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Abstract

Non-isothermal reaction-diffusion (RD) systems control the behavior of many transport and rate processes in physical, chemical, and biological systems. A considerable work has been published on mathematically coupled nonlinear differential equations of RD systems by neglecting the possible thermodynamic couplings among heat and mass fluxes, and reaction velocities. Here, the thermodynamic coupling refers that a flux occurs without its primary thermodynamic driving force, which may be gradient of temperature, or chemical potential, or reaction affinity. This study presents the modeling equations of non-isothermal RD systems with coupled heat and mass fluxes excluding the coupling of chemical reactions using the linear non-equilibrium thermodynamic approach. For a slab catalyst pellet, it shows the dynamic behavior of composition and temperature profiles obtained from the numerical solutions of non-linear partial differential equations by Mathematica for two industrial reaction systems of synthesis of vinyl chloride and dissociation of N_2O .

Keywords: Chemical reaction; Heat and mass transfer; Thermodynamic coupling; Non-equilibrium thermodynamics

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1.0 Introduction

Modeling of spatio-temporal evolution may serve as a powerful complementary tool to experimental non-isothermal reaction-diffusion (RD) systems within a porous catalyst particle and membrane ([Weisz and Hicks, 1962](#), [Hlavecek et al., 1969](#), [Aris, 1975](#), [Froment and Bischoff, 1979](#), [Dekker et al., 1995](#), [Pan and Zhu, 1998](#), [Levent et al., 1998](#), [Levent, 2001](#), [Kafarov et al., 1998](#) and [Burghardt and Berezowski, 2003](#); [Selegny et al., 1995a](#) and [Selegny et al., 1995b](#)). Non-isothermal RD systems represent thermodynamically and mathematically coupled transport and chemical processes, and need a through analysis, as they may evolve multiple steady states with unique dynamic phenomena ([Burghardt and Berezowski, 2003](#)). Here, the coupling refers that a flux occurs without its primary thermodynamic driving force, or opposite to the direction imposed by its driving force, called the active transport. The principles of thermodynamics allow the progress of a process without or against its primary driving force only if it is coupled with another process. This is consistent with the statement of second law that states that a finite amount of organization may be obtained at the expense of a greater amount of disorganization in a series of coupled spontaneous processes.

Although the change in temperature may be small in a RD system ([Weisz and Hicks, 1962](#) and [Froment and Bischoff, 1979](#)), the local gradient of temperature, which is the thermodynamic force, can still induce coupling ([Kutchai et al., 1970](#), [Davis, 1991](#) and [Gas et al., 2003](#)). Also, heat effects can enhance the facilitated membrane transport ([Selegny et al., 1995a](#) and [Selegny et al., 1995b](#)), increase the catalytic membrane activity ([Mita, 2000](#) and [Diano et al., 2000](#)), and induce long-range concentration fluctuations in the absence of any convective instability ([Li et al., 1998](#) and [De Zarate and Sengers, 2004](#)).

2.0 Non-isothermal RD systems

For a steady state, first order RD system ($A \rightarrow$ product), using a non-isothermal catalyst pellet, and considering molecular transport, the mass and energy balances are

$$0 = -\nabla \cdot \mathbf{J} - k_v c, \quad (1)$$

$$0 = -\nabla \cdot \mathbf{J}_q + (-\Delta H_r) k_v c. \quad (2)$$

By using the Fick and Fourier laws in one-dimensional transport in a slab catalyst pellet with, equimolar counter diffusion under mechanical equilibrium, Eqs. (1) and (2) become

$$0 = D_e \frac{d^2 c}{dx^2} - k_v c, \quad (3)$$

$$0 = k_e \frac{d^2 T}{dx^2} + (-\Delta H_r) k_v c. \quad (4)$$

Without the external mass and heat transfer resistances, the boundary conditions with x - coordinate oriented from the centerline ($x=0$) to the surface ($x=L$) are

$$c(L)=c_s, \quad \frac{dc(0)}{dx}=0 \quad \text{and} \quad T(L)=T_s, \quad \frac{dT(0)}{dx}=0. \quad (5)$$

Here ΔH_r is the heat of reaction, and D_e and k_e are the effective diffusivity and thermal conductivity, respectively, and tend to be less than the ordinary gas diffusivity and the thermal conductivity for a non-porous similar solid (Pan and Zhu, 1998). The effective reaction rate ($k_v c$) is based on the total rate of reaction within any small, representative volume.

