

On the equivalence of storage functions in controlled thermodynamic systems

N. Ha Hoang* Denis Dochain**

* *Department of Chemical Process Engineering and Control, University of Technology, VNU-HCM, 268 Ly Thuong Kiet Str., Dist. 10, HCM City, Vietnam (e-mail: ha.hoang@hcmut.edu.vn)*

** *ICTEAM, Université Catholique de Louvain, 1348 Louvain-la-Neuve, Belgium (e-mail: {denis.dochain}@uclouvain.be)*

Abstract: Motivated by thermodynamic concepts strongly related to the second law of thermodynamics, this paper deals with the mathematical foundations of thermodynamics to reconstruct some storage functions usable both for the stability analysis and control of homogeneous chemical processes through the case study of non isothermal continuous stirred tank reactors (CSTRs). Besides, the equivalence of the storage functions in the thermodynamics framework is also shown.

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1. INTRODUCTION

In the field of chemical engineering, thermodynamics plays a central role for the investigation of the behaviors of open reaction systems against spontaneous changes resulting from internal and external circumstances (Glansdorff and Prigogine (1971); Sandler (1999); Callen (1985); Favache and Dochain (2009)). It is shown that any dynamical evolution of the system states (such as temperature and concentration of species) as well as the direction of reversible chemical reactions etc. are directly linked to the energy and entropy transformations. Contrary to the intrinsic conservation of energy as stated by the first law of thermodynamics, the entropy transformation is not conserved due to the presence of the entropy production term (De Groot and Mazur (1962); Ruzskowski *et al.* (2005); Hoang *et al.* (2009, 2012b)). This term is non-negative and therefore, it characterizes the irreversibility of the system as shown in a large number of previous studies (Ydstie and Alonso (1997); Hangos *et al.* (2001); Otero-Muras *et al.* (2008); Dörfler *et al.* (2009); Hoang *et al.* (2010, 2011); Garcia-Sandoval *et al.* (2015)). In addition to the inherent irreversibility, the nonlinearities issued directly from the chemical reaction kinetics may give rise to (local) instabilities of the system (for example, multiple steady states or non-minimum phase behaviors (Favache and Dochain (2010); Hoang *et al.* (2013b))). Nevertheless, it is worth noting that major physical phenomena (such as heat and mass transfers and even, reaction kinetics etc.) taking place in the chemical reactor can be explained and modelled thanks to the frame of thermodynamics on the basis of the non-negative definiteness of the entropy production term (De Groot and Mazur (1962)). Simply speaking, thermodynamics allows to better understand and act more specifically on sources which generate the abnormality of the system dynamics. Consequently, thermodynamics provides a helpful tool and has been extensively used for the dynamical modelling, stability analysis

and control of chemical processes as seen in a large number of references (Dammers and Tels (1974); Tarbell (1977); Georgakis (1986); Srinivasan *et al.* (1998); Alonso and Ydstie (2001); Couenne *et al.* (2006); Jillson and Ydstie (2007); Eberard *et al.* (2007); Hoang *et al.* (2012a); Hudon and Bao (2012); Ramirez *et al.* (2013); Hoang and Dochain (2013a); Rodrigues *et al.* (2015)).

The central objective of this work is to propose some mathematical foundations of thermodynamics that could possibly exhibit a closer connection between the notion of generalized energy functions (i.e., storage functions) of system dynamics with the Lyapunov's stability theory (Khalil (2002)), usable for the stability analysis and control design of chemical reactors. More precisely, the contribution of this paper is twofold. First, we focus our attention on the geometric property of storage functions defined on the basis of the intensive and/or extensive variables which allows to derive candidate Lyapunov functions (CLFs). Second, the equivalence of the proposed storage functions is shown for the case of controlled thermodynamic systems. As shown in (Favache and Dochain (2009)), the continuous stirred tank reactors (CSTRs) belong to (general) thermodynamic systems. Throughout the paper, the CSTR model is reconsidered to illustrate the developments.

This paper is organized as follows. In section 2, the CSTR model and some thermodynamic concepts are reminded. Section 3 is dedicated to the mathematical foundations of thermodynamics required for the developments in this work. This section provides some preliminary results (strongly related to the concavity of the entropy function of homogeneous mixtures) and the one-to-one relationship between the thermodynamic variables which are instrumental in proving the main results of this work. Different thermodynamic storage functions and their equivalence for controlled chemical reactors are proposed in section 4. Section 5 ends the paper with some concluding remarks and perspectives.

Notations: The following notations are considered throughout this paper :

- \mathcal{Z} and \mathcal{W} are Banach space and its dual, respectively.
- $\tilde{\circ}$ denote the deviation form of the variable \circ with respect to some desired reference value \circ^* :

$$\tilde{\circ} = \circ - \circ^*$$
- \mathcal{R}_+^* denotes the set of positive real numbers.

