AN AGENT-BASED FRAMEWORK FOR CONTROL OF REACTOR NETWORKS WITH AUTOCATALYTIC REPLICATORS

Eric Tatara, Fouad Teymour, and Ali Cinar

Department of Chemical and Environmental Engineering, Illinois Institute of Technology, Chicago, IL 60616

Abstract: Several recent studies on autocatalytic reactions in single and coupled continuous stirred-tank reactor (CSTR) networks have demonstrated a rich spectrum of complex behavior. From a control systems perspective, the operating regime of a CSTR network can be manipulated by changing the flow rates between the reactors. Systems of more than one CSTR require multiple controllers and may need transients through several operating regimes to achieve the desired operation. This may require a hierarchical control structure whereby local control objectives can change dynamically in order to achieve the global control objective of the system. An agent-based control system is used to observe and control various aspects of a CSTR network. The primary focus of analyzing complex emergent behavior is demonstrating methods or combinations of methods that influence the behavior and capabilities of the agent-based control system. Simulation studies illustrate scenarios of interest, especially conditions that lead to emergent behavior.

Keywords: Intelligent Agents, Agent-Based Control, Reactor Networks

1. INTRODUCTION

The behavior of continuous stirred tank reactors (CSTRs) has been studied extensively over the past several decades. Fascinating static and dynamic phenomena have been observed for many classes of reactions including autothermal reactions, autocatalytic reactions and polymerization reactions. The analysis of Uppal and Ray (1974) on the behavior of a CSTR with a non-isothermal reaction was one of the first thorough investigations of complex behavior in chemical reaction systems, extending the initial ideas presented by Bilous and Amundson (1955). Complex dynamic behavior has been identified through analytical solutions of the state equations and their stability characteristics. Further investigation of the non-isothermal system (Uppal *et al.*, 1976; Farr and Aris, 1986) using the reactor feed flow rate as a bifurcation parameter yield even more types of complex behavior, such as mushrooms and isolas.

The work of Lin (1981) and Gray and Scott (1983) on the isothermal autocatalytic reaction $A+nB \rightarrow (n+1)B$ with decay $B \rightarrow C$ show that cubic ($n = 2$) and quadratic ($n = 1$) autocatalytic reactions exhibit similar behavior to non-isothermal reactions. The solution multiplicities include isolas, mushrooms and limit cycles. Further work has determined how the various model parameters affect the stability criteria and conditions for multiplicity as well as more sophisticated numerical analysis of the periodic solutions (Gray and Scott, 1984). Birol and Teymour (2000) have studied isothermal autocatalysis when two competing species are introduced to the system. It was shown that with N species, although there may be as many as $2(2^N - 1)$ steady states, only one species can exist stably in the reactor as $t \rightarrow \infty$.

If several identical CSTRs are connected, such that material is exchanged between them, the system becomes spatially heterogeneous compared with a single CSTR. The degree of heterogeneity can be varied by manipulating the interconnections between reactors. Taylor and Kevrekidis (1993) have extensively studied the effects of reactor coupling via numerical bifurcation techniques on the non-isothermal $A \to B$ system. Oscillatory states tend to synchronize when the frequency of the oscillations in each reactor are not too different. Weak coupling of the reactors is usually used, since strong coupling of a reactor network causes the network to behave as one large reactor.

Recent work on multiple reactor configurations with cubic autocatalytic reactions has demonstrated that spatial heterogeneity enlarges the boundaries of species survival (Birol *et al.*, 2002). Furthermore, detailed analysis has shown that networks of reactors with autocatalytic replicators produce highly complex bifurcation structures and that the number of steady states increases exponentially with size of the system (Tatara *et al.*, 2003). With the autocatalytic reaction scheme, larger networks permit more steady states and spatial combinations thereof than smaller networks. Although much of the bifurcation diagram is dominated by unstable steady states, there exists a number of stable steady states for a large range of feed flow rates.

In the case of a single CSTR with competing autocatalytic species, a nonlinear control scheme is necessary to first remove the invading species and then return the host species to the original steady state (Chaivorapoj *et al.*, 2003). Systems of more than one CSTR require multiple controllers and may require transients through several operating regimes to achieve the desired operation. Furthermore, when the system contains multiple reactors, situations arise such that global control objective can be satisfied by several different combinations of local control objectives. This leads to the requirement of a hierarchical control structure whereby local control objectives can change dynamically in order to achieve the global control objective of the system.

