Problem Solving Using CAPE-OPEN Software:
Residue Curves Case Study

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Abstract
Computational simulation is more the rule than the exception in modern process design and analysis. The use of different applications for different purposes is common due to the high specificity of the available software, yet most of the software has the CAPE-OPEN standards that allows its interaction with compatible software. This works uses the generation of the residue curve map as an example to show the potential benefits of combining different applications to solve a time-consuming problem.

Keywords: Residue Curve Map, CAPE-OPEN, Conceptual Design Tools

1 Introduction
Shortcut models are low dimension, deterministic models, that approximate both qualitative and the quantitative behaviors of large scale systems. Usually, shortcut models are used for understanding the process possibilities and confirm the technical
viability of the process. Then, if the viability is confirmed, then the rigorous modelling and simulation followed by experiments are mandatory. One of the most used shortcut models is the residue curve map applied to distillation and reactive distillation processes. It is the model of a hypothetical process in which matter passes differentially from the liquid phase into the vapor phase. It is mathematically described by the following system of nonlinear autonomous differential equations [1]

$$\frac{dx_j}{d\tau} = x_j - y_j \quad j = 1, 2, ..., n - 1$$

(1)

where $x_j$ and $y_j$ are the concentrations of the $j$-th component in the liquid and vapor phases, respectively; $n$ is the number of components in the system and $d\tau = d \ln g$ where $g$ is the amount of the liquid phase. This model is a theoretical simplification of the distillation process.

Residue curve maps are used to assess the separability of any mixture of chemical components by distillation and to conceptually design the distillation column needed to perform the actual separation [2]. The concept of residue curve map was extended to take into consideration more realistic distillation parameters such as reflux and reboil ratios [3], distillations with liquid phase splitting [4] and reactive distillation [5]. It has also been extrapolated to other processes such as reactive membranes [6].

2 The Utility of CAPE-OPEN

CAPE-OPEN is a standard that defines common rules that allow Computer-Aided Process Engineering (CAPE) applications to interact even if they come from different software developers. This allows engineers and undergraduate students to take advantages of the strengths of different applications to solve a problem. One of the most used software in engineering teaching, especially in undergraduate level is Matlab® or for practical purposes any of its clones. It is a versatile software that allows programming in a simple interphase and has an extensive library of accessible numerical routines, yet it lacks the most fundamental thing for chemical engineering calculations, thermodynamic properties. It certainly is a drawback in the teaching process that a student must code its own thermodynamic routines, moreover if the coding is as time consuming as the equilibrium thermodynamic models such as activity coefficients, fugacity coefficient, and excess properties.

Process Simulators usually have all the thermodynamic property calculation subroutines, but the use of this subroutines or property packages is internal and very restricted within the process simulators themselves. Therefore, the student has no opportunity to explore the possibilities of using advanced thermodynamics in less constrictive environments. Although the possible applications of the use of the CAPE-OPEN standard are limitless, the main objective of this work is to illustrate its usefulness by creating a sandbox environment in Matlab® which allows a freer...
exploration of the residue curve map creation instead of the already available pre-packaged options.

3 The Methodology

Three different applications will be used, the CAPE-OPEN to CAPE-OPEN Simulation environment (COCO Simulator) available online (https://www.cocosimulator.org) as the main source for thermodynamic property calculation subroutines, the Amsterchem’s Matlab CAPE-OPEN Thermo Import available online (https://www.amsterchem.com) as a function library that allows calculation of thermodynamic properties from Matlab®, and finally Matlab® as the main platform for the coding. The main idea is to use one of the COCO applications named Thermodynamics for Engineering Applications (TEA-COCO’s) to configure a property package, which is a collection of chemical compounds and calculation methods, that will be accessible from Matlab® using the Matlab Thermo Import.

4 Setting Up a Property Package

The First step is opening the configure TEA application from COCO Simulator and creating a new template. In the new template, a representative azeotropic mix of Acetone, Benzene, and Chloroform will be created by adding the three compounds from the software’s database. On the Advanced Mode, the Peng-Robinson equation of state and the NRTL Activity coefficient model will be chosen as the main calculation methods.

