Rapid Estimation of Life Cycle Inventory

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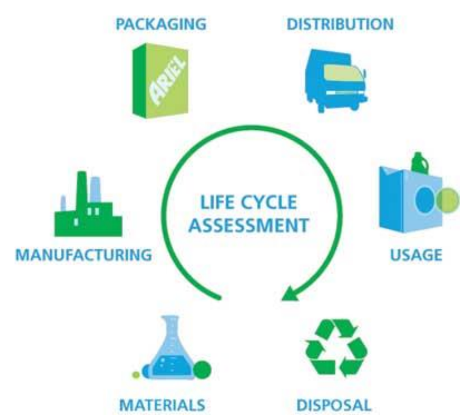

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National Risk Management Research Laboratory
Life Cycle Assessment Center of Excellence

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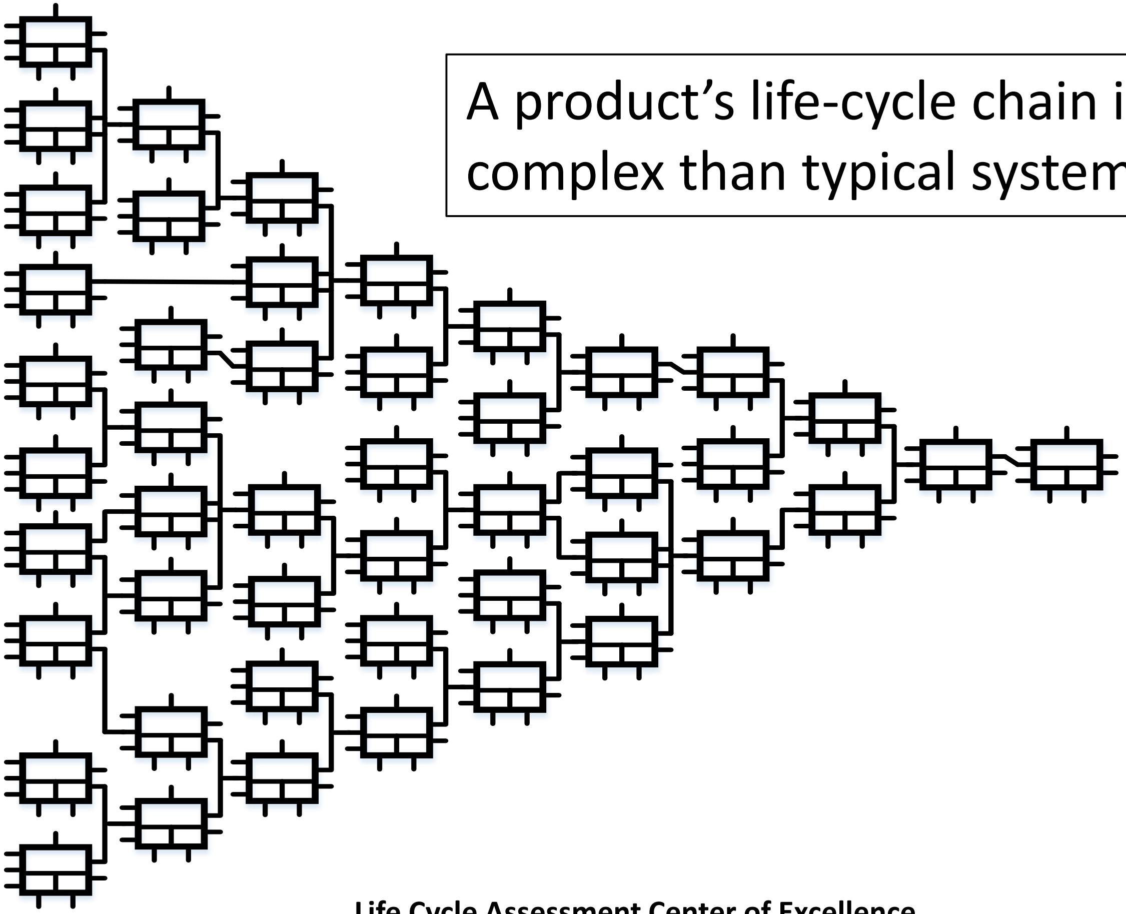
United States Environmental Protection Agency

