International Journal of Mathematics and
Computer Science, **17**(2022), no. 3, 1251–1258

Variational Formulation for Solving Reactive Flash Systems

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(Received March 8, 2022, Accepted April 12, 2022)

Abstract

To represent many chemical processes, systems of higher index differential-algebraic equations (DAEs) are the best choice. So we hypothesize the implicit function theorem to reduce the DAEs of the higher index. Then, using variational formulation theory, it is possible to obtain the solution of higher index DAEs as a critical point of the equivalent variational formulation. We study Reactive Flash to demonstrate the efficiency and good accuracy of the proposed procedure.

1 Introduction

Environmental and Economic considerations motivate industry to utilize technologies based on process intensification. Recently, increasing attention has been given to new developments in chemical engineering, leading to inventories of chemical materials and higher energy efficiency [1]-[4]. Reactive Flash (RF) is one of these chemical processes that can be modeled by DAEs of index-2 [5],[6]. In this case, the most crucial question in solving the RF system is evaluating an easily implemented technique. A parameterization

Key words and phrases: Differential- algebraic equations, Parameterization variational technique, Reactive flash, Variational formulation.
AMS (MOS) Subject Classifications: 34A09, 65L80.
ISSN 1814-0432, 2022, http://ijmcs.future-in-tech.net

variational technique (that is a straightforward extension of [7], [8]) can be utilized to solve a Flash Problem. A simple reactive flash was proposed as an excellent vehicle for introducing the DAE system and indicating the range of this technique developed to solve higher index DAEs, especially for index-2 problems. Therefore, we evaluate the role of the parameterization variational technique (presented previously in [7], [8]) in finding the vapor fraction for a special model of reactive flash.

2 Solving Reactive Flash system using the Variational Formulation

This section is dedicated to discuss reactive flashs solvability using a variational formulation approach. Making implicit equations for the vapor-liquid equilibrium calculations present the modeling of the reactive flash as a DAE system. Therefore, in dynamic conditions and from mass and heat balances, the reactive flash model is calculated. As a particular case of ethylene glycol reactive flash performed in two stages, we give:

- To produce ethylene glycol, the reaction of ethylene oxide and water is as follows:
$$C_2H_4O + H_2O \stackrel{r_1}{\to} C_2H_6O_2$$
- With ethylene oxide, the reaction of ethylene glycol is computed.
$$C_2H_4O + C_2H_6O_2 \stackrel{r_2}{\to} C_4H_{10}O_3$$

The references [1], [5] and [6] illustrate the reactive flash process. We consider the vapor-liquid equilibrium problem:

$$\tau\dot{x}_1 = z_i - x_i - \phi - \tau(x_i - \sum_{j=1}^{r} \gamma_{i,j} r_j) \tag{2.1}$$

$$\tau C\dot{T}(t) = H + q - h_1(1+\tau) + \phi \tag{2.2}$$

$$K_n(1 - x_1 - x_2 - x_3) + K_1x_1 + K_2x_2 + K_3x_3 - 1 = 0 \tag{2.3}$$

With $i = 1, .., n-1, n$ being the number of components in reactive flash Table 1 demonstrate the values of the above parameters.

All these samples are known with appropriate values. For the reader who requires a more detailed overview of the flash system, we recommend the reference [6].

Equations 2.1-2.3 are in index-2 DAEs with $\begin{bmatrix} x_1 & x_2 & x_3 & T \end{bmatrix} y = \phi$ To determine a continuous function ϕ of x_i, T, the implicit function theorem [9], [10] can be used for a differentiation index. Therefore, with respect to time t, equation 2.3 can be differentiated, and one aim is as follows:

$$K_n(1 - \dot{x}_1 - \dot{x}_2 - \dot{x}_3) + K_1\dot{x}_1 + K_2\dot{x}_2 + K_3\dot{x}_3 = 0 \tag{2.4}$$

