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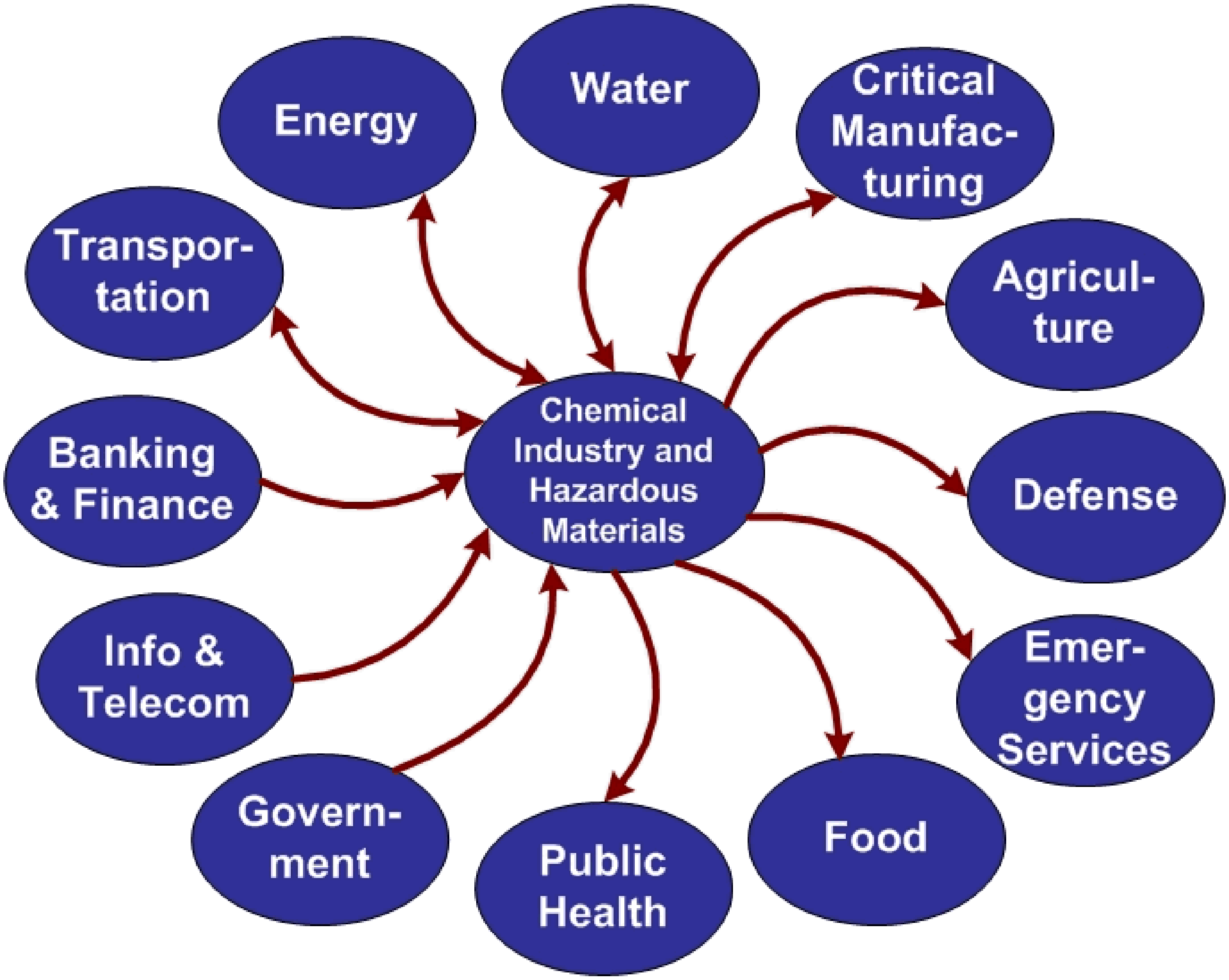

Chemical Supply Chain and Resilience Project: 2009 Capability Report

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Homeland Security

Sandia National Laboratories

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List of Acronyms and Abbreviations

Acronym	Definition
AIChE	American Institute of Chemical Engineers
CDM	Chemical data model
CDR	Chemical Data Review
CEH	*Chemical Economics Handbook*
CIKR	critical infrastructure and key resource
CIP	Critical infrastructure protection
CIR	critical infrastructure resilience
CITF	Critical Infrastructure Task Force
CREATE	Center for Risk and Economic Analysis of Terrorist Events
CSAC	Chemical Security & Analysis Center
DHS	U.S. Department of Homeland Security
DOE	U.S. Department of Energy
DOT	U.S. Department of Transportation
EIA	Energy Information Administration
EPA	U.S. Environmental Protection Agency
E-Plan	Emergency Response Information System
FAIT	Fast Analysis Infrastructure Tool
FASTMap	A NISAC geospatial analysis tool
FTS	Foreign Trade Statistics
GIS	Geographic information system
ID	identifier
IP	Office of Infrastructure Protection
Loki	A NISAC network analysis tool
MIG	Minnesota IMPLAN Group
N-ABLE™	NISAC Agent-Based Laboratory for Economics
NISAC	National Infrastructure Simulation and Analysis Center
R-NAS	Railroad Network Analysis System
S&T	Office of Science and Technology
Sandia	Sandia National Laboratories
TSA	Transportation Security Administration
USGS	U.S. Geological Survey
W-DCP	World Directory of Chemical Producers

Executive Summary

In response to the identification of the U.S. chemical sector as one of the nation's critical infrastructures and key resources (CIKRs), the U.S. Department of Homeland Security (DHS) tasked the National Infrastructure Simulation and Analysis Center (NISAC) with developing a modeling, simulation, and analysis capability that would allow the DHS to assess the vulnerabilities of the chemical sector, its interdependencies with other CIKRs, potential impacts from disruptive events (such as manmade and natural disasters), and its overall economic resilience. Under the direction of the DHS Office of Infrastructure Protection (IP), the NISAC chemical industry project addressed the petrochemical supply chain and reported on that effort in 2007 and 2008 chemical industry project capability reports.[1,2,3,4]

In September 2008, the DHS Science & Technology (S&T) Directorate assumed direction and funding for the chemical sector study beyond petrochemicals into other supply chains. This phase of the multi-year project focused on creating detailed models of the chlorine and ammonia supply chains and on developing an economic resilience methodology that can be applied to all supply chains within the chemical sector.

For the chlorine supply chain, which is composed largely of U.S. producers and users, the project team divided the chlorine derivatives into groups and acquired data on chemical technologies, U.S. chemical plants, and chlorine shipments. For the ammonia supply chain, which relies heavily on ammonia imports from other countries and is also heavily dependent on natural gas, the project team identified and grouped the ammonia derivatives, developed the international and domestic natural gas markets and pipeline flows, and acquired data on technologies and on domestic and foreign chemical plants.

The team participated in a significant effort to compile the various datasets into a consistent form that could be used in the NISAC chemical data model (CDM) to support input requirements for multiple modeling tools. The chlorine and ammonia supply chain capability development focused on the CDM and two of the five simulation modeling tools: Rail Network Analysis System (R-NAS) (transportation analysis) and NISAC Agent-Based Laboratory for Economics (N-ABLE™) (supply chain analysis). The three additional modeling tools were updated by way of additional development within the NISAC CDM: FASTMap (geospatial analysis), Fast Analysis Infrastructure Tool (FAIT) (infrastructure analysis), and Loki (network analysis).

For the second focus of this year's project, the team developed a framework to use in measuring and assessing the economic resilience of the chemical sector. This framework, which has been tested on other projects and will be tested on the chemical project, measures two key indicators of economic

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1 Downes, P. S., W. E. Beyeler, M. A. Ehlen, D. A. Jones, K. L. Stamber, and S. Starks, "National Infrastructure Simulation and Analysis Center Chemical Industry Project: Capability Report 2008," Unpublished Draft, February 2009

2 Downes, P. S., W. E. Beyeler, M. A. Ehlen, and K. L. Stamber, "National Infrastructure Simulation and Analysis Center Analysis of Petrochemical Supply Chain Impacts due to a Scenario Hurricane: Demonstration of Capabilities 2008," February 2009, FOR OFFICIAL USE ONLY

3 Jones, Dean A., Chad Davis, Orr Bernstein, and Mark Turnquist, "National Infrastructure Simulation and Analysis Center: Analysis of Petrochemical Supply-Chain Impacts due to a Rail Transport Embargo, Demonstration of Capabilities 2008, 20 February 2009

4 Downes, P. S., et al., "National Infrastructure Simulation and Analysis Center Chemical Industry Project: Report for Industry Feedback," October 2007

resilience: economic performance, as measured by the difference between actual and targeted economic performance, and recoverability, as measured by the cost or other energies necessary for the chemical sector to economically recover. In cooperation with the National Center for Risk and Economic Analysis of Terrorist Events (CREATE) at the University of Southern California, the team developed and agreed upon a general definition of resilience, as follows:

> *Given the occurrence of a particular disruptive event (or set of events), the resilience of a system to that event (or events) is the ability to efficiently reduce both the magnitude and duration of the deviation from targeted system performance levels.*

Both the supply chain development and the resilience development work were reviewed by U.S. government agencies, chemical industry stakeholders, and university researchers for feedback and comment. Generally, feedback was enthusiastic and positive. In addition to the work in progress, the reviewers identified the following supply chain development needs:

- Validating modeling results,
- Expanding the global supply chain analysis, and
- Encouraging additional cooperation from government agencies, industry associations, and companies to expand and validate data and increase understanding of constraints on the supply chain.

Reviewers also identified the following resilience methodology development needs:

- Evaluating market considerations as part of the resilience methodology,
- Continuing to test and evaluate the resilience metrics in the chemical sector, and
- Reconciling the project resilience definition with definitions of resilience disseminated by other agencies.

1 Introduction

In 2006, the U.S. Department of Homeland Security (DHS) identified the chemical sector as one of the nation's 18 critical infrastructures/key resources (CIKRs) and then tasked the National Infrastructure Simulation and Analysis Center (NISAC) with developing its analytical capabilities for this sector. This project is a multi-year effort because of the size of the sector and its strong interdependencies with many, if not most, of the 18 CIKRs. In 2008, Sandia National Laboratories (Sandia) started to expand this work beyond the petrochemical supply chain to other chemical sectors. Sandia is performing this work under the direction and funding of the DHS Science and Technology (S&T) Directorate.[5]

This report describes capabilities developed and delivered by the S&T chemical supply chain and resilience project between September 2008 and August 2009. This work focused on development and analysis of the chlorine and ammonia supply chains and development and application of metrics for measuring the economic resilience of the chemical sector.

[5] This capability development work is funded by the U. S. Department of Homeland Security's Directorate for Science & Technology, Infrastructure Geophysical Division, under a Technology Transition Agreement between the Infrastructure and Geophysical Division, Science and Technology Directorate, and the Office if Infrastructure Protection and Programs Directorate, dated June 2008, signed July 2008.

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2 Supply Chain Capability Development

The larger goal for the NISAC chemical supply chain capability development project was to identify possible impacts to the chemical industry resulting from manmade and natural disasters. At a minimum, this capability had to provide the consequences of disruptions to chemical production and related manufacturing sectors, including the loss of assets within the chemical industry, outages in a range of critical infrastructures (for example, transportation or electric power), and changes in regulatory and economic conditions.

The supply chains for chlorine and ammonia were developed by the S&T chemical supply chain and resilience project in a multi-year effort to expand the NISAC chemical supply chain capabilities. Both chlorine and ammonia are building-block chemicals; that is, chemicals used in the production of many other chemicals. By focusing on these two supply chains, the project is laying the foundation for the addition of future supply chains. In addition, by adding the chlorine and ammonia supply chains to the petrochemical supply chain already developed by NISAC, the petrochemical capability has also been expanded.

To accomplish the larger goal, the project modeling capability must function across different levels of resolution: individual chemical assets, chemical subsectors, geographic regions, and/or the nation. The chemical project team leverages several of its simulation, modeling, and analytical tools to ensure that the broad set of questions asked about all infrastructures can be answered with respect to the chemical infrastructure.

Supply chains are characterized by a multitude of features: location of plants, production volumes, transportation requirements, and the uses for the goods being produced, to name a few. Employing multiple modeling approaches allows NISAC to provide static, system-wide, short-term approximations that highlight problematic subsectors or regions; and dynamic, facility-level, long-term representations to better understand individual, asset-level concerns.

