A SIMULATION-BASED COMPUTATIONAL FRAMEWORK FOR SUSTAINABILITY ASSESSMENT AND LIFE CYCLE INVENTORY GENERATION

Shuyun Li¹, Selorme Agbleze¹, Gerardo J. Ruiz-Mercado² and Fernando V. Lima¹

¹West Virginia University, Morgantown, WV
²U.S. Environmental Protection Agency, Cincinnati, OH

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Presentation Outline

• Background
  ✓ Motivation and challenges
  ✓ Current Methods: Life Cycle Inventory (LCI) and GREENSCOPE

• Proposed Computational Framework
  ✓ Proposed pollution control unit (PCU) modules
  ✓ Integrated framework
  ✓ PCU simulator example
  ✓ Automated interface with commercial simulators

• Case Study
  ✓ Acetic acid manufacturing process
  ✓ LCI results and radar plots

• Conclusions
Motivation and Challenges

Motivation:

- Chemical industries have begun to shift from economic stand-alone focus to include **sustainability** in the **decision-making** steps.
- **Emissions** have caused serious **environmental** and **sustainability** issues.
- Pollution control is a complex problem arising from the interactions among **environmental**, **economic**, and **social**. So, **Integrated methods/tools** for pollution control and sustainability are needed.

Challenges:

- **Limited capability** of current process simulators in terms of available **pollution control tools**.
- **Data gaps/missing** in current methods.
- **Difficult communication** between process simulators and sustainability assessment tools.

**Objective:** develop an integrated framework to bridge the gap between **process simulators** and **pollution control technologies** for **LCI generation** and **sustainability assessment**.
Current Sustainability Assessment Methods: LCI Data

**Data Sources & Tools**

- **Databases:** Ecoinvent, US LCI, ELCD, LCA food
- **Top-down:** Data Mining & Estimation
- **Bottom-up:** Process simulators

**LCI Data**

- **Utility** (Steam, Fuel, Electricity)
- **Feedstocks**
- **Infrastructure**
- **Land Use**
- **Chemical Processes**
  - Solid Waste
  - Product and Co-Products
  - Water Discharges
- **Air Emissions**

**Limitations** of current methods:

- Missing and incomplete data in databases
- Inventory data gaps (emissions)
- Process simulators have the potential for improving LCI data generation, but currently have limited emission estimation capabilities

**LCA, Sustainability & Risk Assessment**
Current Sustainability Assessment Methods: GREENSCOPE

- Input data: mass & energy flows, operating and equipment data and properties of the involved component
- GREENSCOPE translates process design and performance data into a set of dimensionless indicator scores
- GREENSCOPE can be used to assess new processes or compare different technologies
- Data availability in terms of quality and quantity is very important for the assessment results
- Process simulators have the potential for providing required data, but are limited in emission and data communication

Indicator Score = \frac{|Actual - Worst|}{|Best - Worst|} \times 100\%
Proposed Method for Pollution Control Units (PCUs)

- Process Flow Diagram
- Component Models
- Process Simulations
- LCI Data Collection
- Commercial simulators (e.g., CHEMCAD)
  - Air PCUs: Flare, Thermal Oxidizer, Boiler, Scrubber
  - PM PCU: Baghouse
  - Liquid PCUs: Stripper, GAC
  - Solid PCU: Gasifier/Pyrolysis
- PCUs to augment simulator capabilities
Integrated Framework

- Commercial Simulations (e.g., CHEMCAD, Aspen)
  - air waste streams
  - liquid waste streams
  - solid waste streams

- PCUs
  - Air PCUs
  - PM PCU
  - Liquid PCUs
  - Solid PCU

- LCI Models

- Utility Infrastructure

- PCU LCI Boundaries

- User Interface

- Parameters and Factors Data
  - Economic
  - Efficiency
  - Environmental
  - Energy

- All Indicator Results
A Typical Flare System

Flare Simulator:

- Inputs only require waste stream information and some user-defined parameters (default values are provided)
- Outputs include mass and energy balances, equipment sizing, construction material, utility consumption, land use, and LCI report
PCU Simulators Example (Flare)

Pollution Control Unit (PCU) Modules

All Pollution Control Unit Simulators include Flare, Thermal Oxidizer, Scrubber, and Boiler Units. This simulator allows users to size the necessary equipment, estimate the utility, material of construction, footprint, and the life cycle inventory for the above air pollution control technologies.

Flare is a common unit to deal with VOCs in industrial. In the flaring process, VOCs are added to a remote, usually elevated, location and burned in an open flame using a specially designed burner tip, auxiliary fuel, and steam or air to promote mixing for nearly complete VOC destruction.

Thermal Oxidizer (TO), also called incinerator, is one of the best-known methods of industrial waste disposal. Here TO is designed as a device to control VOCs through thermal or catalytic combustion.

Wet Scrubber is designed to control acid gases, such as HCl, SO2, and NOx, with certain solvent.

Boiler, as one potential air pollution unit, will destroy most VOCs while generating steam.

Instructions

1. Click the "Pollution Control Units" location on the ribbon and select the desired air pollution control unit in the library. Once selected, the unit data input box will appear.
2. Complete all the necessary data on the data input tab.
3. Hold the mouse over certain parameters, a short note will display to help the users define the input value.