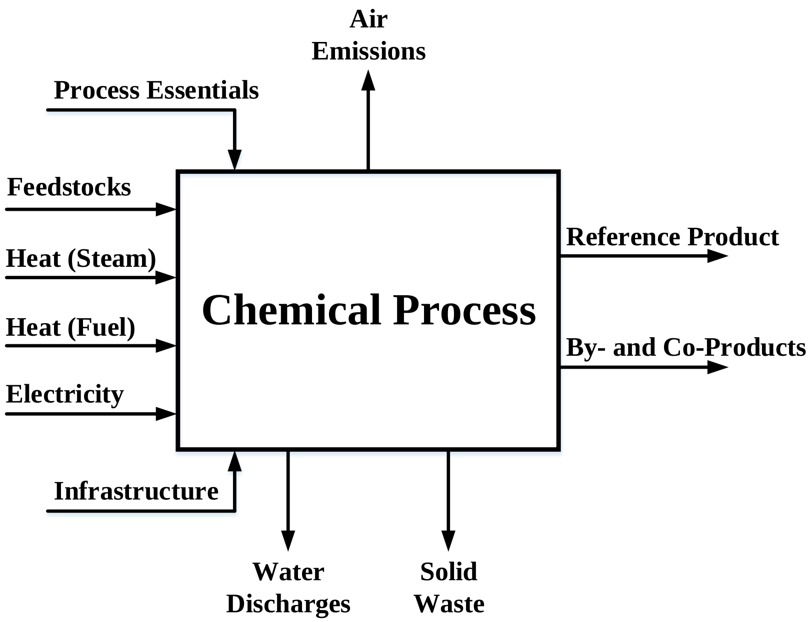
Life-Cycle Chain of Unit Processes



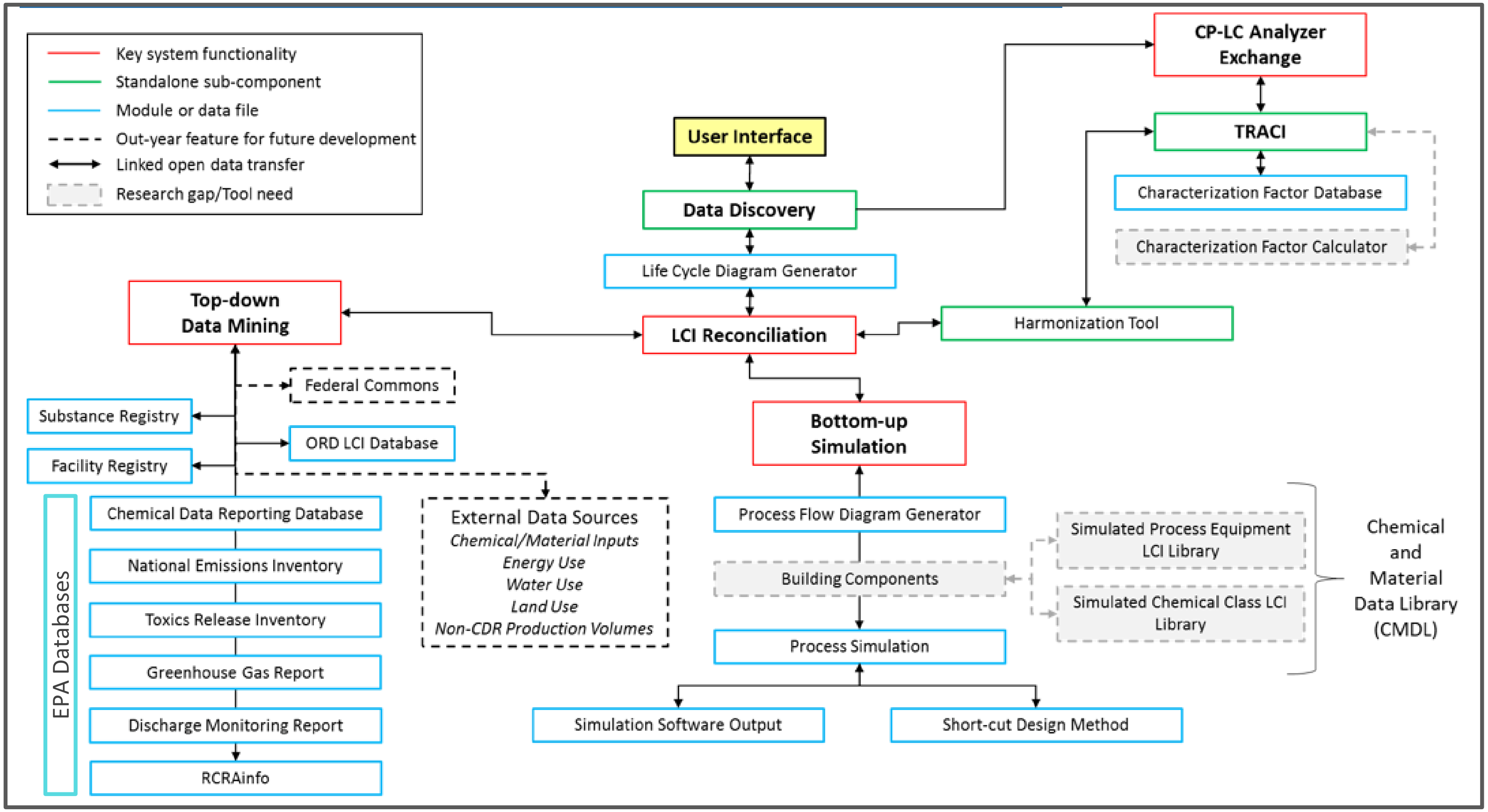
A product's life-cycle chain is much more complex than typical system diagrams.

