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AGENT-BASED CHEMICAL SUPPLY CHAIN MODELS ASSESSING DYNAMIC DISRUPTIONS

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Abstract

The chemical industry is one of the largest industries in the United States and a vital contributor to global chemical supply chains. The U.S. Department of Homeland Security (DHS) Science and Technology Directorate has tasked Sandia National Laboratories (Sandia) with developing an analytical capability to assess interdependencies and complexities of the nation's critical infrastructures on and with the chemical sector. This work is being performed to expand the infrastructure analytical capabilities of the National Infrastructure Simulation and Analysis Center (NISAC). To address this need, Sandia has focused on development of an agent-based methodology towards simulating the domestic chemical supply chain and determining economic impacts resulting from large-scale disruptions to the chemical sector.

Modeling the chemical supply chain is unique because the flow of goods and services are guided by process thermodynamics and reaction kinetics. Sandia has integrated an agent-based microeconomic simulation tool N-ABLE™ with various chemical industry datasets to abstract the chemical supply chain behavior. An enterprise design within N-ABLE™ consists of a collection of firms within a supply chain network; each firm interacts with others through chemical reactions, markets, and physical infrastructure. The supply and demand within each simulated network must be consistent with respect to mass balances of every chemical within the network. Production decisions at every time step are a set of constrained linear program (LP) solutions that minimize the difference between desired and actual outputs.

We illustrate the methodology with examples of modeled petrochemical supply chains under an earthquake event. The supply chain impacts of upstream and downstream chemicals associated with organic intermediates after a short-term shutdown in the affected area are discussed.

Introduction

Domestic events such as hurricanes (Katrina, Ike) and acts of terrorism can potentially have significant impacts on the U.S. chemical industry. Chemical plants, pipelines, rail, and road transportation routes can be damaged indefinitely during these events, thus impacting the ability of chemical facilities to produce, transact, and deliver chemicals. There has been a growing national interest in understanding and estimating the impact of chemical supply chains under natural and man-made events. In doing so, the insight can enhance industry's preparation towards responding to these events. This paper describes an agent-based model of chemical supply chains that is used to estimate supply chain impacts caused by homeland security-related events, including brief descriptions of the mathematical foundation, the chemical sector database, and an illustrated example of supply chains under a natural disruptive event.

Agent-Based Model

As a model, chemical supply chains behave as control-and-adaptation systems in which some components perform as traditional "state-and-control" systems (e.g., in-plant operations, cross-plant logistics networks) while others are more adaptive in nature (e.g., merchant markets with many, heterogeneous buyers and sellers; road transportation systems with many independent vehicles). Agent-based modeling (ABM) is one tool for modeling chemical supply chains as control-and-adaptation systems. ABM has been used widely to capture the structured, complex, and adaptive behavior of collections of economic entities. Examples of seminal ABM work include Palmer et al. (1994), Axelrod (1997), Arthur et al. (2007), and Epstein and Axtell (1996). For homeland security applications, Downes et al. (2005) developed a 3000-firm chlorine supply chain control-and-adaptation model and used it to estimate the impacts to chlorine firms of a rail transport disruption and private policies that reduce impact times by expediting shipments.

ABM has some important benefits over other modeling techniques, including that it can assemble disparate mathematical and network modeling approaches, some basic and others complex, into a single model and simulation environment. In our ABM, individual chemical plants are modeled as synthetic firms that carry out the purchasing, production, scheduling, storage, and sale of chemicals, as illustrated in Fig. 1. Each buyer is responsible for the purchase and inventory management of one chemical. These buyers

