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Smart Manufacturing Experience, Pittsburgh, PA
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What Do We Do?

Discover, integrate, and mature technology solutions to enhance the nation’s energy foundation and protect the environment for future generations.

MISSION

National Energy Technology Laboratory (NETL) is one of 17 U.S. Department of Energy (DOE) national laboratories; producing technological solutions to America’s energy challenges.

- NETL has five locations
- Only National Lab dedicated to carbon research
- Government owned & operated
- One of three applied national labs
- Leader in cutting-edge research in conversion to higher value products
- Flexible Intellectual Property
U.S. Energy Consumption in 2021: 97.3 Quads

Source: LLNL, March 2022. Data is based on DOE/EIA MRE (2021). If this information or a reproduction of it is used, credit must be given to the Lawrence Livermore National Laboratory and the Department of Energy, under whose auspices the work was performed. Net electricity generation does not include self-generation. EIA reports consumption of renewable resources (i.e., hydro, wind, geothermal, and solar) for electricity in MWh-equivalent values by assuming a typical fossil fuel plant heat rate. The efficiency of electricity production is calculated as the total retail electricity delivered divided by the primary energy input into electricity generation. And use efficiency is estimated as 68% for the residential sector, 65% for the commercial sector, 21% for the transportation sector, and 49% for the industrial sector, which was updated in 2017 to reflect DOE’s analysis of manufacturing. Totals may not equal sum of components due to independent rounding. EIA-01072
U.S. Energy-Related CO₂ Emissions in 2021: 4,863 MMt

July, 2021. Data is based on DOE/EIA MED (2019). If this information or a reproduction of it is used, credit must be given to the Lawrence Livermore National Laboratory and the Department of Energy, unless the work was performed. Distributed electricity represents only retail electricity sales and does not include self-generation. EIA reports consumption of renewable resources (i.e., hydropower) and solar for electricity in Btu-equivalent values by assuming a typical fossil fuel plant heat rate. The efficiency of electricity production is calculated as the total retail electricity used by the primary energy input into electricity generation. Total use efficiency is estimated as 45% for the residential sector, 45% for the commercial sector, 21% for the transportation sector, and 45% for the industrial sector, which was updated in 2017 to reflect DOE’s analysis of manufacturing. Totals may not equal sum of components due to independent rounding. LNL-MA-405527
Decision Making for Energy & Manufacturing Systems

Decisions

- Process operation
- Process design
- Technology selection
- R&D priorities

Approaches

- Approximations
- Heuristics
- Spreadsheets
- Simulation
- Optimization
  \[ \min f(x, u) \]
  \[ h(x, u) = 0 \]
IDAES Integrated Platform

Open Source: https://github.com/IDAES/idaes-pse
Lee, et al., 2021
Examples of IDAES Optimization Approach

• Designing carbon capture technologies
  – Incorporating market interactions in system design
  – Family of feasible designs for rapid deployment
  – Reduce technical risk

• Making existing plants more efficient
  – Leverage plant sensor data
  – Build predictive models
  – Optimize plant operations
Multi-scale Surrogate Modeling

Linking models across length/time-scales with minimal loss of accuracy

Should capture system be built? (i.e., Is it cheaper to pay a carbon tax?)

If yes, what is the optimal size and capture rate?

How do various potential market scenarios impact results?
Example Scenarios: Flexible Capture NPV Optimization

Carbon Tax = $150 per ton (Fraction in white denotes the capacity factor)

- 150_CAI SO: Should the capture system be built?
- 150ERCOT: Reduce the capex and opex by 20%
- 150 MISO-W: Must build the capture system
- 150 NYISO: Reduce the capex and opex by 20%
- 150 PJM-W: Must build the capture system
Simultaneous Design of the Entire Process Family

- Select optimal “common” unit sizes and assignment of shared units to process installations simultaneously (MILP formulation)
  - Flexibility across the design range while exploiting opportunities for shared component designs
  - Reducing engineering design costs
  - Reducing manufacturing costs (economies of numbers and learning)
- Ensures each installation is feasible while the entire process family is cost optimal
- **Improved time-to-market and process deployment**

Robust Design to Reduce Technical Risk

Inherent uncertainty in process design models
- Operational uncertainty: e.g., fluctuations in feed
- Economic uncertainty: e.g., cost of utilities
- Epistemic uncertainty: e.g., mass/heat transfer, kinetics

Deterministic design fails to meet CO$_2$ capture performance requirement with a 33% probability

Robust design guarantees CO$_2$ capture in all scenarios; cost increase is kept to the minimum necessary to achieve this

Robustness achieved utilizes smaller equipment overall, putting more emphasis on reboiler and condenser duty control

