

T4P1 - POSTER #1

T4P1 Poster #: 01



Energy Storage Strategies for Large-Scale Chemical Plants Powered by Renewable Energy

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GOALS

PROBLEM STATEMENT

- To facilitate the transition from fossil-based chemical industry to renewable-based chemical industry, it's a crucial step to integrate renewable resource such as solar or wind energy into chemical processes.
- Solar and wind power varies throughout the day and the seasons.
- Challenge:** How to supply a continuous and stable power to large-scale chemical plants to enable load following?

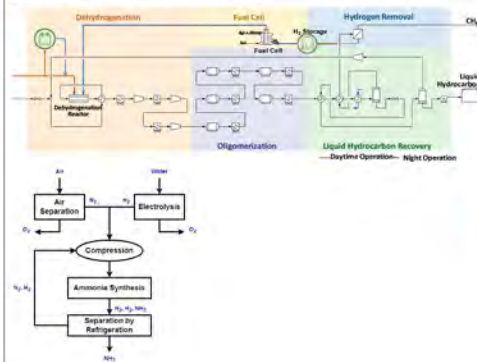
SOLUTION & APPROACH

- The variable renewable electricity of wind and solar requires massive energy to enable load following.
- Strategy 1: No H₂ Storage
- Strategy 2: Minimal Battery Storage
- Strategy 3: H₂ Battery

Innovation

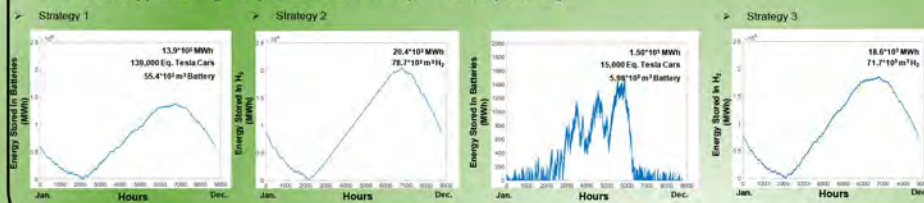
- We systematically evaluate various energy storage strategies for large-scale chemical plants and find the best strategy for minimum storage requirements.
- We illustrate how much of solar and wind energy should be harvested to attain minimum storage based on historical solar and wind intensity data.

PROCESS FLOWSHEET

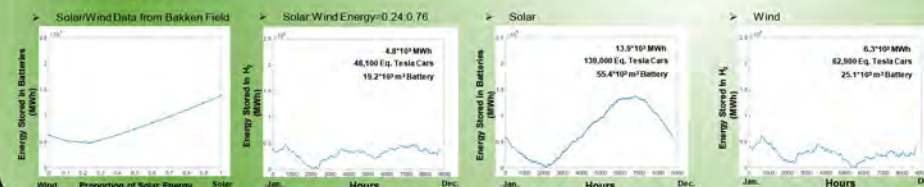


MAIN FINDINGS

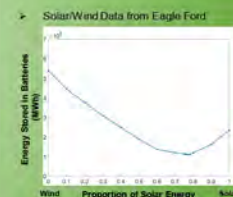
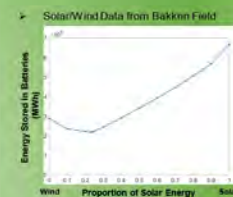
- Battery storage emerges as the optimal choice for minimizing storage volume, given the small difference in energy density between battery and H₂ (0.26 MWh/m³ for H₂ and 0.25 MWh/m³ for battery) and higher process efficiency in battery storage



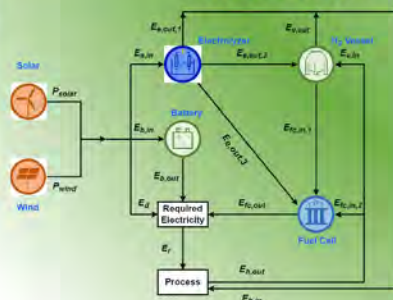
- The combination of solar and wind power in a hybrid system proves to be an effective means to reduce the required storage volume for the decarbonized liquid fuel production and the green ammonia production.



- It's a good way to produce green ammonia to utilize H₂ storage as feedstock and energy supplier simultaneously, considering the existing infrastructure H₂ vessel.



