

Chemical Supply Chain and Resilience Project Workshop

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Arlington, VA

Behind the Scenes: What's in the Dataset

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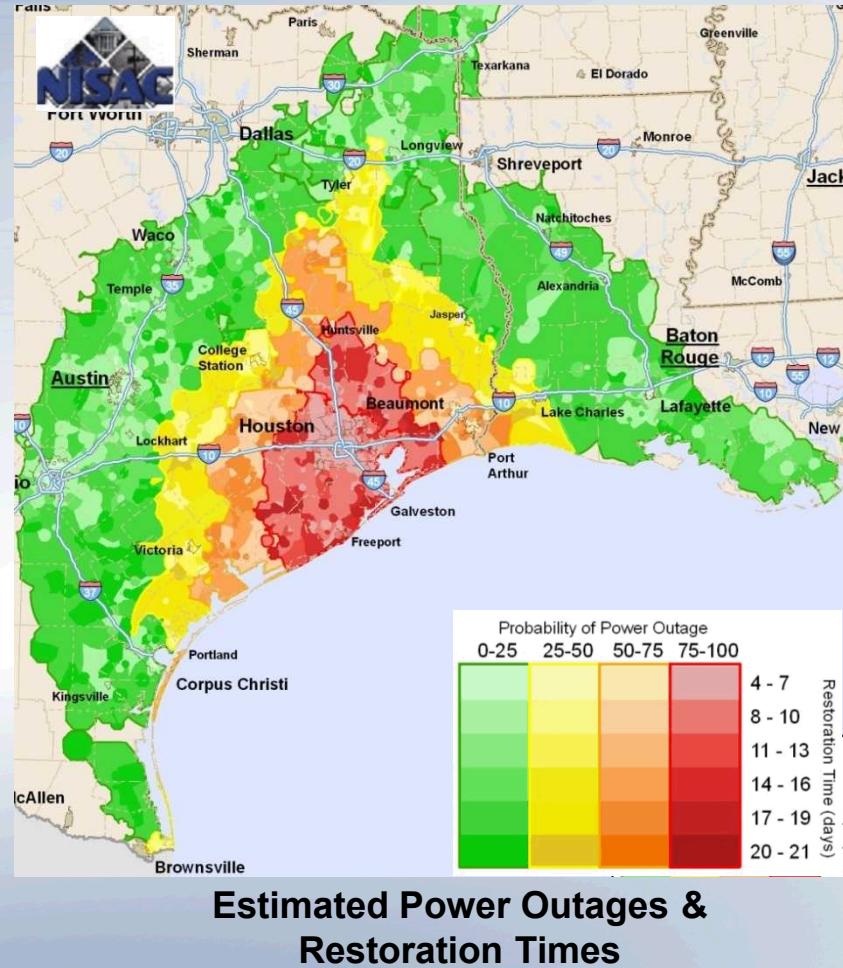
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U.S. Department of Homeland Security
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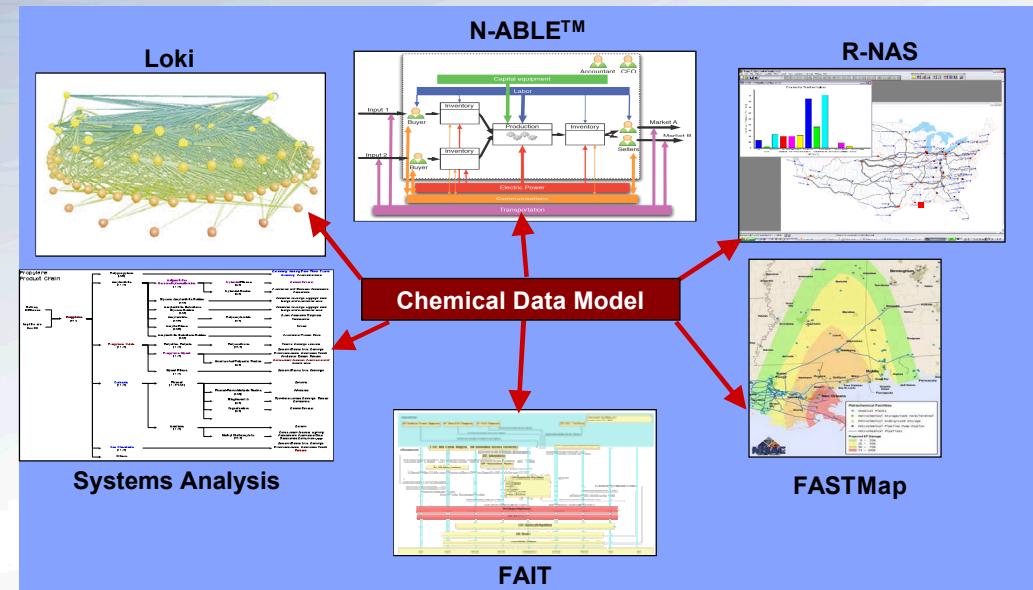
Resilience Analysis

- Goal: Assess the resilience of HCl and HF supply chains to a hurricane
- Analysis needs:
 - ✓ Scenario description
 - Data
 - ✓ Model and simulation capabilities
 - ✓ Integrating framework
- This presentation focuses on meeting the data needs by developing and using the project's chemical database.



The Chemical Data Model (CDM)

- The chemical data model (CDM) provides the data foundation for the project.
- All models are driven from the same set of core input data.
- Differences in model output are due to modeling approaches, not disparate input datasets.
- During this presentation, we will discuss CDM contents and process.

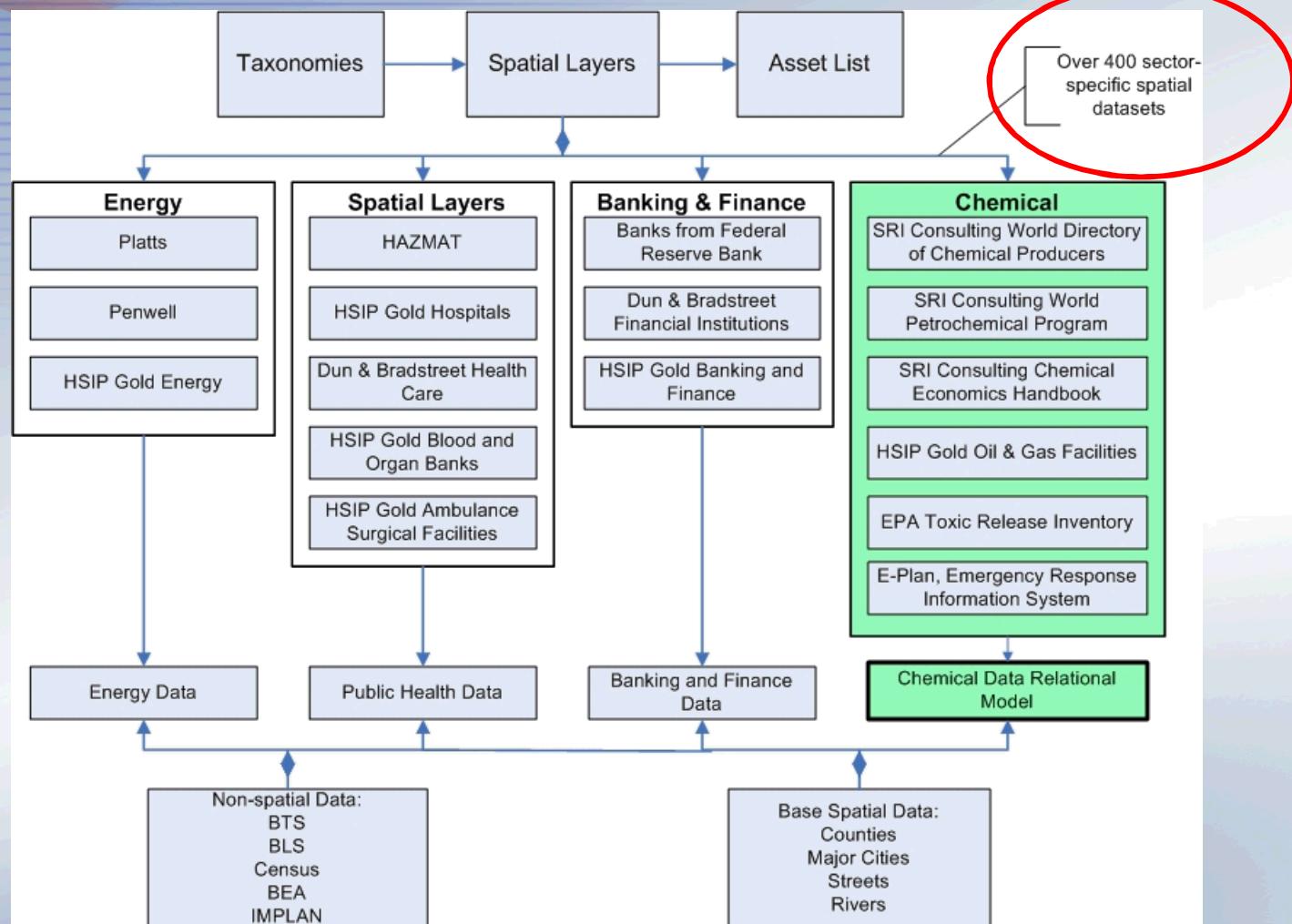


- Project models and analysis tools need the following information:

- Plant facilities
 - Name
 - Location (address and geocodes)
- Facility productions
 - Chemical types
 - Quantities
 - Processes
- Infrastructure dependencies
 - Transportation (rail, pipeline, etc.)
 - Energy (electric power, natural gas, petroleum products)
 - Quantities
- Consumption
 - Categories
 - Locations
 - Quantities
- Imports/exports
 - Locations
 - Quantities
- Other factors
 - Economics
 - Population distribution
 - Emergency services



Integrated NISAC Data Sets



Chemical Source Datasets

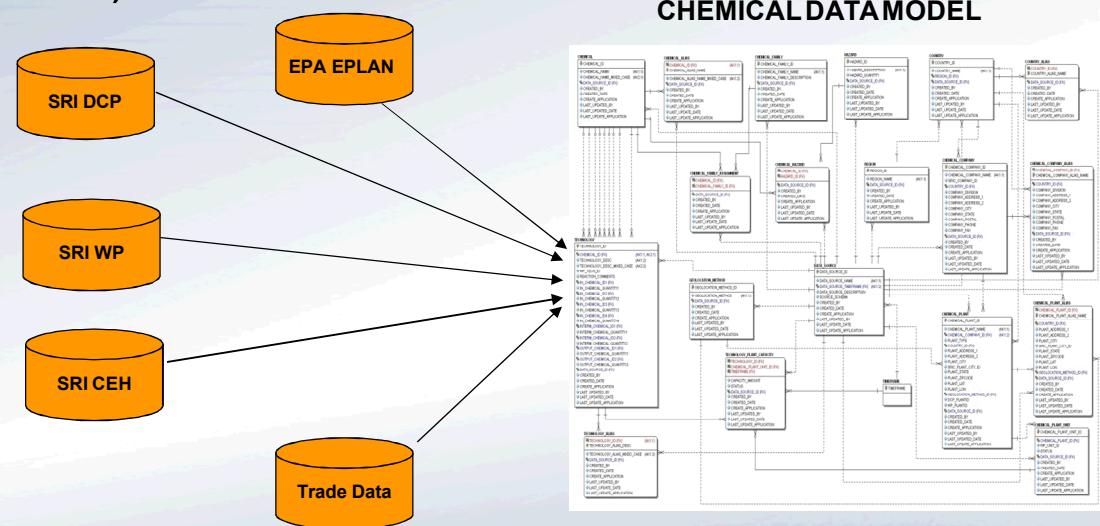
Dataset Name	Provider
World Petrochemicals Program 2009	SRI Consulting
Chemical Economics Handbook 2009	SRI Consulting
Directory of Chemical Producers 2009	SRI Consulting
Oil & Gas Pipelines	NGA HSIP Gold 2008 (PennWell)
Oil & Gas Facilities	NGA HSIP Gold 2008 (PennWell)
United States Census 2000	U.S. Census Bureau
County Business Patterns 2007	U.S. Census Bureau
County Business Patterns Employees Estimation 2007	U.S. Census Bureau
Geographic Names Information System	U.S. Geological Survey
IMPLAN States Summary 2002	Minnesota IMPLAN Group
International Trade Statistics 2007	U.S. Department of Commerce
Refinery Location Data	Argonne National Laboratory*
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	U.S. Environmental Protection Agency/U.S. Department of Homeland Security

* Argonne data were updated using 2007 domestic data from the Energy Information Administration (EIA) and foreign data from SRI Consulting.



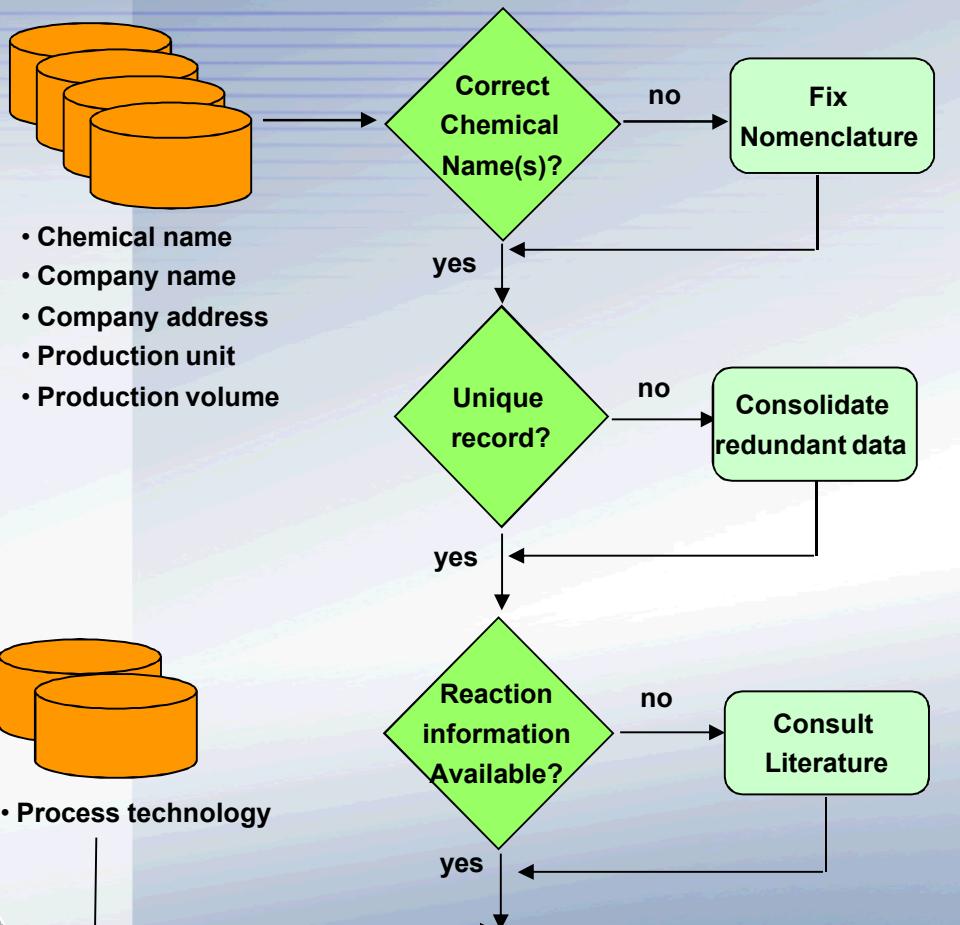
CDM Building Process

- Gather
- Process and integrate
 - Merge datasets into a common, Oracle-based framework
- Authenticate
- Document
 - Ensure traceability
- Test
 - Ensure compatibility with models
- Iterate

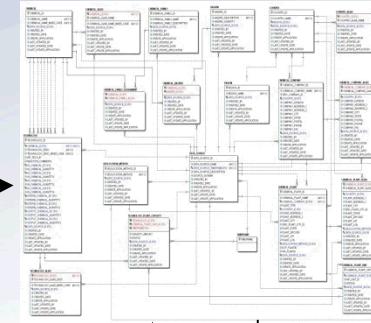


CDM: Data Processing

■ Authentication of data presents multiple challenges



CHEMICAL DATA MODEL



Update needed based on
• Inconsistent mass balance
• Industry feedback
• Transportation limitations
• New processes
• New market, etc.

