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An Alternate Formulation for Calculating Reactive Residue Curve Maps

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Until now, reactive residue curve maps (RRCM) are computed for a liquid phase where either only kinetically controlled reactions, or only chemical equilibrium reactions, take place. We try to model a liquid phase where both kinds of reactions may occur. Using two new transformed composition vectors and the temperature as unknown variables, we provide an alternate formulation for calculating RRCM. The main benefit is a unified and extended framework where one can easily add or remove one or more reactions, and obtain the dynamic model to be integrated. The computational cost of the suggested approach may be less than the previous ones.

1. Introduction

During the last decades, professor Michael F. Doherty and his colleagues provide the main advances, both in the formulation of the differential algebraic equations (DAE) modelling the (reactive) Rayleigh distillation, and in the algorithms for solving them. First, (Doherty and Perkins, 1978) modify the original equations of the simple distillation by replacing the time independent variable, t, by a dimensionless variable, τ, when integrating the partial mass balances under the constraints of thermodynamic equilibria. The resulting dynamic model for calculating a RCM no longer includes the energy balance: in the non-reactive case, it is proved that the residue curve map does not depend on the heating policy.

A dynamic model for RRCM calculation appears in (Barbosa and Doherty, 1988). The DAE, and the graphical representation obtained from its numerical integration, prove to be efficient for providing a “deeper understanding of distillation phenomena” and “the tools for the design and synthesis of reactive distillation columns”. This dynamic model is restricted to one chemical equilibrium reaction. (Venimadhavan et al., 1994) build a DAE modelling a diphasic system with one kinetically controlled chemical reaction in the liquid phase. The Damköhler number, “a dimensionless ratio of a characteristic liquid residence time to the characteristic reaction time” is introduced and the influence of this parameter on the RRCM profiles is discussed.

More general frameworks for simulating several chemical reactions are published later. (Ung and Doherty, 1995a, 1995b) introduce a “new set of composition variables” reducing the dimensionality of the RRCM when a vapor-liquid equilibrium with multiple chemical equilibrium reactions is considered. For such a case, they define a new independent variable τ, and write a DAE using the new set of composition variables. Compared with the non-reactive case, the significance of the independent variable τ changes, and the new composition variables play the role of the molar fractions, but the differential equations look the same. (Venimadhavan et al., 1999) generalize to multiple reactions the model for a single kinetically controlled reaction. Once again, a Damköhler number is defined and allows parametric studies of the RRCM.

Apart from the Doherty papers, some extra publications are worth analyzing. (Almeida-Rivera and Grievink, 2004) summarize the dynamic model for multiple chemical equilibrium reactions as it is commonly adopted since (Ung and Doherty, 1995a). Under the chemical equilibrium assumption, (Sanchez-Daza et al., 2006) introduce an alternate formulation based on the element concept, an element being an atom, a molecule or a fragment of molecule. This element approach leads to RRCM where the vertices are associated to elements. It allows the representation on ternary diagrams of reactive systems with more than three species. (Alloula et

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al., 2013) apply an index reduction technique to an initial DAE in order to provide a DAE more suitable for numerical integration.

From the previous papers, it appears that adequate formulations for modelling either multiple kinetically controlled reactions, or multiple chemical equilibrium reactions exist. However, a formulation for handling both kinds of reactions is missing. In order to build such a framework, part 2 collects the three main DAE models (non-reactive case and two reactive cases). Even if those models can be retrieved in the previously cited papers, a common notation is established for further comparison with the suggested approach. In part 3, this paper introduces an alternate formulation which can be substituted to any of the three usual formulations and, furthermore, can model reactive systems with both kinds of reactions. Part 4 lists the expected benefits of such a new formulation from the points of view of modelling and numerical integration.