Five simulation models were developed by NISAC and are used in the chemical supply chain project. All of these tools use data from the NISAC chemical data model (CDM), or the results from one model are input for another. The chlorine and ammonia supply chain capability development focused on the CDM and two of the five simulation models: Rail Network Analysis System (R-NAS) (transportation analysis) and NISAC Agent-Based Laboratory for Economics (N-ABLE™) (supply chain analysis). Three of these models were updated by way of additional development work on the NISAC CDM design: FASTMap (geospatial analysis), Fast Analysis Infrastructure Tool (FAIT) (infrastructure analysis), and Loki (network analysis). Because the CDM development work is such an integral part of the supply chain development work, it is discussed along with the development of both supply chains.

Long-term studies build these capabilities and provide an opportunity for outreach and engagement with industry and academia. These modeling tools are described in detail in "National Infrastructure Simulation and Analysis Center Chemical Industry Project: Report for Industry Feedback,"[6] October 2007, and "National Infrastructure Simulation and Analysis Center Chemical Industry Project: Capability Report 2008," February 2009.[7]

[6] Downes, P. S., M. A. Ehlen, K. L. Stamber, W. E. Beyeler, T. J. Brown, and A. J. Scholand, "National Infrastructure Simulation and Analysis Center Chemical Industry Project: Report for Industry Feedback," October 2007

[7] Downes, P. S., W. E. Beyeler, M. A. Ehlen, D. A. Jones, K. L. Stamber, and S. Starks, "National Infrastructure Simulation and Analysis Center Chemical Industry Project: Capability Report 2008," Unpublished, February 2009

2.1 Chemical Data

Providing accurate, consistent, and readily accessible data to models and analysts is essential to the project. The NISAC data management platform has been strategically developed over the past 5 years to address the myriad complexities and challenges presented by modeling and simulation efforts on behalf of DHS. The NISAC platform includes data; Oracle® databases; spatial data engines; geographic information system (GIS) applications; and custom-developed tools for data integration, management, and manipulation. This platform, coupled with NISAC's expertise in spatial data management, forms the foundation of the CDM. Table 2-1 lists the data sets, and their sources, used in the CDM.

Table 2-1: Data Sources for the Chemical Data Model (CDM)

Dataset Name	Provider
World Petrochemicals Program 2009[8]	SRI Consulting
Chemical Economics Handbook 2009[9]	SRI Consulting
World Directory of Chemical Producers 2009[10]	SRI Consulting
Oil & Gas Pipelines 2008[11]	National Geospatial-Intelligence Agency (original publisher Penn Well Energy Inc.)
Oil & Gas Facilities 2008[12]	National Geospatial-Intelligence Agency (original publisher Penn Well Energy Inc.)
United States Census 2000[13]	U.S. Census Bureau
County Business Patterns 2007[14]	U.S. Census Bureau
County Business Patterns Employees Estimation 2007[15]	U.S. Census Bureau
Geographic Names Information System[16]	U.S. Geological Survey (USGS)
IMPLAN States Summary 2002[17]	Minnesota IMPLAN Group (MIG)

[8] SRI Consulting, "World Petrochemicals, http://www.sriconsulting.com/WP/Public/ProgramContents.html
[9] SRI International, *Chemical Economics Handbook*, http://library.dialog.com/bluesheets/htmla/bl0359.html
[10] SRI Consulting, *Directory of Chemical Producers* (DCP), http://www.sriconsulting.com/DCP/Public/index.html
[11] National Geospatial-Intelligence Agency Homeland Security Infrastructure Program (HSIP) Gold 2008, http://www.defenselink.mil/policy/sections/policy_offices/hd/assets/downloads/dcip/DCIP_Geospatial_Data_Strategy.pdf
[12] Ibid.
[13] U.S. Census Bureau, *United States Census 2000*, http://www.census.gov/
[14] U.S. Census Bureau News, "California County Shows Biggest Percentage Increase in Jobs and Payroll, *County Business Patterns*, 2007, http://www.census.gov/Press-Release/www/releases/archives/county_business_patterns/000387.html
[15] Ibid.
[16] U.S. Geological Survey, *Geographic Names Information System* (GNIS), U. S. Board on Geographic Names, http://geonames.usgs.gov/
[17] IMPLAN is an input-output model of the U.S. economy. The network model uses IMPLAN data to estimate output in economic sectors that use petrochemicals as inputs. For more information about IMPLAN, see Minnesota IMPLAN Group, Inc., 1725 Tower Drive West, Suite 140, Stillwater, MN, 55082, http://www.implan.com/

Table 2-2: Data sources for the Chemical Data Model (CDM) (continued)

Dataset Name	Provider
International Trade Statistics 2007[18]	U.S. Department of Commerce
Refinery Location Data[19]	Argonne National Laboratory, Energy Information Administration (EIA), SRI Consulting WP 2009
2005 Commodity Flow Survey, Department of Transportation	2005 Waybill Sample, Surface Transportation Board
2007 Class I Railroad Statistics, Association of American Railroads	2007 Producer Price Index, Department of Labor
E-Plan Emergency Response Information System[20]	U.S. Environmental Protection Agency/DHS

The fundamental requirement of the CDM is that it provides the same data across models and analyses and that all modifications are traceable (documented). The focus areas for development of the chemical data model during this effort are the addition of new datasets and development of tools to aid in the review and validation of data for the CDM.

2.1.1 Additional Datasets

There are four primary data additions under this development effort. Information from the World Directory of Chemical Producers (W-DCP), the *Chemical Economics Handbook* (CEH), the DHS's Emergency Response Information System (E-Plan), and Foreign Trade Statistics (FTS) datasets were all incorporated into the CDM. Each of these additions had its own purpose and resulting set of development needs.

World Directory of Chemical Producers

The W-DCP dataset is recognized by the chemical industry as being the most complete source for the identification of global chemical plant locations. The dependence of the U.S. ammonia supply chain on global supply necessitated the addition of global ammonia and ammonia-related chemical plants into the NISAC CDM. The W-DCP presented fewer technical challenges to incorporate; however the dataset does not include geospatial information and, for some plants, the capacity information is not reported. To incorporate geospatial information, the project team used a variety of other sources (e.g., U.S. Environmental Protection Agency [EPA] facility registry) within the greater NISAC data architecture and supplemented by hand, as needed. The process is shown below in Figure 2-1.

[18] U.S. Census Bureau *Foreign Trade Statistics, 2007*
[19] Quarterly dataset produced and distributed by Argonne National Laboratory, updated in 2009 using http://www.eia.doe.gov/oil_gas/petroleum/info_glance/petroleum.html and SRI Consulting, "World Petrochemicals, http://www.sriconsulting.com/WP/Public/ProgramContents.html
[20] Department of Homeland Security's Emergency Response Information System: https://erplan.net/eplan

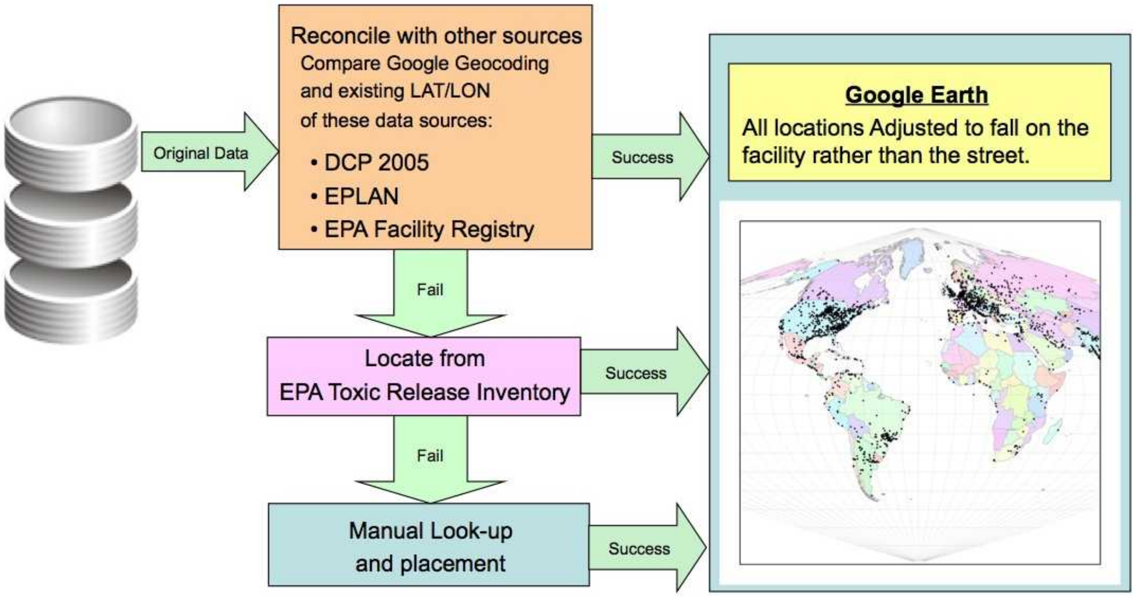

Figure 2-1: Incorporating chemical plant location information

Chemical Economics Handbook

The CEH is a series of industry studies that provide evaluation of supply/demand relationships and analysis of the industry competitive environment for approximately 300 chemical products and product groups. Each study contains the following information:

- Chemical plant and capacity information, if available;
- Aggregate supply and demand for the given chemical market;
- General production yields;
- Demand trend forecasts;
- Aggregate trade information; and
- Price histories.

The CEH is one of the most data-rich sources of chemical information available; however, it presents the largest technical challenge to incorporate into the NISAC CDM. The CEH was never intended to be used electronically and, therefore, it was not designed as such. It is a series of reports that must be read, then the data extracted manually, and then the data entered into the NISAC CDM. The data extracted from CEH were reviewed both by SRI Consulting and by the Fertilizer Institute prior to entry into the NISAC CDM[21]. SRI Consulting and the project team are currently working on ways to collaborate on a solution that will reduce the technical challenges while still providing necessary information.

[21]Personal communications between Sue Downes (SNL) and Pam Guffain (TFI) dated 05/13/2009, 05/14/2009, 05/15/2009, and 05/18/2009, and personal communications between Sue Downes (SNL) and (SRIC) dated 05/11/2009 and 05/20/2009.

Emergency Response Information System Data

The DHS's E-Plan was recommended as a source of data containing information about where chemicals are stored. Chemical storage locations are as important to supply chain analysis as production locations. The E-Plan dataset also provides the project with a good indicator of the distribution of chemicals across the country. E-Plan provides its own set of technical challenges for incorporation into the NISAC CDM. While the E-Plan is a database and should be easy to incorporate, the level of data quality control on data entry is not consistent with that of the NISAC CDM. Because there are multiple entities entering data into E-Plan, there are many issues with merging this dataset into the CDM. Common data entry errors and inconsistencies include

- Multiple spellings for the same chemical (e.g., the word diesel is spelled nine different ways in E-Plan database records);
- Inconsistent formatting for identifier (ID) fields (such as CAS® numbers[22] and latitude and longitude information);
- Duplicate records for the same chemical storage (e.g., data are not always updated, but re-entered as a new record without removing the old); and
- Multiple names for the same chemical (e.g., chemicals with multiple synonyms will have multiple chemical IDs in E-Plan).

In order to incorporate E-Plan data, the project team has created a Chemical Data Review (CDR) tool that allows for a quality check on the data before they are entered. The tool currently checks for multiple spellings and multiple names. Inconsistent formatting and duplicate record identification are currently being designed and developed into the tool, but are not yet available. See Section 2.1.2 for more information on the development of this tool. The E-Plan data are used to determine the storage locations of the intermediates (for all segments of the supply chains). Those locations that were not verified as production plants or storage locations were included as downstream consumers, thus, identifying the distribution of the supply chain nationally. The E-Plan data currently in the NISAC CDM only includes chlorine and ammonia. As the tool is completed, the E-Plan data for other chemicals will be incorporated.

U.S. Foreign Trade Statistics Data

The U.S. Census Bureau's FTS dataset is the easiest to upload into the NISAC CDM, but it too has its issues. The FTS dataset consists of two separate databases of foreign trade information: one for U.S. imports and one for U.S. exports. The trade data are aggregated annually by commodity (in this case, chemicals). The data fields used for the NISAC CDM do not include the entire set of data available within the FTS. The available data fields used within the NISAC CDM are

- Harmonized trade code,
- Commodity description,
- Country of origin (imports),
- Country of destination (exports),

[22] CAS® is a division of the American Chemical Society, http://www.cas.org/aboutcas/index.html

- Imports for consumption,
- 1st unit of quantity for consumption (imports),
- Amount of first unit of quantity (exports),
- Year-to-date,
- Amount, and
- Unit of Measure.

The data in the FTS are for all commodities, not just chemicals. The project analysts worked closely with SRI Consulting to ensure that the chlorine and ammonia information pulled from the FTS was compatible with the less aggregate chemical production and consumption data provided in the other datasets used by NISAC.