MATHEMATICAL MODELLING



- Energy balance of renewable energy
 $P_{solar} + P_{wind} = E_{s,in} + E_{s,out} + E_d$
- Energy balance of required electricity
 $E_r = E_d + E_{b,out} + E_{f,out}$
- Energy balance in electrolyzer
 $E_{e,in} = E_{e,out} + E_{e,loss}$
- Energy balance in fuel cell
 $(E_{f,in,1} + E_{f,in,2} + E_{f,in,3}) \cdot \eta_{fc} = E_{f,out}$
- Mass balance of H₂ entering the process
 $E_{s,in} = E_{s,out} + E_{f,in}$
- Mass balance of H₂ exiting the process
 $E_{s,out} = E_{f,out} + E_{s,in}$
- Converting electricity to hydrogen through an electrolyzer and then back to electricity through a fuel cell is a less efficient process than directly using electricity
 $E_{f,out} < E_{s,in}$
- Battery storage at the kth hour
 $S_k^b = S_{k-1}^b + E_{s,in} - E_{s,out}$
- H₂ storage at the kth hour
 $S_k^h = S_{k-1}^h + (E_{s,in} + E_{f,in,1} + E_{f,in,2} + E_{f,in,3}) \cdot \eta_{fc} - (E_{f,out} + E_{f,in,1})$



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The Poster



SCAN ME

T4P1 - POSTER #2

T4P1 Poster #: 02



Setting Performance Targets For Membranes vis-à-vis Cryogenic Distillation For Ethylene-Ethane Separation

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GOALS

PROBLEM STATEMENT



SOLUTION & APPROACH

- Get the **state-of-the-art process** for cryogenic distillation and membrane cascade
 1. Design a novel energy efficiency cryogenic distillation process
 2. Develop a Mixed Integer Non-linear Program (MINLP) for binary membrane separation
- Compare energy consumption and capital cost of two separation processes on an equivalent basis for two different plant sizes.

INNOVATION

- Access to benchmarks of **permeance, perm-selectivity, and fabrication cost** for membranes
- Provide a tool to **optimize the power consumption and the capital cost** for membrane cascade.

IMPACT & FUTURE

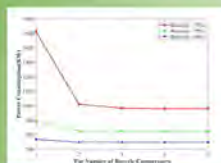
- Set performance targets, including permeance, perm-selectivity, and fabrication cost, for membranes for ethylene/ethane separation.
- Help membrane researchers on how to design membrane cascade for the minimal capital cost or the minimal power consumption.



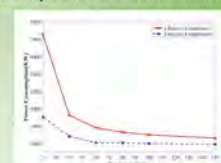
MAIN FINDINGS

If not particularly mentioned, process specifications below are applied to all cases: the number of recycle compressors=2, perm-selectivity=100, feed temperature=25 °C, feed pressure=8.2 bar, feed composition=0.83 C₂H₄/0.17 C₂H₆, feed flowrate=10 MMSCFD, purity=99.9%, recovery=99.0%.

- Beyond 2 compressors, the decreased power consumption is small.



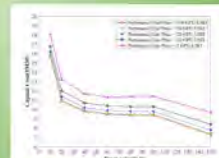
- At low perm-selectivity, the power consumption decreases rapidly. At high perm-selectivity, the power consumption decreases slowly.



- The minimal power consumption and the minimal capital cost generally occur at different pressure ratio.

Pressure Ratio	Power (kW)	Membrane Area (m ²)	Recycle Flowrate (MMSCFD)	Capital Cost (\$MM)
2.0	1326.2	986,517	34.4	39.4
2.7	994.0	226,761	14.1	16.3
3.0	1010.5	156,202	12.2	14.4
4.0	1138.6	72,003	10.0	12.1
5.0	1270.2	46,604	9.3	11.6
6.0	1387.6	35,017	8.9	11.6

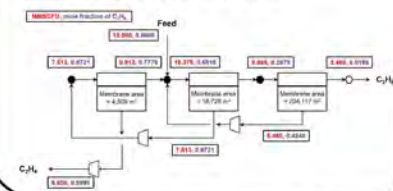
- Case study: recovery=95%, purity=99.9%.
- Distillation capital cost: 10.7 \$MM



OUTCOMES

- New distillation process can decrease the power consumption by 8-23% of the conventional distillation process.
- **Advantages** of the novel distillation process:
 1. High energy efficiency
 2. No external refrigeration
 3. Low pressure operation