Generating more specific and accurate chemical process inventories

- Missed inputs could lead to missing sections of the inventory.
- Missed outputs could lead to missed impact categories.
- Qualitative and quantitative aspects affect data quality.



Project Context

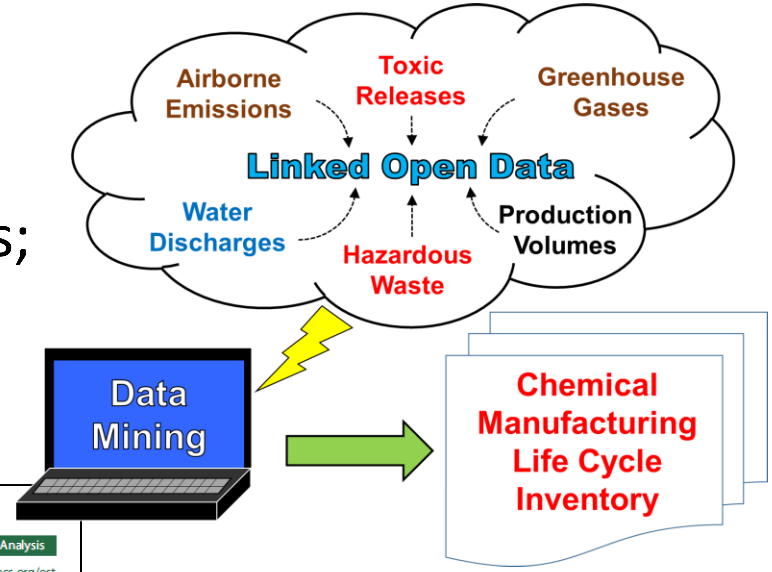


Approaches to Generating Inventory Data

- Existing life-cycle databases
  - Incomplete; proxies
- Top-Down data mining
  - National accounting; facility-level
- Bottom-Up inventory development
  - Process modeling; simulation; complement with emission models

Top-Down: Data Mining & Linked Open Data

Advantages: primary data reported by industry and states; detailed emissions profiles; automation capabilities



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Mining Available Data from the United States Environmental Protection Agency to Support Rapid Life Cycle Inventory Modeling of Chemical Manufacturing

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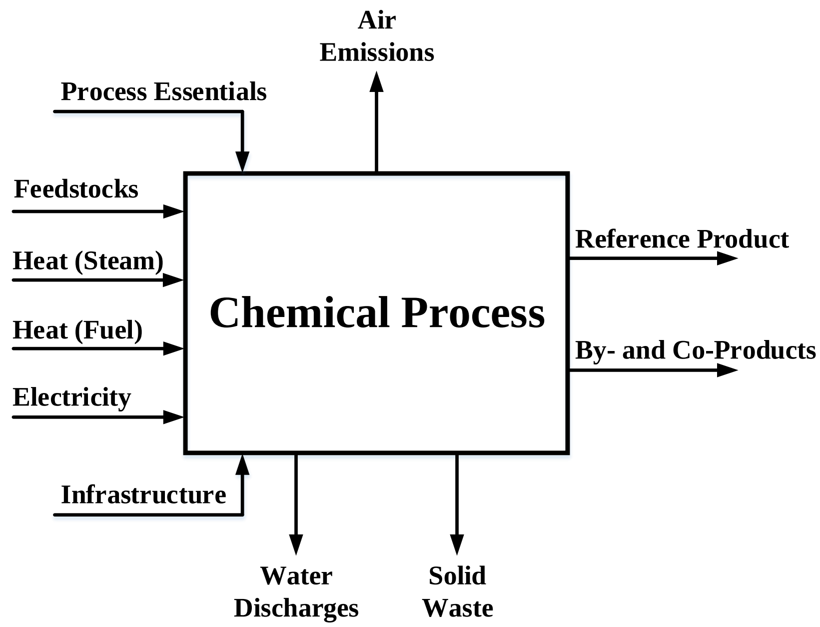
Challenges: multi-chemical facility-level allocation; inventory data gaps; currently limited to TSCA CDR chemicals