2. REACTOR NETWORK MODEL

A network of I interconnected CSTRs is modeled by specifying the mass balance for an individual reactor at position i in the network, where $i = 1..I$. Figure 1 shows the schematic for a system of four CSTRs. The cubic autocatalytic reaction for a single autocatalytic species is

$$R + 2P \xrightarrow{k} 3P \tag{1}$$

$$P \xrightarrow{k_d} D \tag{2}$$

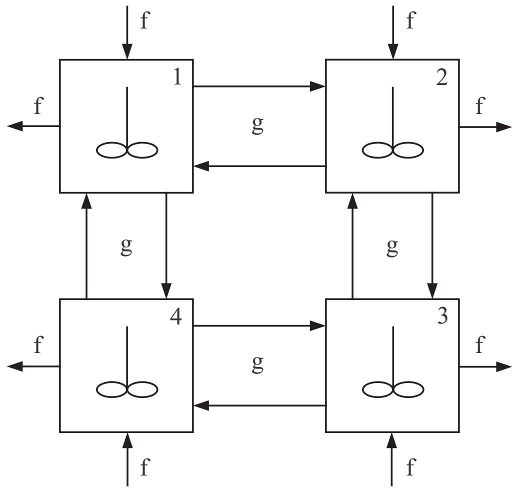

Fig. 1. 4-CSTR network schematic

R is the resource concentration, P is the species concentration, D is a dead (inert) species, k is the species growth rate constant, and k_d is the species death rate constant.

The production rates of the resource and species concentrations for a network of size I are

$$V\frac{dR_i}{dt'} = -VkR_iP_i^2 + F(R_0 - R_i) + G(R_{i-1} + R_{i+1} - 2R_i) \tag{3}$$

$$V\frac{dP_i}{dt'} = VkR_iP_i^2 - P_i(F + Vk_d) + G(P_{i-1} + P_{i+1} - 2P_i) \tag{4}$$

where R_0 is the resource concentration in the feed, R_i is the resource concentration in reactor i , P_i is the species concentration in reactor i, F is the feed flow rate, G is the interconnection flow rate and V is the reactor volume. The feed stream contains only resource. The state equations can be written in dimensionless form as

$$\frac{dr_i}{dt} = -kr_ip_i^2 + f(1-r_i) + g(r_{i-1} + r_{i+1} - 2r_i) \tag{5}$$

$$\frac{dp_i}{dt} = kr_ip_i^2 - p_i(f+d) + g(p_{i-1} + p_{i+1} - 2p_i) \tag{6}$$

by redefining the variables as $r_i = R_i/R_0$, $p_i = P_i/R_0$, $f = F/(VR_0^2)$, $g = G/(VR_0^2)$, $d = k_d/R_0^2$, and $t = R_0^2t'$. For $i > 3$, analytical solutions become intractable, although it should be noted that a single trivial steady state ($r_i = 1$, $p_i = 0$) exists $\forall i$ for every combination of model parameter values. This state represents total extinction in the system. The feed flow rates and interconnection flow rates are treated as manipulated variables. Constraints on the reactor flow rates ensure that material is conserved.

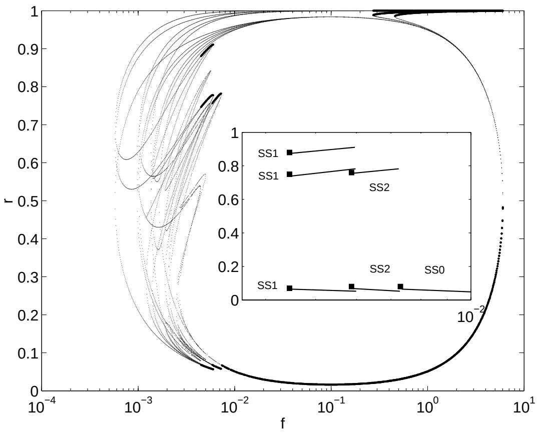

Fig. 2. Bifurcation diagram of r vs f for a 4-CSTR bidirectional network with $k = 25$, $d = 0.1$, and $g = 0.002$. Unstable steady states are indicated with a light line and stable steady states are indicated with a dark line. Inset: stable steady state detail. The ■ symbol represents a Hopf bifurcation point.

