Thermodynamic approach for Lyapunov based control

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Abstract: This paper focuses on non linear control of non isothermal Continuous Stirred Tank Reactors (CSTRs). The model of the CSTR is thermodynamically consistent in order to apply the control strategy based on the concavity of the entropy function and the use of thermodynamic availability as Lyapunov function. More precisely the stabilization problem of continuous chemical reactors is addressed operated at an unstable open loop equilibrium point. The chosen control variable is the jacket temperature. In this paper we propose a state feedback strategy to insure asymptotic stability with physically admissible control variable solicitations. Theoretical developments are illustrated on a first order chemical reaction.

Keywords: Lyapunov based control, Irreversible thermodynamics, Non isothermal CSTR, Multiple steady states, Entropy.

1. INTRODUCTION

Continuous Stirred Tank Reactors (CSTR) have been widely studied in the literature with respect to process control design (Luyben (1990); Alvarez (1999); Hua (2000); Guo (2001); Hoang (2008)). Numerous strategies have been developed to control such non linear systems. Let us cite for example: feedback linearization (Viel (1997)) for control under constraints, nonlinear PI control (Alvarez (1999)), classical Lyapunov based control (Antonellia (2003)), nonlinear adaptive control (Guo (2001)) and more recently thermodynamical Lyapunov based control (Hoang (2008)).

Besides these control problems, observation/estimation strategies have been developed in the case of under sensored CSTRs (Gibon-Fargeot (2000); Dochain (2009)). Usually, the reactor temperature is the only on-line available measurement. Then the purpose is to estimate the missing state variables that are used in the control strategy.

In this paper we focus on the control purposes only and we assume that concentrations and temperature are measured. This control synthesis is based on thermodynamic concepts defined in Callen (1985) and more recently in (Ruszkowski (2005); Ydstie (1997)) and (Hoang (2008)). More precisely, we propose a Lyapunov based approach for the stabilization of CSTR about unstable steady state as in (Hoang (2008)). This is done thanks to the Lyapunov function issued from thermodynamics consideration: the availability function $\mathcal{A}$ (Ruszkowski (2005)).

In Hoang (2008), we proposed feedback laws involving inlet and jacket temperatures as well as inlet flows. These feedback laws were obtained by imposing that the time derivative of the availability $\mathcal{A}$ remains negative, insuring consequently the global asymptotic stability. However, no care was given on the amplitude of the controls. Moreover the temperature of the reactor had to be inverted and the feedback laws had in some case some oscillatory behaviors about the critical point.

The main contribution of this paper with respect to previous work (Hoang (2008)) is the redesign of the exponential asymptotic controller in order to prevent excessive control demand and oscillation problems. In this way the obtained controller is practically more efficient. The price to pay is that global asymptotic stability is obtained on some validity domain only.

This paper is organized as follows: in section 2, we remind thermodynamical concepts and variables necessary to construct thermodynamic availability. This latter function is the Lyapunov candidate of the method. In section 3 the dynamic model of the considered CSTR is presented and analyzed. Section 4 is devoted to the design of the state feedback insuring asymptotic stability. Simulation results are given in section 5. It is shown that the resulting control leads to admissible manipulated control variables.

2. THERMODYNAMIC BASIS FOR AN AVAILABILITY FUNCTION

Irreversible thermodynamics concept will play a leading role in the methodology used for the design of the Lyapunov function (Ruszkowski (2005); Hoang (2008)). In this section we review the main ideas concerning this thermodynamical approach and the construction of the candidate Lyapunov function: the availability function in the case of an homogeneous phase.

In equilibrium thermodynamics, the system variables are divided into extensive and intensive variables, depending on whether their values depend on the "size" of the system or not. The internal energy of a homogeneous system is then expressed in terms of products of pairings of energy conjugate variables such as pressure $P/$ volume V, temperature $T/$ entropy S and chemical potential $\mu_i/$ mole number n_i for each species i of the mixture.

The fundamental relation of thermodynamics expresses the entropy S of a given phase as a function of the so called extensive variables $Z = (U, V, n_i)$ by the Gibbs equation:

$$dS = \frac{1}{T}dU + \frac{P}{T}dV + \sum_{i=1}^{n_c} \frac{-\mu_i}{T}dn_i. \tag{1}$$

It can also be written as:

$$dS = w^T dZ \tag{2}$$

with $w = (\frac{1}{T}, \frac{P}{T}, \frac{-\mu_i}{T})$.

