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The port Hamiltonian approach to modeling and control of Continuous Stirred Tank Reactors

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ABSTRACT

This paper proposes a thermodynamical pseudo-Hamiltonian formulation of Continuous Stirred Tank Reactor model in which takes place some chemical reaction. This is done both in the isothermal and non isothermal cases. It is shown that the Gibbs free energy and the opposite of entropy can be chosen as Hamiltonian function respectively. For the non isothermal case, the so-called Interconnection and Damping Assignment Passivity Based Control method is applied to stabilize the system at a desired state. For this general reaction scheme, the control problem is shown to be easy to solve as soon as the closed loop Hamiltonian function is chosen to be proportional to the so-called thermodynamic availability function. Simulation results based on a simple first order reaction and operating conditions leading to multiple steady states of the CSTR are given to validate the proposed control design procedure.

1. Introduction

Port Hamiltonian framework has been intensively used in electrical, mechanical and electromechanical domains since the initial works of [30,25]. It has been shown to be very powerful especially for the control of nonlinear systems, for example using the Interconnection and Damping Assignment Passivity Based Control (IDA-PBC) method [26]. Indeed the total energy of the system, usable as Lyapunov function for control purpose, is considered as the central element of such formalism. One would have expected that this formulation could generalize to physico-chemical processes thanks to irreversible thermodynamics framework. Unfortunately in the case of irreversible thermodynamic systems the links between thermodynamics and system theory are quite difficult to exhibit from a geometrical point of view [8,9] and remain an open problem even if this subject attracted a large amount of researches these last decades. The first studies pointing out the relations between irreversible thermodynamics and system theory are the pionneering works of [12] in which the stability near of the equilibrium state is analyzed in terms of irreversible entropy production. These works have been later extended to the case of systems far from the equilibrium defining the so-called availability function by [1,35]. Indeed it has been shown that in the case of homogeneous systems the thermodynamic availability function can be used for stability analysis and in some cases for control purpose. Many extensions of these works to the stability analysis of distributed systems or system networks have been proposed during the nineties [35,15,16,2,29,22].

More recently much attention has been paid on the formulation of process systems as port Hamiltonian systems. The first attempts in such modeling proposed an analogy with mechanical or electrical systems [16]. Yet the behavior of irreversible thermodynamic systems is quite different as soon as the thermal domain is considered. Indeed in the mechanical or electrical fields, dynamical models can be derived from the mechanical or electrical energy variations with respect to state variables, a part of this energy being dissipated. In the case of thermodynamic systems, the thermal domain plays an important role (*e.g.* in the kinetics of chemical reactions) and cannot be neglected. Furthermore, from the first principle of thermodynamics stating the strict conservation of energy, the use of the internal energy as Hamiltonian function does not allow to express the irreversible behavior of the system. Many recent works propose appropriate geometric structure and Hamiltonian function to describe in a thermodynamic coherent way irreversible thermodynamic systems. They can be divided in two classes of studies. The first ones [24,34,21], most decoupled from thermodynamics concepts, propose some systematic approach to define pseudo-Hamiltonian structure. The drawback of these approaches is the lack of physical interpretation of the Hamiltonian function for a possible use as closed loop Lyapunov function. The second ones

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