Irreversible thermodynamics and process control

Keywords : Tubular reactor; Distributed parameter systems; Infinite dimensional systems; Control.

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***Abstract* – This research activity deals with the analysis of the link between irreversible thermodynamics, system theory and process control. The objective is to find out new control design paradigms based the knowledge of thermodynamics and its role in the energy representation ic reaction systems.**

The universal character of classical thermodynamics comes from the fact that it does not deal with a restricted class of systems and does not depend on any model nor assumptions on the structure of matter. Unlike other branches of classical science (such as for instance mechanics or electromagnetics), thermodynamics does not try to explain the consequences of some formulated laws (as it is the case with the Newton's laws or the Maxwell's equations). The classical thermodynamic theory relates concepts that seem to be very different such as heat and work, and it explains equally well the working of a combined-cycle gas turbine power plant, of a fridge or of a car engine. Even in biology, thermodynamics shows up to be of primary importance. Indeed most of the exchanges in the human body are based on thermodynamic equilibria (e.g. the essential role of osmotic pressure for the kidneys). In chemical engineering, thermodynamics plays a central role in the modelling of chemical processes. Indeed typical phenomena that are going on in chemical reactors are heat transfers, chemical reactions, mass transfers... These all are phenomena that can be explained and modelled by the thermodynamics.

The analysis and design of control algorithms are largely based on system theory tools, and in particular on the stability "à la Lyapunov" which is indeed intrinsically based and justified on energy considerations. It is therefore natural to consider the thermodynamics theory for the control design of chemical processes. However, if in many situations it is rather easy to describe the Lyapunov theory in terms of energy for electrical and mechanical systems, this is unfortunately not the case for reaction systems. One central idea is to take advantage of the positivity of the state variables to consider Lyapunov functions that are not the classical quadratic functions, that are representative of the energy of mechanical and electrical systems, but not that of reactions systems, for which entropy-based functions are adapted.

Many research progresses have been performed over the past decade. These include in particular the following.

- The design of asymptotic observers, i.e. state observers that do not require the knowledge of the process kinetics, in a thermodynamically rigourous framework [1]
- The stability analysis of the continuous stirred tank reactor (CSTR), the reference case study in process control, by considering several thermodynamics based functions (entropy, entropy production, energy) [4]
- The design of power-shaping controllers by considering the entropy production as the potential function [3]
- The development of a general methodology for deriving the expression of the contact structure elements (i.e. the Legendre submanifold generating function and the contact Hamiltonian function) from the fundamental relation of a thermodynamic system and from its balance equations. Some features of the dynamical behaviour of a system with properties of its contact structure elements have been related [2]. For instance, an equilibrium point of the system is expressed by a critical point of the contact Hamiltonian function. Lyapunov's first stability theorem has also been related to characteristics of the contact Hamiltonian function and of the Legendre submanifold generating function. This has allowed to state a sufficient stability criterion in terms of the contact structure of a system. This stability criterion has then been interpreted using physical considerations.

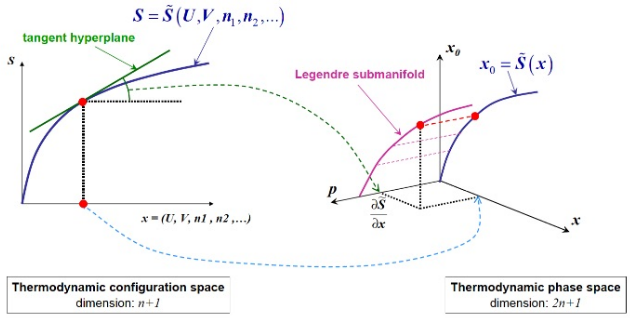

Figure 1: The Gibbs' relation in the thermodynamic state space.

- The derivation of a thermodynamically stable evolution criterion, its use for selecting appropriate potential functions, as well as its use in comparing Hamitonian system representation and Brayton-Moser representation (considered in power-shaping control) [6]
- The analysis of the stability and passivity properties of a class of thermodynamic systems, i.e. those constituted by multiple spatially homogeneous dynamical subsystems modeled by ordinary differential equations, by considering the internal entropy production as a Lyapunov function when the system is isolated and as a storage function when the system interacts with the surroundings [5]

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