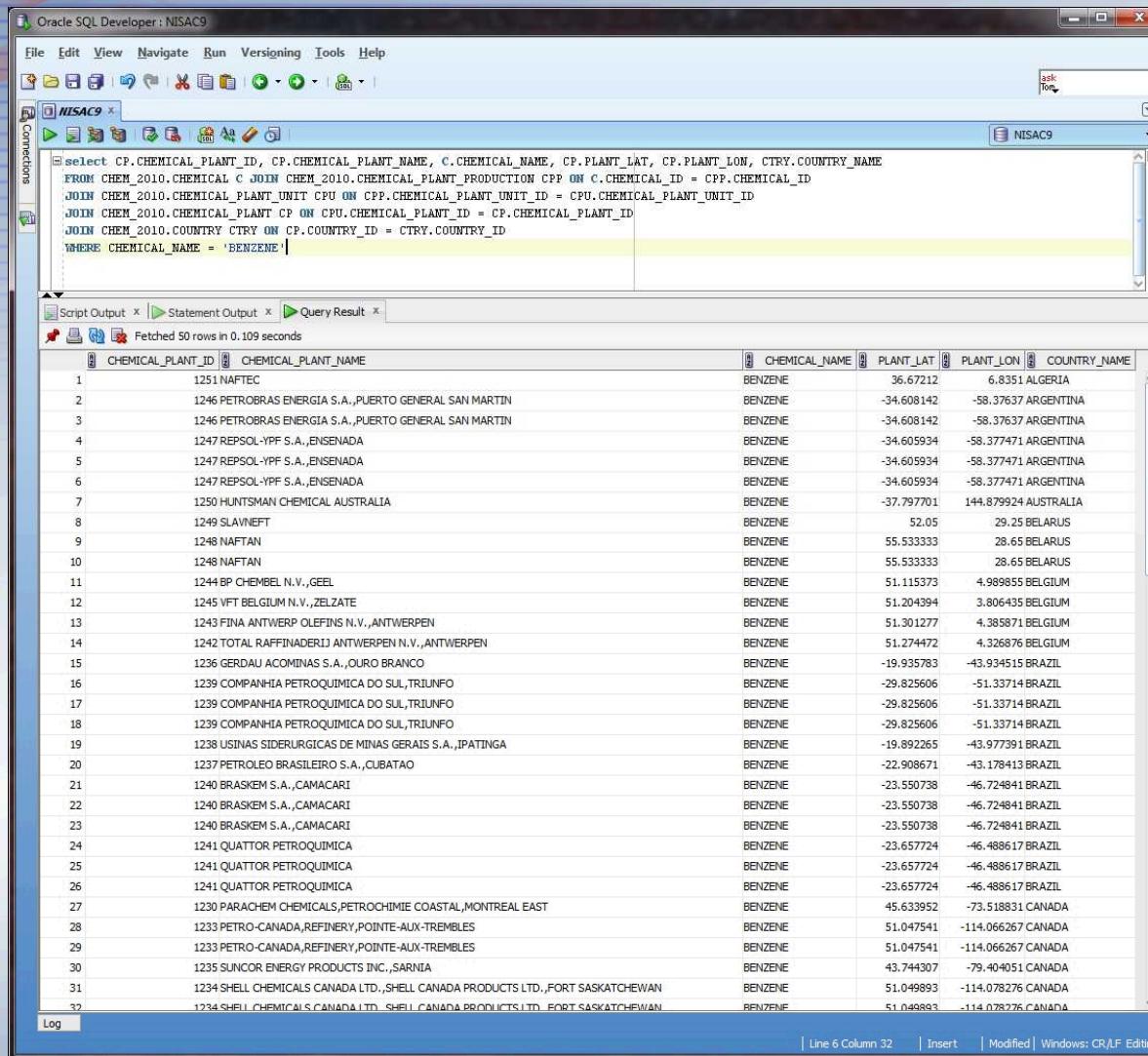
•FAIT
•N-ABLE™
•LOKI



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Example Queries of CDM: Global Benzene Producer Locations



Oracle SQL Developer : NISAC9

File Edit View Navigate Run Versioning Tools Help

Connections

Script Output x Statement Output x Query Result x

Fetched 50 rows in 0.109 seconds

Chemical_Plant_ID	Chemical_Plant_Name	Chemical_Name	Plant_Lat	Plant_Lon	Country_Name
1	1251 NAFTEC	BENZENE	36.67212	6.8351	ALGERIA
2	1246 PETROBRAS ENERGIA S.A.,PUERTO GENERAL SAN MARTIN	BENZENE	-34.608142	-58.37637	ARGENTINA
3	1246 PETROBRAS ENERGIA S.A.,PUERTO GENERAL SAN MARTIN	BENZENE	-34.608142	-58.37637	ARGENTINA
4	1247 REPSOL-YPF S.A.,ENSENADA	BENZENE	-34.605934	-58.377471	ARGENTINA
5	1247 REPSOL-YPF S.A.,ENSENADA	BENZENE	-34.605934	-58.377471	ARGENTINA
6	1247 REPSOL-YPF S.A.,ENSENADA	BENZENE	-34.605934	-58.377471	ARGENTINA
7	1250 HUNTSMAN CHEMICAL AUSTRALIA	BENZENE	-37.797701	144.879924	AUSTRALIA
8	1249 SLAVNEFT	BENZENE	52.05	29.25	BELARUS
9	1248 NAFTAN	BENZENE	55.533333	28.65	BELARUS
10	1248 NAFTAN	BENZENE	55.533333	28.65	BELARUS
11	1244 BP CHEMBEL N.V.,GEEL	BENZENE	51.115373	4.989855	BELGIUM
12	1245 VFT BELGIUM N.V.,ZELZATE	BENZENE	51.204394	3.806435	BELGIUM
13	1243 FINA ANTWERP OLEFINS N.V.,ANTWERPEN	BENZENE	51.301277	4.385871	BELGIUM
14	1242 TOTAL RAFFINADERIJ ANTWERPEN N.V.,ANTWERPEN	BENZENE	51.274472	4.326876	BELGIUM
15	1236 GERDAU ACOMINAS S.A.,OURO BRANCO	BENZENE	-19.935783	-43.934515	BRAZIL
16	1239 COMPANHIA PETROQUIMICA DO SUL,TRIUNFO	BENZENE	-29.825606	-51.33714	BRAZIL
17	1239 COMPANHIA PETROQUIMICA DO SUL,TRIUNFO	BENZENE	-29.825606	-51.33714	BRAZIL
18	1239 COMPANHIA PETROQUIMICA DO SUL,TRIUNFO	BENZENE	-29.825606	-51.33714	BRAZIL
19	1238 USINAS SIDERURGICAS DE MINAS GERAIS S.A.,IPATINGA	BENZENE	-19.892265	-43.977391	BRAZIL
20	1237 PETROLEO BRASILEIRO S.A.,CUBATAO	BENZENE	-22.908671	-43.178413	BRAZIL
21	1240 BRASSEM S.A.,CAMACARI	BENZENE	-23.550738	-46.724841	BRAZIL
22	1240 BRASSEM S.A.,CAMACARI	BENZENE	-23.550738	-46.724841	BRAZIL
23	1240 BRASSEM S.A.,CAMACARI	BENZENE	-23.550738	-46.724841	BRAZIL
24	1241 QUATTOR PETROQUIMICA	BENZENE	-23.657724	-46.488617	BRAZIL
25	1241 QUATTOR PETROQUIMICA	BENZENE	-23.657724	-46.488617	BRAZIL
26	1241 QUATTOR PETROQUIMICA	BENZENE	-23.657724	-46.488617	BRAZIL
27	1230 PARACHEM CHEMICALS,PETROCHIMIE COASTAL,MONTREAL EAST	BENZENE	45.633952	-73.518831	CANADA
28	1233 PETRO-CANADA,REFINERY,POINTE-AUX-TREMBLES	BENZENE	51.047541	-114.066267	CANADA
29	1233 PETRO-CANADA,REFINERY,POINTE-AUX-TREMBLES	BENZENE	51.047541	-114.066267	CANADA
30	1235 SUNCOR ENERGY PRODUCTS INC.,SARNIA	BENZENE	43.744307	-79.404051	CANADA
31	1234 SHELL CHEMICALS CANADA LTD.,SHELL CANADA PRODUCTS LTD.,FORT SASKATCHEWAN	BENZENE	51.049893	-114.078276	CANADA
32	1234 SHELL CHEMICALS CANADA LTD.,SHELL CANADA PRODUCTS LTD.,FORT SASKATCHEWAN	BENZENE	51.049893	-114.078276	CANADA

Log

Line 6 Column 32 | Insert | Modified | Windows: CR/LF Editing



Example Queries of CDM: Merging Multiple Data Sets

Note same facility is listed multiple times with slightly different names

The screenshot shows the Chemical Aliases software interface with three main panels: EPlan, DCP, and WP. Each panel has a search interface with chemical name (BENZENE), state (TX), and company name filters, along with a 'Query' button and a 'Show Unmatched Only' checkbox. The results are displayed in a table format.