3. STEADY STATE BIFURCATION STRUCTURE

The nonlinear solver KINSOL (Hindmarsh and Taylor, 1998) is used to map the bifurcation structure of reactor networks. The steady state solutions are found by sweeping the bifurcation parameter through the region of interest and using a large number of randomized initial guesses in a manner similar to that of Ourique *et al.* (2002). Although this method is more computationally demanding than traditional numerical bifurcation techniques, it removes the constraint of a priori knowledge of the steady state branches. Traditional bifurcation analysis will miss isolated solution branches, unless their location is known beforehand. Stability information is obtained by examining the eigenvalues of the Jacobian matrix.

The steady state bifurcation diagram of r versus f for a single species in 4-CSTR bidirectional ring network is shown in Figure 2. The bifurcation diagram is constructed for all possible steady state values, thus the omission of the reactor number subscript, i. The resource concentration steady states in the bifurcation diagram represent those values that *can* occur in an individual reactor, but not the spatial arrangement of the steady states in the network. The 4-CSTR bidirectional network has two combinations of stable steady states at low feed flow rates in addition to the steady state of the single CSTR. The first combination (SS1) displays three distinct steady states. The spatial pattern consists of one high resource reactor surrounded by two identical lower resource reactors, followed by the lowest resource reactor. Reducing the feed flow rate from SS1 results in the system moving to a periodic regime via a Hopf bifurcation. When the feed flow rate is increased from the SS1, the network displays quasi-periodicity and chaos. Increasing the feed flow rate further causes the network to move to the single CSTR periodic regime in which all reactors synchronize to single CSTR limit cycle. A further increase in the feed flow rate results in the nontrivial single CSTR stable steady state (SS0).

The second reactor configuration (SS2) in the 4-CSTR bidirectional network mimics a 2-CSTR setup through locking neighboring CSTRs in pairs. Note that, though two stable steady states are possible in four reactors, the configuration is always a pair of pairs, as opposed to alternating high and low concentrations. Reducing the feed flow rate from SS2 causes the system to pass through a Hopf bifurcation point and move into a periodic regime. If the feed flow rate is increased from SS2, the system collapses to the nontrivial single CSTR stable steady state because the stability region of the single CSTR SS0 begins just as the stability region of 4-CSTR network terminates. Note that, while for the previous spatial pattern of states in the 4-CSTR network, the system could be moved to an oscillatory regime by increasing the flow rate, in this case, the ending and starting points of the stability region meet, and this does not allow periodic behavior to occur.

4. CONTROL SYSTEM ARCHITECTURE

From a control perspective, reactor networks pose a tough challenge because several different control strategies are necessary to achieve the desired operational goal. Intelligent supervisory control systems (Kendra *et al.*, 1994) adapt to changing process operating conditions, thereby facilitating the control of such processes. Furthermore, the operation of highly nonlinear systems like autocatalytic replicator networks benefit from *evolutionary control* because the optimal operating regime may not be known a priori. Agent-based control systems (Jennings and Bussmann, 2003) provide the capability for localized and global control strategies that are both reactive in controlling disturbances and proactive in searching for more better operational solutions.

Software agents are an extension of object oriented programming in that both agents and objects encapsulate information. The difference between agents and software objects is that agents are semi-autonomous units that employ a form of reasoning to negotiate with other agents - either for self interest or that of the collective (Jennings, 2000). Multi-agent systems have several properties that make them particularly attractive for use with large, complex systems (Lesser, 1999). The first, and usually most impor-

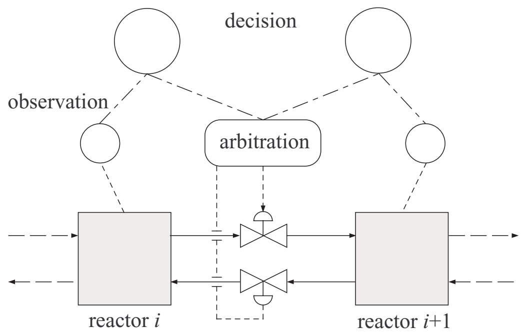

Fig. 3. Control agent architecture.

tant in critical systems, is a high level of reliability. Modularity and scalability also play an important role in multi-agent systems. Software agents often produce different solutions to the same problem. *Solution multiplicity* arises when several agents, using completely independent methods, arrive at different conclusions based on the presented data. Negotiation between agents is therefore required to resolve the situation.