2.1.2 Data Review Tools

To reduce the effort required to merge all these datasets, NISAC is developing a tool that allows data sources to be compared to one another and the NISAC chemical data owner to determine which set of data should be used for a given purpose. The NISAC Chemical Data Review (CDR) tool is a multi-part tool that allows chemical names to be standardized across all datasets and allows for the cross-referencing of chemical synonyms. As data are reviewed, the information is logged for tracking purposes. Once the data have been reviewed and approved, they are loaded into the NISAC CDM.

2.2 The Chlorine Supply Chain

The majority of the chlorine supply chain development covered under the scope of this project was completed at the time of interim report deliverable (March 2009) and is documented in that report. Much of the information contained in that report is repeated in the following sections to provide context for the additional work developed since the issuance of the interim report.

Chlorine is produced at 36 different locations within the United States, and it is used in a variety of other chemical manufacturing processes or direct-use applications at thousands of locations across the county.[23] Because the majority of the production, distribution, and use of chlorine are domestic; this project's efforts focused on the domestic portion of the supply chain. Chlorine supply chain characteristics that are important to ensure proper ties to other infrastructures are mostly concerned with the transportation infrastructure. Approximately one-third[24] of the volume of chlorine produced in the United States is transported predominately by 90-ton rail car (22 percent), with a lesser amount being transported using 4- to 24-inch pipelines (10.2 percent), and less than 1 percent being transported using 15- to 20-ton bulk tank trucks and 1,200-ton barges.[25] These transportation modes are included in the chlorine capability development within N-ABLE™.

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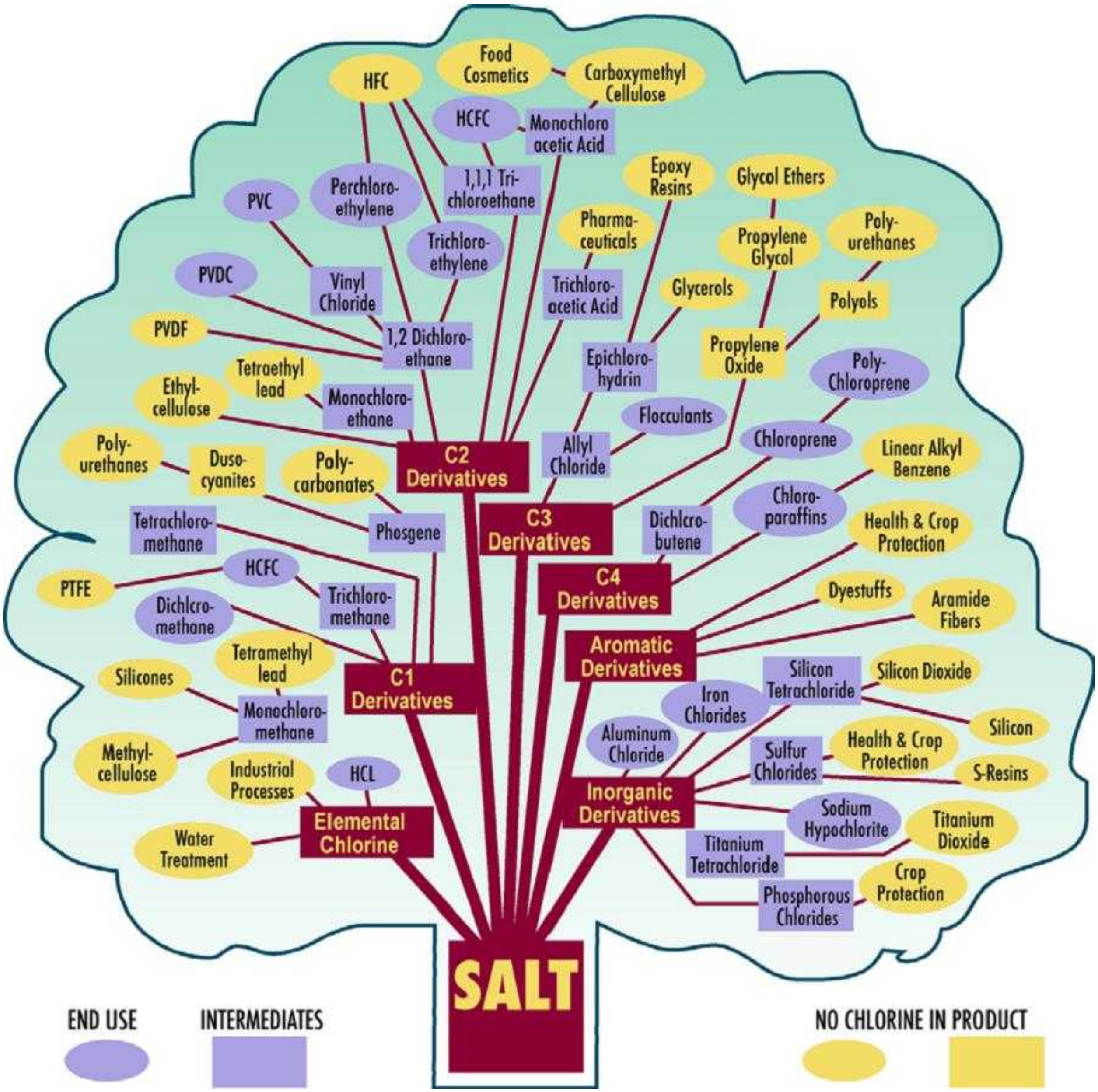
[23] Linak, Eric, Stefan Schlag, and Kazuteru Yokose, *CEH Marketing Research Report: Chlorine/Sodium Hydroxide*, SRI Consulting, September 2008

[24] The percentage of transported chlorine has been reported as high as 46%, reported by The Chlorine Institute for the period 1980-2002.

[25] Source: NISAC Report Titled: *Economic and Public Health and Safety Impacts of Disruptions in Chlorine Transport* dated August 2003.

To represent the widespread, diverse uses of chlorine, the supply chain is divided into derivative groupings, based on the "chlorine tree" (as defined by the American Chemistry Council[26] and shown in Figure 2-2), along with information from SRI Consulting and industry collaborators. The project team's representation of these chemical relationships is shown in Figure 2-3 through Figure 2-8.



Source: American Chemistry Council 2003.

Figure 2-2: American Chemistry Council's chlorine tree

[26] Chlorine Chemistry Division of the American Chemistry Council, http://www.chlorinetree.org/pages/flash.html

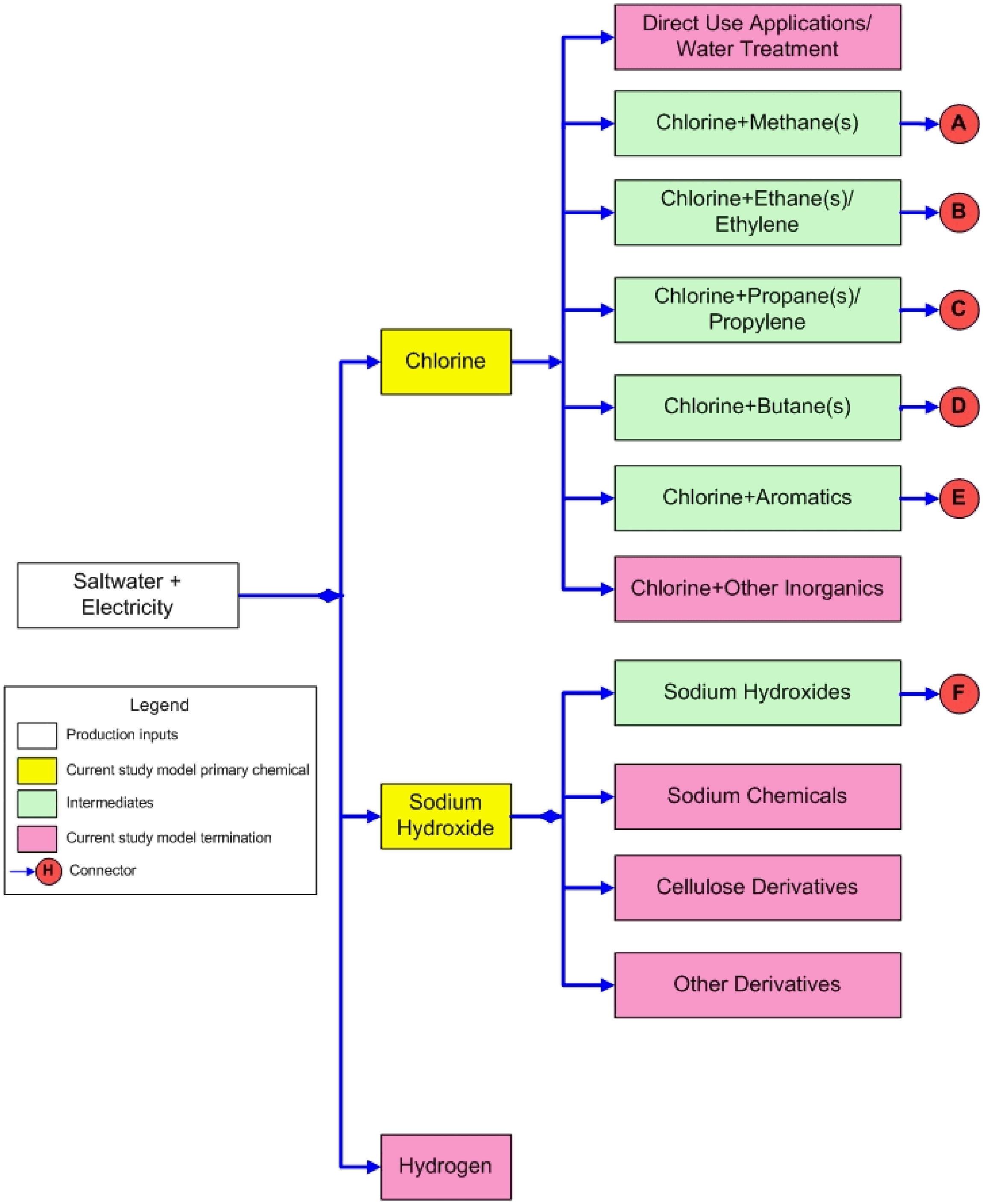


Figure 2-3: Basic chlorine manufacturing derivatives

Figure 2-3 shows the prevalent method for manufacturing chlorine and sodium hydroxide (caustic soda). There are other production methods for both, but very few plants employ them. As stated earlier, there are 36 active chlorine production plants in the United States; 32 of these plants also manufacture sodium hydroxide. The sodium hydroxide portion of the diagram is discussed later in this section.