EPlan Panel:

Company Name	Fac. ID	Facility Name	City	State	CHEM	Chemical
Alon USA LP	404087	Alon USA LP	Big Spring	TX	507540	BENZENE
BASF Corporation - Free	406094	BASF Corporation - Free	Freeport	TX	471668	BENZENE
BASF FINA Petrochemic	423216	BASF FINA Petrochemic	Port Arthur	TX	465323	BENZENE
BP TEXAS CITY CHEMII	424658	BP TEXAS CITY CHEMII	Texas City	TX	472753	BENZENE
BP TEXAS CITY REFINERY	402931	BP TEXAS CITY REFINERY	Texas City	TX	467243	BENZENE
Bayer MaterialScience L	428194	Bayer MaterialScience L	BAYTOWN	TX	455660	BENZENE
Channel Shipyards Comp	407200	Channel Shipyards Comp	Baytown	TX	462197	BENZENE
Chemical Research & Li	423219	Chemical Research & Li	Pasadena	TX	462553	BENZENE

DCP Panel:

ID	Plant Name	City	State	Country	Chem	Chemical Name
14361	ALON USA ENERGY INC., BIG SPRING	Big Spring	TX	United States	0	Benzene
2	14362 BASF FINA PETROCHEMICALS LP, PO	Port Arthur	TX	United States	0	Benzene
3	14363 BP AMERICA INC., TEXAS CITY	Texas City	TX	United States	0	Benzene
4	14364 BP AMERICA INC., TEXAS CITY	Texas City	TX	United States	0	Benzene
5	14365 BP AMERICA INC., TEXAS CITY	Texas City	TX	United States	0	Benzene
6	14366 BP AMERICA INC., TEXAS CITY	Texas City	TX	United States	0	Benzene
7	14367 BP AMERICA INC., TEXAS CITY	Texas City	TX	United States	0	Benzene
8	14369 CHEVRON PHILLIPS CHEMICAL COM	Port Arthur	TX	United States	0	Benzene

WP Panel:

Plant ID	Unit ID	Company Name	Plant Name	City	Country	Chem	Chemical
1814410	970203	Alon		Big Spring	United States	18548	Benzene
2	19032	38603	BASF Fina Petrochemic	Port Arthur	United States	18548	Benzene
3	20482	17370	BP	Texas City	United States	18548	Benzene
4	20482	35344	BP	Texas City	United States	18548	Benzene
5	20482	36920	BP	Texas City	United States	18548	Benzene
6	20482	32655	BP	Texas City	United States	18548	Benzene
7	20482	17371	BP	Texas City	United States	18548	Benzene
8	16973	31145	CITGO	Corpus Christi	United States	18548	Benzene

Benzene-Producing Facilities in Texas



Example Queries of CDM: Benzene Aliases

22 Different Terms for
“Benzene”

Chemical Aliases

File Edit Tools Help

Statistics Chemical Aliases Chemical Names Chemical Families Synonyms Groups EPlan Facilities DCP Facilities WP Facilities Facilities Matching Matched Facilities

AutoWild Fuzzy First 1,000 Show Aliased

Filter: BENZENE Alias Chemical Name Query

Source Name	Alias	Count	Modified	APPROVED
1 BENZENE (DIESEL NO. 2-D)	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
2 BENZENE (1.5%)	BENZENE	2	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
3 BENZENE CONCENTRATE STREAM (DARTMOUTH)	BENZENE	2	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
4 BENZENE (THERMINOL 55 TRANSFER FLUID)	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
5 BENZENE 99%	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
6 BENZENE (CONTINUED)	BENZENE	7	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
7 BENZENE CONCENTRATE	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
8 BENZENE, UNLEAD	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
9 BENZENE - STREAM 26	BENZENE	4	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
10 BENZENE (GASOLINE)	BENZENE	2	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
11 BENZENE (UNLEADED GAS)	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
12 BENZENE, RECOVERED	BENZENE	2	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
13 BENZENE	BENZENE	248	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
14 BENZENE, 100%	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
15 BENZENE PRODUCT - STREAM 15	BENZENE	5	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
16 BENZENE, CRUDE	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
17 BENZENE,100%	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
18 BENZENE (BENZENE CONCENTRATE)	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
19 BENZENE UNLEADED GASOLINE	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
20 BENZENE, (ECA)	BENZENE	3	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
21 BEZENE, DICYCLOPENTADIENE & OTHERS (PYROLYSIS BENZENE	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010
22 BENZENE, 99.9+%, HPLC GRADE (270709)	BENZENE	1	PSDOWNE 10/13/2009	PSDOWNE 4/20/2010