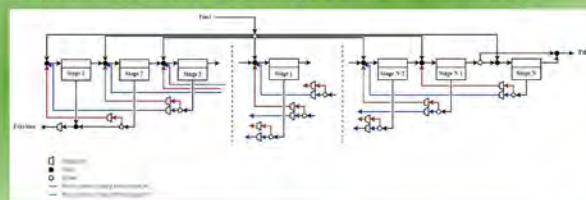
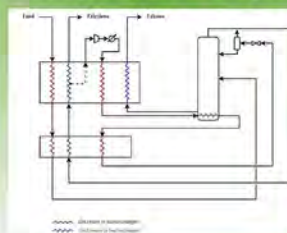
- Feed pressure=8.2 bar, pressure ratio=4, perm-selectivity=100, permeance=100 GPU, unit price of membrane=10 USD/m², purity=99.9%, recovery=99%.



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DISTILLATION & MEMBRANE SCHEMATICS



MODEL CONSTRUCTION

- Construction of the mathematical model:
 1. **Solution-diffusion theory**: model the local flux of each component through the membrane
 2. **Crossflow model**: model the overall permeation process
 3. **Flux equation**: build a relationship between the local flux and the membrane area

T4P8 - POSTER #3



T4P8
Poster #: 03



Multiscale Equation-Oriented Optimization with Embedded Microkinetic Information

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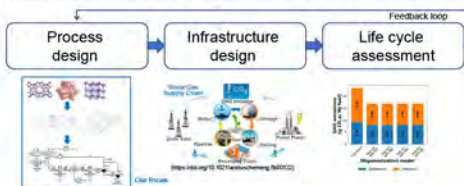
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GOALS

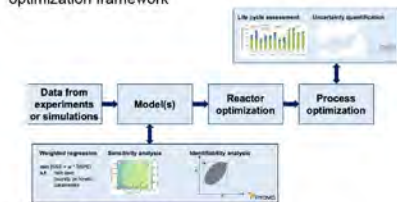
Motivation

How to improve the technical and economic feasibility of the CISTAR process with ongoing research at multiple scales?



Research Aim

Develop a multiscale reactor and process design and optimization framework



Research Questions

- How does the choice of reduced-order kinetic (ROK) model affect model fit quality to microkinetic (MK) model simulation data?
- What is the effect of model-form uncertainty on process-scale reactor design decisions and performance?
- How does model-form uncertainty propagate through process design?

MAIN FINDINGS

ROK models enable the tractable incorporation of MK information in reactor and process design

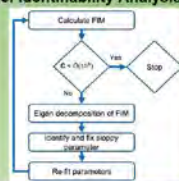
In-Sample Fit Quality:

ROK models differ by functional form of frequency factor, activation energy, adsorption isotherm, and adsorption enthalpy

Model code	No. of fitted parameters	MSLE [log(Pa) ²]
M0	24	3.421
M1	9	5.141
M2	9	3.532
M3	9	3.519
M4	9	4.575
M5	9	4.526

M1 has the worst fit quality

Model Identifiability Analysis:



Model code	FIM condition number		Sloppy parameters
	With sloppy parameters	Without sloppy parameters	
M2	3.87×10^9	1.47×10^7	a_{olig}
M3	7.70×10^9	1.30×10^7	a_{olig}
M4	2.55×10^{21}	2.40×10^6	$\gamma, \delta, E_{\text{olig}}, k_{\text{olig}}$
M5	3.49×10^{21}	1.56×10^6	$\gamma, \delta, E_{\text{olig}}, k_{\text{olig}}$

Condition number decreases
Parameter confidence increases

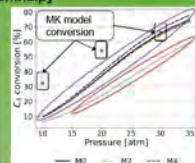


Fig. 1. Quality of fit of ROK models compared to microkinetic model simulation data at $T = 523 \text{ K}$, $P = 10 - 30 \text{ atm}$

According to MSLE, M0 is the model of choice
M0, M2 - M5 capture conversion trends well

Out-of-Sample Behavior:

Industrial-scale operating conditions, Bakken shale basin oligomerization feed composition

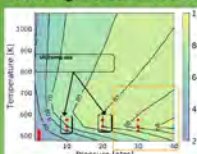


Fig. 2. Conversion to C_4 and heavier olefins at reactor outlet with varying reactor temperature and inlet pressure using representative model M5

