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Chemical supply chain modeling for analysis of homeland security events

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ABSTRACT

The potential impacts of man-made and natural disasters on chemical plants, complexes, and supply chains are of great importance to homeland security. To be able to estimate these impacts, we developed an agent-based chemical supply chain model that includes: chemical plants with enterprise operations such as purchasing, production scheduling, and inventories; merchant chemical markets, and multi-modal chemical shipments. Large-scale simulations of chemical-plant activities and supply chain interactions, running on desktop computers, are used to estimate the scope and duration of disruptive-event impacts, and overall system resilience, based on the extent to which individual chemical plants can adjust their internal operations (e.g., production mixes and levels) versus their external interactions (market sales and purchases, and transportation routes and modes). To illustrate how the model estimates the impacts of a hurricane disruption, a simple example model centered on 1,4-butanediol is presented.

1. Introduction

Disruptive events such as hurricanes (Katrina, Ike) and acts of terrorism have potentially significant impacts on the chemical industry and broader homeland security. Chemical plants, ports, pipelines, and rail and road transportation routes can be damaged, impacting the ability of chemical facilities to produce, transact, and deliver chemicals. The chemical industry and supporting government agencies need to understand these supply chain relationships, dynamics, and cascading effects to improve the sector's resilience to these events, that is, its ability to prepare for, respond to, and recover from them. Important questions include: given an event, will the entire chemical sector be impacted or just parts? Which chemicals, plants, and complexes could be impacted? In which regions of the country? How long will these impacts last?

These and other homeland security mandates indicate the need for new chemical sector modeling and analysis approaches, ones that can accommodate large-scale, whole-system, dynamic analysis. Traditional supply chain models tend to be limited in this regard: they often look at small portions of the chemical sector—for example, a single plant and its suppliers and buyers–and model them with static optimization approaches. For example, Perea-Lopez, Grossmann, Ydtsi, and Tahmassebi (2001) use control-theory techniques to develop an efficient polymers process and distribution network model. Petkov and Maranas (1997), Applequist, Pekny, and Reklaitis (2000), Timpe and Kallrath (2000), Kallrath (2002), Levis and Papageorgiou (2004), and Guillen, Mele, Espuna, and Puigjaner (2006) develop optimization techniques for the efficient operation of chemical plants, including when there is market or other supply chain uncertainty. Chen and Lee (2004) develop a multi-objective optimization of multi-echelon chemical supply chain networks with uncertain product demands and prices. Lababidi, Ahmed, Alatiqi, and Al Enzi (2004) develop a stochastic programming model of a petrochemical supply chain. Yang et al. present stochastic programming techniques for optimizing the yield of a refinery given multiple operation modes. In most cases these models have difficulty extending themselves to large-scale, whole- and dynamic-system analysis, due to the large number of supply chain components and resulting model optimizations and constraints. Furthermore, the assumption of a centralized system controller inherent in optimization becomes less valid.

A dynamic, decentralized, whole-system supply chain model should capture some or all of the following large-system concepts: (1) *distributed control*—how the system is 'controlled' through the distributed actions of individual components; (2) *self-organization*—how system operating conditions are created without any single controlling authority; (3) *emergence*—how system patterns and ultimately performance emerge from smaller, sub-system interactions; and (4) *complex-adaptive* response to disruption—how the system adapts to the disruptive event in complex ways. Models of decentralized supply chain operations

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Nomenclature

Production scheduling

Indices	/sets
$u \in U$	production units within a plant
$g \in G$	a chemical associated with targeted production unit outputs
$h \in H$	a chemical that is a bi-product of a targeted production unit output and that is stored in the warehouse as an intermediate chemical

Variables for a given plant:

p^u	level of production of unit u
$\hat{p}^u$	scheduled production of unit u
I_g	the total draw of chemical g from the warehouse
O_g	the total production of chemical g sent to the warehouse
n_g	the change in inventory of chemical g
e_g	expected amount of chemical g to be removed from the arehouse over the day
w_g	current inventory of chemical g in the warehouse
$f_g^{u \to v}$	the output of chemical g from production unit u that flows directly as an input to production unit v

Parameters

$\bar{p}^u$	production capacity of unit u
$\bar{w}_g$	warehouse capacity for chemical g
i_g^u	amount of chemical g used per unit of production of unit u
o_g^u	amount of chemical g produced per unit of production of unit u
α	penalty weight for the change in inventory for a targeted chemical
β	penalty weight for the change in inventory for a non-targeted chemical