2. THE CSTR CASE STUDY

2.1 The CSTR model

Let us consider a liquid phase reactor modelled with the CSTR in which one first order exothermic chemical reaction involving 2 chemical species A and B (of molar masses M_A and M_B , respectively) takes place. The reaction stoichiometry that represents the (molar) mass conservation is then given as follows (Srinivasan *et al.* (1998); Hoang and Dochain (2013a)) :

$$\nu_A M_A + \nu_B M_B = 0 \quad (1)$$

where ν_A and ν_B are the suitable signed stoichiometric coefficients : $-\nu_A = \nu_B = 1$.

Let us consider the following assumptions :

(H1) The fluid mixture is ideal, incompressible and under isobaric conditions.

(H2) The inlet of the reactor is fed by the only species A with the inlet molar flow rate F_{AI} at a given temperature T_I .

(H3) The heat flow rate \dot{Q}_J coming from the jacket given by the following relation,

$$\dot{Q}_J = \lambda(T_J - T) \quad (2)$$

with $\lambda > 0$ the heat exchange coefficient and the inlet molar flow rate F_{AI} are considered as process inputs.

(H4) The reaction rate is described by the mass action law so that (Luyben (1990)) :

$$rV = k(T)N_A \quad (3)$$

where the function $k(T)$ that depends on the temperature is the kinetics of the liquid phase reaction. The reaction kinetics $k(T)$ is monotone, non-negative and bounded in accordance to the thermodynamic principles by (Favache and Dochain (2010))¹ :

$$k(T) \geq 0, \quad \lim_{T \rightarrow 0} k(T) = 0 \quad \text{and} \quad \lim_{T \rightarrow +\infty} k(T) = k_{\max} \quad (4)$$

2.2 Thermodynamics based view for CSTR modeling

Let us first recall some thermodynamic concepts required for the theoretical developments in this work.

In equilibrium thermodynamics, the system variables are split into the extensive variables (such as the internal energy U , the entropy S , the volume V and the molar number N_i) and the intensive variables (such as the temperature T , the pressure P and the chemical potential

¹ We can easily check that (4) holds for the Arrhenius law given by $k(T) = k_0 \exp\left(\frac{-k_1}{T}\right)$ where k_0 is the kinetic constant and k_1 is the activation temperature.

μ_i). When isobaric conditions are considered, the variation of internal energy U is equal to that of the enthalpy H , given by considering the Gibbs equation (Callen (1985)) :

$$dH = \mu_A dN_A + \mu_B dN_B + T dS \quad (5)$$

From (5), an equivalent expression can be derived as follows :

$$dS = \frac{-\mu_A}{T} dN_A + \frac{-\mu_B}{T} dN_B + \frac{1}{T} dH \quad (6)$$

since the thermodynamic temperature is strictly positive (i.e., $T > 0$).

Similar to the other macroscopic quantities, the entropy S (6) is an extensive variable and is then a homogeneous function of degree 1 with respect to (N_A, N_B, H) . Consequently, one gets by using Euler's theorem (Callen (1985)) :

$$S(N_A, N_B, H) = \frac{-\mu_A}{T} N_A + \frac{-\mu_B}{T} N_B + \frac{1}{T} H \quad (7)$$

(6) can then be rewritten in a compact form as follows :

$$dS = w^T dZ \quad \Rightarrow \quad w(Z)^T = \frac{\partial S(Z)}{\partial Z} \quad (8)$$

where :

$$w(Z) = \left(\frac{-\mu_A}{T}, \frac{-\mu_B}{T}, \frac{1}{T} \right)^T, \quad Z = (N_A, N_B, H)^T \quad (9)$$

and T denotes the transpose operator.

Assume that we hold the total liquid mass constant,

$$m_t = M_A N_A + M_B N_B = \text{const} \quad (10)$$

The reaction system dynamics is then derived on the basis of the energy and material balance equations considered for the extensive variables vector Z (9) which associated to the entropy representation (6) (Sandler (1999)). From the mathematical point of view, the system dynamics is typically described by ordinary differential equations (ODEs) with affine inputs as follows (Favache and Dochain (2009); Hoang *et al.* (2012a); Hoang and Dochain (2013a)) :

$$\frac{dZ}{dt} = f(Z) + g(Z) u \quad (11)$$

with :

$$f(Z) = \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} rV, \quad g(Z) = \begin{pmatrix} \frac{N_B M_B}{N_B M_A} & 0 \\ -\frac{m_t}{N_B M_A} & 0 \\ \left[h_{AI} - \frac{M_A H}{m_t} \right] & 1 \end{pmatrix} \quad (12)$$

and

$$u = \begin{pmatrix} F_{AI} \\ \dot{Q}_J \end{pmatrix} \quad (13)$$

where h_{AI} is the inlet molar enthalpy of the species A .

In what follows, we shall propose some mathematical foundations of thermodynamics which are instrumental in deriving different storage functions usable for both the stability analysis and control design of chemical reactors.

3. THE MATHEMATICAL FOUNDATIONS OF THERMODYNAMICS

3.1 On the concavity of the entropy function

As the reaction mixture is assumed to be homogeneous (i.e., with liquid phase), the entropy function $S(Z)$ de-

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