Staged PBR design and optimization help analyze uncertainty propagation at process-level due to ROK model choice

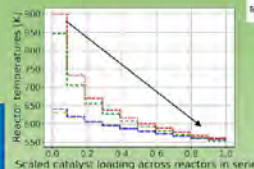


Fig. 3. Optimal temperature profiles along the length of the staged PBR for 10 temperatures

Monotonically decreasing temperature profile: expected behavior for oligomerization

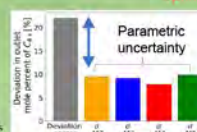
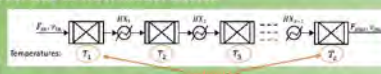


Fig. 4. Uncertainty in optimal C_4 outlet mole percent obtained using first-order error propagation

Model-form uncertainty (22%) supersedes parametric uncertainty (less than 10%)

QR Code for Full Paper



OUTCOMES

Process design with ROK enables confident prediction of oligomerization product portfolio

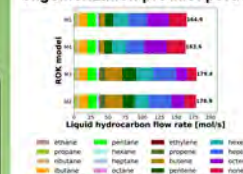


Fig. 5. Outlet product distribution for ROK models M2 - M5

Outlet liquid hydrocarbon flowrate varies by < 9% across ROK models
 C_4 , olefin (high-value product) fraction in outlet liquid hydrocarbon stream varies by < 1% across ROK models

Multiscale optimization identifies emissions reduction opportunity

Optimization formulation

$$\min \text{MSP} = \text{Total annualized cost} + \text{GHG tax} - H_2 \text{ rebate}$$

LHV of liquid hydrocarbon outlet

s.t. mass and energy balances
oligomerization kinetics

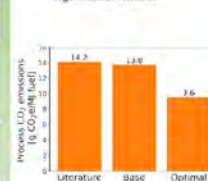


Fig. 6. Downstream process emissions comparison between Literature (no ROK model), Base (with ROK model), and Optimal configurations of the CISTAR process AG2

Process optimization reduces emissions by ~32%

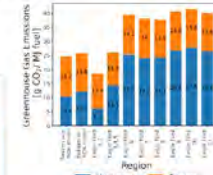


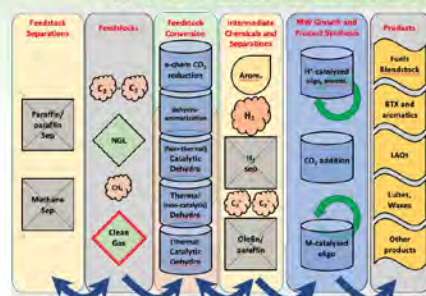
Fig. 7. Process emissions across different shale compositions (Eagle Ford shale basin) from process simulation with embedded ROK models

Process emissions vary with feed composition but are not directly related to feed characteristics (wet or dry gas)

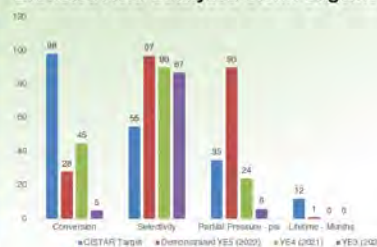
IP & INNOVATION



SYSTEM DESIGN & BENCHMARKS



Brønsted Acid-Catalyzed Olefin Oligomerization



1. Modeling and optimization of membrane-assisted dehydrogenation of membrane reactors for H_2 production

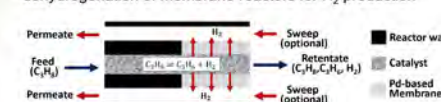


Fig. 8. 1-dimensional schematic of a propane dehydrogenation membrane reactor module

2. Modeling of ethylene oligomerization reaction kinetics through physics-informed machine learning surrogates

T4P9 - POSTER #4



T4P9 Poster #: 4



Integrating CISTAR Processes with Chemical Manufacturing

Qining Chen¹, Qining Wang², Jennifer B. Dunn², David T. Allen¹

¹Center for Energy and Environmental Resources, University of Texas at Austin

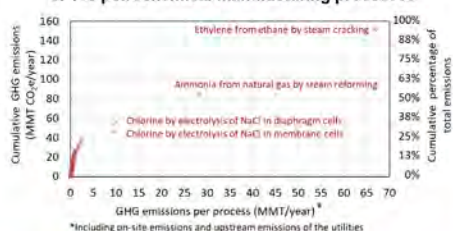
²Department of Chemical and Biological Engineering, Northwestern University