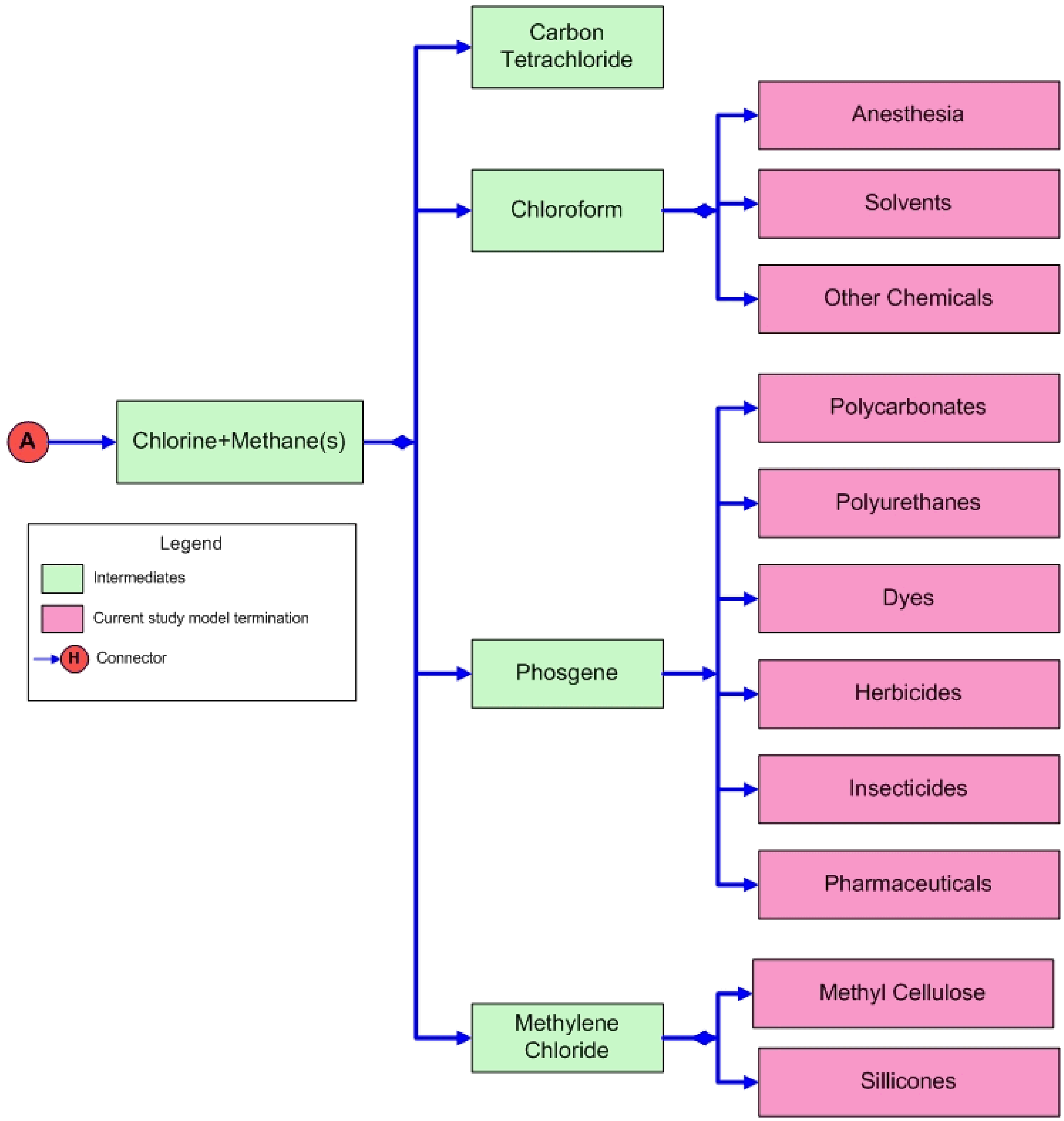


Figure 2-4: Chlorine derivatives related to methane

Figure 2-4 shows the chemicals that can be derived from chlorine and methane. There are 23 plants in the United States manufacturing methylene chlorides, carbon tetrachloride, chloroform, and phosgene. These 23 plants are included in the supply chain modeling development. The remaining portions of the supply chain shown on this diagram are modeled as end-points (pink); therefore, they create the demand for the intermediates (green), but are not taken further (e.g., production of pharmaceuticals is not included, just the demand from the pharmaceutical industry for phosgene).

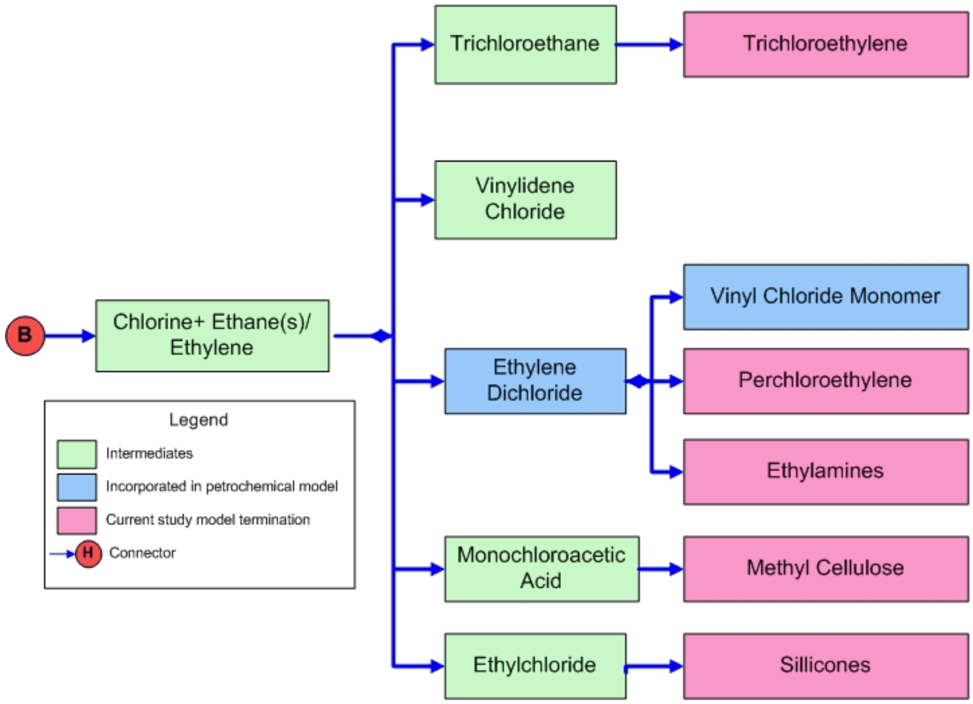


Figure 2-5: Chlorine derivatives related to ethane

Most of the intermediates in the chlorine/ethylene portion of the supply chain (Figure 2-5) were partially represented in the petrochemical supply chain model; this portion of the supply chain serves to more fully represent the coupling of the two supply chains. Methyl cellulose and silicones are considered end-points in the chemical supply analysis at this point in the overall development.

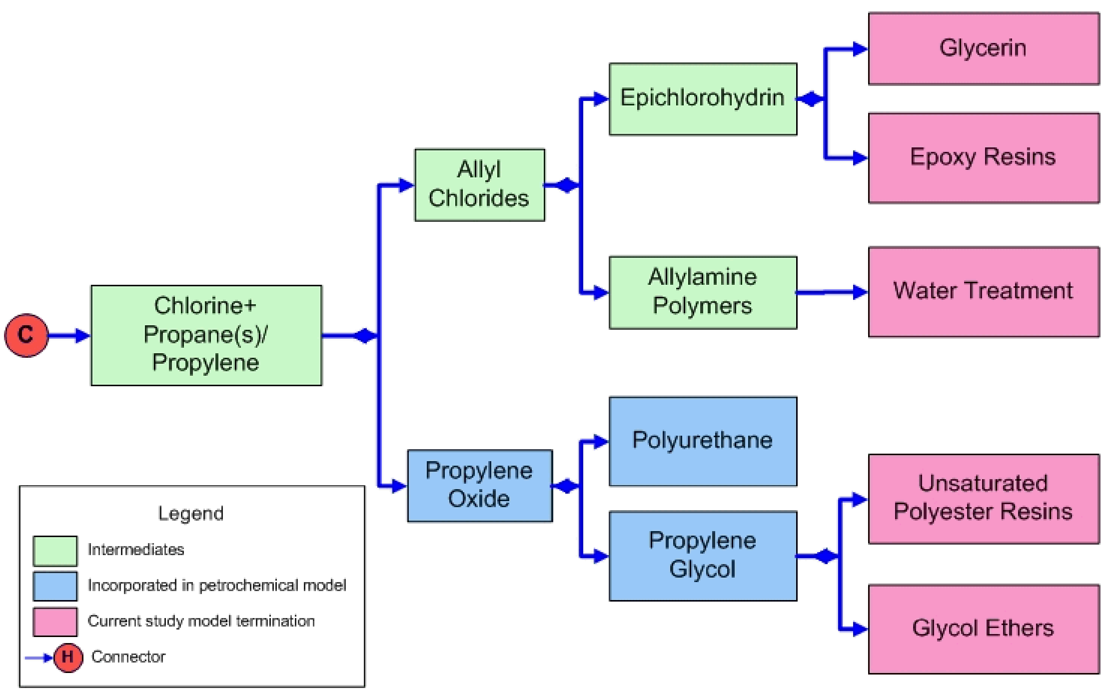


Figure 2-6: Chlorine derivatives related to propane

Similar to chlorine/ethylene, many of the intermediates in the chlorine/propane(s)/propylene supply chain (Figure 2-6) were partially represented in the petrochemical model. The majority of the development needed for this portion of the supply chain is the upstream tie to chlorine production and the further development of the portion of the supply chain that follows the allyl chloride chain through to water treatment.

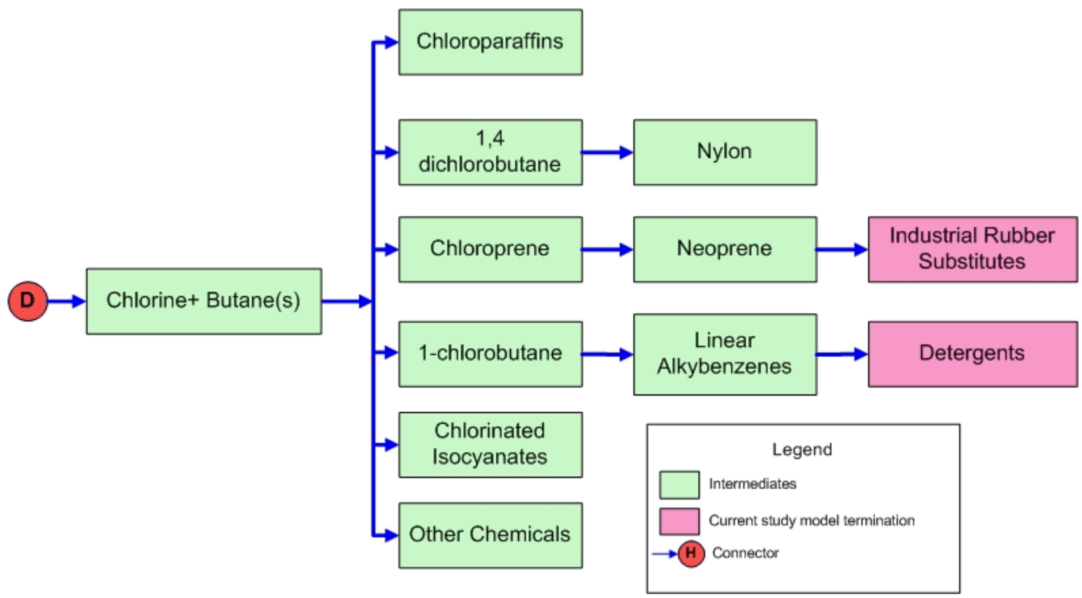


Figure 2-7: Chlorine derivatives related to butane

The majority of the chlorine/butane segment of the supply chain (Figure 2-7) required development in order to incorporate into the modeling efforts. This development allows NISAC to lay the groundwork for the evaluation of substitutability in future resilience work.

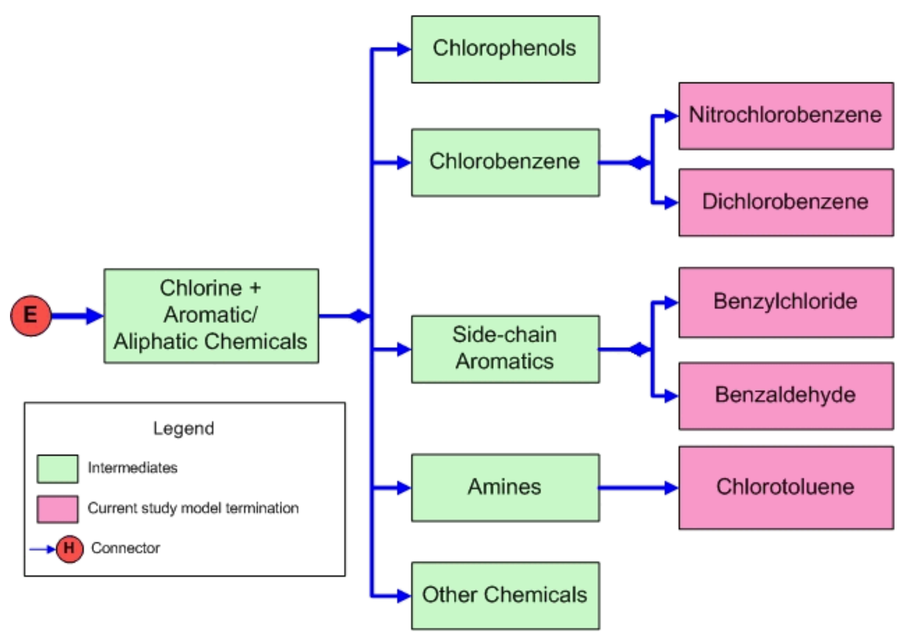


Figure 2-8: Chlorine derivatives related to aromatics and aliphatics

Hydrogen and sodium hydroxide (caustic soda) are co-products of chlorine production, as shown in Figure 2-9. Approximately 1.1 pounds of sodium hydroxide are produced for each pound of chlorine. Sodium hydroxide is used to manufacture other chemicals and in direct applications and is valued more for its neutralizing power as a strong base and as an absorbent, rather than as a source of sodium. Consumption patterns for the direct applications of sodium hydroxide are often difficult to establish because it is routinely used in many plants for acid neutralization and gas scrubbing. For purposes of supply-chain development and modeling, the project team represents the demand for sodium hydroxide with respect to its consumption for manufacturing of other chemicals.