$$K_n[(-\frac{z_1 - x_1 - \phi - \tau(x_1 - \sum_{j=1}^{r}\gamma_{i,j}r_j)}{\tau}) - (\frac{z_2 - x_2 - \phi - \tau(x_2 - \sum_{j=1}^{r}\gamma_{i,j}r_j)}{\tau})$$
$$-(\frac{z_3 - x_3 - \phi - \tau(x_3 - \sum_{j=1}^{r}\gamma_{i,j}r_j)}{\tau})] + K_1(\frac{z_1 - x_1 - \phi - \tau(x_1 - \sum_{j=1}^{r}\gamma_{i,j}r_j)}{\tau})$$
$$+K_2(\frac{z_2 - x_2 - \phi - \tau(x_2 - \sum_{j=1}^{r}\gamma_{i,j}r_j)}{\tau}) + K_3(\frac{z_3 - x_3 - \phi - \tau(x_3 - \sum_{j=1}^{r}\gamma_{i,j}r_j)}{\tau})$$
$$= 0 \tag{2.5}$$

Then, the explicit expression for the vapor fraction ϕ

$$\phi = \frac{\tau K_n - \sum_{i=1}^{3}(K_n - K_i)z_i + \sum_{i=1}^{3}(K_n - K_i)x_i + \sum_{i=1}^{3}(K_n - K_i)\tau(x_i - \sum_{j=1}^{r}\gamma_{i,j}r_j)}{\sum_{i=1}^{3}K_i - 3K_n} \tag{2.6}$$

$$= \psi_1 + \psi_2$$

Table 1: Nominal parameters value in RF

Sample	Represent in Reactive Flash
τ	The reactive flash time constant
z_i	i-th feed mole fraction
x_i	i-th Liquid mole fraction
T	The temperature
r_j	Rate of reaction j
$\gamma_{i,j}$	In reaction j, it is the stoichiometric coefficient of component i
H	Specific enthalpy of liquid exit
ϕ	Vapor fraction
q	2.282kJ/mol
h_1	$\sum_{i=1}^{n} \triangle h_i + C_i(T - 298)$, with $\triangle h_i = -95.7, -285.83$ $-460, -628.5$ and $C_i = 0.0869, 0.0754, 0.1498, 0.2870$ for $C_2H_4O, H_2O, C_2H_6O_2, C_4H_{10}O_3$, respectively.

where

$$\psi_1 = \frac{\sum_{i=1}^{3}(K_n - K_i)x_i + \sum_{i=1}^{3}(K_n - K_i)\tau(x_i - \sum_{j=1}^{3}\gamma_{i,j}r_j))}{\sum_{i=1}^{3}K_i - 3K_n}$$

and

$$\psi_2 = \frac{\tau K_n - \sum_{i=1}^{3}(K_n - K_i)z_i}{\sum_{i=1}^{3}K_i - 3K_n}$$

The reduced form of DAEs 2.1-2.3 is given by:

$$\tau\dot{x_1} + x_i + \psi_1 + \tau(x_i - \sum_{j=1}^{r}\gamma_{i,j}r_j) = z_i - \psi_2 \tag{2.7}$$

$$\tau C\dot{T}(t) + h_1(1+\tau) - \psi_1 = H + q + \psi_2 \tag{2.8}$$

For $i = 1, .., n-1$ with the algebraic constraint

$$-K_n x_1 - K_n x_2 - K_n x_3 + K_1 x_1 + K_2 x_2 + K_3 x_3 - 1 = 1 - K_n \tag{2.9}$$

The class of consistent initial condition by

$$\omega_0 = \left\{ x_i(t_0) | - \sum_{i=1}^{3} k_n x_i^0 + \sum_{i=1}^{3} k_i x_i^0 = 1 - k_n \right\}$$