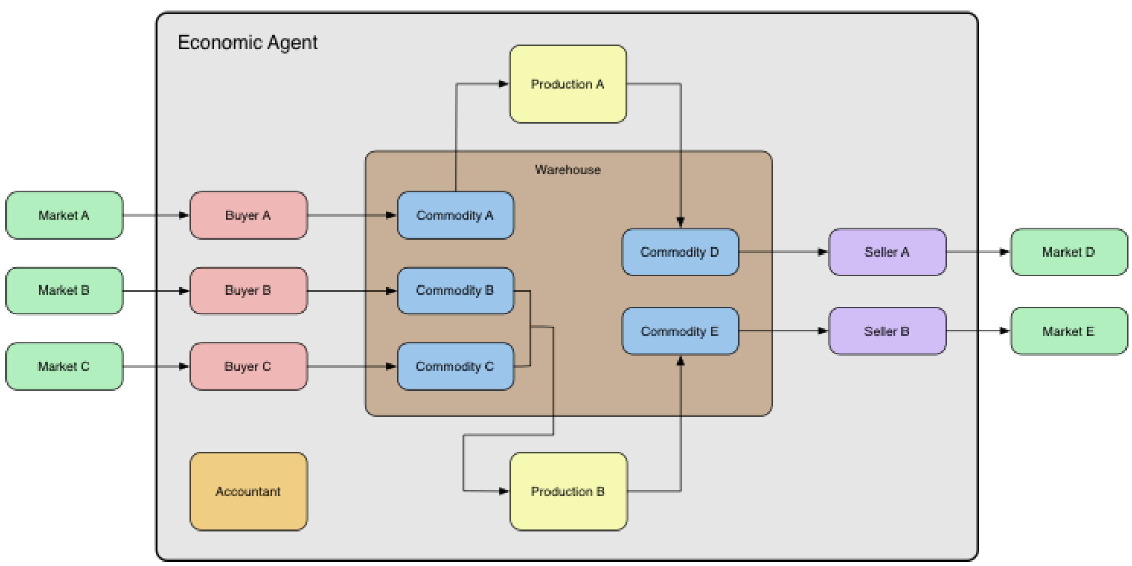

Figure 1. An agent-based chemical plant composed of buyers, productions, warehouses, production scheduler, and sellers.

purchase the chemicals in merchant markets, alongside buyers from other chemical plants, thereby competing for resources. Analogously, the sellers in these plants sell in one or more markets, attempting to set prices that maximize plant profits. Each chemical plant contains one-to-many production units that are managed by a production scheduler that follows the linear program described below, managing inventories of each commodity within the constraints of the warehouse and direct connections between production units.

Chemical Data

Robust and up-to-date information regarding chemical names, chemical manufacturers, economic statistics, and chemical reactions are foundational to conducting a static or dynamic analysis of the chemical supply chain. As such, Sandia has acquired and modified disparate sets of commercial databases over the years to create an in-house suite of application-ready database servers that analysts and software developers can use for software development, fast analysis, and chemical sector statistics. To establish a modeled production market, different layers of data are created to represent different components within a chemical supply chain. Table 1 outlines the different data categories used to represent chemical supply chains.

Table 1. Categories of chemical supply chain data used in constructing supply chain models.

Category	Detailed Information
Plant Information	Parent company; units; geo-location; chemicals; capacities captive production
Infrastructure	Transportation; pipelines;
Chemistry	Process; technologies; stoichiometry
End use	Wholesalers; geo-locations; quantities
Economics	Employees; imports/exports

The fundamental building blocks of chemical data consist of the most current chemical manufacturers information available from SRIC.[1] The Environmental Protection Agency also provides a chemical storage dataset that supplement our knowledge of how the chemicals are stored throughout the U.S.[2] Detailed data sources are described in the next section. The most unique feature of the chemical data is the chemistry information housed within Sandia. Such information relies on years of experience from chemical subject matter experts and hours of data recording to create a stoichiometric table that enables the analysts to link facility-level production data with their perspective end consumers.

