

454b Process Networks with Chemical Engineering Applications

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A large number of natural and engineered systems can be modeled using networked representations. The dynamics at each node of these representations have a finite dimensional state description and the flows between nodes are driven by a potential difference. Our paper will deal with a certain class of networks called process networks. In a process network, there exists a convex scalar potential which can be interpreted as the entropy of the node. This formulation is broad enough to include a wide range of applications, including networks made up of interconnected chemical processes, biological networks, and supply chain networks.

The structural properties of the network are defined using a graph with three general classes of elements: nodes, terminals, and flows. These classes allow for descriptions of the interactions within the network and between multiple networks, as well as chemical/physical manipulation at the various well-mixed units that make up the network.

The flow and storage of material and energy are defined using vectors of inventories that can represent extensive variables. Examples of inventories include total mass, energy, number of particles, or other discrete components. At each node, the state is uniquely defined by the vector of inventories. Also, a vector of intensive variables is defined at each node related to the inventories by a partial derivative of the entropy function. The difference of these potentials between connected nodes act as driving forces for flow, similar to the relationship between current and voltage in electrical networks.

By considering only the topology of the system and basic conservation principles, a result analogous to Tellegen's Theorem of electrical circuit theory is produced. This development shows the orthogonal relationship between flow and potentials throughout the network. Using this result and passivity theory, a network is shown to converge to a stationary point when the flow relationships are positive. We show that the classical Joule-Thompson flow satisfies such a relationship.

An example network was developed to show passivity. This network represents a plantwide process system consisting of a reactor, a 15 stage distillation column, a mixer and a splitter. Each process unit, distillation plate, reboiler and condenser can be modeled as nodes in a complex network which can be extended to include more detail and more units. By introducing inventory and flow controllers for each unit while satisfying degree of freedom requirements, the system inventories are controlled to set-points when disturbances are introduced to the system. These set-points include the overall mass in each process unit, and the purity of the product flows, while the disturbances are introduced by varying the inlet feed rate and a change to the product purity requirement.