Eliminating the reaction terms from Eqs. (3) and (4), and integrating twice with the boundary conditions given in Eq. (5), temperature is related to concentration by

$$\varphi = 1 - \beta(\theta - 1), \quad (6)$$

where

$$\theta = \frac{c}{c_s}, \quad \varphi = \frac{T}{T_s}, \quad \beta = \frac{(-\Delta H_r)D_e c_s}{k_e T_s}.$$

Eq. (6) is valid for any particle geometry under steady-state conditions, and can be used to eliminate θ or φ from one of the differential equations (3) and (4).

The value of β is a measure of non-isothermal effects; for increasing values of β , non-isothermal effects may become important (Froment and Bischoff, 1979 and Tavera, 2005). Heat of reaction is strongly nonlinear function of temperature. For any interior points within the pore where the reactant is largely consumed, the maximum temperature difference for an exothermic reaction becomes

$$\Delta T_{\max} = (T - T_s)_{\max} = \frac{(-\Delta H_r)D_e c_s}{k_e} = \beta T_s. \quad (7)$$

Using the dimensionless parameters

$$z = \frac{x}{L}, \quad \tau = \frac{D_e t}{L^2}, \quad \phi^2 = \frac{L^2 k_0 \exp(E/RT_s)}{D_e},$$

$$\gamma = \frac{E}{RT_s}, \quad Le = \frac{k_e / \rho C_p}{D_e} = \frac{\alpha_e}{D_e}$$

the transient forms of Eqs. (3) and (4) become

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial z^2} - \phi^2 \theta \exp[\gamma(1 - 1/\varphi)], \quad (8)$$

where Le is the modified Lewis number, and α_e is the effective thermal diffusivity. The initial and boundary conditions are

$$\theta(0, z) = 1, \quad \theta(\tau, 1) = 1, \quad d\theta(\tau, 0)/dz = 0, \quad (10)$$

$$\varphi(0, z) = 1, \quad \varphi(\tau, 1) = 1, \quad d\varphi(\tau, 0)/dz = 0. \quad (11)$$

After using Eq. (6) in Eq. (8), steady and non-isothermal concentration profile becomes

$$\frac{d^2\theta}{dz^2} = \phi^2 \theta \exp\left(-\frac{\gamma\beta(\theta-1)}{1-\beta(\theta-1)}\right). \quad (12)$$

3.0 RD systems with thermodynamically coupled heat and mass transfer

Non-isothermal RD systems represent open, non-equilibrium systems with thermodynamic forces of temperature gradient, chemical potential gradient, and affinities. In a non-equilibrium system, temperature and internal energy are well defined in an elemental volume containing a sufficient number of molecules. Therefore a local equilibrium exists, and the thermodynamic properties are related to the state variables in the same manner as in equilibrium ([Prigogine, 1967](#), [Wisniewski et al., 1976](#), [Kondepudi and Prigogine, 1999](#), [Demirel, 2002](#) and [Demirel and Sandler, 2004](#)); the total entropy S and energy U are expressed by entropy s and energy u densities:

$$S = \int_V s[T(x), n_i(x)] dV.$$

$$U = \int_V u[T(x), n_i(x)] dV$$

and hence the local variables become $(\partial S/\partial U)_m=1/T(x)$ and $(\partial S/\partial N_i)_u=-\mu(x)/T(x)$. Mostly, the internal relaxation processes in a fluid or material are much faster than the rate of change imposed upon the state variables, and the local equilibrium concept is valid for a wide range of transport and rate processes of usual fluid systems ([Sieniutycz, 1992](#), [Kondepudi and Prigogine, 1999](#), [Demirel and Sandler, 2001](#) and [Demirel and Sandler, 2004](#)).