[1] SRI Consulting: Directory of Chemical Producers, World Petrochemicals, and Chemical Economic Handbook
[2] Environmental Production Agency, E-Plan Chemical and Facility Hazards Data https://erplan.net/eplan/login.htm

Building a supply chain not only relies on accurate chemical producer information but also technology information that links the manufacturers to their perspective consumers. Each producing facility must transport its chemical product to another chemical user, and so on. The chemical user at the end of the chemical network chain can either be a chemical producer or an end consumer (such as a distributor or a wholesaler or a consumer product manufacturer). Figure 2 illustrates a simple example that centers around 1,4-butanediol. The upstream step shows the four different reaction pathways representative of how 1,4-butanediol is manufactured from different chemical raw materials. Likewise, three different processes then use 1,4-butanediol to manufacture other chemicals, mostly polyurethane and tetrahydrofuran. Overall, eleven chemicals are immediately tied to 1, 4-butanediol while approximately fifty-three domestic facilities are directly impacted by the flow of these eleven chemicals. The collection of chemical data, known as the Chemical Data Model (CDM) allows different application software to access the chemical manufacturing data and their respective technology information for analysis at different granularities from individual facilities to global chemical supply chain networks.

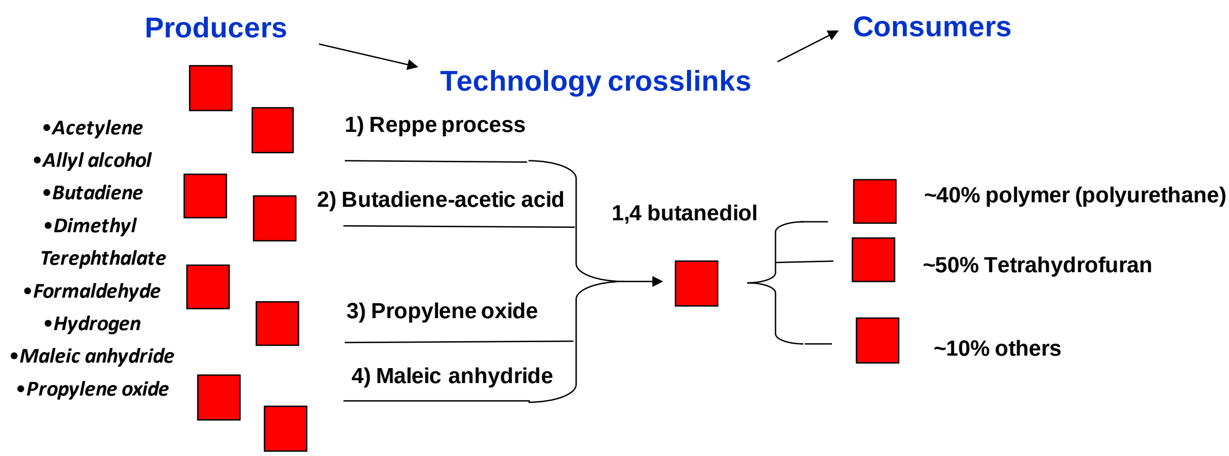

Figure 2. Chemicals directly impacted by the production of 1,4-butanediol.

Earthquake Scenario

This capability demonstration study analyzes the impacts on the chemical industry of an earthquake scenario centered around the New Madrid Seismic Zone (NMSZ). Figure 3 shows the impact area in different magnitudes.

