Extended Irreversible Thermodynamics (E.I.T.) for Chemical Reactor Stability Analysis

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The concept of stability is of particular importance to the optimal design and successful control of numerous traditional as well as novel unit operations in modern chemical process industries. Despite the fact that the stability of processes described as Lumped Parameter Systems (LPS) can be reliably established on the basis of ordinary differential equation (ODE) formulations, the respective procedure for examining the stability of Distributed Parameter Systems (DPS) need inevitably rely on first-principle partial differential equation (PDE) formulations, whose stability is an open and hard problem in the field of Applied Mathematics and Numerical Analysis. Industrial data-driven control approaches are of course more amenable to statistical processing, but cannot compensate for the lack of understanding produced by discounting process physics. Conversely, first-principle conservation laws can yield very complex PDE models of systems. We call multiphysics DPS the systems that feature strong interdependence of at least two PDEs. The complexity of PDEs results in a lack of explicit criteria for their spatiotemporal stability, often necessitating expensive PDE simulations just to draw conclusions about simpler questions. A meaningful endeavor is thus to take a step deeper into the generality of thermodynamic laws, in order to capitalize on our intuition regarding the conservation and availability of energy. Therefore, a Lyapunov-like energy function is defined via entropy and used for stability analysis. Thermodynamic laws, phenomenological equations and energy methods can thus provide the physical insight required for stability analysis and control, if the DPS process is well understood.

Classical (CIT) and Extended (EIT) Irreversible Thermodynamics Theory (Jou et al., 1996) rely on the generality of the First and Second Thermodynamic Laws that govern LPS and DPS alike. The basis of a CIT/EIT mathematical formulation for examining stability is the entropy balance, the monotonic increase of the entropy function and the monotonic decrease of its time derivative. Entropy can be considered an additional state variable, with a custom-defined total differential: the touchstone is the completeness of the problem-specific entropy function (sigma) postulated. Phenomenology is thus vital, but this only means one cannot study a DPS inadequately known.

In the present study we develop a systematic methodology aimed at quantitative stability investigation for two specific process examples from the realm of chemical reactor engineering. The first system is an irreversible CSTR reactor (coupled heat and molar balances, multiplicity); the second system is a irreversible exothermic PFR reactor (coupled heat and molar balances). These prototype systems have been modeled both as approximate ODE and as 1D-PDE systems, employing a variety of tools (phase plane analysis, explicit PDE simulation via FEMLAB v. 3.0, and mathematical analysis that relies on defining all the intensive and conjugate thermodynamic variables, and manipulating the relevant Lyapunov-like storage function via the Second Law).