64e Integrating Physics and Process Control

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Computational chemistry provides a methods for anlysis In this paper we integrate the passivity theory of nonlinear control, molecular, non equilibrium molecular dynamics and statistical mechanics using inherent passivity property of distributed parameter chemical process systems. We show that the operator mapping flows to inventories in a coarse grained (macroscopic) system is passive. This demonstrate that this leads very naturally to control systems that focus on the controlling average system properties and methods for control that can be linked to thermostating in molecular dynamics. Input Strictly Passive (ISP) feedback can therefore be used to achieve input-output stability. Examples of ISP controllers include the PID controller, parameter adaptive feedforward control, optimal controllers and many nonlinear and gain scheduling controllers. Input output stability and convergence of inventories like total mass and energy guarantee that other internal state variables belong to invariant sets. But, this does not necessarily imply convergence since a stabilizability condition, known as strict state passivity, must be satisfied. In this paper we use the 2nd law of thermodynamics to develop sufficient conditions for strict state passivity in the space of intensive variables. The theory relies on the following two assumptions: (1) The hypothesis of local equilibrium and (2) That a local entropy is defined using semi-classical statistical mechanics. These assumptions allow us to define a local entropy function for the coarse grained system which is homogeneous degree one, concave and has positive temperature. Subject to these conditions we develop stability theory for conjugate variables like temperature, pressure and chemical potential in infinite dimensional reaction-diffusion-convection systems. In classical irreversible thermodynamics this type of analysis assumes linearity and symmetry of transport relations. The use of Gibbs tangent plane condition allows us to define a Lyapunov like storage function for passivity design which gives stability criteria for nonlinear problems. The resulting sufficient condition for stability can be expressed in terms of dimensionless groups, similar to the (second) Damkohler number. Simple simulation examples illustrate the application of the theory.

Keywords: Process Control, Coarse graining, Distributed Parameter System, Irreversible Thermodynamics, Feedback, Passivity, Invariant set, Stability, Entropy, Reciprocity relations, Nonlinear, Convexity, Minimum Entropy Production.