Bottom-Up Simulation

Advantages: potential for improved LCI compared to commercial databases; includes storage and fugitive emissions; process-specific



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Coupling Computer-Aided Process Simulation and Estimations of Emissions and Land Use for Rapid Life Cycle Inventory Modeling

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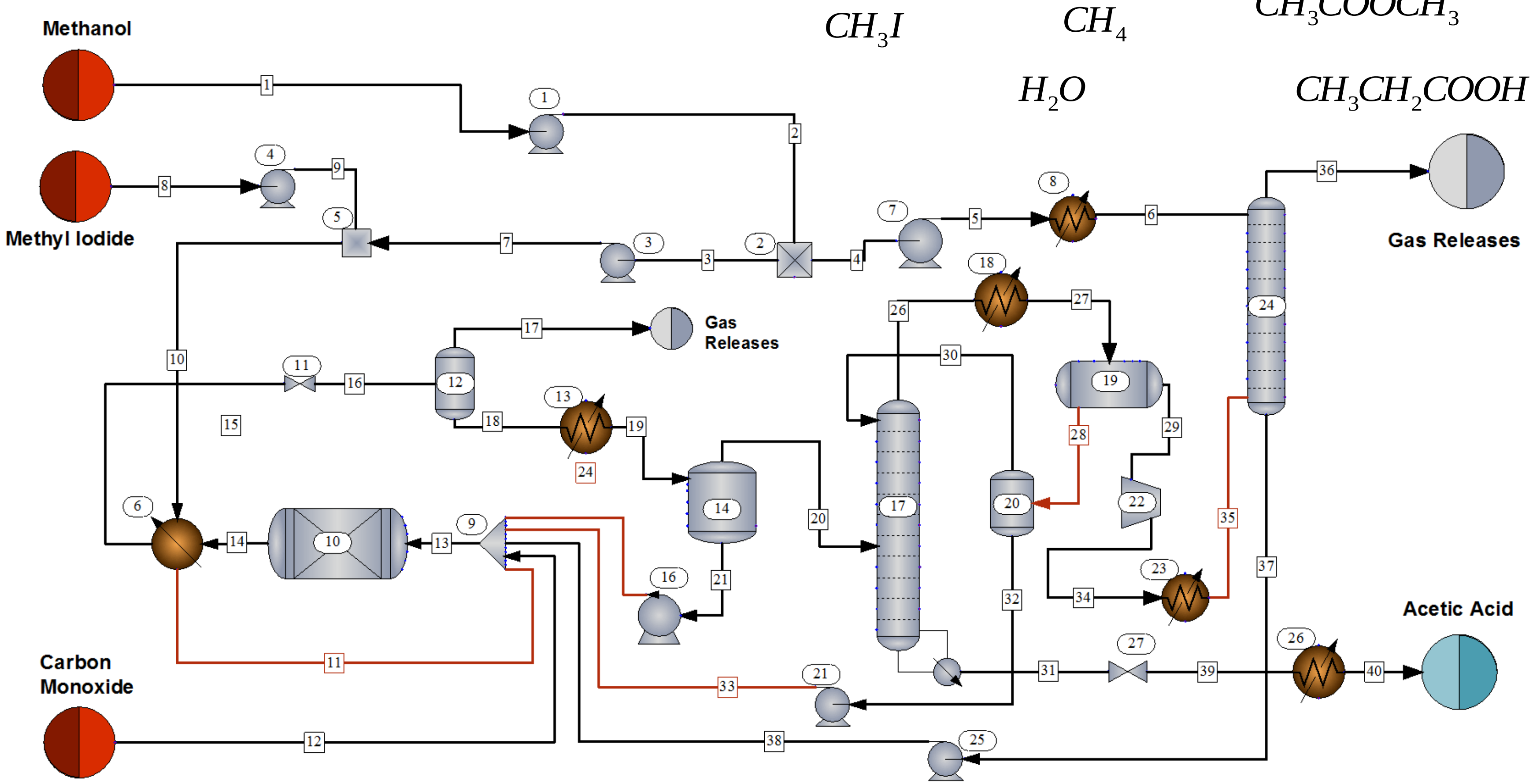
Challenges: knowledge of engineering design; need for chemical synthesis details; establishing assumptions