The rate of entropy production Φ due to irreversible processes is always positive, and calculated in terms of conjugate forces X and fluxes J as

$$\Phi = (d_i S/dV dt) = \sum J_k X_k \geq 0$$

within a system. For a multicomponent fluid system under mechanical equilibrium with n species and N_r number of chemical reactions, the dissipation function Ψ is obtained from

the general balance equations including the entropy balance and the Gibbs relation ([De Groot and Mazur, 1985](#), 1985; [Wisniewski et al., 1976](#) and [Demirel and Sandler, 2001](#))

$$\begin{aligned} \Psi &= T \dot{\Phi} \\ &= \left(-\frac{1}{T} \mathbf{J}_q \nabla T - \sum_{i=1}^n \mathbf{J}_i (\nabla \mu_i) + \sum_{j=1}^{N_r} J_{rj} A_j \right) \geq 0 \end{aligned} \quad (13)$$

where, \mathbf{J}_q is the vector of reduced heat flux ([Demirel and Sandler, 2001](#)), and \mathbf{J}_i is the vector of mass fluxes, μ_i is the chemical potential of species i , A is the affinity $A = -\sum \nu_i \mu_i$, ν is the stoichiometric coefficients, and J_r is the reaction velocity. Eq. (13) consists of scalar processes of chemical reactions and vectorial processes of heat and mass transfer, while it excludes viscous flow flux, electrical, and magnetic effects.

In the dissipation-phenomenological equation (DPE) approach ([Demirel and Sandler, 2001](#)), Eq. (13) identifies a set of independent conjugate fluxes J and forces X to be used in the following linear phenomenological equations when system is not far away from global equilibrium:

$$J_i = \sum_{k=1}^m L_{ik} X_k. \quad (14)$$

The phenomenological coefficients L_{ik} ($i, k=1, 2, \dots, m$) can be determined experimentally ([Rowley, 1989](#) and [Demirel and Sandler, 2002](#)). The values of L_{ik} satisfy that $L_{ii} L_{kk} - L_{ik} L_{ki} \geq 0$ and $L_{ii} \geq 0$; $L_{kk} \geq 0$, and Onsager's reciprocal relations state that the cross (coupling) coefficients are symmetric $L_{ik} = L_{ki}$; ($i \neq k$) for a set of independent conjugate fluxes and forces identified by the dissipation function or the rate of entropy production ([Wisniewski et al., 1976](#), [Kondepudi and Prigogine, 1999](#), [Demirel and Sandler, 2001](#) and [Demirel, 2002](#)). Onsager's relations are based on microscopic reversibility, and are independent of the state of a system or any other microscopic assumptions ([De Groot and Mazur, 1985](#); [Kondepudi and Prigogine, 1999](#)).

Excluding the coupling of chemical reaction with the heat and mass transfer, and using $\nabla \mu_1 = (\partial \mu_1 / \partial c_1) \nabla c_1$, we identify the fluxes and forces for a binary mixture from Eq. (13)

$$\Psi = -\frac{1}{T} \mathbf{J}_q \nabla T - \mathbf{J}_1 \lambda_{T,P} \nabla c_1 \geq 0, \quad (15)$$

where

$$\lambda_{T,P} = \left(1 + \frac{\bar{V}_1 c_1}{\bar{V}_2 c_2} \right) \left(\frac{\partial \mu_1}{\partial c_1} \right)_{T,P},$$

and \bar{V}_i is the partial molar volume of component i . Assuming that the RD system is not far from global equilibrium, the linear phenomenological equations based on Eq. (15) are

$$-\mathbf{J} = L_{11} \lambda_{T,P} \nabla c + \frac{1}{T} L_{1q} \nabla T = D_e \nabla c + D_{S,e} \nabla T, \quad (16)$$

$$-\mathbf{J}_q = L_{q1} \lambda_{T,P} \nabla c + \frac{1}{T} L_{qq} \nabla T = D_{D,e} \nabla c + k_e \nabla T, \quad (17)$$

where $D_{D,e}$ is a coefficient in $\mathbf{m}^2 \mathbf{J} / (\mathbf{mol} \text{ s})$ related to the effective Dufour effect, and $D_{S,e}$ is a coefficient in $\text{mol}/(\text{m s K})$ related to the effective Soret effect (thermal diffusion). When there is no volume flow, the mass flux \mathbf{J}_1 is: $\mathbf{J} = -L_{11} \lambda_{T,P} \nabla c$, and comparing it with Fick's law $\mathbf{J} = -D_e \nabla c$, the coefficient L_{11} is related to the effective diffusion coefficient by $L_{11} = D_e / \lambda_{T,P}$. Using Fourier's law $\mathbf{J}_q = -k_e \nabla T$ in Eq. (17), the primary coefficient L_{qq} is related to the effective thermal conductivity k_e by $L_{qq} = k_e T$. The thermal diffusion coefficient for species 1 is $D_T = L_{1q} / (cT)$. For liquids the diffusion coefficient D is of the order of $10^{-5} \text{ cm}^2/\text{s}$, and the thermal diffusion coefficient D_T is of the order of $10^{-8} - 10^{-10} \text{ cm}^2/\text{s}$. For gases the order of magnitude for D is $10^{-1} \text{ cm}^2/\text{s}$ and $10^{-4} - 10^{-6} \text{ cm}^2/\text{s}$, respectively (Wisniewski et al., 1976).