22 Records

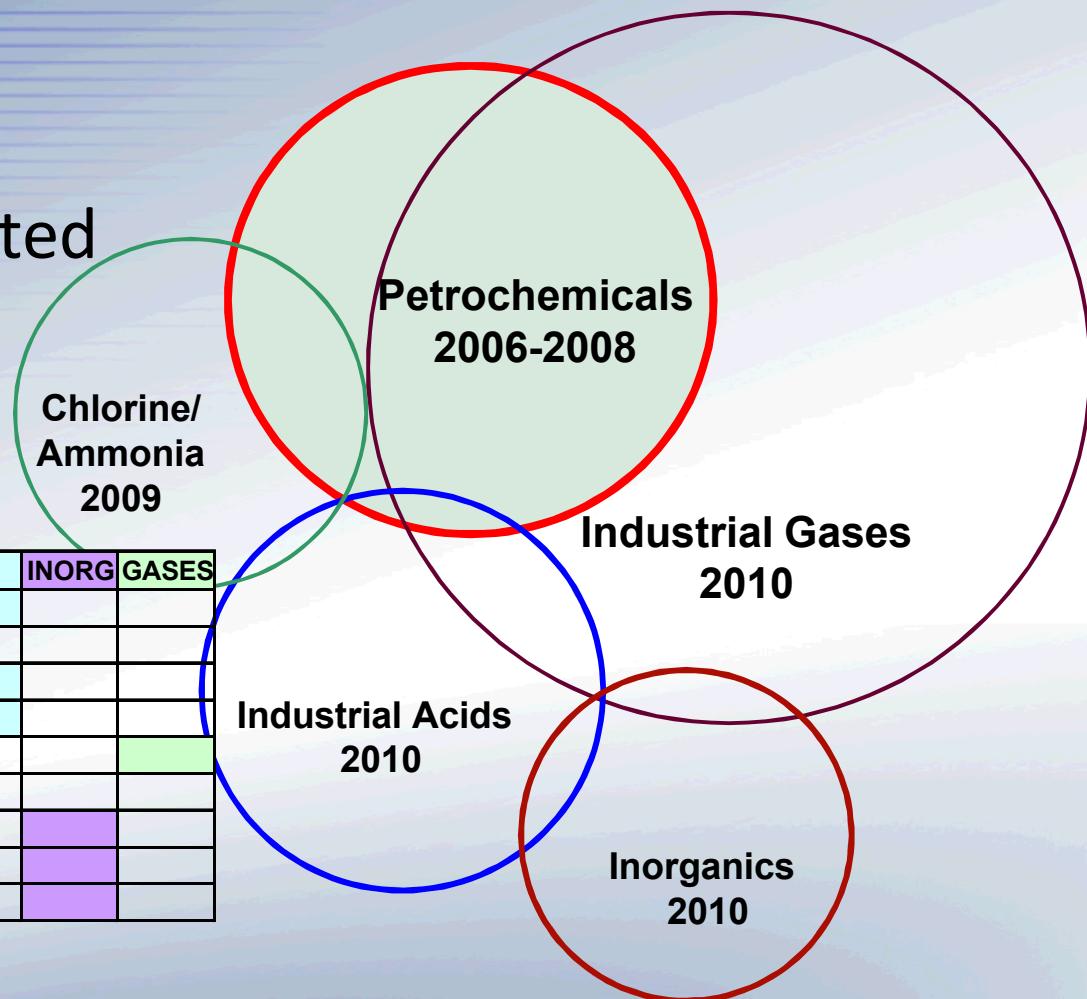


Relative Overlap of Chemical Supply Chains

- Anticipated overlap among different targeted chemical classes

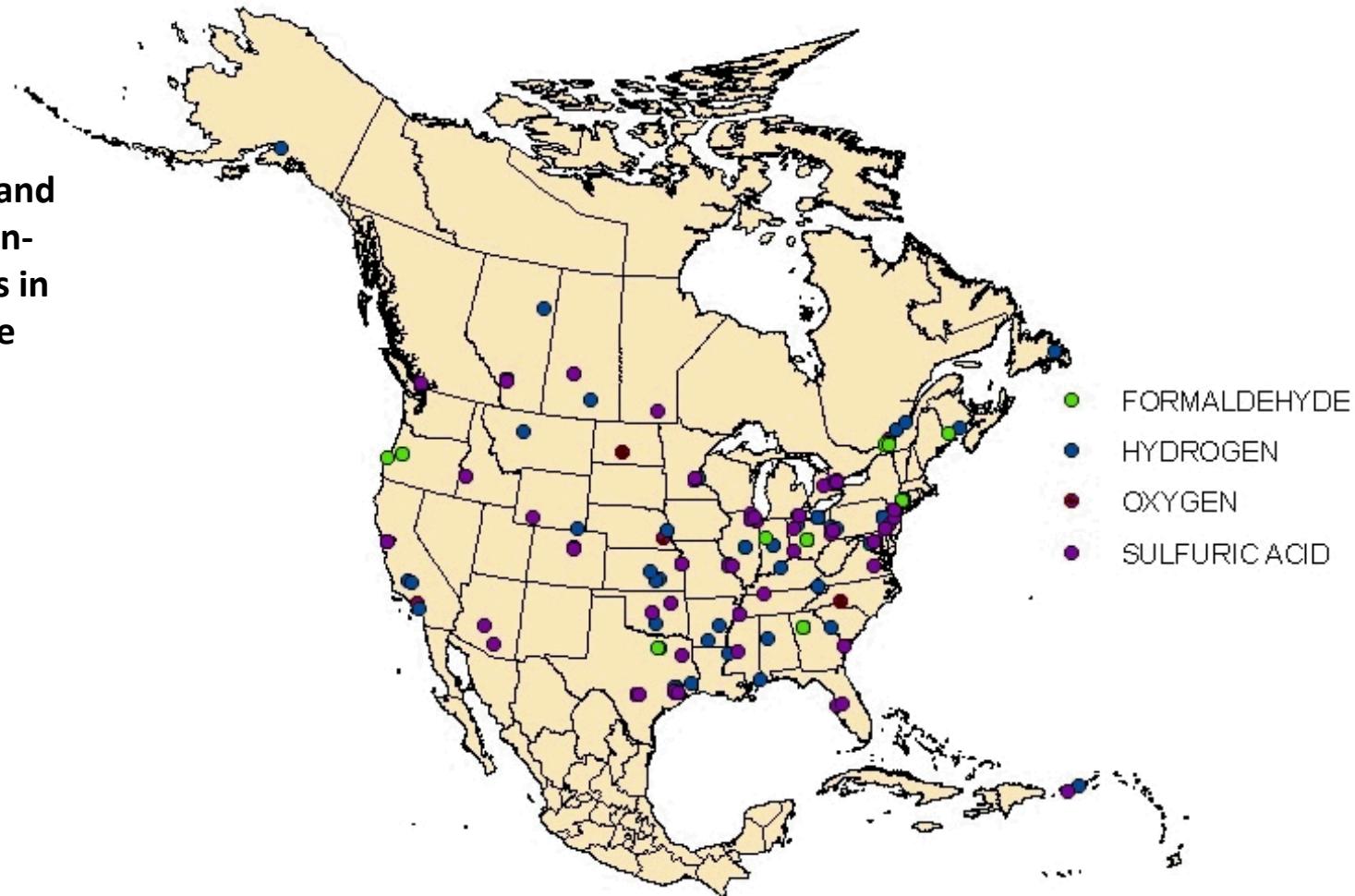
Example of chemicals associated with HF/HCl supply chains

CHEMICAL NAMES	CHC	CFC	FC	INORG	GASES
1,1,1,2-tetrafluoroethane					
1,1,1-Trichloroethane	■				
1,1,2-trichloro-2,2,1 trifluoroethane	■	■	■		
1,2-dichlorotetrafluoroethane	■	■	■		
Acetylene				■	
Allyl Chloride	■				
alumina				■	
aluminum fluoride				■	
aluminum hydroxide				■	



Example Queries of CDM: Plant Locations

Locations of CFC and
CHC supply chain-
related chemicals in
Canada and the
United States



CDM: Additional Attributes

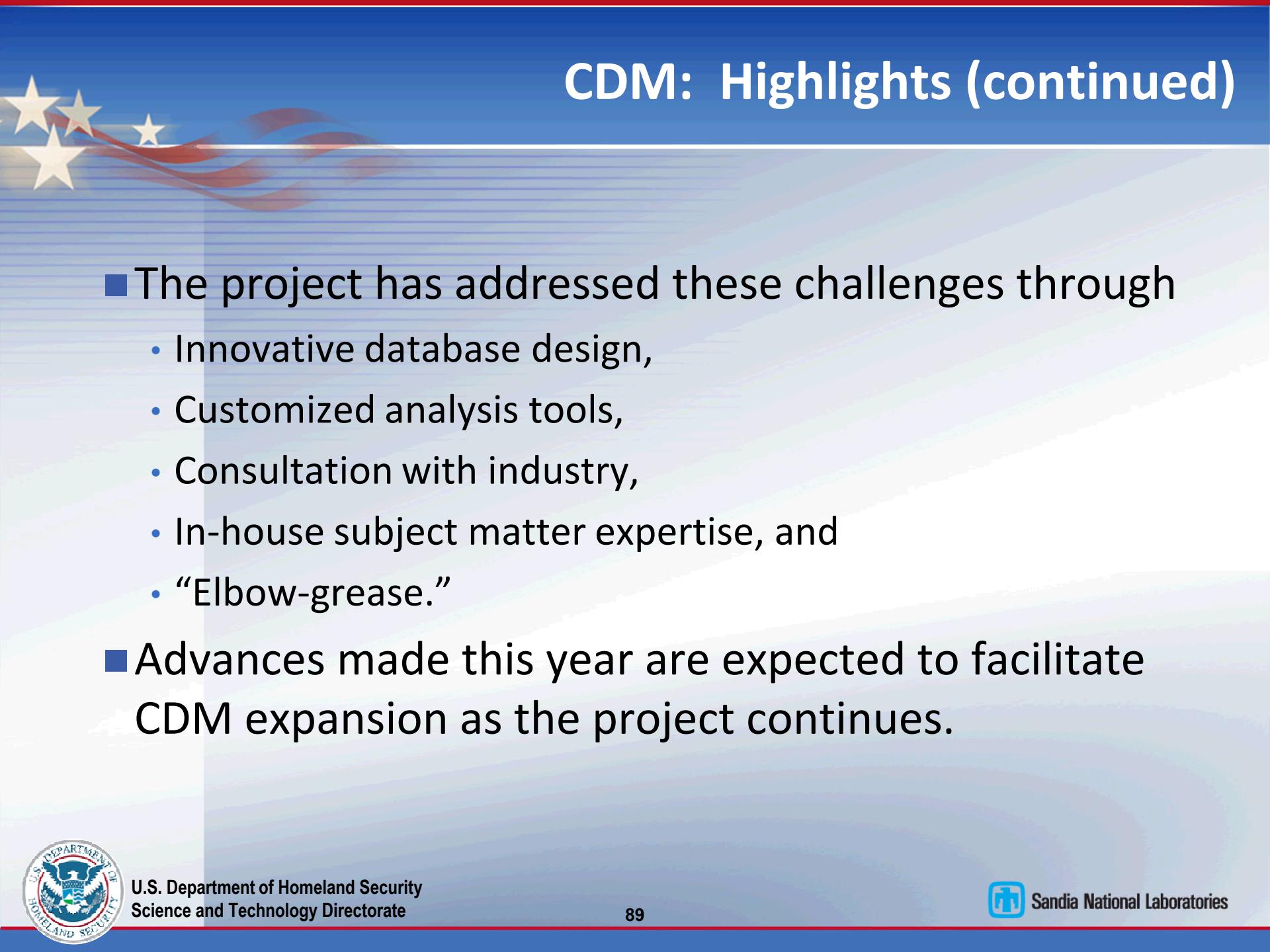
- Data are secure (only approved users allowed to access), and data are backed up on a regular basis.
- The majority of data structures are simple and allow for ad-hoc query analysis outside of the modeling tools.
- Customized Oracle “views” of data are created to simplify the more complicated data queries and relationships (such as derived summary data).
- Oracle tables are indexed for performance. Most queries will return instantly.



CDM: Highlights

- The chemical data model provides the foundation for all models and analyses.
- Integrity of the CDM is paramount to ensuring validity of project efforts.
- CDM development provides many challenges, such as
 - Disparate datasets,
 - Multiple names and aliases,
 - Sparse data, and
 - Verification.





CDM: Highlights (continued)

- The project has addressed these challenges through
 - Innovative database design,
 - Customized analysis tools,
 - Consultation with industry,
 - In-house subject matter expertise, and
 - “Elbow-grease.”
- Advances made this year are expected to facilitate CDM expansion as the project continues.