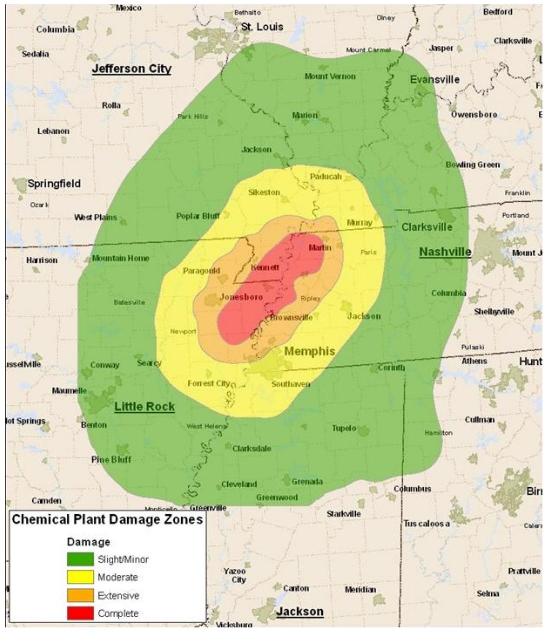

Figure 3. Impacted zones in different magnitudes for New Madrid Seismic zone.

N-ABLE Results

The N-ABLE model was built on 80 chemicals and 900 manufacturing facilities; a subset of those contained in the CDM. The 900 chemical facilities were comprised of both CDM plants and synthetic firms that act as “sources” and “sinks” at the boundaries of the supply chain. The analysis was focused on changes in supply chain structure and performance caused by the disruption. The length of the disruption is the primary factor determining supply chain-wide impacts. Changes in structure do not automatically result in changes in performance due to supply chain inventories and market liquidity. The analysis includes that of an individual chemical plant, a particular chemical in the supply chain, and across the entire supply chain.

Sample Plant

An individual chemical plant is linked to the supply chain through the markets by which it purchases and sells chemical. When the plant is unable to operate, its ability to purchase and produce is reduced. Internally, a plant’s response to a disruption may include shutdown, restart, and accumulation or depletion of inventories. Figure 4 shows the mass of input chemical shipments over a period of time that includes the disruption. Each chemical this facility uses is represented by a color band in Figure 4. Day 1 is the beginning of the disruption and it takes approximately 50 days to return to baseline shipment levels. The decline in shipments is not immediate upon the disruption because in-transit shipments continue to arrive. Once the disruption is over, shipments levels rise above the previous baseline to make up for those lost during the disruption.