The agent-based control system architecture consists of several sub-systems, each of which are highly modularized (Figure 3). At the process level, network elements such as reactors and valves interface with the higher level agents via low level agents. Each reactor is monitored by an *observation* agent that is responsible for sampling data requested by other agents as well as storing the data in a history for some specified time. Data collection occurs asynchronously with data requests from other agents. Upon instantiation, the frequency at which an observation agent samples data from the process is set by a superior agent. The observation agent maintains the process history and provides data to superior agents when queried. The interconnection flow rates are manipulated by *actuation* agents (not shown) that receive commands from superior control agents.

The next layer in the control hierarchy is the *local decision* layer. Local decision agents are responsible for monitoring control functions and proactively improving the overall performance of the network based on the control objectives of the individual agents and the network as a whole. Due to the number of control responsibilities of decision agents, each agent may use sub-agents. For example, the local control decision agent requires information regarding the state of the process. A sub-agent is therefore tasked with checking whether the system is at steady state, on a limit cycle, or a quasi-periodic regime.

During network operation, local decision agents attempt to satisfy their individual control objectives. An objective may be to maximize a specific species concentration for example. However, in most cases, a decision agent can never fully reach it's desired objective due to conflicts with other agent's control objectives. If an agent desires to modify the interconnection flow rate between a reactor and its neighbor in order to meet a control objective, the adjacent reactor will be affected as well. Naturally, disputes will arise as to the value of the interconnection flow rates between neighboring reactors.

Arbitration agents serve both as a communication channel between decision agents as well as a means to resolve disputes between agents. The arbitration agents receive requested operational procedures from the local decision agents and then presents a solution to them. For example, a decision agent must maximize the species concentration in a reactor and attempts to do so by manipulating the interconnection flow rate. The decision agent sends a set of acceptable values for the manipulated variables to the arbitration agent which then tries to match the desired operational values for neighboring decision agents. If the arbitration agent cannot find an acceptable solution to the control requests from two or more decision agents, then the control move is not permitted. Finally, *supervision* agents function as the topmost layer in the control system hierarchy. This layer is responsible for setting the desired global operating conditions for the entire network.

Considering the nonlinearity of reactor networks, it is difficult to predict how the bifurcation structure of the system changes when the system parameters are manipulated. Consequently, one cannot easily predict how to change operating conditions of the network by manipulating the flow rates. Decision agents are given the task of increasing the concentration of the autocatalytic species in their reactor by manipulating the interconnection flow rates between neighboring reactors. Various methods may be used to guide the decision agents in planning their control strategies including dynamic exploration of the parameter space, rule-based heuristic models, or first-principles based models.

Decision agents may exploit a model of the reactor network, say by knowing the precise location of stable branches and oscillatory regimes. For example, the complete bifurcation structure shown in Figure 2 would be quite valuable to the decision agents in formulating a control strategy. However, since the number of steady states increases exponentially with the size of the system, this method is not scalable to larger systems. An effective solution is provided via rule-based heuristic models coupled with dynamic exploration techniques.

A heuristic model of the reactor networks consists of rules that describe how the manipulated variables effect the system behavior. For example, in the four reactor network bifurcation diagram