Buyers and sellers

Indices	/sets
$m \in M$	modes of transportation available to buyers and sellers
$r \in R$	market regions in which buyers and sellers transact
$\{g,r,\{m\}\}$	market map of chemical g, market r, and transportation modes $\{m\}$ available to given buyer or seller

Variables for a given buyer:

d_g	number of days on buyer calendar for chemical g
e_g	buyer's expectation of daily warehouse withdrawal of chemical g
c^s	per-item shipping cost from seller s
$c^{s:h}$	per-item shipping cost from seller s for shipment h

Parameters for buyer

ω	chemical withdrawal moving-average term
σ	shipping cost moving-average term

Variables for a given seller:

$\rightarrow \rho, \leftarrow \rho, \leftrightarrow \rho$	probabilities of increasing price, decreasing price, or leaving price unchanged, respectively

include Prabhu and Duffie (1995), Androulakis and Reklaitis (1999), Gjerdrum, Shah, and Papageorgiou (2001), Garcia-Flores and Wang (2002), Kaihara (2003), Lou, Zhou, Chen, and Ai (2004), and Mondal and Tiwari (2003).

One approach that accommodates the four requirements above is the agent-based model (ABM).[1] Unlike the preceding traditional approaches that model a subset of the overall chemical supply chain as a globally controlled set of plants, an ABM models the entire supply chain as essentially an uncontrolled collection of plants. An ABM accommodates the above four concepts through at least three fundamental characteristics of its own: (1) *autonomy*—chemical-plants can be functionally autonomous in scheduling and execution of tasks; (2) *local* views—no plant has global knowledge of the entire supply chain; and (3) *decentralization*—there is no single system-controlling plant or other authority. An ABM can capture how chemical supply chain properties emerge through non-centralized processes, and how the entire supply chain collectively and dynamically adapts to and recovers from disruptive events. Julka, Karimi, and Srinivasan (2002) use ABM techniques to model the supply chain operations of a refinery including crude procurement, demand tracking, and retrofit analyses. Garcia-Flores, Wang, and Goltz (2000) develop an ABM for information flow between chemical supply chain components. Garcia-Flores and Wang (2002) describe an ABM of a paints and coatings chemical supply chain with intra-enterprise production, scheduling, and regional inter-firm locations and transport. Ito and Abadi (2002) develop a similar ABM of material and inventory planning. Adhitya et al. develop hybrid optimization and ABM techniques for managing disruptions to supply chains. More examples of agent-based modeling of chemical supply chains, some of which specifically target disruption management, can be found in Srinivasan, Bansal, and Karimi (2006), Gao, Shang, and Kokossis (2009), van Dam, Lukszo, and Srinivasan (2009), Aslam and Ng (2010), Mishra, Kumar, and Chan (2010), Giannakis and Louis (2011), and Sinha, Aditya, Tiwari, and Chan (2011). None of these, however, attempt to model the plant-level components and whole-system dynamics of large chemical supply chains.

This paper describes an agent-based model of large, firm-level chemical supply chains, and the larger framework used to assess the impacts of disruptive events on these chemical plants and supply chains. As compared with larger, more complex agent-based models, this model can run simulations in minutes on desktop computers. Reflecting the general distributed nature of agent-based models, the overall model is a collection of constrained-optimization, adaptive-learning, and network-theoretic models, each of which captures the essential dynamics of the supply chain component.

Section 2 describes the mathematical models of chemical-plant production scheduling; the spatial-economic models of chemical buying, selling, and shipping; and the multi-modal network models of chemical transport. Section 3 describes the baseline and disruption characteristics of a small chemical supply chain model subject to a disruptive event. Section 4 concludes.

2. Modeling approach

2.1. Chemical production agent

In the ABM, each chemical plant is modeled as an enterprise-firm agent composed of internal sub-agents that carry out distributed tasks within the plant, including the purchase and inventory management of input chemicals, the coordinated production of chemicals, and the sale of chemicals in merchant markets (Fig. 1).

Each chemical plant has a production supervisor who sets daily production levels for each production unit$u \in U$, based on

[1] Seminal ABM work includes Palmer et al. (1994), Axelrod (1997), Arthur et al. (2007), and Epstein and Axtell (1996).