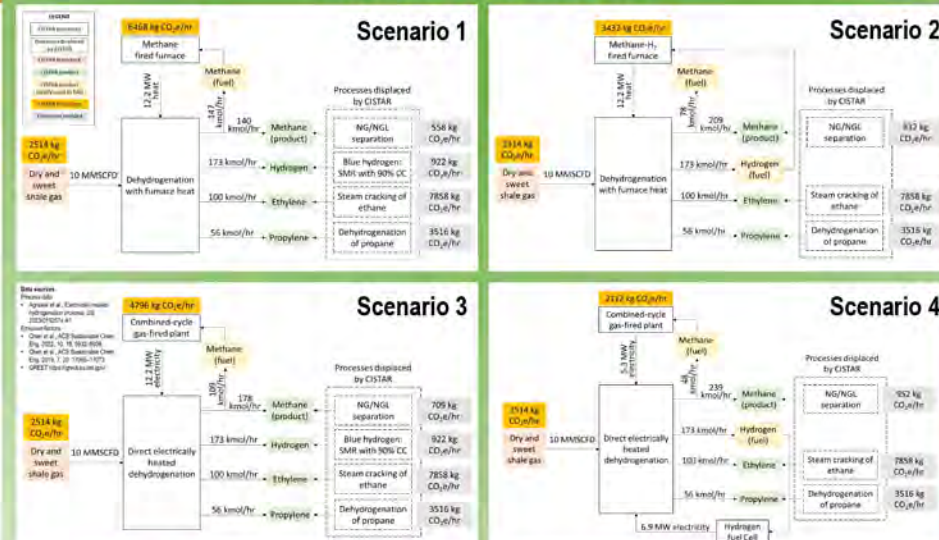
GOALS

- Ethylene production from ethane by steam cracking and ammonia production from natural gas by steam reforming contribute >60% total GHG emissions of 135 commodity petrochemical manufacturing processes in the U.S. (Chen et al., ACS Sustainable Chem. Eng. 2022, 10, 18, 5932–5938)
- This project evaluates net GHG benefits of replacing conventional high emission intensity production of alkenes (via steam cracking) and hydrogen (via steam methane reforming) with various CISTAR processes

Total greenhouse gas emissions per year of 135 petrochemical manufacturing processes



MAIN FINDINGS



Energy consumption scenarios assumed for CISTAR dehydrogenation (Base case: 100% carbon recovery rate and 0 emissions from separation of co-products)		Net GHG (tonne CO ₂ e / MMSCF shale gas input)
Scenario	Description	
1	Heat from methane fired furnace using 51% CH ₄ produced	-9.3
2	Heat from methane-H ₂ fired furnace using all H ₂ and 27% CH ₄ produced	-15
3	Electrified dehydrogenation; electricity from gas-fired plant using 38% CH ₄ produced	-14
4	Electrified dehydrogenation; electricity from fuel cell (all H ₂ used) and gas-fired plant using 17% CH ₄ produced	-18

OUTCOMES

Sensitivity Analyses

- GHG benefits achieved by replacing conventional alkene / hydrogen production with CISTAR dehydrogenation processes are sensitive to carbon recovery rates and emissions from co-product separation
- Minimum carbon recovery rates and maximum energy consumption rates for co-product separation for achieving GHG benefits from process displacements above are back calculated

Thresholds for achieving GHG benefits by replacing conventional alkene and hydrogen production by CISTAR dehydrogenation, under different energy consumption scenarios assumed for CISTAR

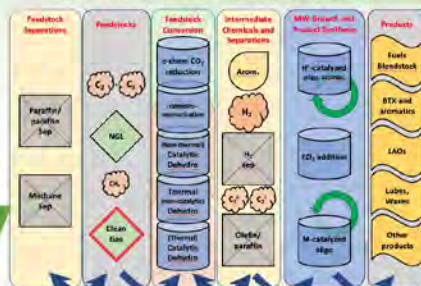
Thresholds for achieving GHG benefits	Energy consumption scenarios			
	1	2	3	4
Minimum C2/C3 recovery rate	69%	45%	54%	33%
Maximum heat consumption for separating product streams (BTU/SCF shale gas input)	13	21	19	26
Maximum power consumption for separating product streams (BTU/SCF shale gas input)	8	13	12	16