Deterministic Solution
Cost: $7.25$ MM/yr
Second-stage Cost: $5.19$ MM/yr

Robust Solution
Cost: $10.90$ MM/yr
Expected Second-stage Cost: $5.51$ MM/yr

Nominal Capture = 85%
Worst-case Capture = 63%
Prob. of Satisfactory Capture = 58%

Nominal Capture = 92%
Worst-case Capture = 85%
Prob. of Satisfactory Capture = 100%

Used with permission from Isenberg et al., 2021
Examples of IDAES Optimization Approach

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### Data Reconciliation

“Ensure data is reliable”

Minimize \( \sum_{\text{data}} (\text{error}_{\text{meas}})^2 \)

subject to
- Flowsheet connectivity
- Mass and energy balances
- Physical property calculations

\[
\text{error}_{\text{meas}} = \frac{\text{measurement} - \text{model prediction}}{\text{measurement uncertainty}}
\]

### Parameter Estimation

“Make models predictive”

Minimize \( \sum_{\text{data}} (\text{error}_{\text{meas}})^2 \)

subject to
- Flowsheet connectivity
- Mass and energy balances
- Physical property calculations
- Performance equations for unit models

### System-wide Optimization

“Identify optimal operation”

Minimize \( \sum_{\text{data}} (\text{error}_{\text{meas}})^2 \)

subject to
- Flowsheet connectivity
- Mass and energy balances
- Physical property calculations
- Performance equations for unit models
- Load = Target Load
- Operational Constraints (e.g., \( T < T_{\text{max}} \))
- Emissions < Emission Limits

"Ensure data is reliable"

"Make models predictive"

"Identify optimal operation"
Data Reconciliation Allows Characterizing Variability in Measured and Unmeasured Quantities

Hourly data: Jan 10, 2019 – Apr 8, 2019

**Main Steam Measurements (Measured)**

- **Net Load (MW)**
- **Flow Rate**
- **Temperature**
- **Pressure**

**Steam extraction flow rates (Not Measured)**

- **FHW 1 Flow Rate**
- **FHW 2 Flow Rate**
- **FHW 3 Flow Rate**

Outliers

Median

75%-ile

95%-ile

Median

75%-ile

95%-ile
Improving Existing Fleet Operations

Maximize \( \text{Plant Efficiency} \) 
\[
\{\text{temps, pressures, flows}\}
\]

subject to
- Flowsheet connectivity
- Mass and energy balances
- Physical property calculations
- Performance equations for unit models
- Load = Target Load

Ball-park model size (1 time point):
- ~80 process streams, ~25 unit models
- ~2700 variables, constraints
- Initialization time: ~ 1-3 minutes
- CPU time: ~ 3-30 sec
- Standard desktop CPU
- Solver: IPOPT

0.6 %-point (2% overall) improvement achievable with steeper sliding pressure
Software Development & Release Management

• Mature Software Development, Test, & Release Processes
  – Open-Source Software repository at GitHub
    https://github.com/IDAES/idaes-pse
  – Continuous development, testing & documentation updates
  – Quarterly release schedule
    • 22 Releases in past 4 years on the 1.X line
  – 2.0 Release schedule for November 2022
    • Major organizational and API improvements
    • As learned over the past years of development
  – February's 1.13 release last of the 1.X line
    • May & August will each have 2.0.0 alpha releases to ease migration to 2.0
Open Source Platform

Website: https://idaes.org/
GitHub repo: https://github.com/IDAES/idaes-pse
Support: idaes-support@idaes.org
    Ask questions, subscribe to the user and/or stakeholder email lists
Documentation: https://idaes-pse.readthedocs.io
    Getting started, install, tutorials & examples
Overview Video
    https://youtu.be/28qjcHb4JfQ
Tutorial 1: IDAES 101: Python and Pyomo Basics
    https://youtu.be/_E1H4C-hy14
Tutorial 2: IDAES Flash Unit Model and Parameter Estimation (NRTL)
    https://youtu.be/H698yy3yu6E
Tutorial 3: IDAES Flowsheet Simulation and Optimization; Visualization Demo
    https://youtu.be/v9HyCiP0LHg
Summary

• Trends Requiring Innovation in Decision Support Tools & Multi-scale optimization
  – Evolving energy ecosystem requires new system designs
  – Expanding and decarbonizing U.S. industry
  – Efficient designs through intensification & modularization

• Need for Advanced, Optimization-Based Modeling Platform
  – Decision support for nonlinear, interacting flexible systems
  – Multi-scale from molecular to process/plant to enterprise
  – Leverage 30 years of progress in algorithms, hardware, modeling

• Examples of IDAES Optimization Approach
  – Carbon Capture System Design
  – Improve existing plant performance through optimization
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References