2. Usual formulations for calculating residue curve maps

2.1 Non-reactive residue curve maps

Throughout this paper, we consider that two phases exist, there is no vapour retention and no chemical reactions in the vapour phase. The vapour phase is considered to be ideal. Heat and pressure policy remain free. Table 1 gives a list of all the symbols appearing in the forthcoming model. According to the previous assumptions, and following the given notations, a mathematical model of the non-reactive Rayleigh distillation may be written as:

$$\begin{cases} \forall i \in \{1,\dots,N\}; \overset{\cdot}{\overbrace{x_i \cdot U_l}} = -V \cdot y_i \\ \overset{\cdot}{\overbrace{h_l(T,P,x) \cdot U_l}} = Q - V \cdot H(T,P,y) \\ \forall i \in \{1,\dots,N\}; y_i = K_i(T,P,x) \cdot x_i \\ \sum_{i=1}^{N} x_i = 1 \\ \sum_{i=1}^{N} y_i = 1 \end{cases} \tag{1}$$

This model consists of N partial mass balances, 1 energy balance, N thermodynamic equilibria, and 2 definitions of molar fractions. Derivatives are with respect to the independent variable t. The unknown vector can be defined as $(U_l, T, x, y, V)'$. Q and P remain user-defined variables. The overall mass balance $\dot{U}_l = -V$ can be deduced from $\sum_{i=1}^{N} x_i = 1$ by adding all the partial mass balances. Then, combining the overall mass balance with each partial mass balance, one obtains the following differential equations:

$$\forall i \in \{1,\dots,N\}; \frac{U_l}{V} \cdot \dot{x}_i = x_i - y_i \tag{2}$$

These equations suggest the introduction of a dimensionless variable τ, satisfying:

$$d\tau = \frac{V}{U_l} dt \tag{3}$$

From this variable change one obtains the differential algebraic system usually integrated for producing a RCM:

$$\begin{cases} \forall i \in \{1,\dots,N-1\}; \frac{dx_i}{d\tau} = x_i - y_i \\ \forall i \in \{1,\dots,N\}; y_i = K_i(T,P,x) \cdot x_i \\ \sum_{i=1}^{N} x_i = 1 \\ \sum_{i=1}^{N} y_i = 1 \end{cases} \tag{4}$$

In (4) the unknown vector can be defined as $(T, x, y)'$. From the initial equation system, U_l and V have been eliminated, and two equations –one partial mass balance and the energy balance- have been dropped.

2.2 Kinetically controlled reactions only

For R kinetically controlled reactions only, a reactive Rayleigh distillation model may be written as:

$$\begin{cases} \forall i \in \{1,\dots,N\}; \overset{\cdot}{\overbrace{x_i \cdot U_l}} = \sum_{j=1}^{R} \left(\nu_{i,j} \Delta_j(T,P,x)\right) - V \cdot y_i \\ \overset{\cdot}{\overbrace{h_l(T,P,x) \cdot U_l}} = Q - V \cdot H(T,P,y) - \sum_{j=1}^{R} \left(Qr_j(T,P) \cdot \Delta_j(T,P,x)\right) \\ \forall i \in \{1,\dots,N\}; y_i = K_i(T,P,x) \cdot x_i \\ \sum_{i=1}^{N} x_i = 1 \\ \sum_{i=1}^{N} y_i = 1 \end{cases} \tag{5}$$

Applying the same variable change and elimination process as in the non-reactive case, one obtains a reduced differential algebraic system modelling the reactive Rayleigh distillation:

$$\begin{cases} \forall i \in \{1,\dots,N-1\}; \frac{dx_i}{d\tau} = x_i - y_i + \frac{U_l}{V} \cdot \sum_{j=1}^{R} \left(\nu_{i,j} - \left(\sum_{k=1}^{N} \nu_{k,j}\right) \cdot x_i\right) \cdot \delta j(T,P,x) \\ \forall i \in \{1,\dots,N\}; y_i = K_i(T,P,x) \cdot x_i \\ \sum_{i=1}^{N} x_i = 1 \\ \sum_{i=1}^{N} y_i = 1 \end{cases} \quad (6)$$

