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Reconfiguration of Chemical Reactor Networks Using a Hierarchical Agent-based System

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***Abstract*— Controlling reactors in distributed manufacturing processes producing different grades of a product requires intelligent reconfiguration strategies. Agent-based approaches are ideal for such cases, since they can provide flexible, robust, and emergent solutions during dynamically changing process conditions. A hierarchical, agent-based system with local and global control agents is developed to control networks of interconnected chemical reactors. This paper proposes a multi-layered, multiagent framework based on a decentralized approach for the supervision of grade transitions in autocatalytic reactor networks. The values for the manipulated variables are chosen to give the least disturbance to the system. The case studies show that the approach is successful in controlling the reactor network and being able to keep the desired grade even after the need of shutting down some of the reactors.**

I. INTRODUCTION

Agent-based systems are one of the emerging approaches for supervision and fault tolerant control of distributed networked processes. Agent-based models have been used since the mid-1990s to solve a variety of business and technology problems. Examples of applications include supply chain optimization and logistics, modeling of consumer behavior, including social network effects, distributed computing, workforce management, traffic management, and portfolio management. In these applications, the system of interest is simulated by capturing the behavior of individual agents and their interconnections. The increasing interest in agent-based frameworks for control applications is because of their ability to adapt to dynamically changing system conditions and self-organize the system to to give rise to solutions, which cannot be guessed beforehand. This self-organizing behavior can be achieved via a highly modular framework, where local modules are designed such that they encapsulate knowledge and solution techniques specific to that region of the network they operate. To achieve an intelligent control behavior, agents with organizational rules are crucial in serving as higher level coordination mechanisms, which will harmonize local control actions. A layered control structure interfaced with complex arrays of sensors and actuators provides a flexible supervision and control platform that can deal with local and global challenges.

We are investigating the advantages and limitations of agent-based control mechanisms in large scale, complex networked manufacturing processes producing different grades of products. Usually, the desired end-product qualities such as density, molecular weight distribution, pH, etc. are known, however the process configuration that produces the desired product may not be known a priori or there may be more than one system configurations that lead to the specified end-product qualities required. Generating production campaigns of different grade products may usually result in off-spec products during transition from one product to another. It is usually desired to complete the grade transitions by implementing the least amount of disturbance to the process as possible.

Two alternative techniques can be used to develop coordination mechanisms [1]. The first is a centralized approach that relies on a special coordinator agent responsible for detecting interdependencies between the local agents' activities at successive levels of abstraction. This approach is contrasted by a decentralized stance where no such special agent exists and local agents interact laterally. The agents are endowed with the knowledge to discover inconsistencies between their intended actions and interchange messages to mutually adopt their local decisions so as to converge on one or several sets of consistent local control plans. The former coordination model leads to a hierarchical integration of control plans as determined by the upper level functions, while in the latter this integration emerges from agent interactions.

This paper mainly focuses on the logic behind decentralized approach and proposes an adaptive multi-agent based control framework for the supervision of a distributed chemical manufacturing process and investigates benefits and limitations of it by using different case studies. The decentralized approach has some advantages over the centralized one considering that the fully centralized approach may be less reliable, as the consequences may be catastrophic if the centralized controller is disabled or malfunctions and the information that needs to be exchanged may be too demanding of communication resources in the case of large systems with many manipulated variables. The decentralized scheme also gives the opportunity to resume the plant operation, even in the case of maintenance to different section of the plant, since it does not rely on a central operation and can continue working while satisfying the local objectives.

The chemical process being studied in the paper is an interconnected CSTR (continuous stirred tank reactor) network. This reactor network can represent many population dynamics problems when specific types of chemical reactions take place in them. We use autocatalytic reactions in the network to formulate surrogates for predator-prey, virus propagation in a distributed population, multiple species of animals that rely on the same resources, or chemical manufacturing problems. Reactor networks exhibit highly complex behavior, with multiple steady state operating regimes, and have a large pool of candidates for manipulated variables [2]. Recent work on multiple reactor configurations with cubic autocatalytic reactions has demonstrated a rich spectrum of static and dynamic behavior [2]. The topography of interconnected CSTR networks has been shown to drastically affect the steady state bifurcation structure of the system [2], [3]. Spatial inhomogeneity of the network can be increased by increasing the number of reactors in the network as well as manipulating the interconnection flow rates of the network. It has also been shown that the number of stable and unstable steady states increase with the inhomogeneity of the network. Larger networks permit more steady states and spatial combinations 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 reactor feed and interconnection flow rates.