By using the fluxes \mathbf{J}_i and \mathbf{J}_q from Eqs. (16) and (17), respectively in Eqs. (1) and (2), and with the coupled values of temperature T' and concentration c' , we have

$$0 = \nabla \cdot (D_e \nabla c' + D_{S,e} \nabla T') - k_v c', \quad (18)$$

$$0 = \nabla \cdot (D_{D,e} \nabla c' + k_e \nabla T') + (-\Delta H_r) k_v c'. \quad (19)$$

As before, elimination of the reaction terms from Eqs. (18) and (19) yields

$$\varphi' = 1 - \beta'(\theta - 1), \quad (20)$$

where

$$\theta' = \frac{c'}{c_s}, \quad \varphi' = \frac{T'}{T_s} \quad \text{and} \quad \beta' = \frac{(D_e(-\Delta H_r) + D_{D,e})c_s}{(k_e + D_{S,e}(-\Delta H_r))T_s} \quad (21)$$

and the maximum temperature difference becomes

$$\beta' \approx (\varphi_{\text{center}} - 1) = \frac{\Delta T'_{\text{max}}}{T_s}. \quad (22)$$

The modified dimensionless group β' represents the ratio between the rate of heat of chemical reaction and the rate of heat conduction when the heat and mass fluxes are coupled only. By neglecting the coupling effects, we would have $\beta' = \beta$.

Using Eqs. (18) and (19) with the Arrhenius equation $k_v = k_0 e^{-E/RT}$ we have the transient forms of the coupled heat and mass fluxes for a single component

The initial and boundary conditions are the same with those given in Eqs. (8) and (9). For a simple plane geometry and one-dimensional unsteady state equimolar diffusion, Eqs. (23) and (24) become

$$\frac{\partial c'}{\partial t} = \nabla \cdot (D_e \nabla c' + D_{S,e} \nabla T') - (k_0 e^{-E/RT'}) c', \quad (23)$$

$$\begin{aligned} \rho C_p \frac{\partial T'}{\partial t} = \nabla \cdot (D_{D,e} \nabla c' + k_e \nabla T') \\ + [-(\Delta H_r)] (k_0 e^{-E/RT'}) c'. \end{aligned} \quad (24)$$

$$\frac{\partial \theta'}{\partial \tau} = \frac{\partial^2 \theta'}{\partial z^2} + \varepsilon \frac{\partial^2 \phi'}{\partial z^2} - \phi^2 \theta' \exp \left[\gamma \left(1 - \frac{1}{\phi'} \right) \right], \quad (25)$$

$$\frac{1}{Le} \frac{\partial \phi'}{\partial \tau} = \frac{\partial^2 \phi'}{\partial z^2} + \omega \frac{\partial^2 \theta'}{\partial z^2} + \beta' \phi^2 \theta' \exp \left[\gamma \left(1 - \frac{1}{\phi'} \right) \right], \quad (26)$$

where

$$\varepsilon = \frac{D_{S,e} T_s}{D_e c_s}, \quad \omega = \frac{D_{D,e} c_s}{k_e T_s}.$$

All the other non-dimensional parameters are the same with those in Eqs. (8) and (9). Eqs. (25) and (26) represent the modeling of RD systems with the thermodynamically coupled heat and mass fluxes excluding the coupling effects due to reaction when compared with Eqs. (8) and (9). After combining Eq. (20) with Eqs. (25) and (26), steady-state balance equations for a RD system with the coupled heat and mass transfer become

$$(1 - \beta' \varepsilon) \frac{d^2 \theta'}{dz^2} = \phi^2 \theta' \exp \left(-\frac{\gamma \beta' (\theta' - 1)}{1 - \beta' (\theta' - 1)} \right), \quad (27)$$

$$\left(\frac{\omega}{\beta'} - 1 \right) \frac{d^2 \phi'}{dz^2} = \beta' \phi^2 \left(1 - \frac{\phi' - 1}{\beta'} \right) \exp \left[\gamma \left(1 - \frac{1}{\phi'} \right) \right]. \quad (28)$$