Assuming that some heating policy can maintain the ratio $\frac{U_l}{V}$ to its initial value $\frac{U_l(0)}{V(0)}$, and evaluating one of the forward reaction rate constants (k_1 for example) at a reference temperature $T_{reference}$ (Venimadhavan et al., 1999), the kinetically controlled residue curve map is computed from:

$$\begin{cases} \forall i \in \{1,\dots,N-1\}; \frac{dx_i}{d\tau} = x_i - y_i + D_a \cdot \sum_{j=1}^{R} \left(\nu_{i,j} - \left(\sum_{k=1}^{N} \nu_{k,j}\right) \cdot x_i\right) \cdot \frac{\delta j(T,P,x)}{k_1(T_{reference})} \\ \forall i \in \{1,\dots,N\}; y_i = K_i(T,P,x) \cdot x_i \\ \sum_{i=1}^{N} x_i = 1 \\ \sum_{i=1}^{N} y_i = 1 \end{cases} \quad (7)$$

In the multiple kinetically controlled reaction case, the Damköhler number can be defined as $D_a = \left(\frac{U_l(0)}{V(0)}\right) / \left(\frac{1}{k_1(T_{reference})}\right)$, ratio of a characteristic residence time $\frac{U_l(0)}{V(0)}$ to a characteristic reaction time $\frac{1}{k_1(T_{reference})}$. The RRCM depends on D_a, that is to say on the conditions offered to the chemical reactions. When D_a goes to 0, the dynamic model (7) goes to the non-reactive model (4). When D_a goes to $+\infty$, all the reactions can be viewed as a chemical equilibrium reaction.

2.3 Chemical equilibrium reactions only

For R chemical equilibrium reactions only, a reactive Rayleigh distillation model may be written as:

$$\begin{cases} \forall i \in \{1,\dots,N\}; \overbrace{x_i \cdot U_l}^{\cdot} = \sum_{j=1}^{R} \left(\nu_{i,j} \dot{\xi}_j(T,P,x)\right) - V \cdot y_i \\ \overbrace{h_l(T,P,x) \cdot U_l}^{\cdot} = Q - V \cdot H(T,P,y) - \sum_{j=1}^{R} \left(Qr_j(T,P) \cdot \dot{\xi}_j(T,P,x)\right) \\ \forall i \in \{1,\dots,N\}; y_i = K_i(T,P,x) \cdot x_i \\ \forall j \in \{1,\dots,R\}; K_{c\,j}(T,P) = \prod_{i=1}^{N} a_i(T,P,x)^{\nu_{i,j}} \\ \sum_{i=1}^{N} x_i = 1 \\ \sum_{i=1}^{N} y_i = 1 \end{cases} \quad (8)$$

$\dot{\xi}_1, \dot{\xi}_2, \dots, \dot{\xi}_R$ no longer have an explicit expression. They become additional variables. (8) is saturated thanks to R chemical equilibrium equations. (Ung and Doherty, 1995a) details how $\dot{\xi}_1, \dot{\xi}_2, \dots, \dot{\xi}_R$ are eliminated, and how new variables $X_1, X_2, \dots, X_{N-R}$ are defined in terms of $(\nu_{i,j})$ and $x_1, x_2, \dots, x_N$. New variables $Y_1, Y_2, \dots, Y_{N-R}$ are also defined in terms of $(\nu_{i,j})$ and $y_1, y_2, \dots, y_N$. These "transformed composition variables" satisfy $\sum_{i=1}^{N-R} X_i = 1$, $\sum_{i=1}^{N-R} Y_i = 1$, and $N - R - 1$ partial mass balances:

$$\forall i \in \{1,\dots,N-R-1\}; \mathrm{f}(\nu) \cdot \frac{U_l}{V} \cdot \dot{X}_i = X_i - Y_i \quad (9)$$

where f(ν) depends only on stoichiometric coefficients.

(9) suggests the introduction of the dimensionless variable τ, satisfying:

$$d\tau = \frac{V}{U_l \cdot \mathrm{f}(\nu)} dt \quad (10)$$

As mentionned in (Ung and Doherty, 1995b), the differential equation "has exactly the same functional form as the simple distillation equation for non-reacting mixtures in terms of mole fractions":

$$\begin{cases} \forall i \in \{1,\dots,N-R-1\}; \frac{dX_i}{d\tau} = X_i - Y_i \\ \forall i \in \{1,\dots,N\}; y_i = K_i(T,P,x) \cdot x_i \\ \forall j \in \{1,\dots,R\}; K_{c\,j}(T,P) = \prod_{i=1}^{N} a_i(T,P,x)^{\nu_{i,j}} \\ \forall i \in \{1,\dots,N-R\}; X_i = \alpha_i(\nu,x) \\ \forall i \in \{1,\dots,N-R\}; Y_i = \beta_i(\nu,y) \\ \sum_{i=1}^{N-R} X_i = 1 \; or \; \sum_{i=1}^{N} x_i = 1 \\ \sum_{i=1}^{N-R} Y_i = 1 \; or \; \sum_{i=1}^{N} y_i = 1 \end{cases} \quad (11)$$