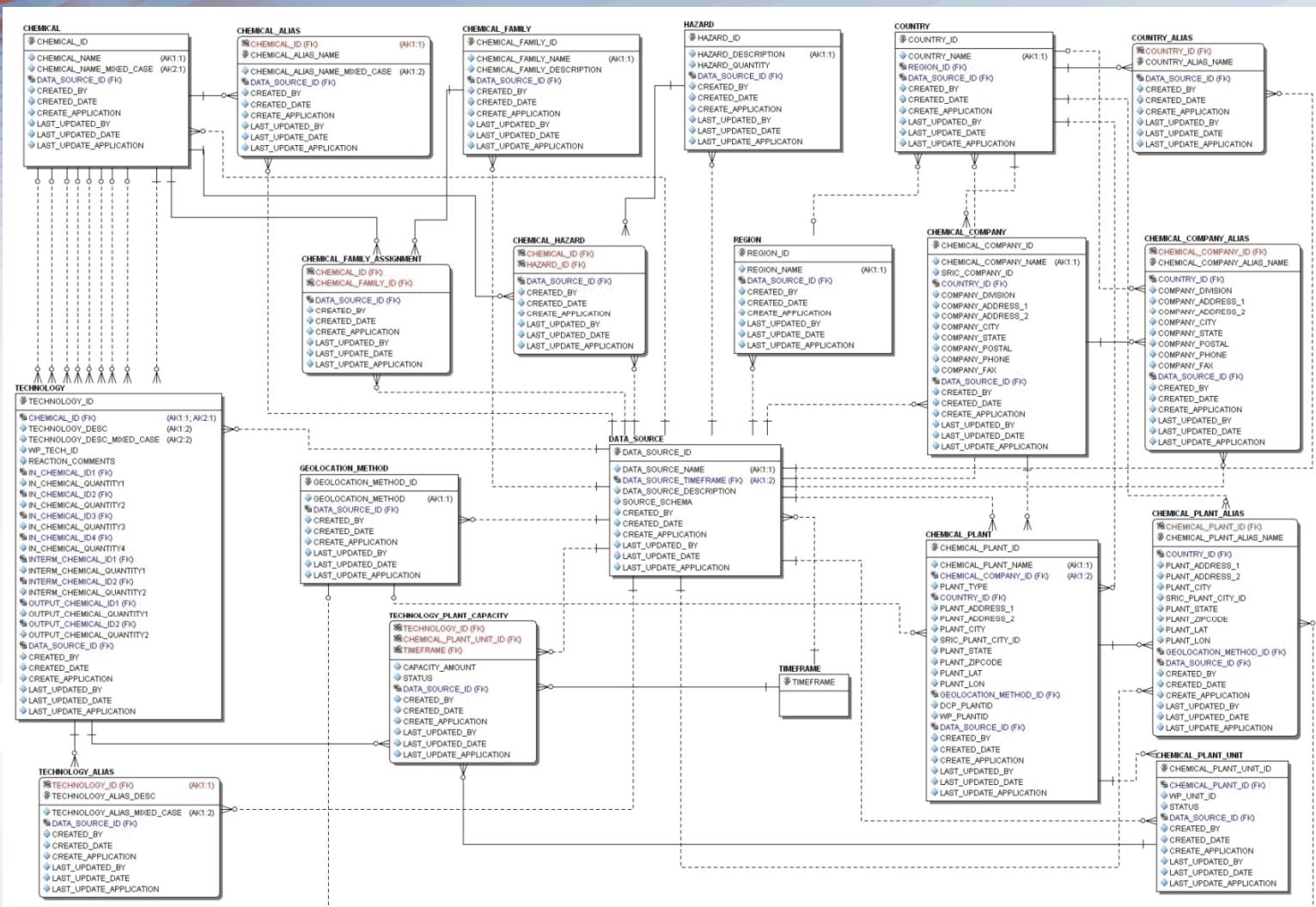


Backup Slides

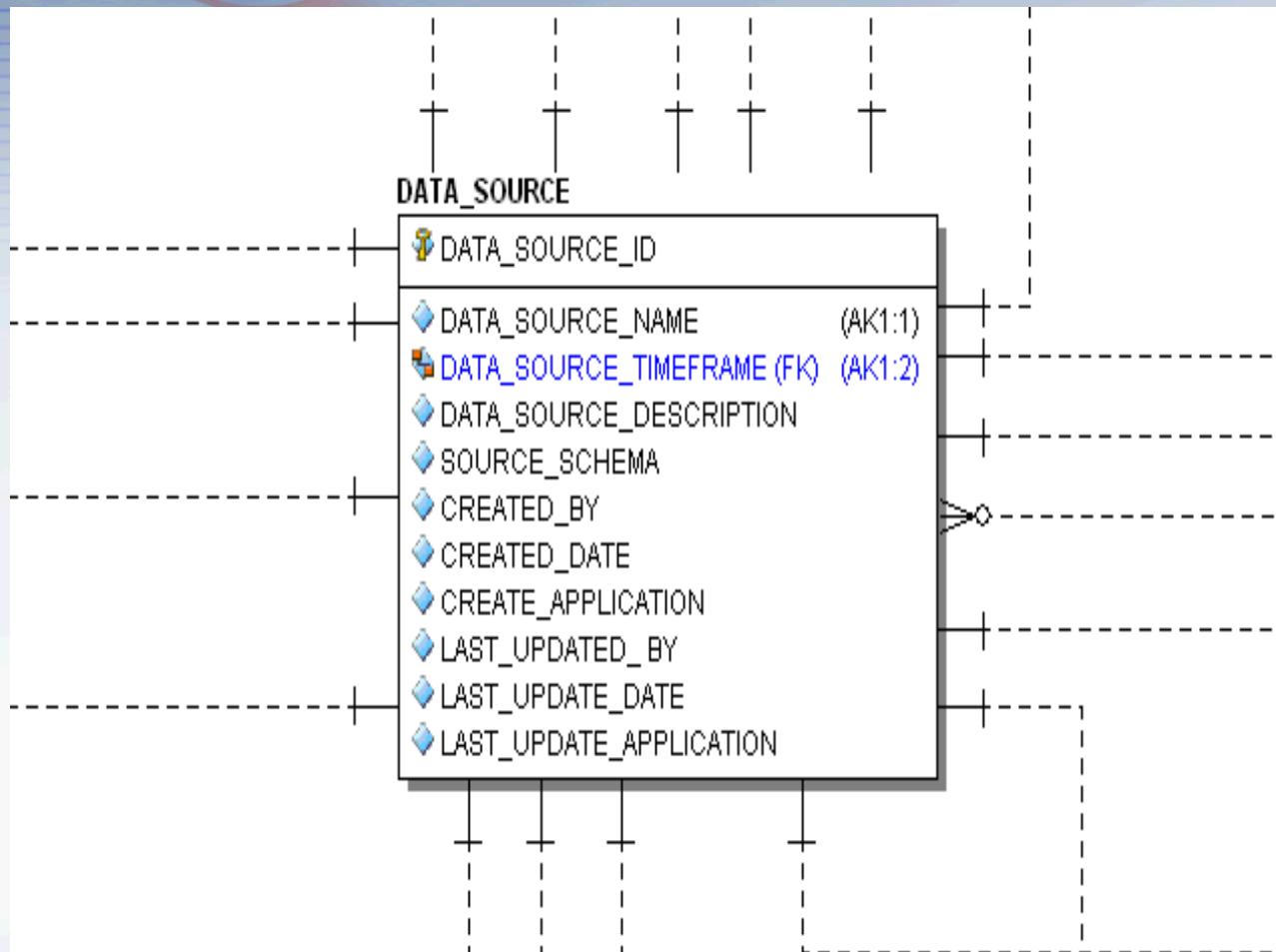


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CDM: Data Traceability

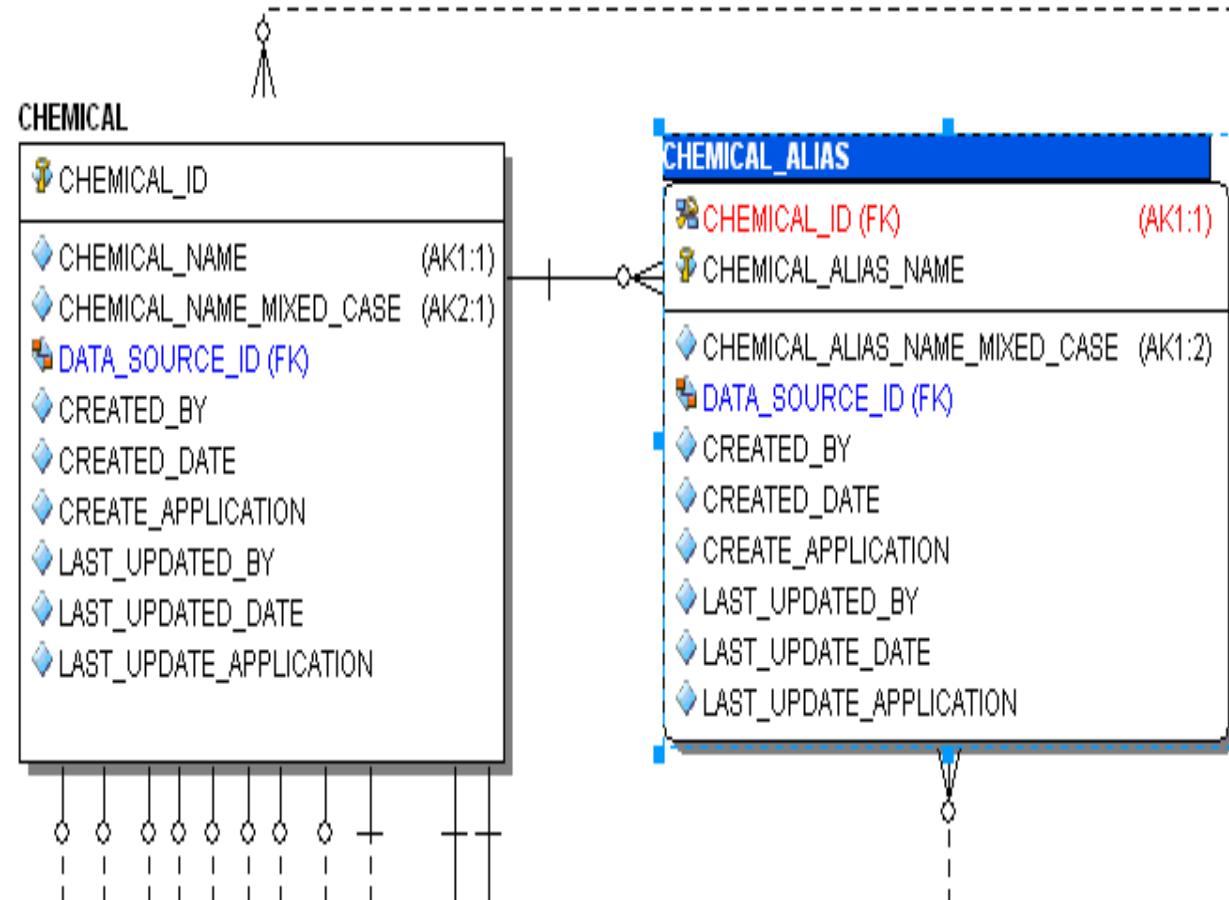


Every record in the CDM can be traced back to its source dataset. This allows us to merge disparate datasets while allowing for drill-down back to the detailed source if required.

