VLE equations affects the shape of these curves. To understand why the curves take these shapes we plot the phase plane diagrams of the underlying difference equations. The phase plane diagrams suggest how the profiles would evolve starting from a given location. Students can use sliders to study how the landscape changes with reflux ratio. They can also observe how the fixed points of the profiles move upon changing reflux ratio. Figure 3 shows two plots made using this notebook.

Example IV: Extractive distillation



(a) (b)

Figure 4: These are two sets of plots from example IV where a student can vary the feed stage of the entrainer. In the left the operating conditions are such that the middle-section profile (green) does not connect the rectifying (red) and stripping (blue) profiles and therefore the separation is infeasible. In the right we have a case where the middle section profile acts a staple connecting the rectifying and stripping profiles indicating that separation is feasible. The phase planes of the rectifying, middle-section and stripping difference equations for both cases are also shown. Students can use sliders to observe how modifying reflux ratio and feed rate of the entrainer changes the landscape of the phase planes.

The last notebook is on extractive distillation of the Acetone Methanol Water system. This is a technique commonly used to separate azeotropic (Acetone/Methanol) mixtures. Typically a heavy solvent (Water) called the entrainer that does not introduce any new azeotropes to the phase diagram is introduced at the top of the column. The entrainer leaves the column at the bottom with one (methanol) of the two components of the azeotrope. The other component (acetone) leaves at the top in an almost pure form. Due to the presence of two feeds there are three sections in the column; rectifying, middle-section and stripping. Each of these sections can be modeled using a difference equation that arises due to the stage-wise mass balance. More details on these equations can be found in[5,4]. In the interactive notebook students can use sliders to understand how (i) the location of the feed stage of the entrainer (ii) flow rate of the entrainer and (iii) reflux ratio affect the rectifying, middle-section and stripping profiles. There is an upper bound and lower bound for both entrainer feed rate and reflux ratio within which separation is feasible. In addition this notebook also describes why a single feed distillation column cannot be used for this separation.

In order for a column to be feasible for a chosen distillation and bottoms composition there must be overlap between the rectifying and middle-section profiles and middle-section and stripping profiles. The middle-section profile must act as a staple linking the rectifying and stripping profiles. This will imply that there is a path from the bottom composition to the distillation composition via the stages in the middle-section. Figure 4 shows interactive plots from this example.

Summary and Future Work

We are currently introducing these notebooks in our Process Design with Aspen Plus course. Based on student feedback we will refine these notebooks and our code-base. We will require our students to use this code-base to design distillation columns before they start designing columns in Aspen Plus. We plan to host these notebooks on a remote server so that it is accessible online. The code is freely available for download via this Github link. The code base has been written such that it is easy to create new Jupyter notebooks. It is also relatively straightforward to add more activity coefficient models. We also plan to add a few more Jupyter Notebooks on ternary and quaternary mixture separation.

References

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[5] Michael F Doherty and Michael F Malone. *Conceptual design of distillation systems*. 2001.