3. Alternate formulation for calculating residue curve maps

Assuming that a mixture contains N components, a DAE modelling the non-reactive Rayleigh distillation may consist of N partial mass balances, 1 energy balance, N thermodynamic equilibria, and 2 molar fraction definitions. In the reactive case, $\dot{\xi}_1, \dot{\xi}_2, \dots, \dot{\xi}_R$ modify the partial mass balances, and R additional equations, either algebraic (chemical equilibrium reaction), or differential (kinetically controlled reaction) are added. (12) is a generic DAE modelling a system with both kinetically controlled and chemical equilibrium reactions:

$$\begin{cases} \forall i \in \{1, \dots, N\}; \overset{\cdot}{\overbrace{x_i \cdot U_l}} = \sum_{j=1}^{R} \left(\nu_{i,j} \dot{\xi}_j(T,P,x) \right) - V \cdot y_i \\ \overset{\cdot}{\overbrace{h_l(T,P,x) \cdot U_l}} = Q - V \cdot H(T,P,y) - \sum_{j=1}^{R} \left(Qr_j(T,P) \cdot \dot{\xi}_j(T,P,x) \right) \\ \forall i \in \{1, \dots, N\}; y_i = K_i(T,P,x) \cdot x_i \\ \forall j \in \{1, \dots, R\}; K_{c\,j}(T,P) = \prod_{i=1}^{N} a_i(T,P,x)^{\nu_{i,j}} \quad or \quad \dot{\xi}_j(T,P,x) = \Delta_j(T,P,x) \\ \sum_{i=1}^{N} x_i = 1 \\ \sum_{i=1}^{N} y_i = 1 \end{cases} \tag{12}$$

The alternate formulation for calculating a RRCM from (12) is based on the elimination of $\dot{\xi}_1, \dot{\xi}_2, \dots, \dot{\xi}_R$. The elimination process is very similar to the one detailed in (Ung and Doherty, 1995a). However, here we write the set of partial mass balances using n, the numbers of moles of each species in the liquid, instead of using the liquid molar fractions x. Adopting a vectorial notation, the N partial mass balances may be written:

$$\dot{n} = \nu.\dot{\xi} - V.y \tag{13}$$

We start by isolating R partial mass balances, for example the last R ones.

$$\dot{\underline{n}} = \underline{\nu}.\dot{\xi} - V.\underline{y} \tag{14}$$

In (14), $\underline{n}$ stands for the last R lines of the n vector, $\underline{y}$ stands for the last R lines of the y vector, and $\underline{\nu}$ is the RxR submatrix built from the last R lines of the NxR stoichiometric matrix ν. Provided that $\underline{\nu}$ is not singular:

$$\dot{\xi} = \underline{\nu}^{-1}.\left(\dot{\underline{n}} + V.\underline{y}\right) \tag{15}$$

Using a notation analoguous to the previous one, the first $N - R$ partial mass balances may be written:

$$\dot{\overline{n}} = \overline{\nu}.\dot{\xi} - V.\overline{y} \tag{16}$$

or, after replacing $\dot{\xi}$ by its value from (15):

$$\dot{\overline{n}} = \overline{\nu}.\underline{\nu}^{-1}.\left(\dot{\underline{n}} + V.\underline{y}\right) - V.\overline{y} \tag{17}$$

In (17) variables can be grouped in the following way:

$$\overset{\cdot}{\overbrace{\overline{n} - \overline{\nu}.\underline{\nu}^{-1}.\underline{n}}} = -V.\left(\overline{y} - \overline{\nu}.\underline{\nu}^{-1}.\underline{y}\right) \tag{18}$$

