Thermodynamic-based contributions on modeling and control by Prof. Antonio A. Alonso

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ABSTRACT

In this manuscript, we summarize some of the works initiated, developed and supervised by Prof. Antonio A. Alonso in the context of process and bioprocess engineering. In particular, we focus on those works related to modeling, optimization and control in which the Thermodynamics played a key role, namely: (i) the thermal sterilization of food products using steam and super-heated water retorts; (ii) modeling, model reduction and control based on first and second laws of thermodynamics; and (iii) plant-wide control of large dimensional systems using the link among thermodynamics, passivity and Lyapunov theory.

1. FOOD STERILIZATION PROCESS

Modeling, simulation, control and optimization of the thermal sterilization of food products have been regular research fields since the beginning of Prof. Antonio A. Alonso's career (Alonso et al., 1997, 1998, 2013, 2021). In particular, he focused on the thermal sterilization using a steam retort. In this type of retorts, there is a mixture of steam, water and air. The model of the sterilization unit was derived by combining mass and energy balances, thermodynamic properties of steam-air mixtures, equilibrium relationships, empirical formulas to compute the fluid flow through the valves, among other. The mass of water exchanged between the liquid and vapor phases was calculated, in an iterative process, by assuming equilibrium between the two phases. Despite the assumptions made in order to improve the efficiency of the simulations, validation using experimental data obtained in a pilot-scale retort demonstrated the predictive capabilities of the model under a wide range of operating conditions. Modeling and optimization of industrial super-heated water retorts were also considered (Pitarch et al., 2021). The sterilization section consisted of two units: a plate heat exchanger (PHE) that used steam to produce super-heated water; and the retort that used such super-heated water to sterilize the food products. In this case, the phase change from steam to water was produced in the PHE so, the modeling approach of this unit was similar to the *steam sterilizer*.

2. THERMODYNAMIC-BASED MODELING AND ROBUST CONTROL

Typically, the approach to derive the structure of a white-box mathematical models is based on the macroscopic balances of fundamental quantities (mass, energy and momentum). In the PhD Thesis by Vilas (2008), supervised by Prof. Alonso, a different, although equivalent, approach was followed. In this regard, the first law of thermodynamics, together with some well known mathematical theorems (such as Gauss, Taylor, Reynolds transport, Cauchy's second law of motion, among other) were used to derive the mathematical structure of the model that was completed with the relationships between the density fluxes (heat, mass, momentum) and thermodynamic forces (gradients of temperature, concentration, fluid velocity) impulsing such fluxes. Such relationships are known as the *constitutive equations.* The second law of thermodynamics provided us the framework to establish them. Such law states that there exists a state function called *entropy* (extensive magnitude) and its variation, that can be split into two contributions, one related to the internal changes on the system and the other related to the exchanges with the surroundings. The Gibbs equation was used to obtain the structure of the entropy production term and to define the variables known as *intensive variables.* With these preliminaries the constitutive equations were obtained, and a first order (linear) Taylor series approximation was derived. Finally, the second law was employed to obtain the constraints on the coefficients of the linear version of the constitutive equation. Thermodynamics allowed us not only to derive the mathematical structure of a model in an elegant way but it was also used as the connecting thread between the different tasks of such thesis. In particular, use was made of the dissipative nature of diffusive process to derive reduced order models and to design control laws that dealt with model uncertainties.

3. PLANT-WIDE CONTROL

This topic attracted the attention of Prof. Antonio A. Alonso as a challenging problem that arises when the dimension of the system to be controlled increases and the classical control design approaches become unsolvable for these large systems. In this aim, in the work by Antelo et al. (2007), we made use of the existing link thermodynamics with passivity and Lyapunov theory, process networks and systems theory (Alonso and Erik Ydstie, 1996; Ydstie and Alonso, 1997; Hangos et al., 1999) to derive robust decentralized controllers (Alonso and Ydstie, 2001), that ensure complete plant stability. As a first step, the considered process system is decomposed into abstract mass and energy inventory networks, a graph representation of the process flowsheet defined by a given number of well mixed homogeneous material regions connected by material and energy fluxes we will refer to as nodes, plus an extra region which represents the environment. In this framework, conceptual inventory control loops are then designed for the mass and energy layers to guarantee that the states of the plant, both in terms of extensive and intensive properties, will converge to a compact convex region defined by constant inventories. This result by itself does not ensure the convergence of intensive variables to a desired operation point as complex nonlinear dynamic phenomena such as multiplicity of steady states may appear in the invariant set. In order to avoid these phenomena, thermodynamics naturally provides the designer, in these convex regions, with a legitimate storage or Lyapunov function candidate, the entropy (which has a definite curvature – concavity, and it has a well-defined maximum in those regions), that can be employed to ensure global stability. Based on this, the control structure design procedure is completed with the realization of the conceptual inventory and intensive variable control loops over the available degrees of freedom in the system. Finally, the entropy balance is revealed as a powerful tool to analyze the stability or instability of the potential steady states existing on a process system.

In the work by Antelo et al. (2008), we successfully applied the previously described plant-wide control methodology based on thermodynamics to the highly non-linear, open-loop unstable Tennessee Eastman Process (TEP) benchmark by Downs and Vogel (1993). Decentralized control structures for both sections we defined in the TEP (reaction and separation networks) as well as for the overall process were designed, ensuring simultaneously stabilization of both plant extensive and intensive variables. However, the dynamic performance tests carried out indicated that proposed inventory control design is not enough to ensure the global stability of the TEP since there exists problems with the dissipative capacity of the reactor network due to the fact that the coolant it is unable to extract all the reaction heat generated in the reactor. As a consequence, the need for intensive variable control (which preserves the dissipative property of a network) emerges as the next step in the design procedure in order to avoid stability problems, ensuring the appropriate convergence rate and satisfying quality, safety and/or environmental requirements. We proposed a different approach for the intensive variable loops realization by considering the set points of the inventory control loops as the manipulated variables in the composition loops. Finally, the decentralized thermodynamic based control control structure was tested dynamically against selected disturbances and step changes in defined set points showing a proper performance.

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