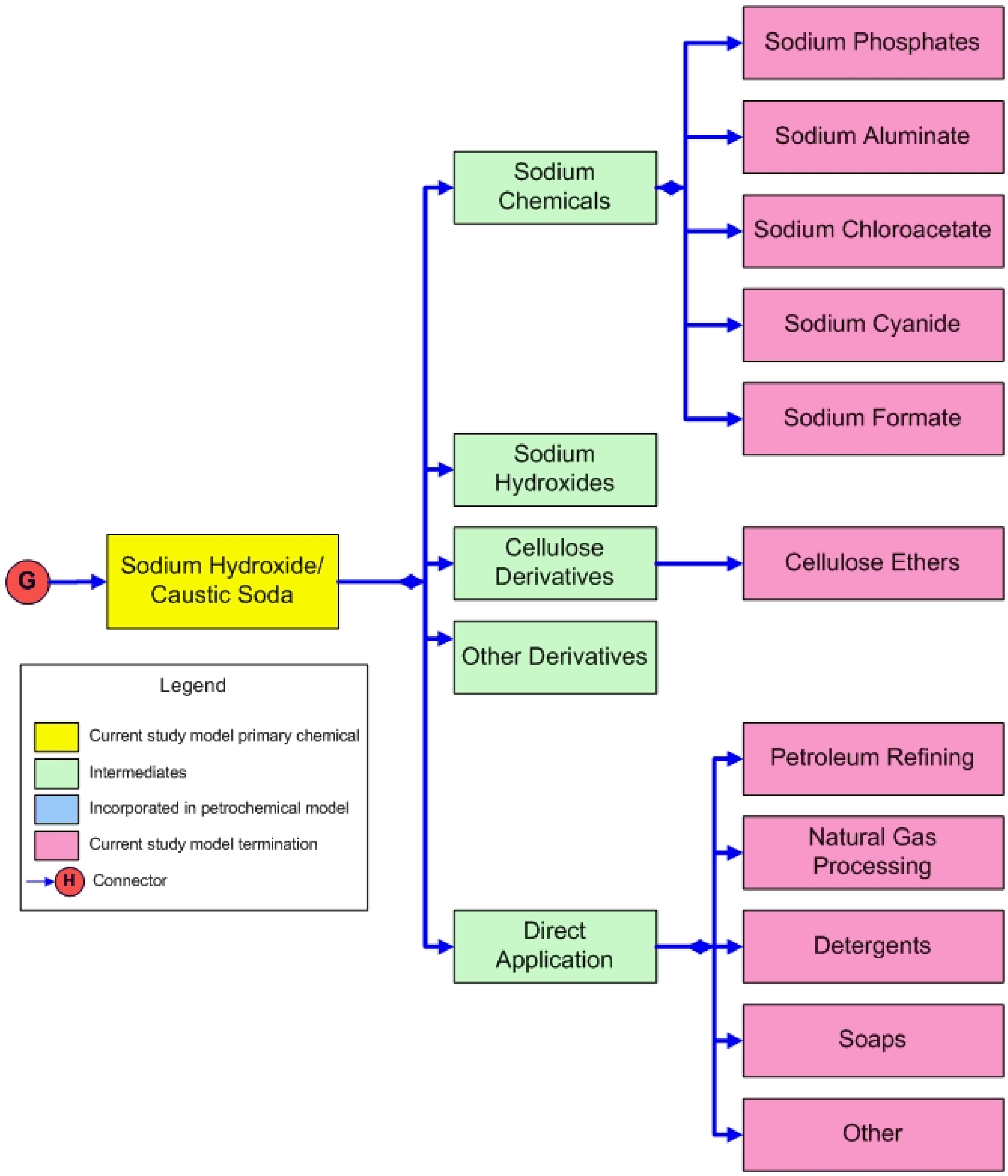


Figure 2-9: Basic Sodium hydroxide manufacturing derivatives

Figure 2-9 shows a simplified layout of the sodium hydroxide tree.[27] This figure represents the direct application consumption of sodium hydroxide, as a portion of the total sodium hydroxide production

[27]This tree was created by adapting the sodium hydroxide tree developed by Chlorine Chemistry Division of the

consumed, but exact locations of direct application are limited to the information within the E-Plan data and may not fully represent the direct application consumption.

The amount of hydrogen produced during chlorine and sodium hydroxide production is small, approximately 3 percent by weight. The majority of hydrogen produced in this manner is used on-site by the producing plant for fuel and other chemical manufacturing needs. The captive uses are represented through analysis of the E-Plan data. Non-captive (sold hydrogen) will be considered in the next scope of work for the supply chain capability development.

The chlorine supply chain development includes more than just locating plants and consumers. Because all of these chemicals are derived from the same base chemical, disruptions to one portion of the supply chain can, and do, affect other portions of the supply chain, which can cascade through the supply chain, connected infrastructures, and ultimately the economic markets. As a result, the project team has done significant work on the economic portion of the supply chains as well (Section 2.4).

2.3 The Ammonia Supply Chain

Ammonia is produced at 22 different locations within the United States. It is the primary source of nitrogen for large-scale industrial agriculture in North America, Western Europe, and many other agricultural producing regions of the world. Ammonia accounts for a significant portion of the production cost for many U.S. agricultural crops. Fertilizers (direct or ammonia-based) represent 80 percent of the ammonia used in the United States. Ammonia is also used in commercial and industrial processes and, in particular, as a building block in the production of many pharmaceuticals. It is also used to produce explosives, plastics fibers and resins, and animal feed.

Characteristics of the ammonia supply chain that are important to include in the project development effort are its dependency on the rail transportation system, the staging of inventories, and the large imports of ammonia into the United States. Ammonia consumed within the United States is transported by rail, truck, barge, and pipeline. Rail, truck, and barge transportation modes each represent approximately 29 percent of the transported volume, while 12 percent is transported by pipeline.[28]

The demand for ammonia for agriculture use is seasonal; however, production is not. Ammonia producers supply agriculture "stage" or store inventories close to agricultural users during the off-season so that during the spring planting season, it will be readily available to all growers. For industrial uses, supplies are distributed continuously throughout the year.

Unlike the U.S. chlorine supply, the U.S. ammonia supply is dependent on both domestic and foreign production. This is primarily a result of the dependence on natural gas to produce ammonia. As the cost of natural gas increases domestically, production is moving offshore to areas where natural gas prices are more amenable. As a result, the total domestic ammonia production capacity has declined and continues to trend downward.

American Chemistry Council, http://www.chlorinetree.org/pages/flash.html; along with SRI International's *Chemical Origins and Markets: Flowcharts and Tables,* 6th Edition, Chemical Marketing Research Center, Kirtland E. McCaleb, ed, 1993

[28] Source: *Rail Transportation of Fertilizer*, The Fertilizer Institute. http://www.tfi.org/. TransportPolicy.pdf, access date, May 2009

For this project, Sandia extended the natural gas analytic capability developed by NISAC in 2008 to include the natural gas economic markets. This modeling effort was described in detail in the 2008 capability report.[29] This newly expanded modeling capability is being used in ammonia and chlorine supply chain test cases.

To represent the widespread, diverse uses of ammonia, the supply chain is divided into derivative groupings, as shown in Figure 2-10).

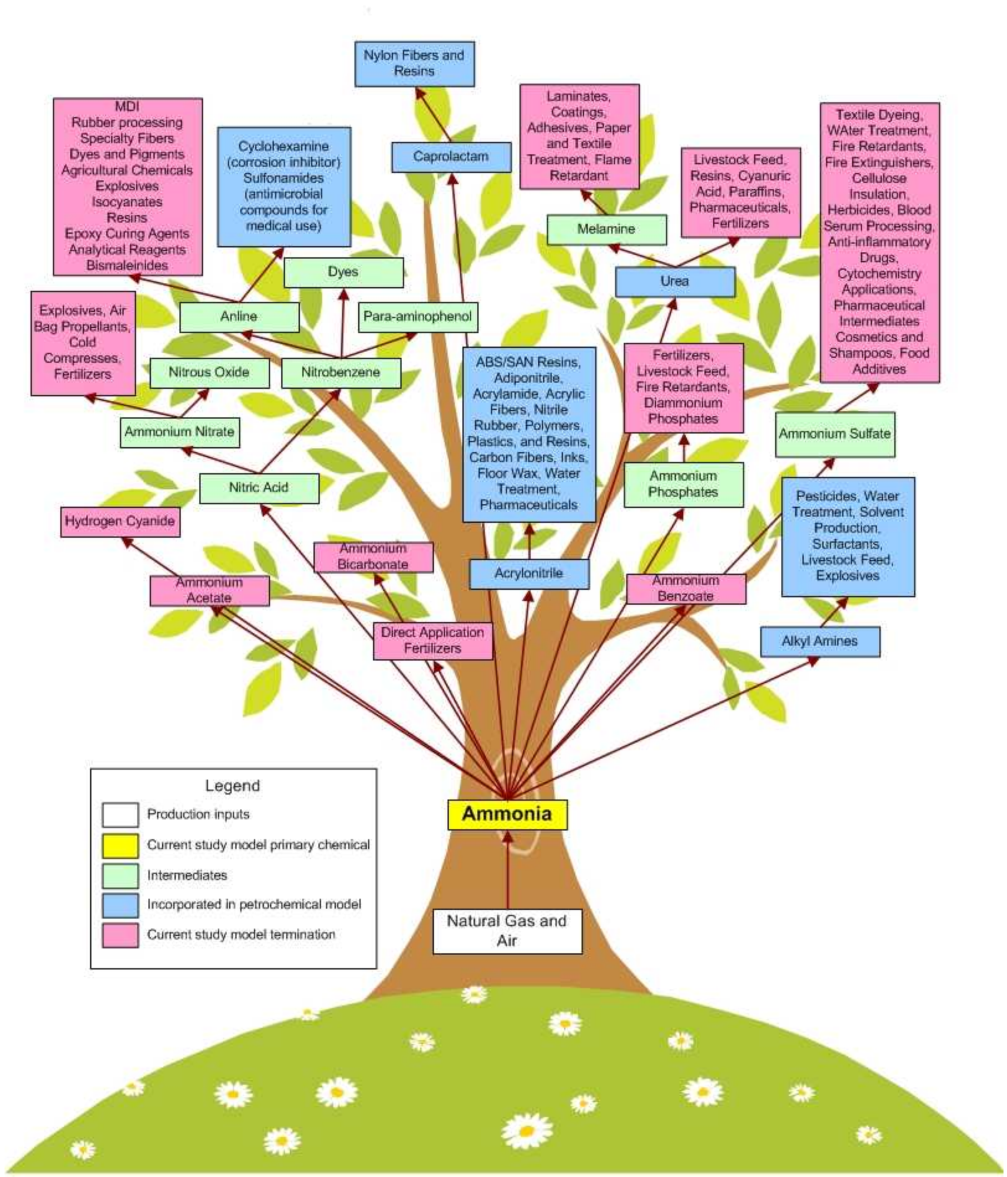


Figure 2-10: Chemical supply project representation of the ammonia tree

[29] Downes, P. S., W. E. Beyeler, M. A. Ehlen, D. A. Jones, K. L. Stamber, and S. Starks, "National Infrastructure Simulation and Analysis Center Chemical Industry Project: Capability Report 2008," Unpublished Draft, February 2009

Figure 2-11 shows the basic ammonia derivatives, and Figure 2-12 through Figure 2-19 show additional detail. As with the chlorine supply chain, the ammonia supply chain is connected to the petrochemical supply chain. The NISAC petrochemical supply chain held placeholders for the ammonia feedstock, or in some cases, placeholders for ammonia-based intermediates that are now incorporated in the larger chemical supply chain model.