Controlling the spatial distribution of autocatalytic species in a network of reactors requires simultaneous manipulation of interconnection flow rates within the system. Numerical experiments suggest that individual CSTRs in networks are capable of hosting only a single dominant species, while other competing species may be present only in trace quantities [4]. Consequently, if the control objective calls for one species to be replaced with another, a nonlinear control scheme must be used. For a single CSTR with competing autocatalytic species, one strategy may be to modify the reactor residence such that the undesirable species is washed out of the system, and then set to an appropriate value that is favorable to the existence of the desired species [5], [6]. Obviously, there is usually more than one strategy to achieve such control objectives. An agent-based framework provides the flexibility to implement multiple control strategies to local agents and coordinate their local strategies through communication between agents.

The general approach used throughout this work relies on the fact that in order to change the dominant species within a reactor, some amount of the desired species must be transported to the target reactor from another one, to which it is connected. This procedure results in the transported species becoming the dominant one because of its higher concentration than the previously dominant species.

The organization of paper is as follows: Section II provides the background of autocatalytic CSTR networks. Section III describes the the decentralized framework developed and its integration to the reactor network. Section IV is dedicated to giving information about the simulation environment and case studies. Section V concludes the paper.

II. CSTR Networks

A network of I interconnected isothermal CSTRs (Fig. 1a) is modeled by specifying the material balance for each individual reactor i (Fig. 1b) in the network, where $i = 1..I$. The cubic autocatalytic reaction for N autocatalytic species is given in (1), where R is the resource, P_n is the n^{th} species, and D is a dead (inert) species. Reaction rate constants k_n and k_{dn} characterize the growth and death rates of the n^{th} species respectively.

$$\begin{aligned} R + 2P_n &\xrightarrow{k_n} 3P_n \\ P_n &\xrightarrow{k_{dn}} D \end{aligned} \tag{1}$$

The rates of change of the resource and species concentrations for a reactor i in network of I identical reactors of constant volume can be written as

$$\begin{aligned} \frac{dr_i}{dt} = -\sum_{n=1}^{N} k_n r_i p_{ni}^2 + f_i - r_i \left[fo_i + \sum_{j=1}^{I} g(i,j) \right] \\ + \sum_{j=1}^{I} r_j g(j,i) \end{aligned} \tag{2}$$

$$\begin{aligned} \frac{dp_{ni}}{dt} = k_n r_i p_{ni}^2 - p_{ni} d_n + f_i p_{fni} \\ - p_{ni} \left[fo_i + \sum_{j=1}^{I} g(i,j) \right] \\ + \sum_{j=1}^{I} p_{jn} g(j,i) \end{aligned} \tag{3}$$

by defining the variables as $r_i = R_i/R_0$, $p_{in} = P_{ni}/R_0$, $f = F/(VR_0^2)$, $fo = Fo/(VR_0^2)$, $d_n = k_{dn}/R_0^2$, and $t = R_0^2 t'$, where R_0 is the resource concentration in the feed, P_0 is the species concentration in the feed, R_i is the resource concentration in reactor i, P_{ni} is the n^{th} species concentration in reactor i, F is the feed flow rate, Fo is the exit flow rate, and V is the reactor volume. The interconnection matrix g defines the strength of the interconnection flow rates between networked reactors, such that $g(i,j)$ is the interconnection flow rate from reactor i to reactor j.

In the case studies provided, the interconnection flow rates are used as manipulated variables. The system is operated with constant volume, thus, constraint equations are formulated on the reactor flow rates to ensure that material is conserved. The reactor flow inputs include the reactor feed and the interconnection flows from the neighboring reactors. Outflow rates from each reactor include the interaction outflows to neighboring reactors as well as the drain. The constraints include a lower bound such that all flow rates are non-negative and an upper bound that ensures the equality of total inflow and total outflow. The implication for a controller