Since the entropy S is an extensive variable, it is a homogenous function of degree 1 of Z (Callen (1985)). From Euler's theorem we get:

$$S(Z) = w^T Z \tag{3}$$

Equation (2) can also be applied in irreversible thermodynamics as soon as the local state equilibrium is assumed: it postulates that the present state of the homogeneous system in any evolution can be characterized by the same variables as at equilibrium and is independent on the rate of evolution. So (2) can also be applied at any time.

Moreover, it is well known that balance equations can be established for Z= (U, V, n_i) as well as for the entropy S but this latter is not conservative: in irreversible thermodynamics there is a source term σ which is always positive from the the second law of thermodynamics. This term represents the irreversible entropy production: the energy $T\sigma$ associated to this term represents the energy lost from material, space or thermal domains and that will never more contribute to some physical works. As a consequence of (2), the entropy balance can alternatively be written as:

$$\frac{dS}{dt} = w^T \frac{dZ}{dt} \tag{4}$$

Finally let us notice that for homogeneous thermodynamical systems (one phase only), the entropy function $S(Z)$ is necessarily strictly concave (see Callen (1985)) as shown in Fig. 1.

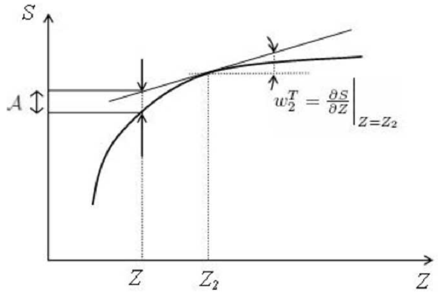

Fig. 1. Entropy and availability functions w. r. to Z.

From these observations, it can be shown (see Ydstie (1997)) that the non negative function:

$$\mathcal{A}(Z) = S_2 + w_2^T(Z - Z_2) - S(Z) \geq 0 \tag{5}$$

where Z_2 is some fixed reference point (for example the desired set point for control), is a measure of the distance between entropy $S(Z)$ and its tangent plane passing through Z_2. It is geometrically presented in Fig. 1. The slope of the tangent plane is related to intensive vector $w(Z)$ calculated at $Z = Z_2$.

As soon as we consider homogeneous mixture, S remains concave and then $\mathcal{A}$ remains also non negative. As a consequence, A is a natural Lyapunov candidate. It remains to build a feedback law to insure:

$$\frac{d\mathcal{A}}{dt} \leq 0. \tag{6}$$

3. CASE STUDY: A NON ISOTHERMAL CSTR MODEL

3.1 Assumptions of the model

We consider a jacketed homogeneous CSTR with the following first-order chemical reaction: $A \rightarrow B$. The temperature of the jacket T_w is supposed to be uniform and is used for the control purpose. The dynamics of the CSTR is deduced from volume, material and energy balances.

The following assumptions are made:

- The fluid is incompressible and the reaction mixture is supposed to be ideal.
- The two species are supposed to have the same partial molar volume v.
- At the inlet of the reactor, the pure component A is fed at temperature T_e.
- The reaction volume V is supposed to be constant.
- The heat flow exchanged with the jacket is represented by $\dot{Q} = \lambda(T_w - T)$.
- The kinetics of the liquid phase reaction is modelled thanks to the Arrhenius law. The reaction rate r_v is given by $k_0 \exp(\frac{-k_1}{T})\frac{n_A}{V}$.

In Tables (1,2) are given the notations and numerical values that will be used for modelling and simulation. Finally let us notice that constant volume assumption implies that the total number of moles n_T is constant since the two species have the same partial molar volume.

Notation	unit	
F_{Ae}	mol/s	Inlet molar flow rate of A
F_A	mol/s	Outlet molar flow rate of A
F_B	mol/s	Outlet molar flow rate of B
F	mol/s	Total outlet molar flow rate
h_{Ae}	J/mol	Inlet molar enthalpy of A
h_i	J/mol	Molar enthalpy of species i $(i = A, B)$
H	J	Total enthalpy of the mixture
n_A	mol	Mole number of species A
n_B	mol	Mole number of species B
T	K	Temperature in the CSTR
n_T	mol	Total mole number
r_v	$mol/m^3/s$	Reaction rate
U	J	Internal energy
$x_i = \frac{n_i}{n_T}$		Molar fraction of species i, $i = A, B$

Table 1. Notation of the variables of the model.

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