Since the dynamic behavior of a RD system may be more apparent with the state-space diagrams, the temperature and concentration profiles are replaced with the spatial integral averages obtained from

$$\theta'(\tau) = \int_0^1 \theta'(z, \tau) dz, \quad (29)$$

$$\phi'(\tau) = \int_0^1 \phi'(z, \tau) dz. \quad (30)$$

4.0 Results

Non-isothermal reaction diffusion systems considered are the synthesis of vinyl chloride and dissociation of N_2O reactions. [Table 1](#) shows some of the experimental and assumed values of the parameters ([Hlavecek et al., 1969](#)) considered for these reaction systems, which have large values of β , and hence display relatively strong non-isothermal effects. The thermal diffusion coefficient is usually smaller by a factor of 10^2 – 10^3 than the ordinary diffusion coefficient for non-electrolytes and gases. Therefore, for the present analysis the values for ε and ω are assumed to be 0.001 for the both reaction systems. The Mathematica is used to solve the partial differential equations of mathematically and thermodynamically coupled systems of Eqs. [\(25\)](#) and [\(26\)](#) simultaneously. The numerical solutions from Mathematica are obtained with a ‘precision goal’ of 0.1, ‘maximum step size’ of 0.0005, and ‘maximum steps’ of infinity.

Table 1.

Experimental ([Hlavecek et al., 1969](#)) and assumed values of parameters used in the thermodynamically coupled model for the two industrial reaction systems

Reaction	φ	$\beta \approx \beta'$	γ	Le	ε^a	ω^a
Synthesis of vinyl chloride	0.27	0.25	6.5	0.1	0.001	0.001
Dissociation of N_2O	5.0	0.64	22.0	0.01 ^a	0.001	0.001

^a Assumed values.

[Figs. 1](#) and [2](#) show the dynamic behavior of concentrations and temperatures for the synthesis of vinyl chloride reaction and dissociation of N_2O reaction, respectively. In both the reaction systems, the surface of temperature closely follows the change in concentrations. As expected, the rise of temperature is relatively larger as the value of β increases in dissociation of N_2O reaction as seen in [Fig. 2](#).

Fig. 1 Dynamic behavior of thermodynamically coupled non-isothermal reaction-diffusion system of diffusion system of synthesis of vinyl chloride reaction: (a) concentration surface, (b) temperature surface. The parameters used are in Table1