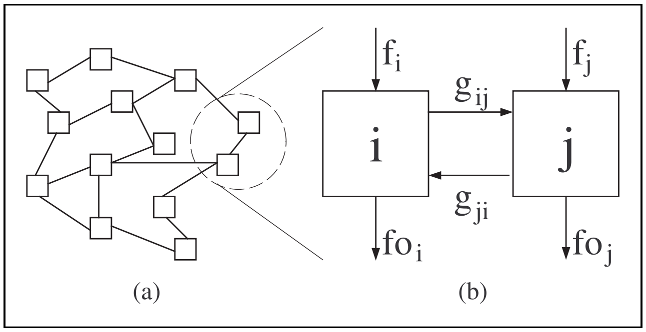

Fig. 1. (a) Network of interconnected reactors. Feed and exit streams are not shown. (b) Detail view of interconnection flows between reactors with feed and exit streams.

scheme that manipulates interconnection flow rates is that the action taken will not violate the constraints and the volume is kept constant all the time.

III. Use of Perceptron-Based Learning in Multi-Agent Systems for the Grade Transition Problem

The decentralized agent-based control framework proposed consists of a spatial reconfiguration technique by using a combination of heuristics and perceptron learning in order to maintain the grade set in the reactor network. The method is different from the previous work [7] not only algorithmically, but also by being able to reject disturbances as well as resuming the operation during maintenance periods.

The model is hierarchical and the control layer resides on top of the observer layer, which is responsible for getting data from the physical layer. The physical layer is composed of reactors, valves, pipes, sensors etc. There are as many local controller agents as the number of the reactors. They are responsible of keeping control of the dominant species in the reactor under their control via communicating with other local controller agents, which they are connected with. The connections among the local controller agents are governed by the layout of the physical system. The arbitrators are resolving any issue that might show up because of some dispute between two local controller agents arising due to a conflict of local objectives. All local controller agents are connected to a global controller agent, which is responsible for keeping track of the global objective and sharing global information with the local controllers. The described layout is shown in (Fig. 2) in detail.

The approach used in each local controller is a combination of heuristics and perceptron-based learning. The manipulated variables are the interconnection flow rates. The controller agents use a conservative approach in changing the flow rates in order not to disturb the system more than necessary. The decision mechanism used is relying on perceptrons and it is basically a binary classifier to determine if an attack to a neighboring reactor is needed. The classifier is shown in (Fig. 3) in detail. The input layer consists of the cells, which indicate the number of neighbors with the same dominant species, the number of neighbors with a different

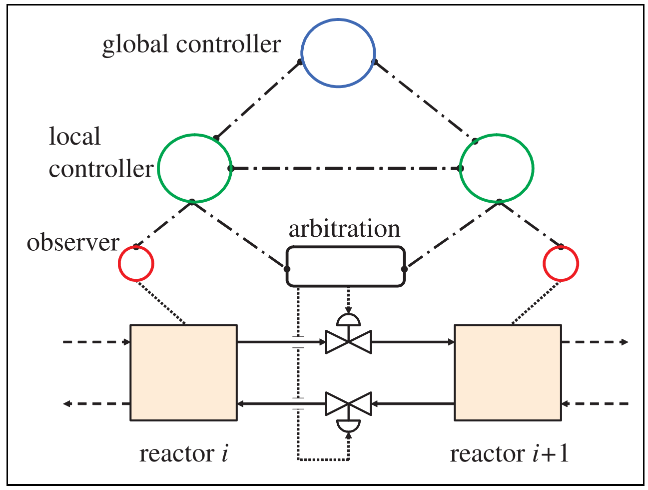

Fig. 2. Hierarchical layers of controller framework.

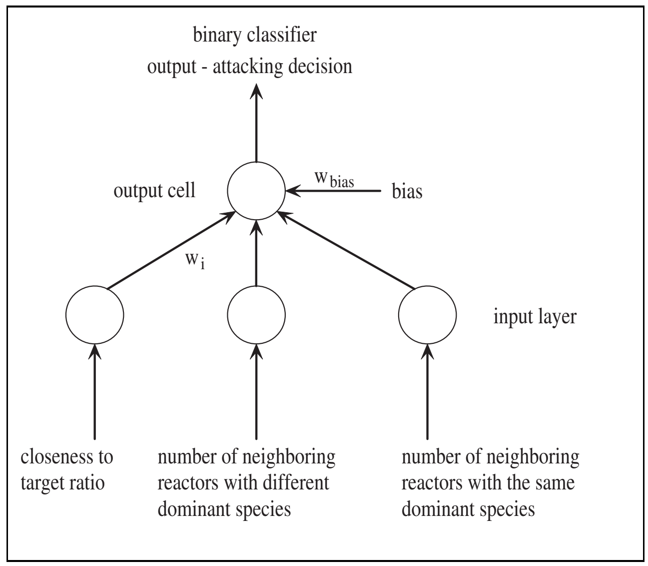

Fig. 3. Binary classifier used in each local controller agent.