Main Air Pollution Control Technologies

<table>
<thead>
<tr>
<th>DEVICE</th>
<th>INLET CONC.</th>
<th>EFFICIENCY</th>
<th>ADVANTAGES</th>
<th>DISADVANTAGES</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSORPTION</td>
<td>250</td>
<td>90</td>
<td>Especially good for inorganic acid</td>
<td>Limited applicability</td>
</tr>
<tr>
<td></td>
<td>1000</td>
<td>95</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>5000</td>
<td>90</td>
<td></td>
<td></td>
</tr>
<tr>
<td>THERMAL OXIDIZER</td>
<td>20</td>
<td>95</td>
<td>High destruction efficiency, wide applicability, can recover heat energy</td>
<td>No organics can be recovered</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>90</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FLARE</td>
<td>&gt; 98</td>
<td>&gt; 98</td>
<td>High destruction efficiency, no additional</td>
<td>No organics can be recovered</td>
</tr>
<tr>
<td>BOILER</td>
<td>&gt; 98</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

For more details on Air Pollution Control Units.

LCI Report

Equipment, Utility and Emission Results

- Utility Type
- Utility rate limits
- LCI Utility Index
- Construction Material
- Amount
- LCI Material Index
- Footprint
- Area
- LCI Footprint Index
Integrated Simulator for Data Collection

- The integrated simulator allows **data collection and processing more efficiently** for different scenarios.
- This framework enables the **automatic generation of LCI data and sustainability assessment results** from process simulations.
- Load CHEMCAD
- Load CHEMCAD simulation file
- Identify waste stream ID and upload waste stream to PCU
Benefits of Novel Automated Interface

- Allows PCU modules to be directly connected with waste streams from process simulators
- Enables users to open and run simulation files in Excel so that LCA practitioners can collect data without need of prior process simulation knowledge
- Improves the information search and data collection processes as well as data accuracy

Acetic Acid Manufacturing Process in CHEMCAD
Case Study: Acetic Acid Process*

## LCI Monitoring Results

<table>
<thead>
<tr>
<th>LCI Inputs</th>
<th>Unit</th>
<th>Simulation</th>
<th>Simulation with emission control</th>
<th>Percentage change</th>
</tr>
</thead>
<tbody>
<tr>
<td>Natural Gas</td>
<td>scm/kg AA</td>
<td>0</td>
<td>2.34E-2</td>
<td>∞</td>
</tr>
<tr>
<td>Steam</td>
<td>kg/kg AA</td>
<td>7.79E-1</td>
<td>-2.84E-1</td>
<td>−37%</td>
</tr>
<tr>
<td>Purge Gas</td>
<td>scm/kg AA</td>
<td>0</td>
<td>1.24E-3</td>
<td>∞</td>
</tr>
<tr>
<td>Electricity</td>
<td>kW/kg AA</td>
<td>5.60E-3</td>
<td>1.40E-4</td>
<td>3%</td>
</tr>
<tr>
<td>Construction Material</td>
<td>kg/kg AA</td>
<td>2.03E-6</td>
<td>1.49E-5</td>
<td>733%</td>
</tr>
<tr>
<td>Footprint</td>
<td>kg/kg AA</td>
<td>1.02E-4</td>
<td>2.42E-6</td>
<td>2%</td>
</tr>
</tbody>
</table>

### LCI Outputs

<table>
<thead>
<tr>
<th></th>
<th>Unit</th>
<th>Simulation</th>
<th>Simulation with emission control</th>
<th>Percentage change</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td>kg/kg AA</td>
<td>1.97E-4</td>
<td>1.09E-9</td>
<td>−100%</td>
</tr>
<tr>
<td>CO₂</td>
<td>kg/kg AA</td>
<td>5.45E-4</td>
<td>1.36E-1</td>
<td>24868%</td>
</tr>
<tr>
<td>CO</td>
<td>kg/kg AA</td>
<td>4.39E-2</td>
<td>8.73E-4</td>
<td>−98%</td>
</tr>
<tr>
<td>HI</td>
<td>kg/kg AA</td>
<td>1.84E-3</td>
<td>0</td>
<td>−100%</td>
</tr>
<tr>
<td>H₂S</td>
<td>kg/kg AA</td>
<td>2.60E-02</td>
<td>1.00E-03</td>
<td>−96.15</td>
</tr>
<tr>
<td>H₂O</td>
<td>kg/kg AA</td>
<td>0</td>
<td>3.89E-2</td>
<td>∞</td>
</tr>
<tr>
<td>CH₃OH</td>
<td>kg/kg AA</td>
<td>3.10E-5</td>
<td>0</td>
<td>−100%</td>
</tr>
<tr>
<td>AA</td>
<td>kg/kg AA</td>
<td>5.89E-4</td>
<td>0</td>
<td>−100%</td>
</tr>
<tr>
<td>PM (&lt; 1 μm)</td>
<td>kg/kg AA</td>
<td>0</td>
<td>1.63E-6</td>
<td>∞</td>
</tr>
</tbody>
</table>
Comparison between scenarios with/without pollution control units shows that pollution treatment units do not decrease majority of indicator scores. Only scores of MP (Mass productivity) and MRP (Material Recovery Parameter) are decreased.
Comparison between scenarios with/without pollution control units shows that pollution treatment units do not have much impact on the economic performance.
Comparison between scenarios with/without pollution control units shows that all the energy indicators keep the same scores except REI (Energy Intensity), $\eta_{Ex}$ (Resource-Exergy Efficiency) and Extotal (Exergy Consumption) change slightly.
there are three areas of scores improved: hazardous materials involved (indicators 1-3); global warming and smog potential (indicators 23-24, 27-28); water quality (indicators 36-37).
Conclusions

- Proposed framework can bridge existing gaps between sustainability and process systems engineering (commercial simulators).
- The developed PCU modules can improve process data collection and have potential for automation with commercial software.
- An automated interface between PCUs and commercial simulators was developed to reduce the effort for collecting and processing data.
- The effectiveness of proposed framework was illustrated through acetic acid manufacturing process example.
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Thank you!

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