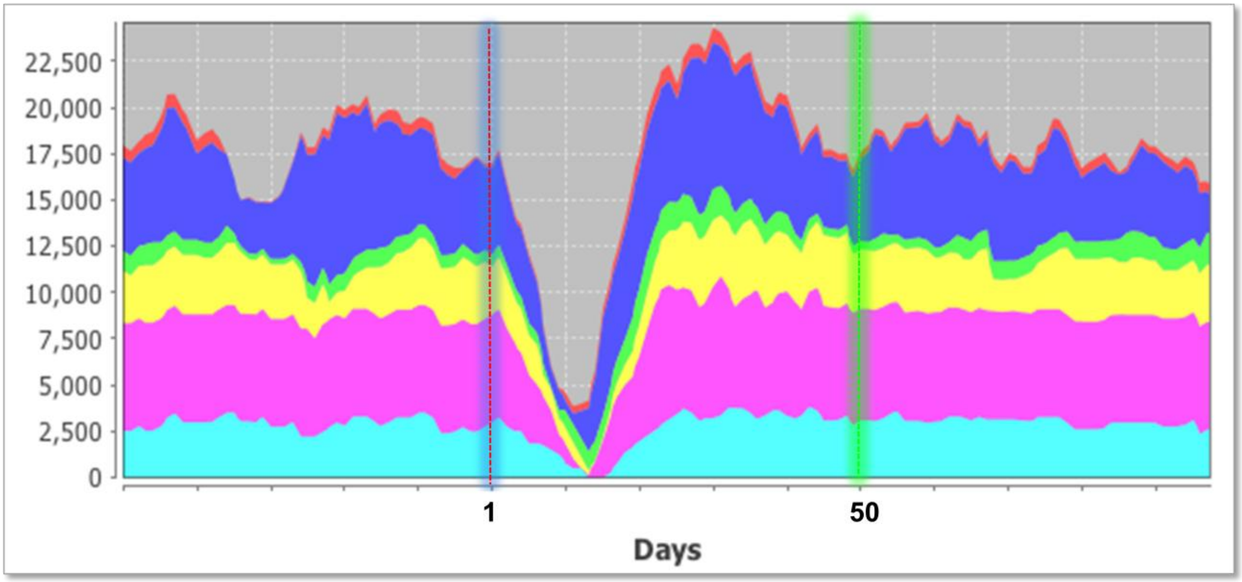

Figure 4. Input shipments by chemical

Sample Commodity

N-ABLE provides analysis of individual commodities (chemicals) by aggregating the production of this chemical across all the facilities where it is manufactured. For example, chemical ‘A’ is produced by approximately 30 plants, most of whom experience a direct or indirect impact from the earthquake, as seen in Figure 5. During the disruption, aggregate supply decreased by approximately 50%. Although most plants experienced significant decreases in production, in a few cases, plants increased production during the disruption to compensate for an overall decreased supply.

The nature of the chemical ‘A’ market during the disruption also changed. Buyer-seller relationships before the earthquake were changed by the disruption and new relationships were created during the disruption. Figure 6 shows the flow of chemical ‘A’ on A) a base line day B) day1 of the disruption and C) on day 200 of the disruption. The gray cylinders are buyers and sellers, with their height and diameter representative of production level and inventory, respectively. The turquoise arcs show transactions; the lighter end is the seller and the darker end the buyer. N-ABLE shows that some firms impacted by the earthquake do not return to their pre-disruption status. Furthermore, during the disruption several cross-country arcs are established as firms seek buyers and sellers outside the damage zone. Finally, N-ABLE also shows that in some cases buyer-seller relationships established during the disruption continue post disruption.

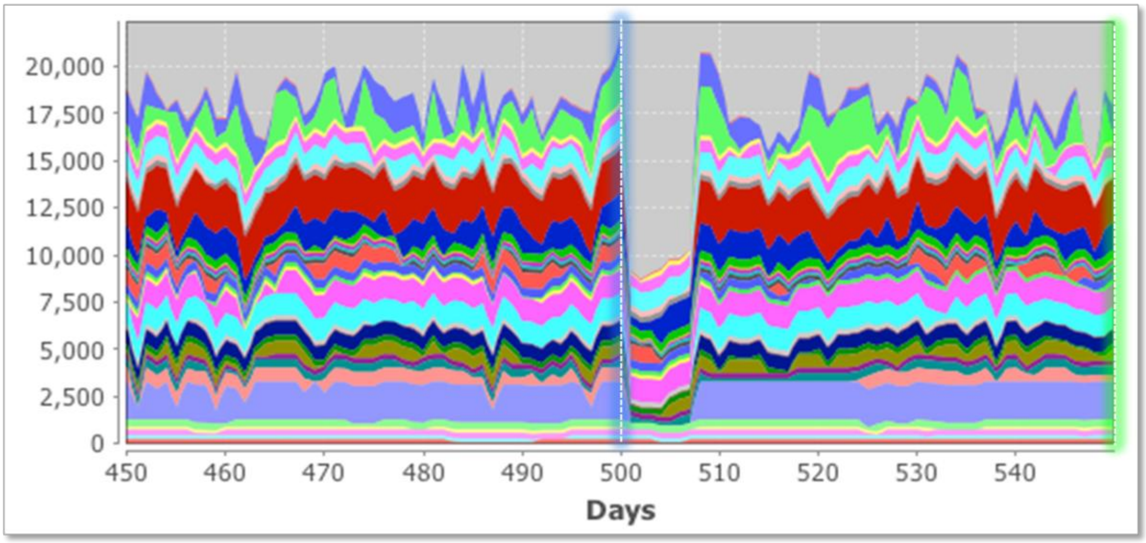

Figure 5. Chemical 'A' production by plant

Supply Chain-Wide Impacts

The disruption impacted chemicals across the product network, which indicates potentially wide-spread changes in market conditions. Figure 7 shows graphically how the chemicals are networked. During the first week of disruption, the supply chain experiences a 30 percent decline in production by mass. The overall supply-chain production levels return to normal after approximately 30 days, though some individual chemicals take much longer, see Figure 8. Sales experienced a 15 percent decline and take approximately 20 days to recover. The reduction in sales is less than in production due to sales from inventory for those markets that are not supply constrained during baseline and short duration conditions.