dominant species and the closeness to the target grade in terms of the dominant species of the reactor itself. The information of the current grade and the global objective is obtained from the global controller agent. The decision given determines if the local controller agent should take an action or not, where the action is to attack a neighboring reactor by increasing the interconnection flow rate to that particular one. The weights in the classifier are initially assigned semi-randomly, that is, the interval of the weights are given in such a way that the decision will start to make sense at the beginning. They are updated after each step, depending on the change of the spatial configuration, where a step is a large dimensionless time interval to give the system enough time to reach the steady state.

If the local controller agent should act in the controlling scheme, the neighboring reactor, to which the interconnection flow rates should be increased, is picked after communicating with other local agents, which are controlling the neighboring reactors. The decision to pick a reactor and to attack to

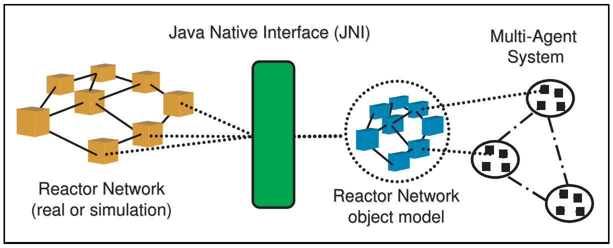

Fig. 4. Layout of the reactor network model and agent-based control framework

it via changing the interconnection flow rates is based on the difference between closeness to the target grade and the difference between the dominant species concentrations in both attacking and the attacked reactors and the number of the neighboring reactors with the same dominant species as the attacked one. The last parameter is needed in order to be very conservative and give the system the least amount of disturbance as possible, since this approach relies on the independent actions of the local controllers acting at the same time and it tries not to put any limits to them in their actions, as long as they are in agreement with the global objective. Because of these simultaneous and conservative actions, the steady state is reached very fast and there are almost no or minimal amount of oscillations in our test cases.

IV. SIMULATION ENVIRONMENT AND CASE STUDIES

The reactor network model and agent-based control framework proposed are implemented in Java and using the open source agent modeling and simulation environment RePast [8]. The RePast toolkit is a Java-based framework for agent simulation and provides features such as an event scheduler and visualization tools. The control agents created interact with virtual representations of the physical reactor network. The virtual network objects map the states of the physical system to objects that can be manipulated by control agents. The interface between the physical network and the agent environment can take the form of a data acquisition system in the case of a real process, or in this case, a simulator of a chemical reactor network. The ordinary differential equations that describe the autocatalytic reactions in each CSTR are solved numerically using CVODE libraries [9], whereas all the variables are made dimensionless. The solver code is written in C and linked to RePast via the Java Native Interface (JNI). The layout is shown in (Fig. 4).

The agent-based control structure explained can be used in a wide range of control related application problems in distributed networked systems. The applications vary from minor configuration changes to satisfy final product quality desired where a small number of units in the network is affected, to major product grade transition applications where the whole network is affected and the transition trajectory to be followed is not apparent a priori. The control structure is also quite resistant to disturbances and changes in the network, such as multiple reactors becoming inoperable or are shut down for maintenance or repair.

Fig. 5. Initial reactor network configuration before grade transition starts. The configuration is consisting of 30% of species 1 represented with red (gray), 30% of species 2 represented with green (light gray) and 40% of species 3 represented with blue (dark gray) - (For interpretation of the references in color in this figure legend, the reader is referred to the web version of this article).

This study provides two different case studies to test and compare the effectiveness of the proposed framework. Simulations are generated on a network that has twenty (4x5 grid) chemical reactors hosting three autocatalytic species competing with each other. The growth and death rate parameters for the species are chosen to be equal in order to eliminate the possibility of one species having advantage over the other ones. Initially all feed flow rates and all interconnection flow rates are uniform for all reactors. Initial species concentrations in the reactors are selected randomly. The network is simulated for some time, allowing each reactor to reach a steady state before the agent-based controller framework starts to manipulate the system.