Additionally, each record contains an audit trail that details information about record creation as well as any subsequent changes.



CDM: Chemicals

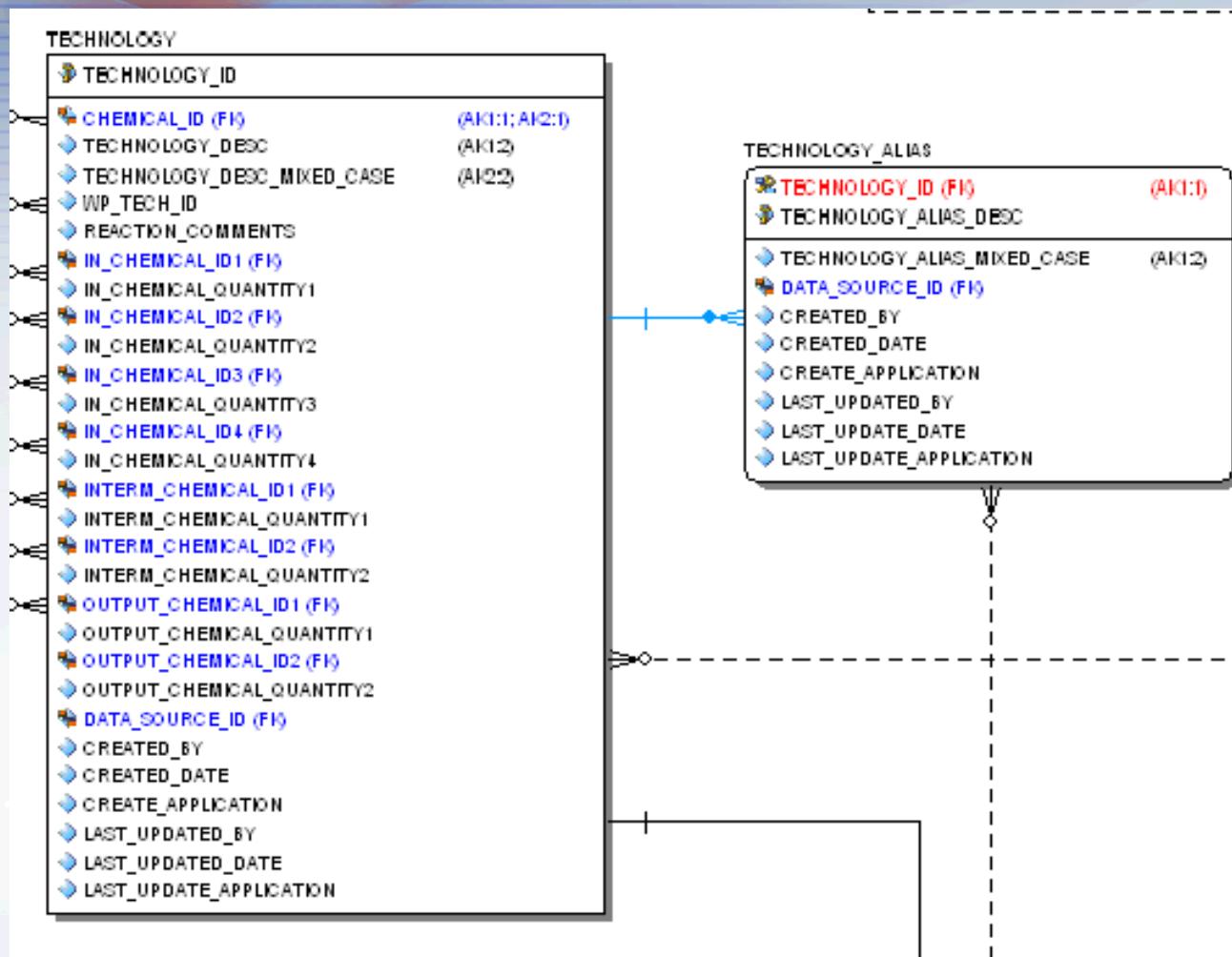


Data Source: SRI World Petrochemicals (WP) /Directory of Chemical Producers (DCP)

Alias names are stored to deal with AKAs, abbreviations, and alternate spellings. Storing aliases is an absolute must when loading from disparate data sources.



CDM: Technology



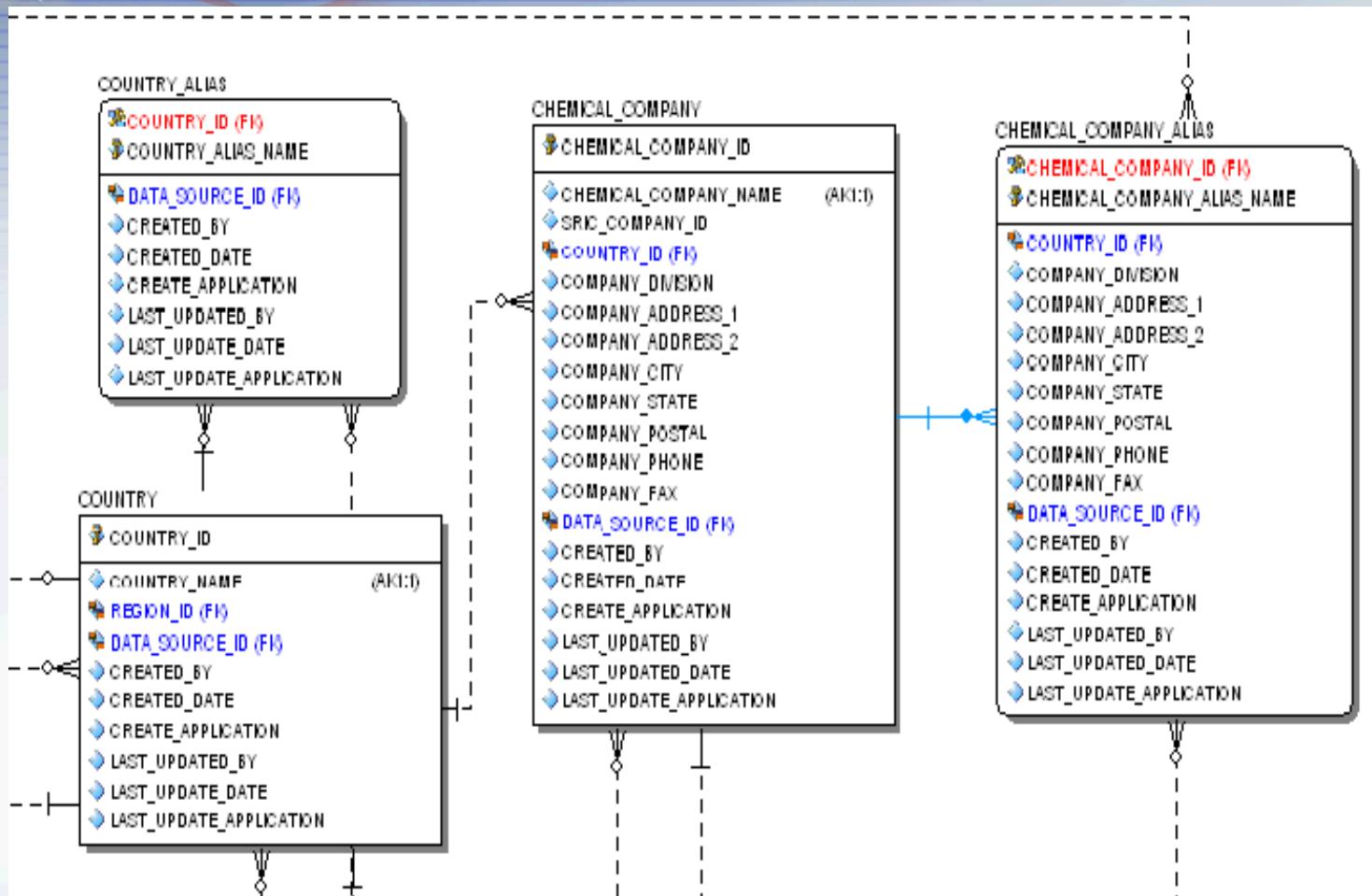
Technologies tell us the relationships among chemicals (inputs and outputs).