Aggregate unmet demand stabilizes after an estimated 80 days, although there is unmet demand for certain chemicals that remain. Longer term unmet demand for certain chemicals is expected due to the lack of production of particular chemicals even after the overall supply-chain production levels return to normal. Finally, shipment levels experienced a reduction during the disruption, followed by a surge immediately after, and return to baseline conditions after about 80 days. N-ABLE indicated that some firms in the impacted areas will have production processes out of service for six months or more. However, beyond the core damage area, most production flows return to normal status after 25-50 days.

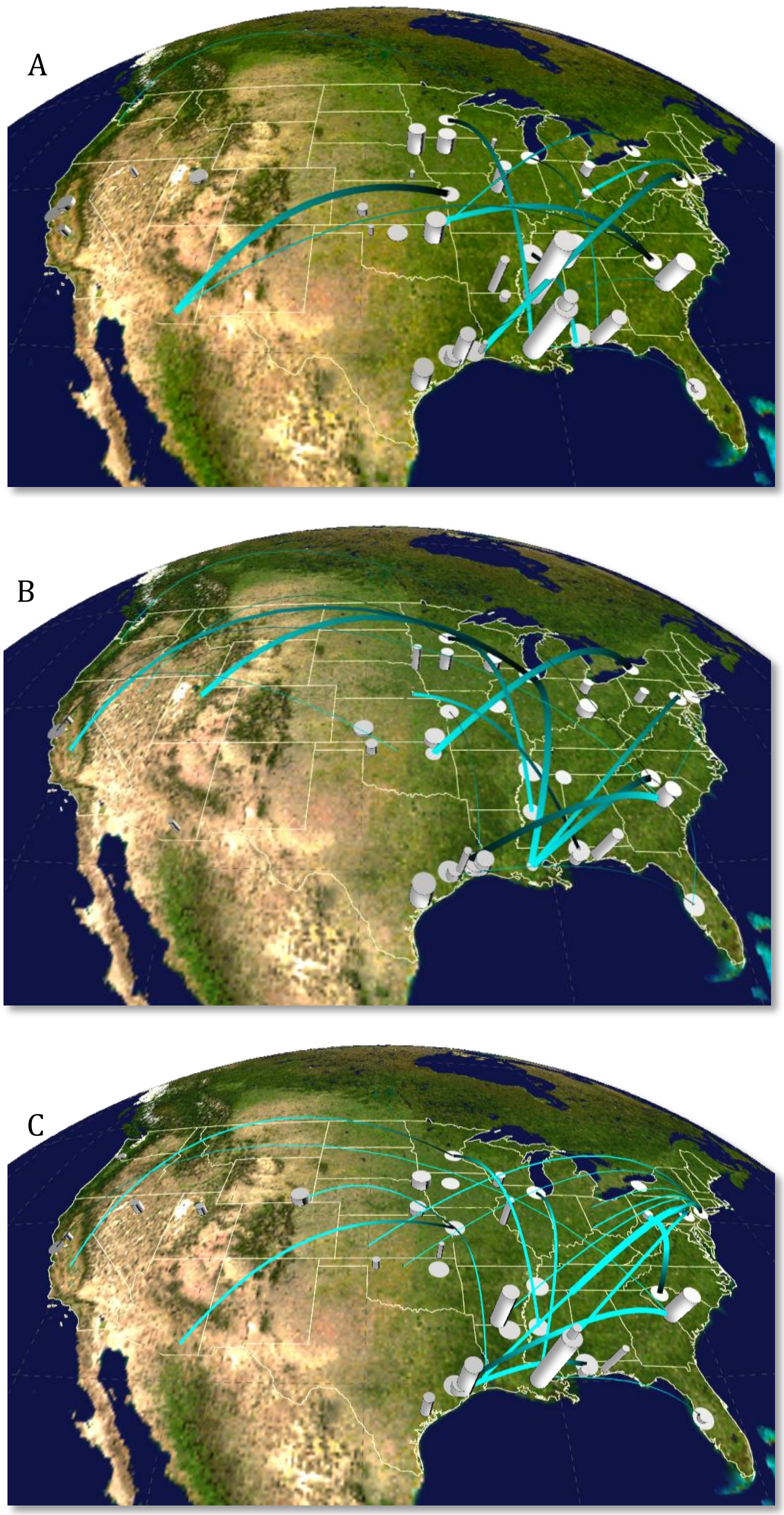

Figure 6. Chemical ‘A’ market A) baseline day, B) day 1 of disruption, and C) day 200 of disruption