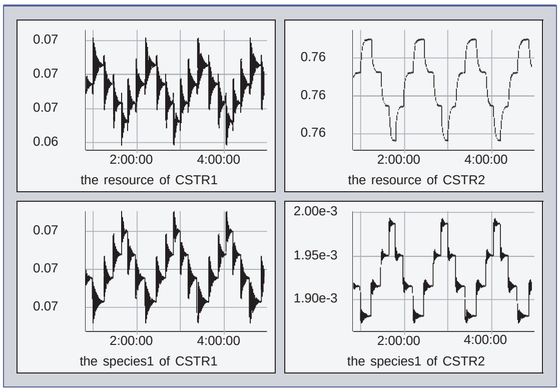

Fig. 4. Non-cooperative agent control strategy

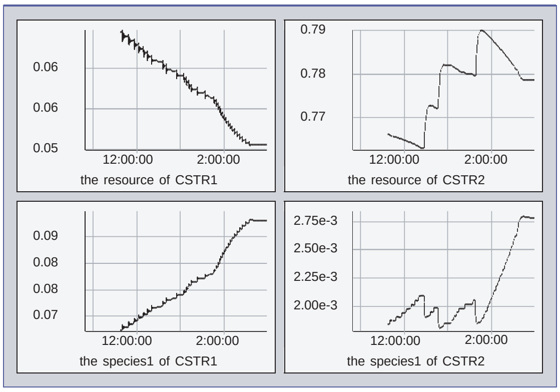

Fig. 5. Cooperative control strategy performance

shown in Figure 2, the stable steady states occupy only certain portions of the diagram. This information is provided to the decision agents in the form of rules to guide their control actions. Furthermore, the decision agents are allowed to "probe" the system by making small, temporary changes to the manipulated variables and observing the resulting system behavior. This dynamic exploration provides additional flexibility to the decision agents when the generalized heuristic model cannot explain system behavior.

The software agents have been developed in G2 (Gensym, 2003), which is a graphical knowledge base development environment for creating intelligent real-time applications. G2 provides an excellent platform for the development of agent-based monitoring and control systems. The ordinary differential equations that describe the autocatalytic reactions in each CSTR are solved numerically using the CVODE solver (Cohen and Hindmarsh, 1994). The solver code is written in C and linked to the G2 agent-based system via a custom software bridge. The reactor class definition in G2 is designed such that the reactor objects have the same attributes as defined in the ODE model. For example, the feed rate to any particular CSTR object is mapped to the specific array location in the ODE solver. When the simulator is initialized, the user may specify the size of the reactor network, initial conditions and inputs. The appropriate number of reactor objects are automatically created by the agent-based system and the reactor objects are modified to include the initial conditions. The CVODE solver simply requires the initial states and parameters to describe the system. The solver then dynamically creates the appropriate equations internally and returns the output to G2, where the states are then mapped back to the reactor objects.

5. EFFECTS OF CONTROL STRATEGY

The performance of two different control strategies is examined in case studies of agent interactions between neighboring reactors. The reactor network is operated initially on a stable steady state. The control objective for the two neighboring decision agents is to maximize the concentration of autocatalytic species in their respective reactors. A competitive strategy is defined by allowing the decision agents to make selfish control moves without regard for its neighbor. In contrast, a cooperative strategy permits the neighboring agents to coordinate their control decisions by allowing a temporary degradation in performance in return for a long-term performance gain.

The result of using a purely competitive strategy on neighboring reactor concentrations is shown in the time series charts of Figure 4. Initially the network is located on steady state SS2 (Figure 2). The competitive control strategy used by the local decision agents allows each to agree on a new operating regime only if both agents see a improvement in their reactor. As shown in Figure 4, the agents are able to improve the operating conditions (increase in species concentration) only slightly before the performance begins to degenerate once again. The control strategy gets stuck in the parameter space and will oscillate indefinitely unless halted by the supervision agents.

A more robust approach to this problem is to permit the local decision agents to suffer some performance loss, but only for a small number of control moves. Figure 5 shows the concentrations of neighboring reactors when the decision agents are designed to cooperatively optimize the network performance. The rules governing the arbitration agent permit a decision agent to make a control move that is detrimental to its neighbor for only one iteration, otherwise it must return to its previous state. This strategy proves to be very effective at improving the network performance. Although the performance of CSTR 2 occasionally suffers while the performance of CSTR 1 improves continuously, this loss is only relative to the previous move and ultimately results in a net gain in performance for the whole network.

6. CONCLUSIONS

Interconnected networks of CSTRs with an autocatalytic reaction mechanism produces highly complex static and dynamic behavior. The extent of the complexities in the bifurcation structure of the system cannot be understood simply by examining a few regions of the parameter space and network configurations. These uncertainties naturally result in complications in controlling the system, either in disturbance rejection or changing the operational regimes of the system.