A. Case Study: Reconfiguration of the reactor network for grade transition

The first case study demonstrates a complete grade transition using the decentralized agent-based framework. The initial configuration of the network is shown in (Fig. 5). The objective is starting from a product grade composition of 30% of species 1 represented with red, 30% of species 2 represented with green and 40% of species 3 represented with blue to reach a grade consisting of 20% of species 1 (red), 30% of species 2 (green) and 50% of species 3 (blue). The final network configuration is given in (Fig. 6).

After the initiation of the control framework, the system succeeds in reaching the desired grade as the figures show. There are either no or minimal oscillations in the transition grades, hence a minimal disturbance is applied to the system.

B. Case Study: Controlling the grade after some of the reactors shut down

The second case study aims to see how the control framework will behave in the case of a multiple reactor shut down. This might be happening because of the need

Fig. 6. Final reactor network configuration after grade transition is performed. The configuration is consisting of 20% of species 1 represented with red (gray), 30% of species 2 represented with green (light gray) and 50% of species 3 represented with blue (dark gray) - (For interpretation of the references in color in this figure legend, the reader is referred to the web version of this article).

Fig. 7. Initial reactor network configuration after half of the reactors are shut down. Grade transition controller is active all the time, hence it tries to meet the set grade to satisfy the global objective. The configuration is consisting of 40% of species 1 represented with red (gray), 30% of species 2 represented with green (light gray) and 30% of species 3 represented with blue (dark gray) - (For interpretation of the references in color in this figure legend, the reader is referred to the web version of this article).

of planned reconfiguration due to maintenance or repair, or even because some part of the network becoming inoperable due to loss of power. The initial network configuration is given in (Fig. 6). The control framework stays always active after the initiation, so it will try to maintain the desired grade no matter what is happening throughout the simulation. This case study is in combination with the first one, since the simulation is running continuously after reaching the desired grade of 20% of species 1 (red), 30% of species 2 (green) and 50% of species 3 (blue). After the system has reached the steady state, half of the reactors are randomly shut down. The network configuration at that time is given in (Fig. 7) and the shut down reactors are shown in white. Since the control framework is active all the time, the objective of it is again to maintain the grade mentioned with the initial configuration consisting of 40% of species 1 (red), 30% of species 2 (green) and 30% of species 3 (blue).

The agent-based control framework succeeds in reaching the desired grade and the final network configuration after the global objective is met, is shown in (Fig. 8). There are either no or minimal oscillations in the transition grades, which again suggests that the system is disturbed minimally.

The concentration profiles in CSTR 5 and CSTR 6 are shown in (Fig. 9) and in (Fig. 10) respectively. The mentioned reactors are subject to bigger changes in the second case study because of the transitions they have to undergo in order to fulfill the objective of reaching the desired grade in the network.

C. General remarks on both case studies

In both case studies, different runs of the simulation with the same parameters may produce different final configurations because of the random values in initial species concentrations in the network of reactors. There are some test runs, which show minor amount of oscillations until steady state is reached. One example of oscillations in CSTR 6, encountered in the first case study is shown in (Fig. 11).

Fig. 8. Final reactor network configuration after grade transition controller satisfied the global objective. Half of the reactors are still shut down. The configuration is consisting of 20% of species 1 represented with red (gray), 30% of species 2 represented with green (light gray) and 50% of species 3 represented with blue (dark gray) - (For interpretation of the references in color in this figure legend, the reader is referred to the web version of this article).

V. Summary and Conclusions

The decentralized agent-based control framework proposed gives the ability to control reconfiguration of chemical reactor networks. Local controller agents have a decision making and learning capability, which results from the combined implementation of the heuristics and perceptrons. Each local controller agent is responsible from one reactor and is in communication with the other local controller agents,