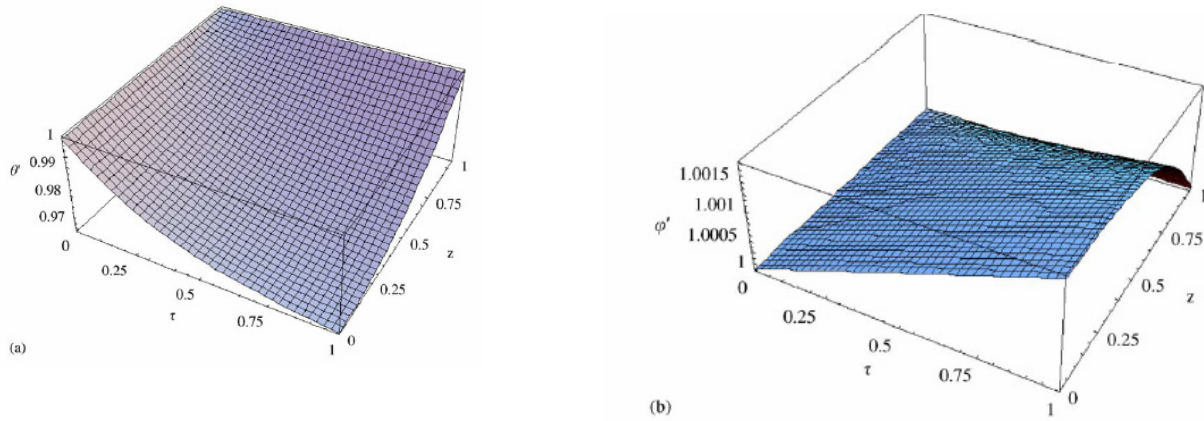
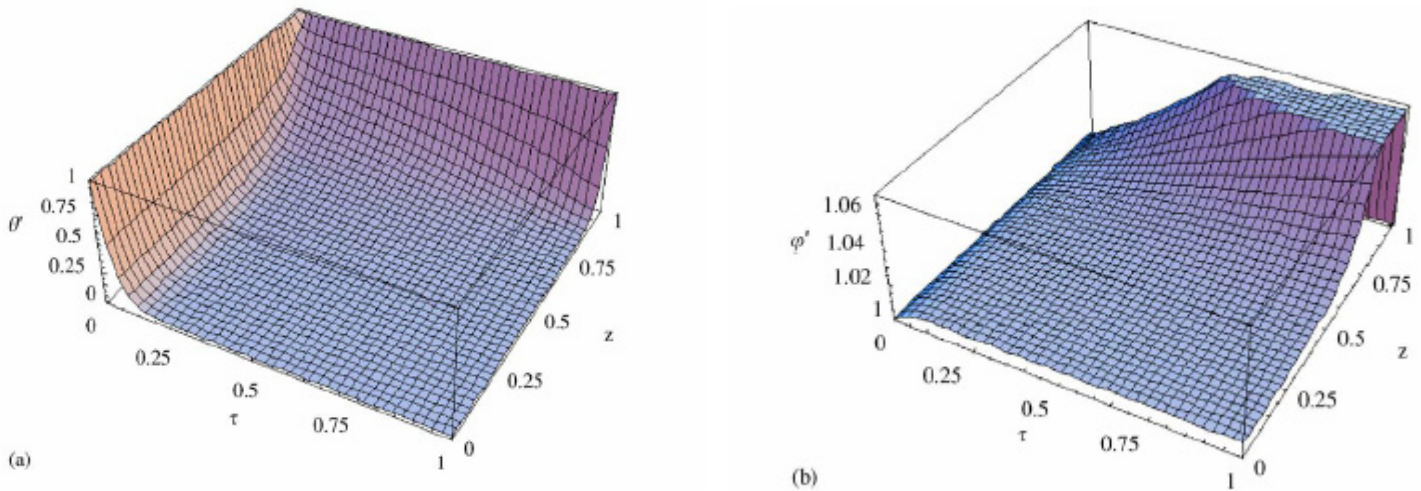


Fig. 2. Dynamic behavior of thermodynamically coupled non-isothermal reaction-diffusion system of dissociation of N_2O reaction: (a) concentration surface, (b) temperature surface. The parameters used are in [Table 1](#).



[Figs. 3](#) and [4](#) show the changes of the spatial integral averages of concentration and temperatures with time for the systems considered. [Figs. 3\(c\)](#) and [4\(c\)](#) show the state-space representation of temperature versus concentration when the time changes from zero to one. For the synthesis of vinyl chloride reaction system, temperature reaches its maximum value when the dimensionless concentration is around 0.97, as seen in [3 \(c\)](#)

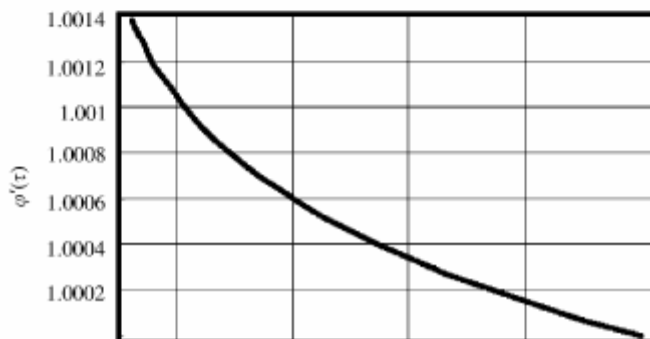
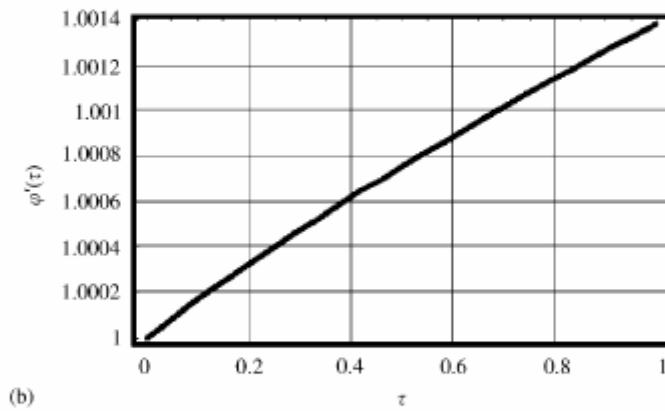
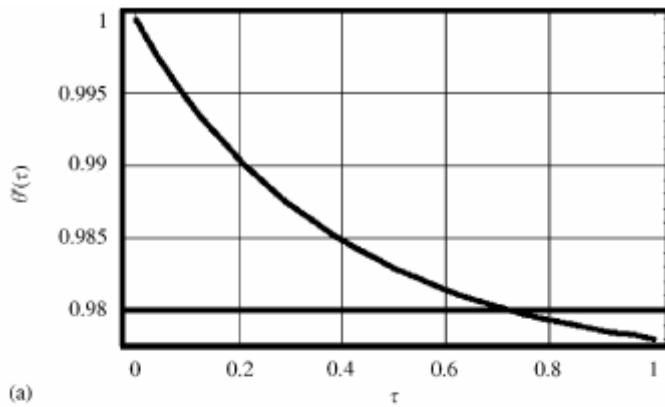