The concept of agent-based control has been successfully applied to a reactor network to improve the overall performance of the system. The multi-agent control system is able to explore the parameter space of the network and intelligently manipulate the network flow rates such that the specified goal is achieved.

Furthermore, it was shown that cooperative relationships between the decision agents provide a more effective paradigm for improving the network performance than selfish relationships. The overall network performance is improved, despite the fact that individual reactors may see a temporary decrease in performance.

Acknowledgment: This material is based upon work supported by the National Science Foundation under Grant No. CTS-0325378.

REFERENCES

Bilous, O. and N.R. Amundson (1955). Chemical reactor stability and sensitivity. *AIChE Journal* **1**(4), 513–521.

Birol, I. and F. Teymour (2000). Statics and dynamics of multiple cubic autocatalytic reactions. *Physica D* **144**, 279–297.

Birol, I., S.J. Parulekar and F. Teymour (2002). Effect of environment partitioning on the survival and coexistence of autocatalytic replicators. *Physical Review E* **66**, 051916.

Chaivorapoj, W., I. Birol, A. Cinar and F. Teymour (2003). Feedback control of a continuous-flow stirred tank reactor with competing autocatalators. *Industrial and Engineering Chemistry Research* **42**, 3765–3785.

Cohen, S.D. and A.C. Hindmarsh (1994). *CVODE User Guide*. LLNL Report UCRL-MA-118618.

Farr, W.W. and R. Aris (1986). Yet who would have thought the old man to have had so much blood in him?-reflections on the multiplicity of steady states of the stirred tank reactor. *Chemical Engineering Science* **41**(6), 1385–1402.

Gensym (2003). *G2 Reference Manual*. Gensym Corporation, Boston, MA.

Gray, P. and S.K. Scott (1983). Absence of restrictions on permissible paths for changing the efficiencies of operation of flow reactors. *Journal of Physical Chemistry* **87**(11), 1835–1838.

Gray, P. and S.K. Scott (1984). Autocatalytic reactions in the isothermal, continuous stirred tank reactor: Oscillations and instabilities in the system $A + 2B \rightarrow 3B; B \rightarrow C$. *Chemical Engineering Science* **39**(6), 1087–1097.

Hindmarsh, A.C. and A.G. Taylor (1998). Pvode and kinsol: Parallel software for differential and nonlinear systems. *Lawrence Livermore National Laboratory technical report UCRL-ID-129739*.

Jennings, N.R. (2000). On agent-based software engineering. *Artificial Intelligence* **117**, 277–296.

Jennings, N.R. and S Bussmann (2003). Agent-based control systems. *IEEE Control Systems* **23**, 61–73.

Kendra, S.J., M.R. Basila and A. Cinar (1994). Intelligent process control with supervisory knowledge-based systems. *IEEE Control Systems* **14**, 37–47.

Lesser, V.R. (1999). Cooperative multiagent systems: A personal view of the state of the art. *IEEE Transactions on Knowledge and Data Engineering* **11**(1), 133–142.

Lin, K.F. (1981). Multiplicity, stability and dynamics for isothermal autocatalytic reactions in cstr. *Chemical Engineering Science* **36**(9), 1447–1452.

Ourique, C.O., E.C. Biscaia and J.C. Pinto (2002). The use of particle swarm optimization for dynamical analysis in chemical processes. *Computers and Chemical Engineering* **26**, 1783–1793.

Tatara, E., I. Birol, F. Teymour and A. Cinar (2003). Static and dynamic behavior of autocatalytic replicators in heterogeneous reactor networks (paper 457f). *AIChE Annual Meeting*. San Francisco, CA, November 16-21.

Taylor, M.A. and I.G. Kevrekidis (1993). Couple, double, toil and trouble: A computer assisted study of two coupled CSTRs. *Chemical Engineering Science* **48**(11), 2129–2149.

Uppal, A. and W.H. Ray (1974). On the dynamic behavior of continuous stirred tank reactors. *Chemical Engineering Science* **30**, 967–985.

Uppal, A., W.H. Ray and A.B. Poore (1976). The classification of the dynamic behavior of continuous stirred tank reactors-influence of reactor residence time. *Chemical Engineering Science* **31**, 205–214.