These partial mass balances may be viewed as the generalization to the reactive case of the partial mass balances in the non-reactive case. With the following definition:

$$\begin{cases} \overline{\mathcal{N}} = \overline{n} - \nu.\underline{\nu}^{-1}.\underline{n} \\ \overline{\mathcal{Y}} = \overline{y} - \nu.\underline{\nu}^{-1}.\underline{y} \end{cases} \tag{19}$$

the first $N - R$ partial mass balances take the form:

$$\dot{\overline{\mathcal{N}}} = -V.\overline{\mathcal{Y}} \tag{20}$$

If we generalize the definition (19) of $\overline{\mathcal{N}}$ and $\overline{\mathcal{Y}}$ with:

$$\begin{cases} \underline{\mathcal{N}} = \underline{n} \\ \underline{\mathcal{Y}} = \underline{y} \end{cases} \tag{21}$$

we obtain two new transformed composition vectors, $\mathcal{N}$ and $\mathcal{Y}$, which are in bijective correspondence with n and y. There is not such a bijective correspondence for the usual "transformed composition variables" X and Y from (Ung and Doherty, 1995b). Using $\mathcal{N}$ and $\mathcal{Y}$, and taking into account the fact that $N + 1$ variables U_l, $x_1, \dots, x_N$, are replaced by N variables $\mathcal{N}_1, \dots, \mathcal{N}_N$, (12) becomes:

$$\begin{cases} \forall i \in \{1, \dots, N - R\}; \dot{\overline{\mathcal{N}}}_i = -V.\overline{\mathcal{Y}}_i \\ \overset{\cdot}{\overbrace{h_l(T,P,x) \cdot U_l}} = Q - V \cdot H(T,P,y) - \sum_{j=1}^{R} \left(Qr_j(T,P) \cdot \left[\underline{\nu}^{-1}.\left(\dot{\underline{n}} + V.\underline{y}\right)\right]_j \right) \\ \forall i \in \{1, \dots, N\}; y_i = K_i(T,P,x) \cdot x_i \\ \forall j \in \{1, \dots, R\}; K_{c\,j}(T,P) = \prod_{i=1}^{N} a_i(T,P,x)^{\nu_{i,j}} \quad or \quad \left[\underline{\nu}^{-1}.\left(\dot{\underline{n}} + V.\underline{y}\right)\right]_j = \Delta_j(T,P,x) \\ \sum_{i=1}^{N} y_i = 1 \end{cases} \tag{22}$$

Finally, defining τ from $d\tau = V.dt$, and assuming that some heat policy can make the vapour flowrate V vary in the same rate as the liquid retention $U_l = \sum_{i=1}^{N} \mathcal{N}_i$, lead to the DAE to be integrated for generating the RRCM:

$$\left\{\begin{array}{c} \forall i \in \{1,\dots,N-R\}; \frac{d\overline{\mathcal{N}}_i}{d\tau} = -\overline{\mathcal{Y}}_i \\ \forall i \in \{1,\dots,N\}; y_i = K_i(T,P,x) \cdot x_i \\ \forall j \in \{1,\dots,R\}; \left\{\begin{array}{c} K_{c_j}(T,P) = \prod_{i=1}^{N} a_i(T,P,x)^{\nu_{i,j}} \\ or \\ \left[\underline{\nu}^{-1}.\left(\frac{d\underline{n}}{d\tau} + \underline{y}\right)\right]_j = D_a \cdot \frac{k_j}{k_1(T_{reference})} \cdot \left(\prod_{i=1}^{\tilde{R}} a_i^{-\nu_{i,j}} - \frac{1}{Kc_j} \prod_{i=\tilde{R}+1}^{N} a_i^{\nu_{i,j}}\right) \end{array}\right. \\ \sum_{i=1}^{N} y_i = 1 \end{array}\right. \tag{23}$$

The heat policy assumption removes one degree of freedom in the physical system and makes it possible to drop one of the equation -the energy balance- from (22). In (23), there are only $2N+1$ unknown variables. x and y appear in several equations, but (19) and (21) give the bijective correspondence between n and $\mathcal{N}$, and between y and $\mathcal{Y}$. Consequently, (23) may be solved with respect to T, $\mathcal{N}$ and $\mathcal{Y}$.