Figure 1. TEA Configure interphase to configure the property package for the Benzene- Acetone-Chloroform Mixture
5. Performing Equilibrium Calculations in Matlab®

Once Matlab Thermo Import is installed, it will automatically register itself on Matlab to be used. Once in Matlab® and after entering valid license code the application is ready to use. The first step will be to create a Matlab® object named a handle, which will be an identifier of the property package, so anytime this handle is used by a function it will use the property package that was created.

Once the handle is created, it is possible to use a vast collection of functions of the Matlab Thermo Import for the calculation of thermodynamic properties. Figure 2 shows an example of the calculation of some equilibrium properties of the selected mixture. Figure 2 also shows that the software is not only capable of performing equilibrium property calculation, but it is also capable of calculating the all equilibrium properties of a mixture once composition and two properties are fixed.

Figure 2 Examples of equilibrium and equilibrium property calculation for the for the Benzene- Acetone-Chloroform Mixture
6. Generating a Residue Curve Map

The residue curve map is the phase portrait of equation (1), the integration of this differential equations where \( x_i \) an \( y_i \) are in physical equilibrium, would not be possible as straightforward as is done in this work, if calculation subroutines were not already available.

**Code 1: Matlab code for the residue curve map equation**

```matlab
function [dx]=RCMODE(t,x)
global handle
[phases,phaseFracs,phaseCompositions,T]=capeOpenEquilibrium(handle,[x(1)
x(2) 1-x(1)-x(2) ],'vaporFraction',0.0,'pressure',101325);
dx(1,1)= x(1)- phaseCompositions(1,1);
dx(2,1)= x(2)- phaseCompositions(1,2);
```

Code 1 shows how simplified equations (1) implementation becomes once, it is implemented using the tools discussed in this work. Normally an undergraduate student takes almost half the semester to acquire the necessary concepts and the skills to implement the thermodynamic property calculations and the physical equilibrium solvers to be able to perform the integration of this system. The next step is to integrate this function using a proper solver.

**Code 2: Matlab® Code for generating residue curve maps**

```matlab
for i= 0:0.02:0.5
    X1=i;
    X2=i;
    [t,y]=ode23s(@RCMODE,[0 10],[X1,X2]);
    [t,y1]=ode23s(@(t,x) -RCMODE(t,x),[0 20],[X1,X2]);
    plot(y(:,1),y(:,2),'b')
    plot(y1(:,1),y1(:,2),'b')
    hold on
end
axis([0 1 0 1])
line([0 1],[1 0])
```

Code 2 is a repetitive integration using ode23s form the ode suite of Matlab®, that allows tracing all the residue using the curve \( y = x \), from \( x = 0 \) to \( x = 0.5 \) as initial conditions. This algorithm integrates the residue curve map equation implemented in Code 1 and its negative form \((-RCMODE(t,x))\) from 0 to a sufficiently high number in this case 20 (which was picked arbitrarily) to generate the curve map.
Figure 3 show the results of the running Code 2 in Matlab® once Code 1 is already implemented, for simplicity it was plotted on a right triangle diagram. The residue curve map qualitatively agrees with the ones reported in [7]. Although the search for azeotropes is not in the scope of the work, the diagram suggest that the max boiling point azeotrope reported is present, validating the results.

7 Conclusions

Although, residue curve map calculations are available in several process engineering software, its implementation outside of these black box environments is time consuming. Nevertheless, to show it was possible to generate a residue curve map using CAPE-OPEN applications with Matlab® was not the only purpose of this work, it was also to demonstrate that the combined use of specialized software can result in considerable efficiency boost for the process engineering labor, moreover, to boost the learning of undergraduate students and the direct application of thermodynamics to their assignments. In a certain way the modular use of applications can encourage the creative problem solving and independent work, making the student create its own solutions rather than to adapt to what is already available in a process simulator framework. Finally, it is important to remark that
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this is just a little example of all the capabilities and all the possibilities of the use the thermodynamics interphases in Matlab® and similar software.

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References


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