Acetic Acid Production

$$CH_3OH + CO \xrightarrow{\text{catalyst}} CH_3COOH$$



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Simulation and Emission Model Outputs

LCI Outputs	Simulation			Simulation and Emission Models		
Acetic Acid Product (kg/kg)	Fugitive	Storage	Vents	Fugitive	Storage	Vents
Carbon monoxide			2.18E-02	1.77E-05		4.36E-02
Carbon dioxide			1.72E-03	7.94E-07		3.50E-03
Methane			6.37E-04	2.90E-07		1.27E-03
Methanol			1.90E-03	1.52E-05	1.85E-04	1.90E-03
Acetic acid				3.17E-05	5.07E-05	7.15E-04
Methyl Iodide			6.92E-03	2.78E-05	2.29E-05	8.13E-03
Hydrogen iodide			2.02E-03	1.07E-06		2.09E-03
Methyl acetate			1.33E-03	1.10E-05		2.23E-03
Water			5.18E-07	2.64E-05		6.93E-06
Propionic acid				1.83E-08		3.12E-07

Comparing Inventory Inputs

LCI Inputs	Units	Simulation	Simulation and Emission Models	Percent Change
Carbon monoxide	kg/kg	5.088E-01	5.093E-01	0.08%
Methanol	kg/kg	5.389E-01	5.395E-01	0.12%
Methyl Iodide	kg/kg	1.225E-02	1.351E-02	10.32%
Steam	MJ/kg kg/kg	1.751+00 7.785E-01	1.752E+00 7.791E-01	0.08%
Cooling water	MJ/kg kg/kg	3.058E+00 4.361E+01	3.060E+00 4.365E+01	0.08%
Electricity	MJ/kg	5.598E-03	5.602E-03	0.08%
Steel	kg/kg	3.095E-04	3.097E-04	0.08%
Land Use	m^2/kg		1.023E-04	∞

Acetic Acid: Emissions Availability

United States Environmental Protection Agency

		Inventory Source					TRACI Impact Category									
	Emission	Simulation	Simulation and Emission Modeling	Data Mining[1]	USLCI[2]	ecoinvent[3]	AP	EP	ODP	SFP	GWP	HHR	HHC	HHNC	ETP
Emission	Acetaldehyde														
	Acetic acid														
	Acrolein														
	Acrylic acid														
	Ammonia														
	Butadiene														
	Butane														
	Butanol														
	Carbon Dioxide														
	Carbon monoxide														
	Chromic Acid														
	Chromium III														
	Chromium VI														
	Cobalt														
	Ethyl acetate														
	Ethylene glycol														
	Formaldehyde														
	Heat, waste														
	Hexane														
	Hydrogen														
	Hydrogen Iodide														
	Maleic Anhydride														
	Manganese														
	Methane														
	Methane, bromo-, Halon 1001														
	Methanol														
	Methyl Acetate														
	Methyl Iodide														
	Propionic Acid														
	TOC, Total Organic Carbon														
	VOC, volatile organic compounds														
	Water														
TRACI Impact Categories (number of flows)	AP				1										
	EP				1										
	ODP			1											
	SFP	4	6	12	2	7									
	GWP	2	2	1	1	2									
	HHR	1	1	1	2	1									
	HHC	1	1	6	1	2									
	HHNC	1	1	10	1	3									
	ETP	2	4	9	1	4									

Emission or impact is included in column category

Emission or impact is not included in column category

Smith, R.L. et al. (2017). Coupling computer-aided process simulation and estimations of emissions and land use for rapid life cycle inventory modeling. *Sustainable Chem. Eng.* 5 (5): 3786-3794, SI.

Reconciliation of Methods

- **Reconciliation** of Top-Down Data Mining and Bottom-Up Simulation methods can produce inventories that are qualitatively and/or quantitatively better than either method alone.
  - **Top-Down** Data Mining uses EPA databases, but facility data requires allocation.
  - **Bottom-Up** Simulation provides inputs and alleviates need for allocation, but time and knowledge requirements are intensive.
- **Reconciliation** will combine aspects of both approaches.

Conclusions

- Top-Down data mining uses linked open data from national emissions databases. Facility-level data usually requires allocation.
- Bottom-Up method assumes simulation and emission models represent actual facilities; inventory data is process-specific.
- Chemical process simulation can be used to determine inputs and some releases. Addition of emission models complete the releases.
- **Future Work**: Further development of reconciliation methods and potential for automation.

Thank you!

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