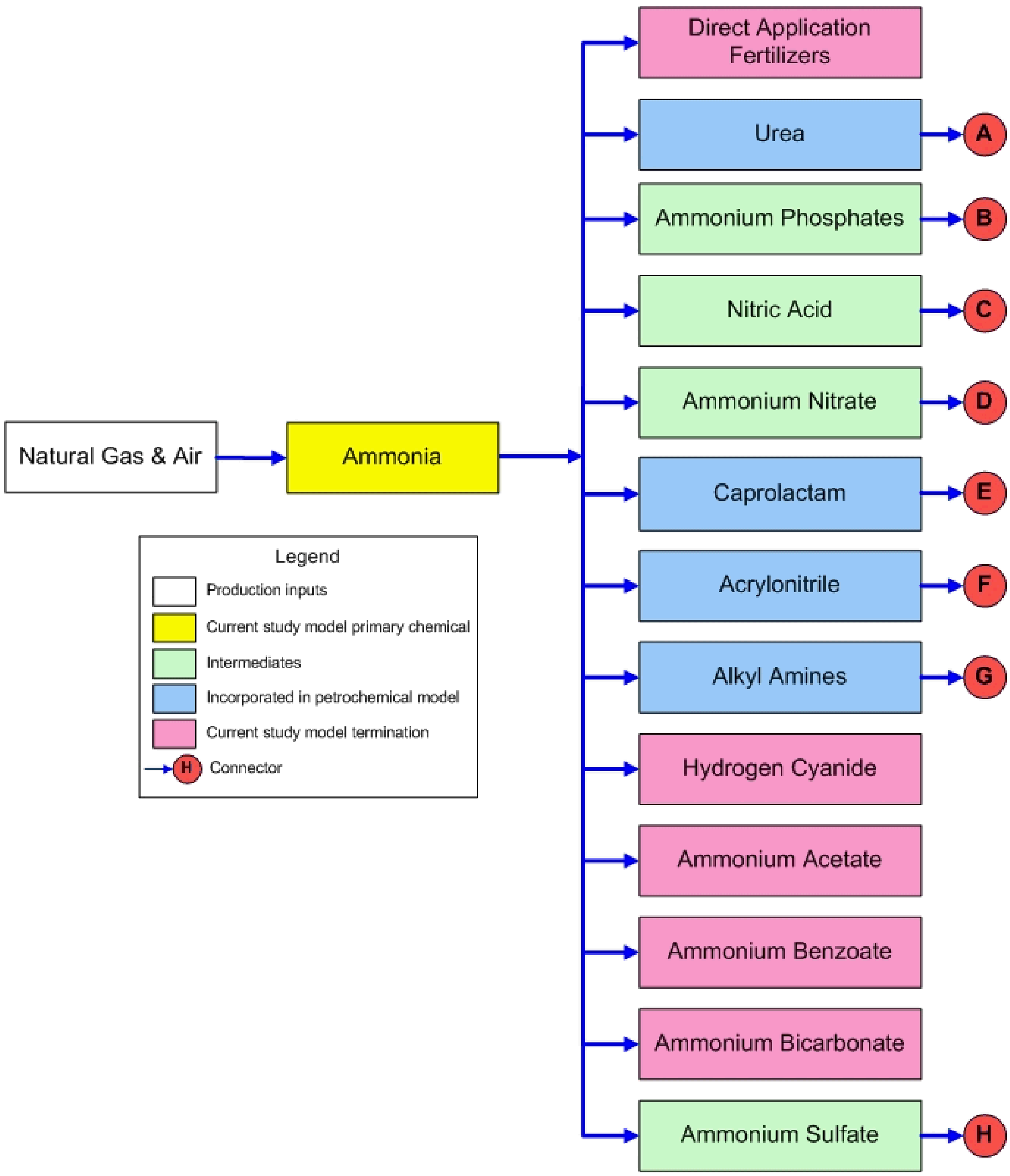


Figure 2-11: Basic ammonia derivatives

The ammonia supply chain is relatively straightforward. Production inputs are primarily natural gas and air from the atmosphere. This yields anhydrous ammonia, the key feedstock for downstream nitrogen products including urea, the primary nitrogen fertilizer product. Liquid forms of urea and ammonium nitrate are combined into nitrogen solutions used in agriculture. The solid product, ammonium nitrate, is made from nitric acid recombined with ammonia.

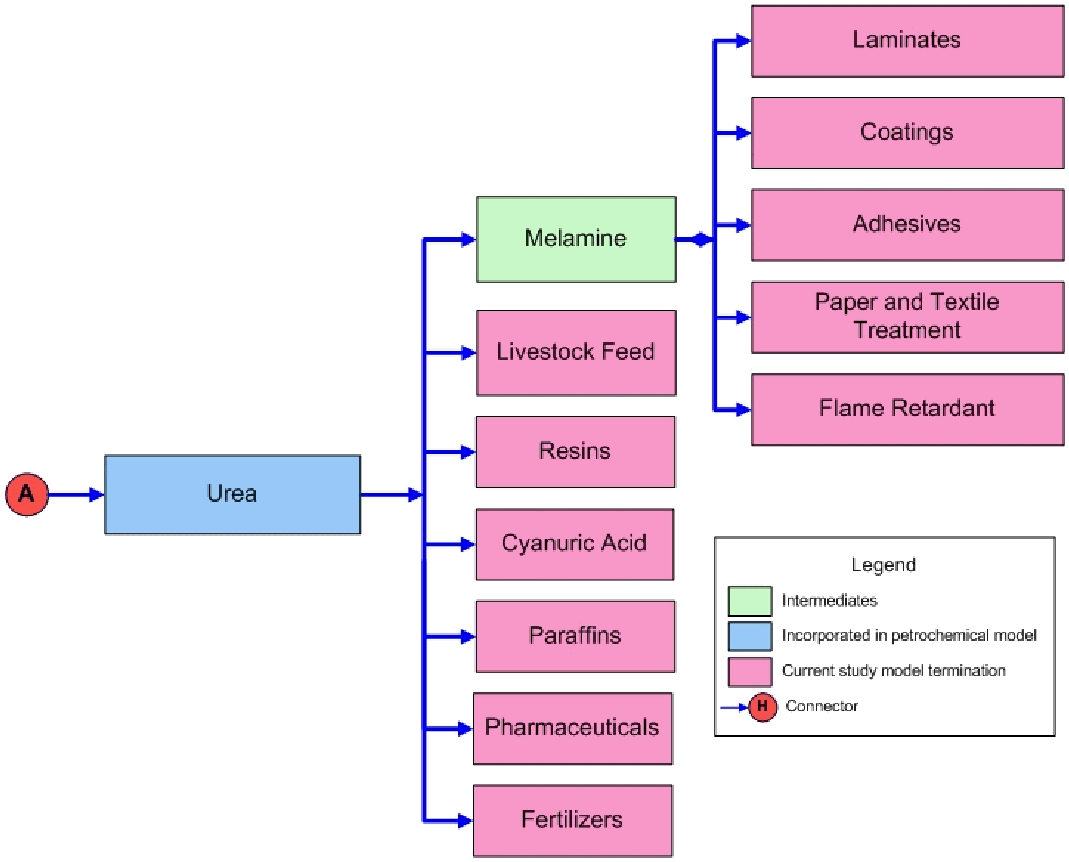


Figure 2-12: Urea derivatives

Urea, as noted on Figure 2-12, was included in previous petrochemical supply chain development, but it was a terminating point for that model. All of the downstream chemicals shown on Figure 2-12 are new development under the ammonia supply chain model. Fertilizer distribution was represented using analysis of E-Plan data.