For example, the data show 10 different ways to make/recover acetone.

Data Source:
SRI CEH



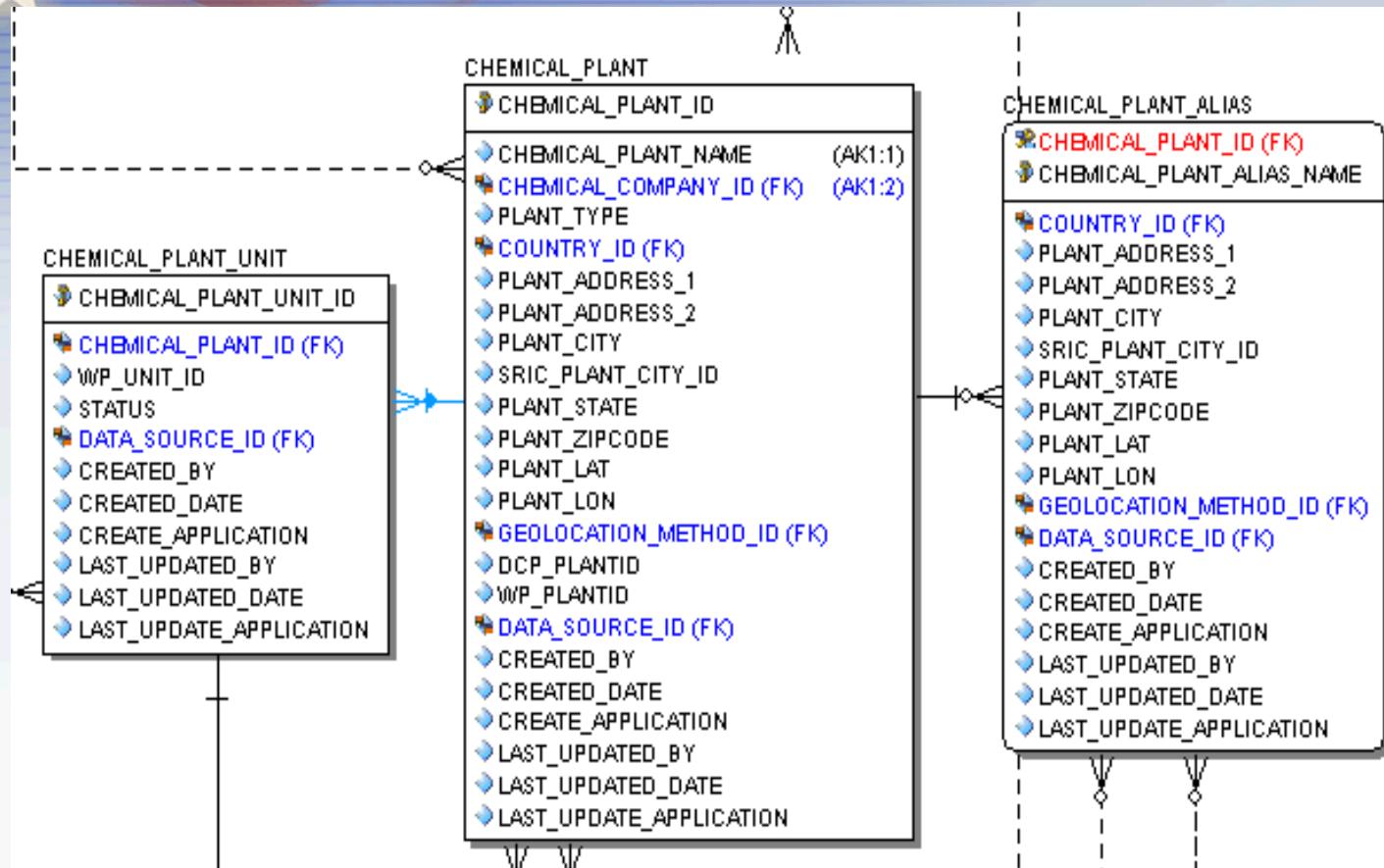
CDM: Countries and Companies



Data Source:
SRI WP/DCP and
Trade Statistics
Data



CDM: Chemical Plants and Units



Chemical plant locations are geocoded

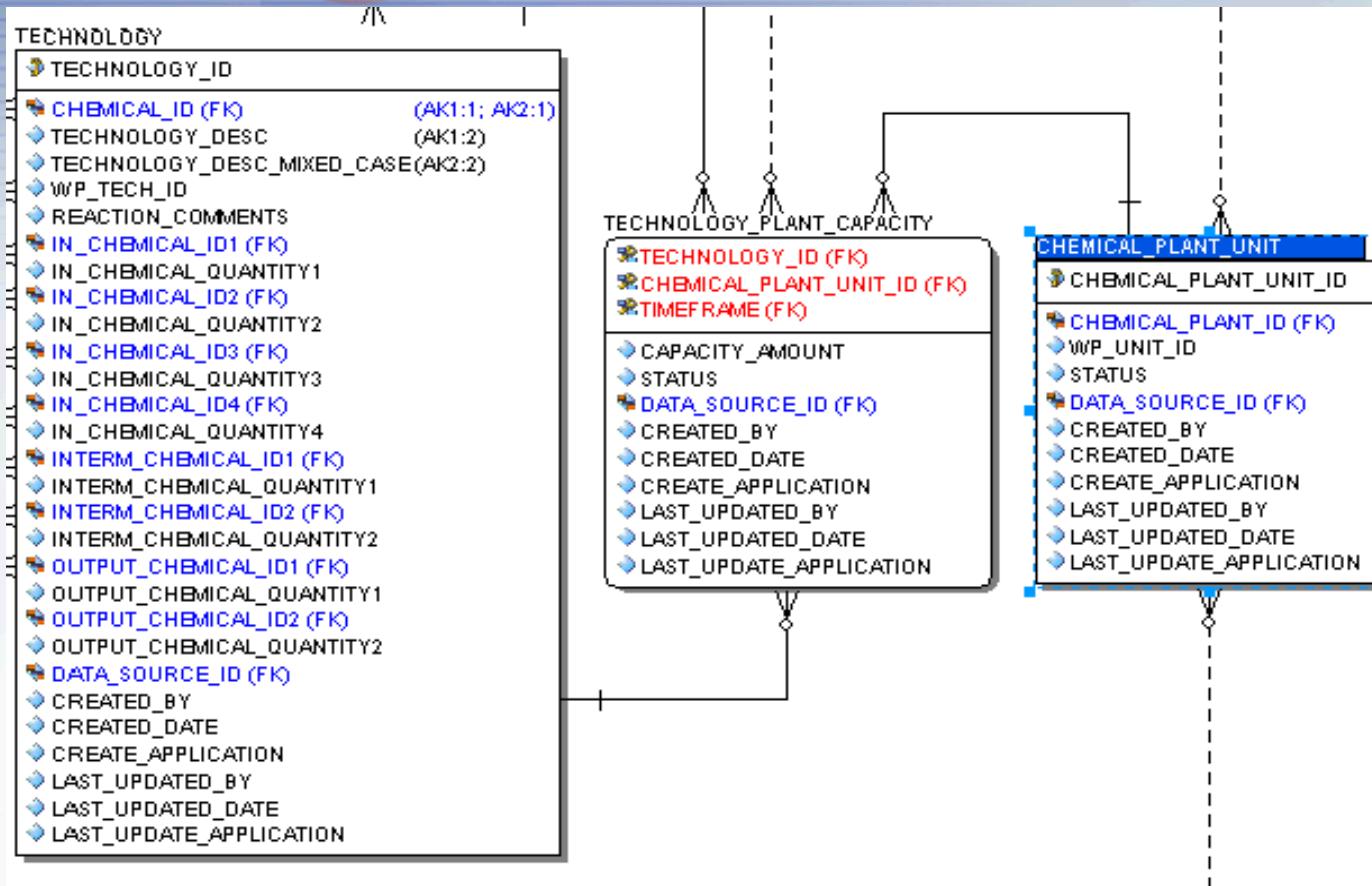
Currently storing 5,659 distinct chemical plants

Each plant may support multiple chemical processing capabilities (units)

Data Source: SRI WP/DCP



CDM: Capacities/Production



Source data capacity information is only available at the plant unit/technology level (e.g., There are X metric tons of capacity to produce Chemical A using Technology B at Plant Unit C).

Data Source:
SRI WP



CDM: Industrial Acids Supply Chain Statistics

Category	# of Records (06/2010)
Chemicals	100
Companies	400
Units	800
Process reactions	200