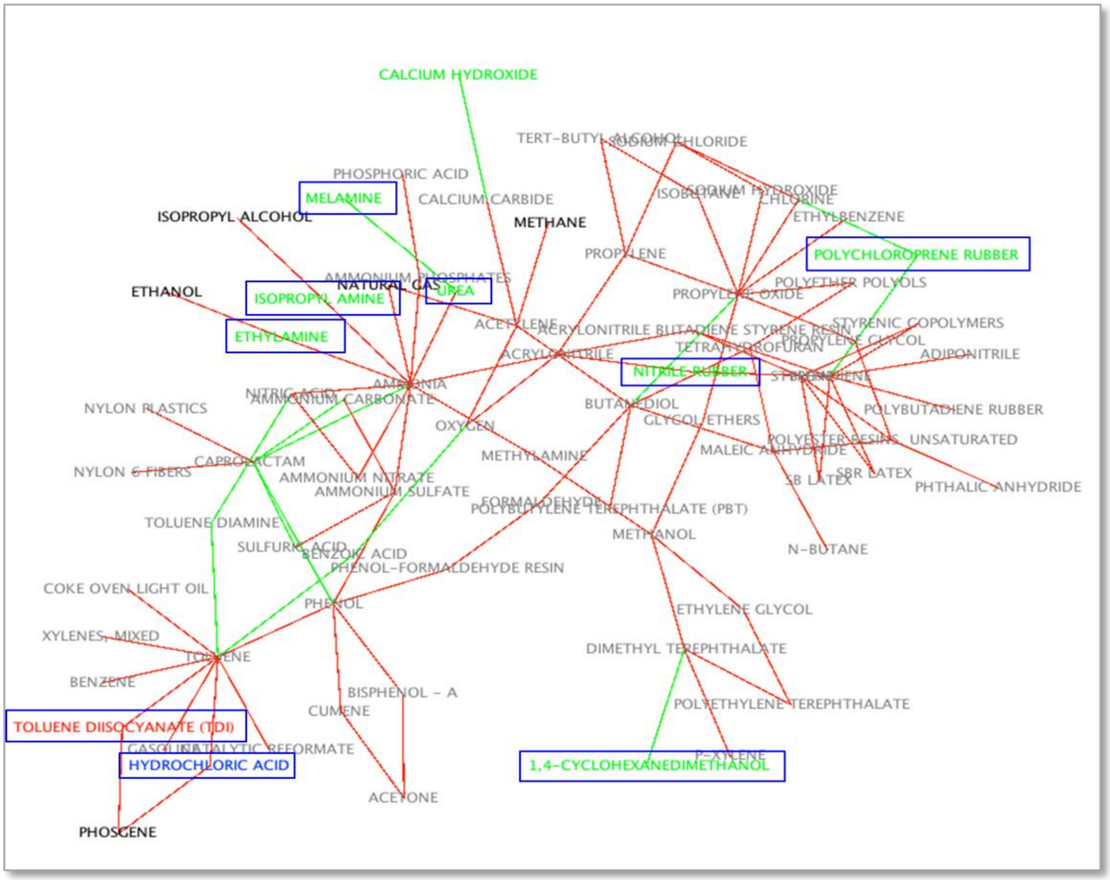

Figure 7. Chemical markets

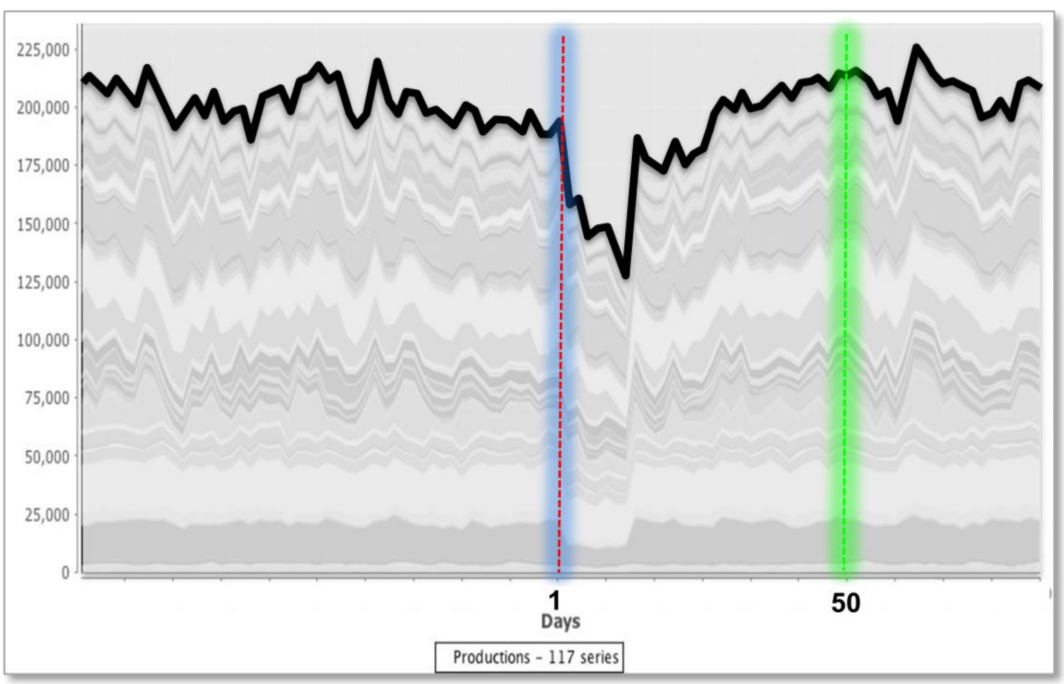

Figure 8. Chemical production

Summary

Sandia has developed an agent-based tool, N-ABLE, capable of simulating the domestic chemical supply chain that can be sued to estimate economic impacts resulting from large-scale disruptions to the chemical sector. N-ABLE draws upon various chemical industry datasets to simulate firms within a supply chain network where each firm interacts with others through chemical reactions, markets, and physical infrastructure. The supply and demand within each simulated network is consistent with respect to mass balances of every chemical within the network. Production decisions at each time step are a set of constrained linear program (LP) solutions that minimize the difference between desired and actual outputs.

The methodology is demonstrated through the simulation and analysis of an 80 chemical supply chain disrupted by an earthquake in the New Madrid Seismic Zone. It was found that disruptions impact chemicals across the product network, suggesting potentially wide-spread changes in chemical plants' operations, aggregate output declines by 30 percent and recovers in about 2 months, and sufficient capacity exists in the system to adapt and recover from lost capacity, despite the assumed total loss of some facilities.

Acknowledgement

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