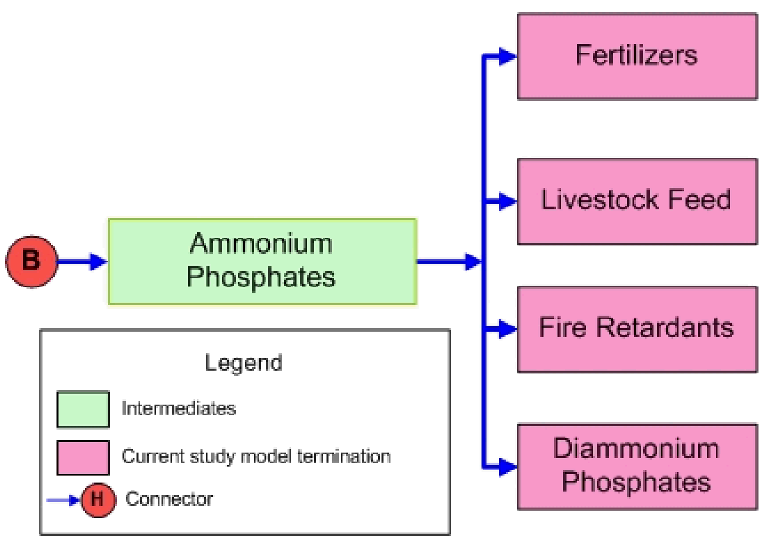


Figure 2-13: Ammonium phosphate derivatives

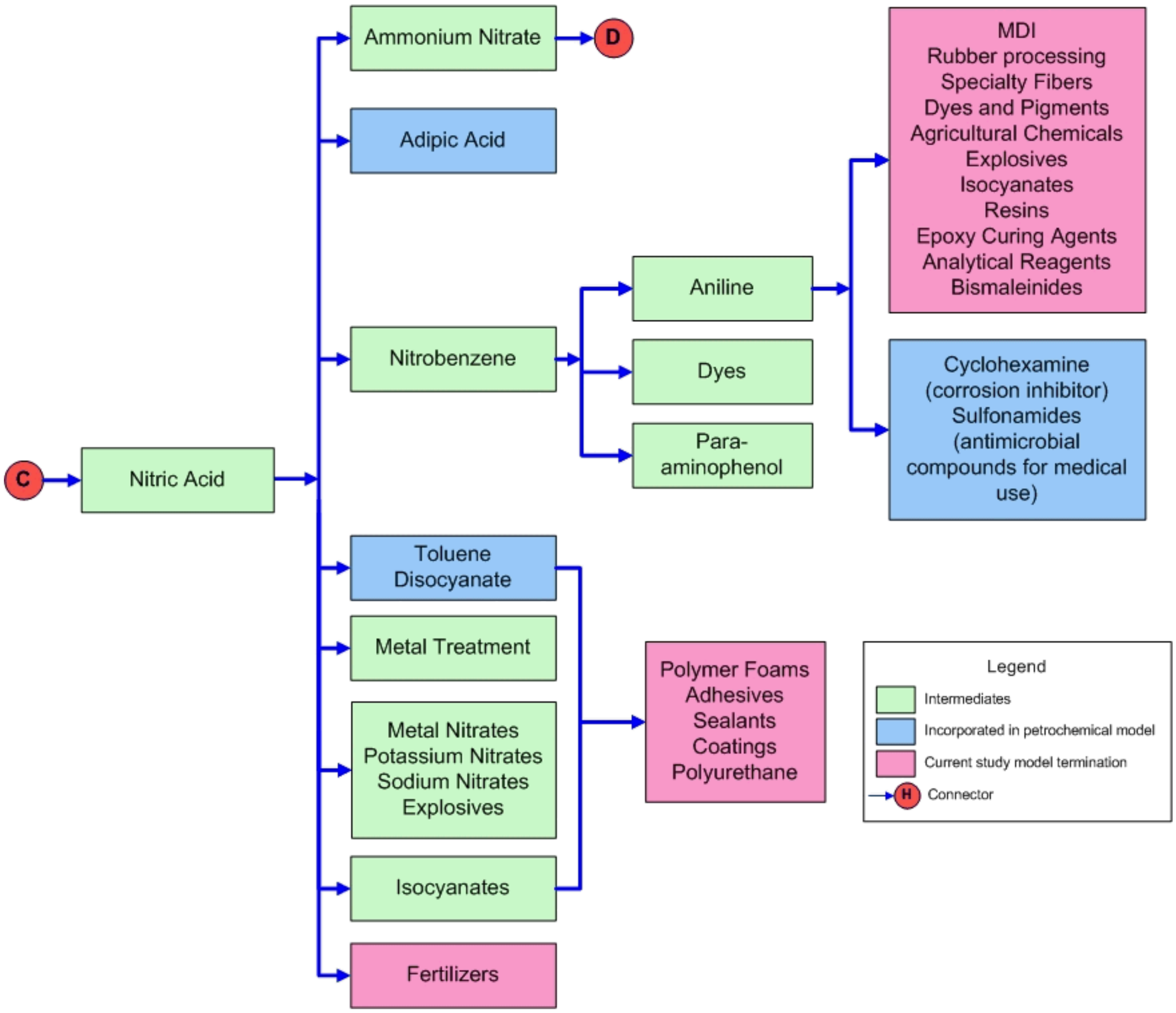


Figure 2-14: Nitric acid derivatives

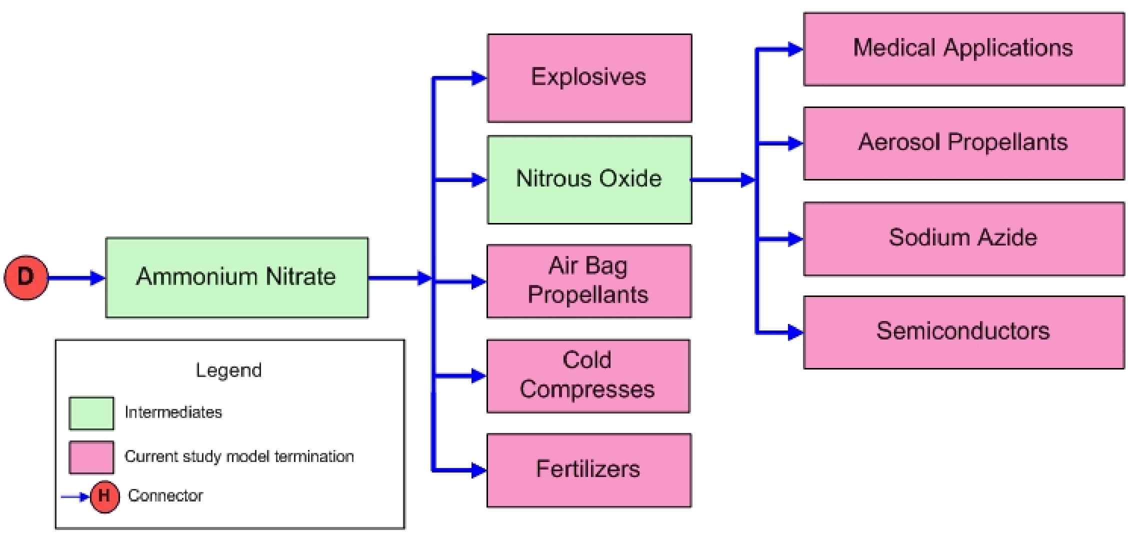


Figure 2-15: Ammonium nitrate derivatives

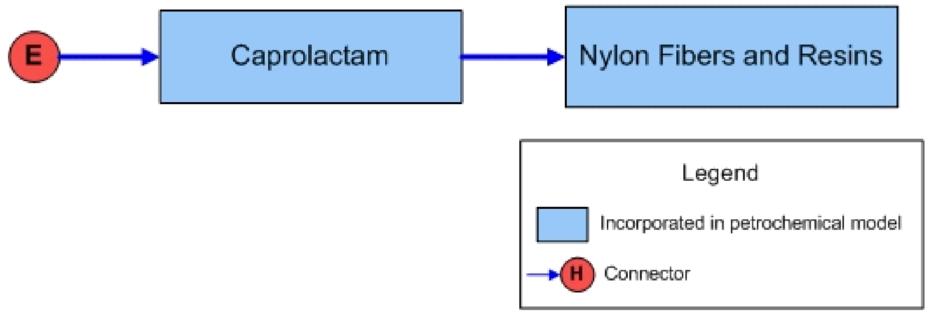


Figure 2-16: Caprolactam derivatives

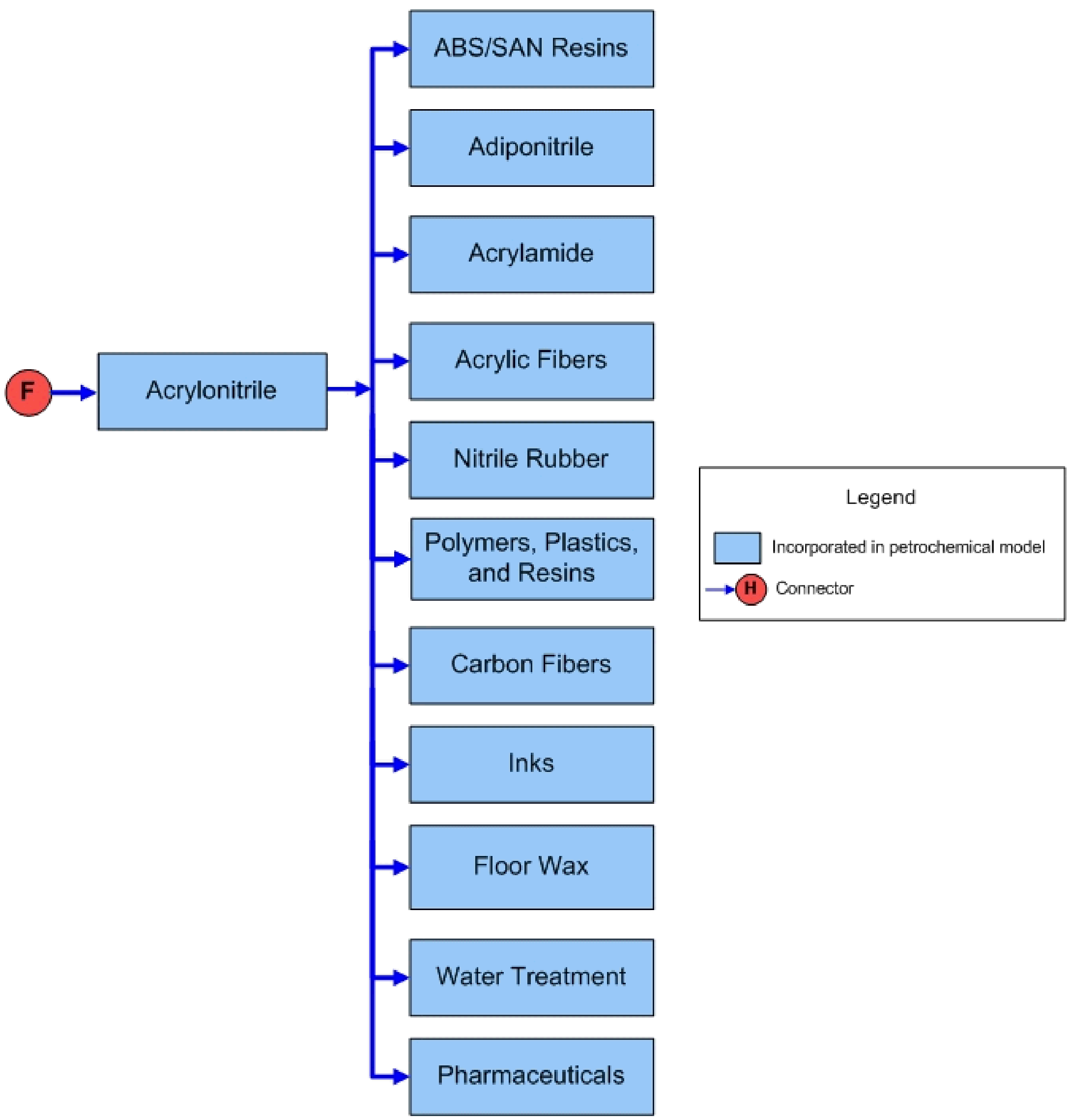


Figure 2-17: Acrylonitrile derivatives

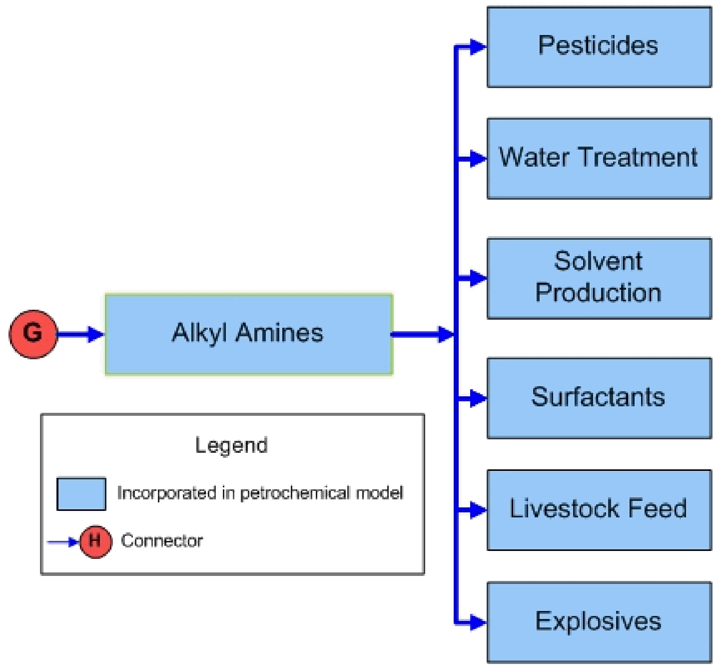


Figure 2-18: Alkyl amines derivatives

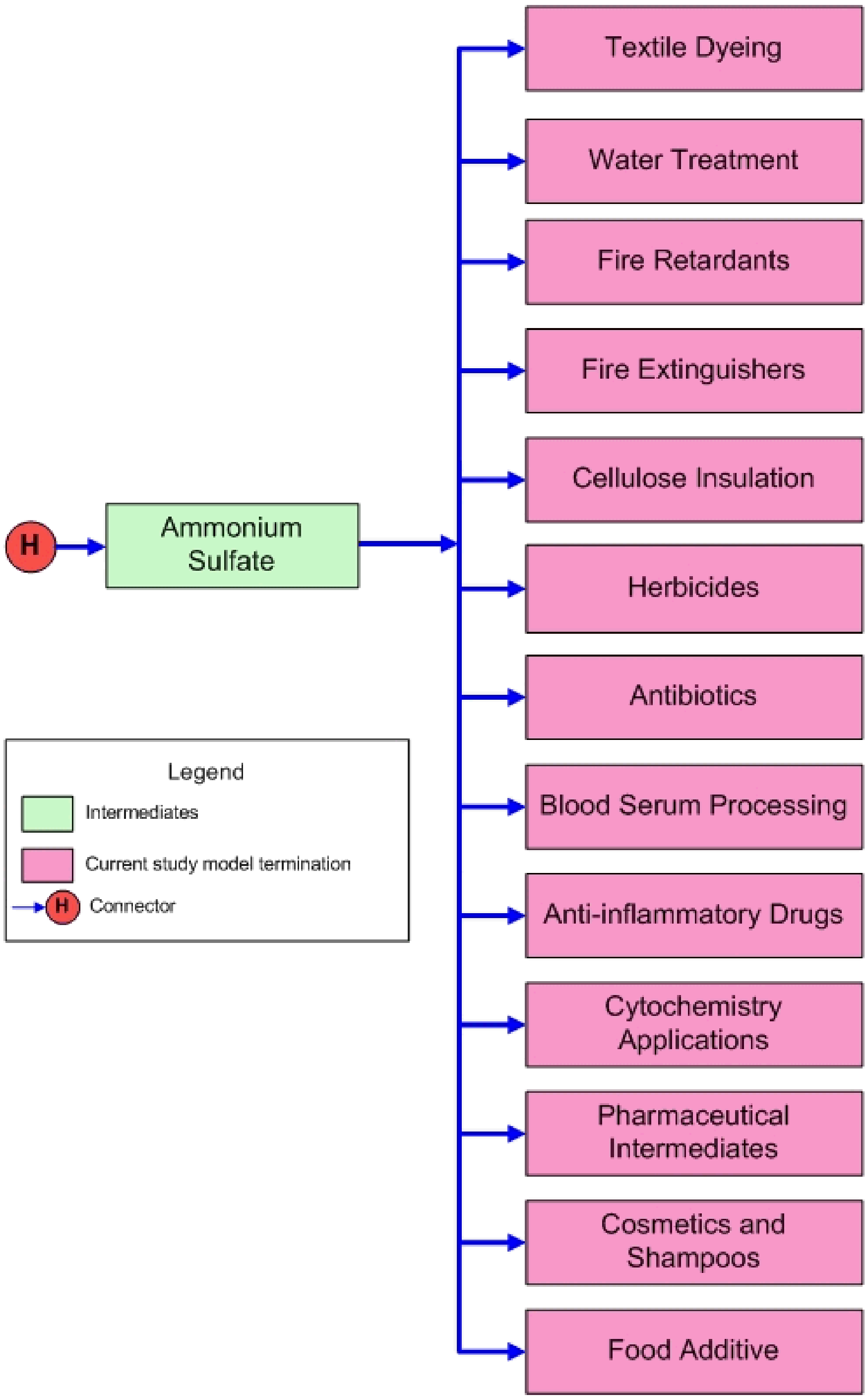


Figure 2-19: Ammonium sulfate derivatives

Industry collaborators reviewed these supply chain representations during the 2009 chemical supply chain and resilience project workshop held at Sandia on June 16 through 18. Sandia has updated the representations based upon their feedback (see Section 2.4).