Fig. 3. Spatial integral averages for the synthesis of vinyl chloride reaction system: (a) change of concentration with time, (b) change of temperature with time, (c) change of temperature with concentration when the time varies between 0 and 1. The parameters used are in [Table 1](#).

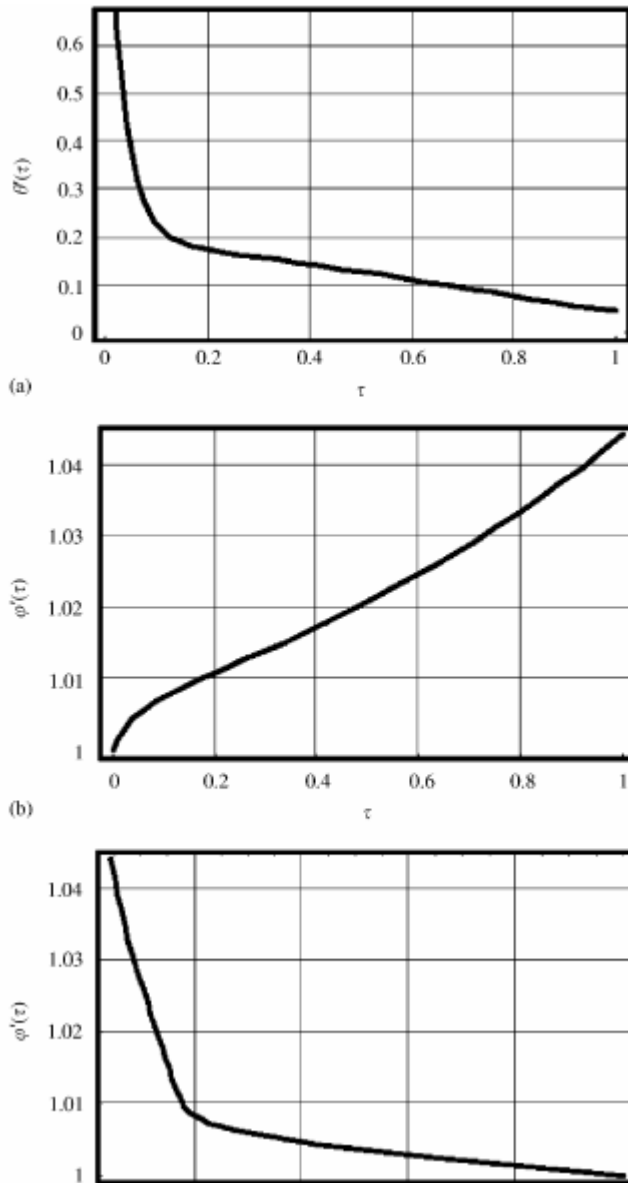


Fig. 4. Spatial integral averages for synthesis of dissociation of N_2O reaction system: (a) change of concentration with time, (b) change of temperature with time, (c) change of temperature with concentration when the time varies between 0 and 1. The parameters used are in [Table 1](#).

5.0 Conclusions

This analysis considers the thermodynamic coupling between heat and mass fluxes in the two industrial RD systems of synthesis of vinyl chloride and dissociation of N_2O reaction systems. The modeling with the coupling effects of Soret and Dufour would open the path to describe more complex RD systems by adding the two new controlling parameters into their dynamic behavior. The linear non-equilibrium thermodynamics approach can provide the quantified description of the fully coupled phenomena for systems not far from global equilibrium.

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