Define the operator $L : D(L) \subset H \to R(L) \subset H$, with $\overline{D(L)} = H$, where H is an appropriate Hilbert space (e.g., $H = L_2(T); T = [t_0, t_f], t_0 < t_f)$ by $Lx = F(t)$. The differential and algebraic operator is defined by L, which can be formulated as follows:

$$\begin{bmatrix} \tau & 0 & 0 & 0 \\ 0 & \tau & 0 & 0 \\ 0 & 0 & \tau & 0 \\ 0 & 0 & 0 & \tau C \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{dx_1}{dt} \\ \frac{dx_2}{dt} \\ \frac{dx_3}{dt} \\ \frac{T}{dt} \end{bmatrix} + \begin{bmatrix} \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \\ \alpha_5 & \alpha_6 & \alpha_3 & \alpha_4 \\ \alpha_5 & \alpha_2 & \alpha_7 & \alpha_4 \\ \alpha_5 & \alpha_2 & \alpha_3 & \alpha_8 \\ K_1 - K_n & K_2 - K_n & K_3 - K_n & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ T \end{bmatrix} \tag{2.10}$$

where α_i is given in table 2. By using the parameterization variational technique in 2.7, 2.8 to obtain functional corresponding to 2.10, one can define the following:

$$\mathcal{F}_{\omega_0} = \frac{1}{2}\int_{t_0}^{t_f} [[\tau\dot{x}_1 + \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3 + \alpha_4 T]^T [\tau\dot{x}_1 + \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3 + \alpha_4 T]$$

$$-2[F_1]^T[\tau\dot{x}_1 + \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3 + \alpha_4 T]$$

$$+[\tau\dot{x}_2 + \alpha_5 x_1 + \alpha_6 x_2 + \alpha_3 x_3 + \alpha_4 T]^T[\tau\dot{x}_2 + \alpha_5 x_1 + \alpha_6 x_2 + \alpha_3 x_3 + \alpha_4 T]$$

$$-2[F_2]^T[\tau\dot{x}_2 + \alpha_5 x_1 + \alpha_6 x_2 + \alpha_3 x_3 + \alpha_4 T]$$

$$+[\tau\dot{x}_3 + \alpha_5 x_1 + \alpha_2 x_2 + \alpha_7 x_3 + \alpha_4 T]^T[\tau\dot{x}_3 + \alpha_5 x_1 + \alpha_2 x_2 + \alpha_7 x_3 + \alpha_4 T]$$

$$-2[F_3]^T[\tau\dot{x}_3 + \alpha_5 x_1 + \alpha_2 x_2 + \alpha_7 x_3 + \alpha_4 T]$$

$$+[\tau\dot{x}_4 + \alpha_5 x_1 + \alpha_2 x_2 + \alpha_3 x_3 + \alpha_8 T]^T[\tau\dot{x}_4 + \alpha_5 x_1 + \alpha_2 x_2 + \alpha_3 x_3 + \alpha_8 T]$$

$$-2[F_4]^T[\tau\dot{x}_4 + \alpha_5 x_1 + \alpha_2 x_2 + \alpha_3 x_3 + \alpha_8 T]$$

$$+[(K_1-K_n)x_1+(K_2-K_n)x_2+(K_3-K_n)x_3]^T[(K_1-K_n)x_1+(K_2-K_n)x_2+(K_3-K_n)x_3]$$

$$-2[F_5]^T[(K_1 - K_n)x_1 + (K_2 - K_n)x_2 + (K_3 - K_n)x_3]$$

$$+[(K_1-K_n)x_1^0+(K_2-K_n)x_2^0+(K_3-K_n)x_3^0]^T[(K_1-K_n)x_1^0+(K_2-K_n)x_2^0+(K_3-K_n)x_3^0]$$

$$-2[F_5]^T[(K_1 - K_n)x_1^0 + (K_2 - K_n)x_2^0 + (K_3 - K_n)x_3^0]]dt, \qquad (2.11)$$

Where F_1, F_2, F_3, F_4, F_5 are the nonhomogeneous part of equations 2.7-2.9. By setting $x_1 = \sum_{i=0}^{5} s_i t^i$,$x_2 = \sum_{i=0}^{5} b_i t^i$,$x_3 = \sum_{i=0}^{5} h_i t^i$,$T = \sum_{i=0}^{5} f_i t^i$, we can approximate the solution of the linear algebraic equation $A(\overrightarrow{s}, \overrightarrow{b}, \overrightarrow{h}, \overrightarrow{f}) = B$. The functional simulations 2.11 were numerically carried out in computer programming by solving
$(\overrightarrow{s}, \overrightarrow{b}, \overrightarrow{h}, \overrightarrow{f}) = A^{-1}B$ to obtain the approximate solution (x_1, x_2, x_3, T). Figures 1 and 2 show the vapor fraction for the reactive flash:

Table 2: α_i values

α_i	equal to
α_1	$1 + (K_n - K_1)(1 + \tau)$
α_2	$(K_n - K_2)(1 + \tau)$
α_3	$(K_n - K_3)(1 + \tau)$
α_4	$-(K_n - K_2)\tau \sum_{j=1}^{r} \gamma_{i,j} r_j$
α_5	$(K_n - K_1)(1 + \tau)$
α_6	$1 + (K_n - K_2)(1 + \tau)$
α_7	$1 + (K_n - K_3)(1 + \tau)$
α_8	$C_i(1 + \tau)$

3 Conclusions

In this article, we evaluated the role of parameterization variational technique in finding the vapor fraction of a reactive flash. The experiments demonstrated that the technique is efficient and applicable in finding a fraction of a reactive flash. In the beginning, the problem of index-2 DAEs has been transformed into a reduction system. Then, in the corresponding variational formulation, the critical point has been found, which led to determining the solution of DAEs of index-2. Consequently, the vapor fraction of a reactive flash was determined.

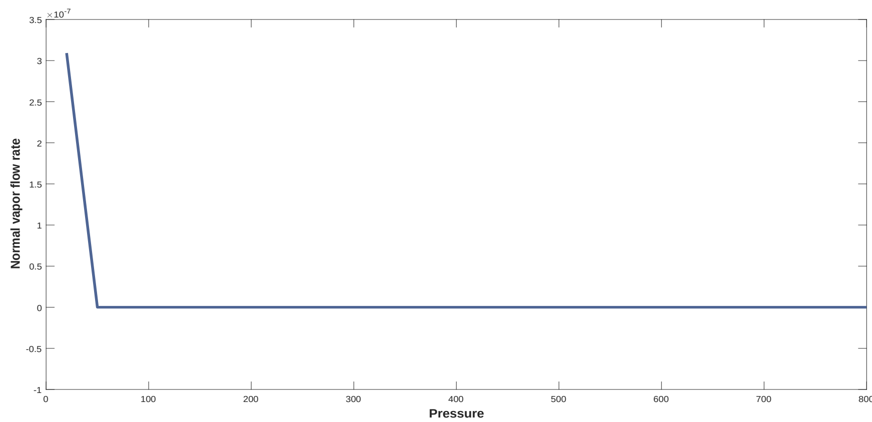

Figure 1: Effect of pressure on amount of vapor

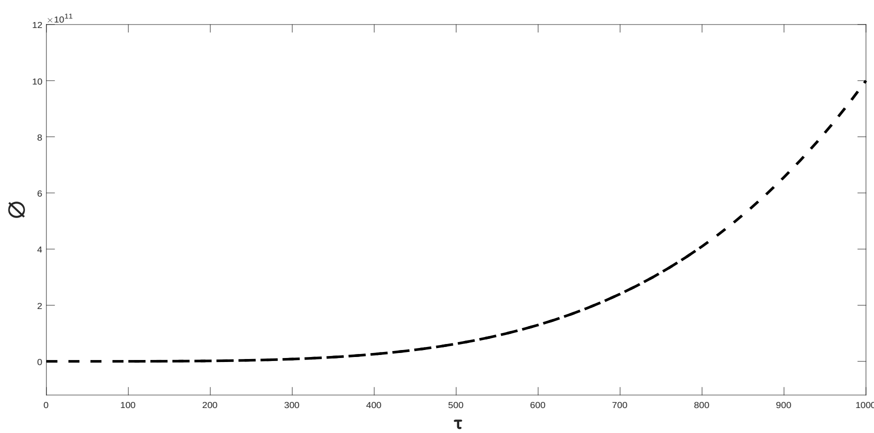

Figure 2: Vapor fraction state

Acknowledgment. The authors would like to thank Mustansiriyah University (www.uomustansiriyah.edu.iq) Baghdad, Iraq for its support in the present work.

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