2.4 The Economic Resilience Methodology

Until recently, the federal government's traditional policy toward critical infrastructure protection (CIP) has focused on "physical protection" and "asset hardening." In 2005, the DHS Critical Infrastructure Task Force (CITF) recommended that DHS focus on critical infrastructure resilience (CIR) as its top-level strategic objective.[30] In addition to the supply chain analysis development undertaken in this project, Sandia was tasked with developing a framework for defining and assessing the resilience of the chemical infrastructure and economic systems. This framework is not intended to replace CIP, but rather to act as an *integrating objective* designed to foster *systems-level* thinking and provide a quantifiable objective. The project team spent considerable effort in defining resilience in this context and developing a methodology and quantifiable measures that could be applied to CIR. This work was conducted in collaboration with the National Center for Risk and Economic Analysis of Terrorism Events (CREATE). The working definition is presented below. The associated methodology and quantifiable measures document will be released in October 2009.

> *Given the occurrence of a particular disruptive event (or set of events), the resilience of a system to that event (or events) is the ability to efficiently reduce both the magnitude and duration of the deviation from targeted system performance levels.*

To further explain the subtleties of the definition, abridged descriptions are provided for the following terms:[31]

- **All-hazards**: Applicable to all types of hazards, natural and manmade. When applying the definition to the resilience of a system, it should be considered in the context of a particular disruptive event.
- **Multiple infrastructures**: General enough to apply to multiple CIKR systems. Different infrastructure systems will use different units of analysis to measure terms like "system performance levels" and "efficiency."
- **Systems focus**: Generally applicable to infrastructure and economic systems; that is, sets of related and often interconnected entities that form a whole. Engineered systems—such as infrastructure systems—have a precise, collective, measurable purpose.
- **Efficiency**: The value of resources and how those resources are used for recovery. Depending on the domain under consideration, these resources could be dollars, repair man-hours, infrastructure replacement assets, or time.
- **Preparation (pre-disruption actions)**: Actions performed in anticipation of the disruptive event to reduce system losses and expedite recovery processes. These actions can include implementing system redundancies and taking other steps to reduce vulnerabilities and consequences.
- **Recovery**: Recovery may occur by way of the system's internal mechanisms or by mechanisms provided by external entities (e.g., government entities). The efficiency of the recovery considers recovery actions by both internal and external mechanisms.

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[30] Homeland Security Advisory Council, 2006, *Report of the Critical Infrastructure Task Force*, January 2006 http://www.dhs.gov/xlibrary/assets/HSAC_CITF_Report_v2.pdf

[31] Vugrin, E. D., D. E. Warren, M. A. Ehlen, A. Z. Rose, and A. M. Barrett, "Chemical Supply Chain and Resilience Project: A Resilience Definition for Use in Economic and Critical Infrastructure Resilience Analysis," Unpublished, 24 August 2009

- **System performance**: Given the flexibility of many systems to adjust to and reconfigure from a disruptive event, maintaining system structure is not as important as maintaining system performance.
- **Targeted system performance**: System output levels that are reasonable and acceptable following a disruptive event. In general, these levels do not necessarily refer to pre-disturbance levels. They may vary according to the disruption type and change over time. This performance level provides a reference point for comparing actual system performance.

3 Collaboration and Outreach

From the outset of the chemical analysis infrastructure development, NISAC has taken the position that the effort cannot be successfully completed without collaboration and assistance from a variety of government agencies, industry organizations, and private-sector companies. It is through these interactions that the project:

- Receives feedback on the depth and breadth of the capability,
- Resolves data obscurity issues,
- Identifies infrastructure dependencies not included in existing data, and
- Receives recommendations for the path forward in the chemical sector development.

Within the last year, the focus has been on chlorine and ammonia and, therefore, most of the collaboration and outreach has been focused on entities either involved with or directly part of those industries. During the early part of this effort, the project team met with representatives of The Fertilizer Institute and subsequently received a review of the ammonia supply chain data from that perspective. The team also had conference calls with The Chlorine Institute during this same period and received feedback on development of the chlorine supply chain.

3.1 American Institute of Chemical Engineers (AIChE) Annual Conference

One of the largest outreach efforts the team makes each year is to host an annual workshop that includes government agency representatives, chemical company and trade association representatives, and academia. To increase participation in this year's workshop, the team participated in the American Institute of Chemical Engineers (AIChE) annual conference as a way to communicate to the community at large what the DHS and Sandia are undertaking. Project personnel and S&T personnel prepared handout material, manned a booth, and attended conference sessions to meet members of the AIChE community, listen to their concerns, and request their input and attendance at the workshop.

3.2 The Chemical Supply Chain Workshop

This year's Chemical Supply Chain and Resilience Project workshop hosted approximately 40 participants for 3 days. Participants included individuals from the following organizations:

- CREATE
- Cornell University
- Morgan State University
- SRI Consulting
- The Dow Chemical Company
- Olin Corporation
- Terra Industries
- Agrium, Inc.

- The Chlorine Institute (U.S.)
- The American Chemistry Council
- The Fertilizer Institute (U.S.)
- The Fertilizer Institute (Canada)
- The U.S. Department of Energy (DOE)
- The DHS Chemical Security & Analysis Center (CSAC)
- The DHS Chemical Sector Specific Agency
- The Federal Bureau of Investigation
- The U.S. Department of Transportation's (DOT's) Transportation Security Administration (TSA)

The Chemical Supply Chain Workshop is designed to create discussion among the participants about the appropriateness of the data, simulation and data analysis tools, generated results, and even the types of analyses being considered. Participants were shown the chlorine and ammonia supply chains as the project team has defined them, the prototype resilience definition and measurement methodology, and three demonstration scenarios using the developed supply chain capabilities. The demonstration scenarios were amalgamations of typical analytical requests received by NISAC that have components related to the chemical infrastructure. The three demonstration scenarios discussed in the following sections, along with specific feedback related to each scenario. The three scenarios cover a rail transportation disruption, a facility-level analysis, and a large hurricane analysis.

Actual results are not presented in this document for any of these scenarios because they were specifically designed to stimulate a dialogue between the federal entities and the private sector participants, rather than to evaluate the validity of results. Additional general comments and feedback from the participants are included in Section 3.2.

3.2.1 The Transportation Scenario

The transportation scenario was designed to show how NISAC answers questions about the impact of rail transportation infrastructure disruptions on the chemical sector. The scenario showed a disruption in a segment of rail line between Virginia and Maryland for a specific chemical. NISAC's R-NAS[32] was used to evaluate the change in commodity flow for that specific chemical and the change in transportation costs associated with the disruption. The results of this scenario analysis are documented in a report entitled "Disruption of Rail Transportation of Ammonia and Chlorine: Implications for the Chemical Supply Chain."[33]

Discussion on the results of the scenario focused less on the actual results and more on current trends in rail transport commodity flows in response to recent transportation security regulations. Industry participants voiced concerns that, as the chemical industry and the transportation industry respond and adjust to transportation security regulations, the historical commodity flow patterns of chemicals

[32] Additional information on R-NAS can be found at http://www.sandia.gov/nisac/net_op.html

[33] Jones, Dean A., Chad E. Davis, Orr Y. Bernstein, and M. A. Turnquist, "Disruption of Rail Transportation of Ammonia and Chlorine: Implications for the Chemical Supply Chain," Unpublished (in review), 11 August 2009

along the nation's rail lines may change significantly. They indicated that NISAC may need to pay particular attention to this area over the next few years.

3.2.2 The Facilities Scenario

The facilities scenario was designed to expand the dialogue about resilience beyond the formal definition and into the area of practicality. The scenario consisted of four production units making the same chemical at different locations. All four units are assumed to be disrupted simultaneously. None of the four units in the analysis produces large quantities of the specific chemical and there are other plants nationally producing the same chemical. However, the plant-level supply chain analyses showed that there is a niche market that is being supported by each of the four plants.

There was lively discussion between the federal entities and the private sector about the role that each has in strengthening the resilience of the chemical sector. There were issues raised about the dependency of the United States on global supply of various chemicals and the desire by all for the resilience methodology to be capable of quantifying these types of dependencies in addition to those that include multiple infrastructures. The project team and CREATE have already begun to incorporate global dependencies into the resilience analysis.

3.2.3 The Hurricane Scenario

When NISAC performs analysis of a chemical infrastructure disruption, the first step is to determine what the event is and what characteristics of the chemical industry may be important, given what happened. This allows NISAC to focus the analysis quickly. For the workshop, NISAC created Hurricane Scenario Quintin by combining characteristics of two real hurricanes: Charlie and Ivan, which both made landfall in 2004. The path is similar to that of Hurricane Ivan, while the windspeed at U.S. landfall is similar to Hurricane Charlie. Scenario Hurricane Quintin makes U.S. landfall in late September as a Category 4 hurricane. Quintin cuts quite a path before making landfall, however, as shown in Figure 3-1. Quintin crosses Trinidad & Tobago and the Virgin Islands before making final landfall in Tampa, Florida. The analysis begins at U.S. landfall and works backward along Quintin's path.

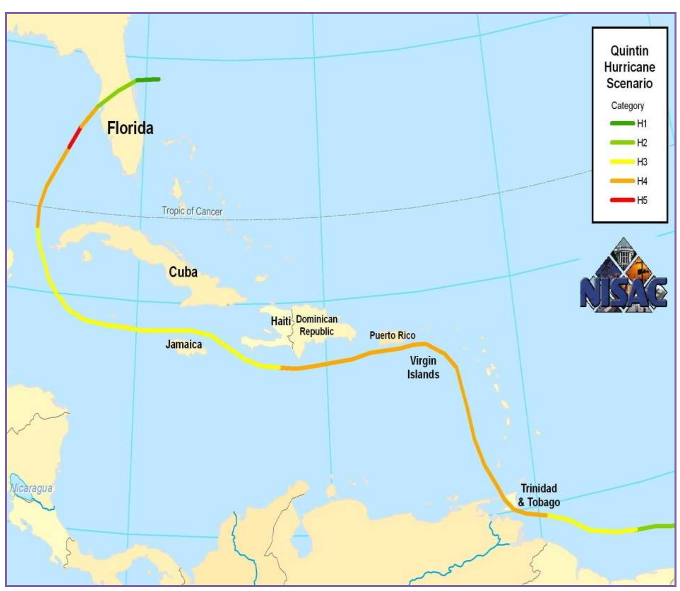

Figure 3-1: Hurricane Quintin's scenario path

Much of the discussion and comments from the participants focused on the cascade of losses to other supply chains and infrastructures such as the agriculture and water sectors. While all participants were pleased by the progress made during this stage of development, the consensus is that more work is needed to develop the supply chains more fully and roll the resilience work into the cascading impact analysis.

3.3 General Workshop Feedback

Feedback was enthusiastic and positive. Some of the general areas of concern include the following:

- Government participants wanted better access to the information that NISAC and the S&T chemical project are developing. The reasons for the interest vary. The FBI sees a potential to use these tools and analytical capability to identify facilities at higher risk so that planning and training for protection can be better prioritized among the many chemical facilities. The DHS/TSA representative would like to use these tools to aide in policy making. Various branches of DHS would like access to NISAC chemical capabilities analysis during emergency and non-emergency conditions to make more informed emergency response and policy decisions.
- A major focus of many of the industry session remarks was concern that once government agencies had access to these models, tools, and analyses, they would use them to formulate long-term (non-emergency) policy. Industry noted that these tools were designed to analyze disruptions and emergency conditions, and not normal conditions. Industry also noted that they would have no objections to the use of the models and tools in support of decision-making during emergency conditions.
- Both industry and government participants want better informed policies that ensure safety and security while simultaneously maintaining functional U.S.-based chemical production capabilities.

Participants identified the following specific supply chain development needs:

- Validating modeling results,
- Expanding the global supply chain analysis, and
- Encouraging additional cooperation from government agencies, industry associations, and companies to expand and validate data and increase understanding of constraints on the supply chain.

Participants also identified the following resilience methodology development needs:

- Evaluating market considerations as part of the resilience methodology,
- Continuing to test and evaluate the resilience metrics in the chemical sector, and
- Reconciling the project resilience definition with definitions of resilience disseminated by other agencies.

4 Summary and Path Forward

NISAC has completed the development of the chlorine and ammonia supply chains and is currently addressing those issues and concerns that are within its prevue brought forth during the workshop. The chlorine and ammonia capability is scheduled to be transferred to the DHS Office of Infrastructure Protection (IP) in October 2009.

The S&T Directorate has already tasked the Chemical Supply Chain and Resilience project with the next set of development activities. These activities will refine more of the petrochemical capability to include dependencies on the production and supply of industrial gases and acids. Preliminary work on selected inorganic chemical supply chains will also begin. The CDR tool will be completed with respect to the current datasets. Should there be new datasets identified while developing the new supply chains, those will need to be incorporated into the tool. The resilience methodology will be more fully tested and exercised.

Because there are so many with interest in this capability development, S&T is working through the integrated product teaming process within DHS to determine the set of tasking to be completed in fiscal year 2011. A determination will be made in December 2009.

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