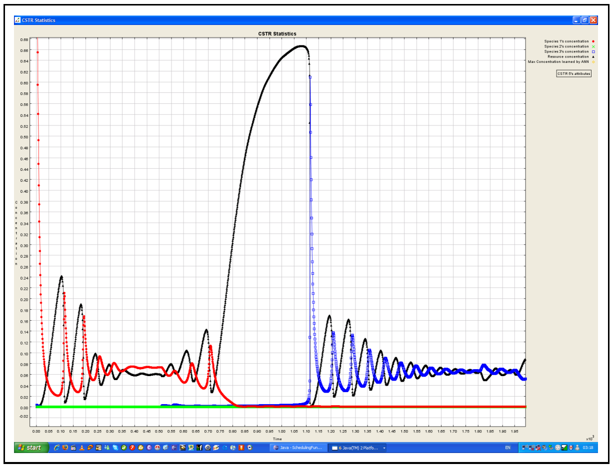

Fig. 9. Resource and species concentrations in CSTR 5. Concentration of species 1 is represented with red (gray), concentration of species 2 represented with green (light gray) and concentration of species 3 represented with blue (dark gray). The resource concentration is represented with black. The horizontal x-axis shows time in the interval of 0 and 2000 and the vertical y-axis is showing concentrations between 0 and 0.68. - (For interpretation of the references in color in this figure legend, the reader is referred to the web version of this article).

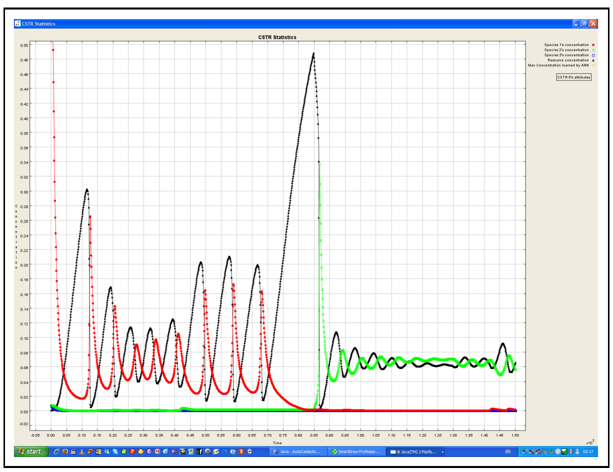

Fig. 10. Resource and species concentrations in CSTR 6. Concentration of species 1 is represented with red (gray), concentration of species 2 represented with green (light gray) and concentration of species 3 represented with blue (dark gray). The resource concentration is represented with black. The horizontal x-axis shows time in the interval of 0 and 1500 and the vertical y-axis is showing concentrations in the interval of 0 and 0.50. - (For interpretation of the references in color in this figure legend, the reader is referred to the web version of this article).

which are responsible from the reactors to which its own reactor connected to. They also communicate with the global controller agent to check the closeness to the global objective and whether it is met.

It has been shown that the decentralized multi-agent control system developed is able to reconfigure the reactor network intelligently for a grade transition in the operation and it is maintaining the desired production grade after some reactors are randomly shut down, which is simulating a maintenance period in the reactor network. The decentralized system proposed in the paper will be useful in large scale and complex reconfiguration cases where multiple reactors

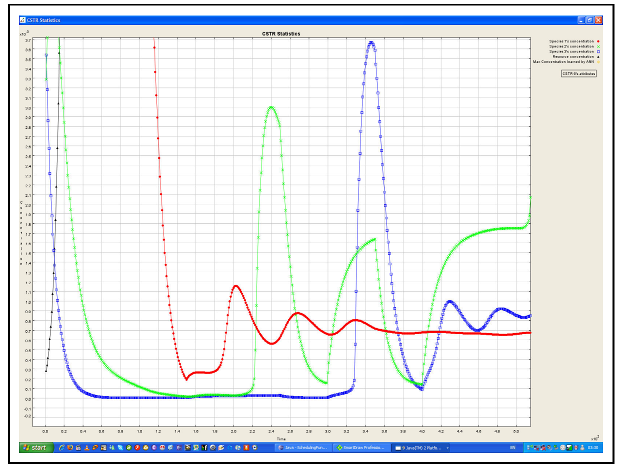

Fig. 11. Oscillations observed in CSTR 6 in the early stages of the simulation until steady state is reached. Concentration of species 1 is represented with red (gray), concentration of species 2 represented with green (light gray) and concentration of species 3 represented with blue (dark gray). The resource concentration is represented with black. The horizontal x-axis shows time in the interval of 0 and 500 and the vertical y-axis is showing concentrations in the interval of 0 and 4×10^{-3}. - (For interpretation of the references in color in this figure legend, the reader is referred to the web version of this article).

are reconfigured concurrently.

VI. Acknowledgment

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