4. Expected benefits

4.1 Single modelling framework

This alternate formulation unifies and extends the three usual ones. A generic DAE (23) consists of $N-R$ partial mass balances written in terms of new transformed composition variables, N thermodynamic equilibria, and 1 definition for the vapour molar fractions. Each chemical equilibrium reaction adds 1 algebraic constraint. Each kinetically controlled reaction adds 1 differential equation. Instead of providing a DAE whose size may be $2N+1$ or $4N-2R+1$, the suggested approach always leads to fixed size $(2N+1)$ system. Instead of defining either the molar fractions or the “transformed composition variables” as dependent variables, the suggested approach always integrates the new transformed composition variables $\mathcal{N}$ and $\mathcal{Y}$. Instead of using different definitions for the independent variable τ, the suggested approach always uses the same definition: $d\tau = V.dt$.

The alternate formulation is more versatile than the usual ones. According to (23) an arbitrary number of kinetically controlled chemical reactions and/or chemical equilibrium reactions can be modelled within a single framework.

4.2 Reduced computational effort

Finally, the numerical integration based on this alternate formulation may be less costly. With the usual formulation, in the chemical equilibrium case, $2(N-R)$ definitions of the “transformed composition variables” are integrated by a DAE solver as algebraic equations, or may be part of a non linear equation system defining Y in terms of X. Whatever integration method is selected, the computation time in the usual approach should be greater than the one obtained with the new formulation. Here T, $\mathcal{N}$ and $\mathcal{Y}$ are the only integrated variables; the reactive liquid composition X is only used after numerical integration, for producing graphical representations.

5. Conclusions

After reviewing the different DAE models used for generating RCM and RRCM, we introduce an alternate formulation. Within this new modelling framework, the number of equations $(2N+1)$ depends only on the number of components, and the unknown variables are always the temperature T and a set of new transformed composition variables $\mathcal{N}$ and $\mathcal{Y}$. From a generic DAE, one can easily build a specific DAE in order to model a liquid phase with an arbitrary number of chemical equilibrium reactions and/or kinetically controlled reactions. When simulating this resulting DAE, we take the view that the new approach will prove to be not only versatile, but also cost-effective due to its reduced computational complexity.

Nomenclature

Symbol name	Meaning	Unit
N	Number of components	
R	Number of chemical reactions	
$\tilde{R}$	Number of reactants	
t	Time, independent integration variable	s
τ	Dimensionless independent integration variable	
U_l	Liquid retention	mol
V	Vapour flow rate	$mol.s^{-1}$
x_i	Liquid molar fraction of component i	
y_i	Vapour molar fraction of component i	
X_i	Transformed composition variable in the liquid phase *(Ung and Doherty, 1995b)*	
Y_i	Transformed composition variable in the vapor phase *(Ung and Doherty, 1995b)*	
$\mathcal{N}_i$	New transformed composition variable in the liquid phase	
$\mathcal{Y}_i$	New transformed composition variable in the vapor phase	
T	Temperature	K
P	Pressure	atm
h	Molar liquid enthalpy	$J.mol^{-1}$
H	Molar vapour enthalpy	$J.mol^{-1}$
Q	Heating power	$J.s^{-1}$
K_i	Thermodynamic equilibrium constant for component i	
$\nu_{i,j}$	Stoichiometric coefficient for component i in reaction j	
ξ_j	Extent of reaction j	mol
Qr_j	Heat of reaction j	$J.mol^{-1}$
a_i	Activity of component i	
Kc_j	Chemical equilibrium constant of reaction j	
k_j	Reaction rate constant of reaction j	s^{-1}
D_a	Damköhler number	
δj	$k_j\left(\prod_{i=1}^{\tilde{R}} {a_i}^{-\nu_{i,j}} - \frac{1}{Kc_j}\prod_{i=\tilde{R}+1}^{N} {a_i}^{\nu_{i,j}}\right)$	s^{-1}
Δ_j	$\delta j \cdot U_l$	$mol.s^{-1}$

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