IP & INNOVATION

Replacing conventional alkene and hydrogen processes with CISTAR processes reduces greenhouse gas emissions from chemical manufacturing



SYSTEM DESIGN



IMPACT & FUTURE

- Selectivities of dehydrogenation and emission burdens from co-product separation are crucial in defining GHG benefits of CISTAR
- Future research will combine environmental and economic analyses in evaluating the integration of CISTAR processes into chemical manufacturing

- For example, for Scenario 1, at least 69% C2/C3 alkenes need to be converted to C2/C3 alkenes, with zero GHG burdens from co-product separation
- Or if 100% selectivity can be achieved and co-product separations need extra energy input, maximum allowed heat or power consumption is 8-13 BTU/SCF shale gas input

T4P9 - POSTER #5

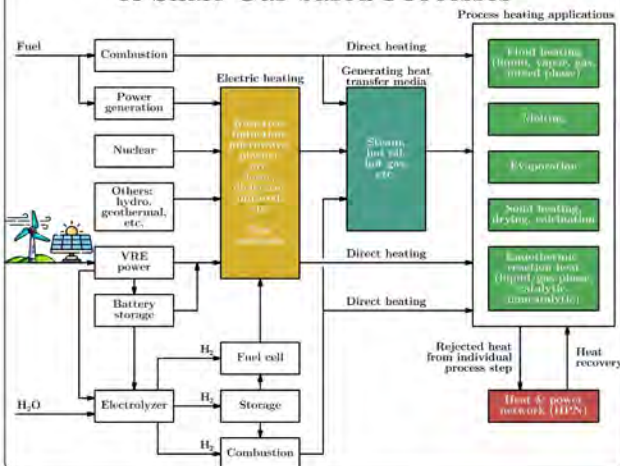


Re-Imagining Ethylene & Liquid Hydrocarbon Production From Shale Gas

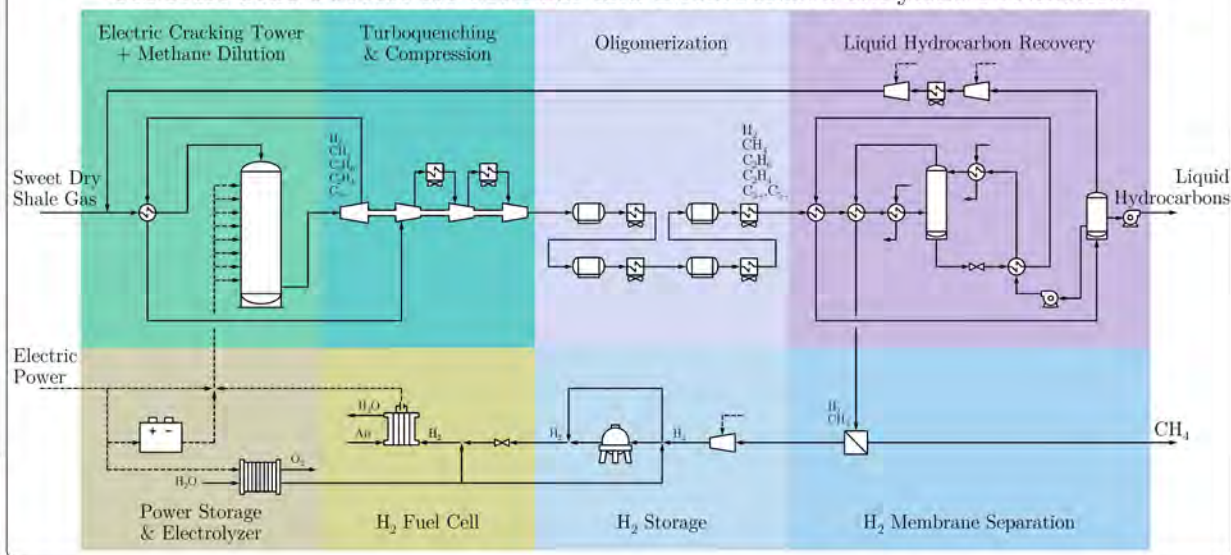
Edwin Rodriguez, Rakesh Agrawal



The goal is to Develop Comprehensive Energy and Process Systems to Enable the Decarbonization of Shale Gas-based Processes



CISTAR 2023 Process for Modular and Decarbonized Ethylene Production

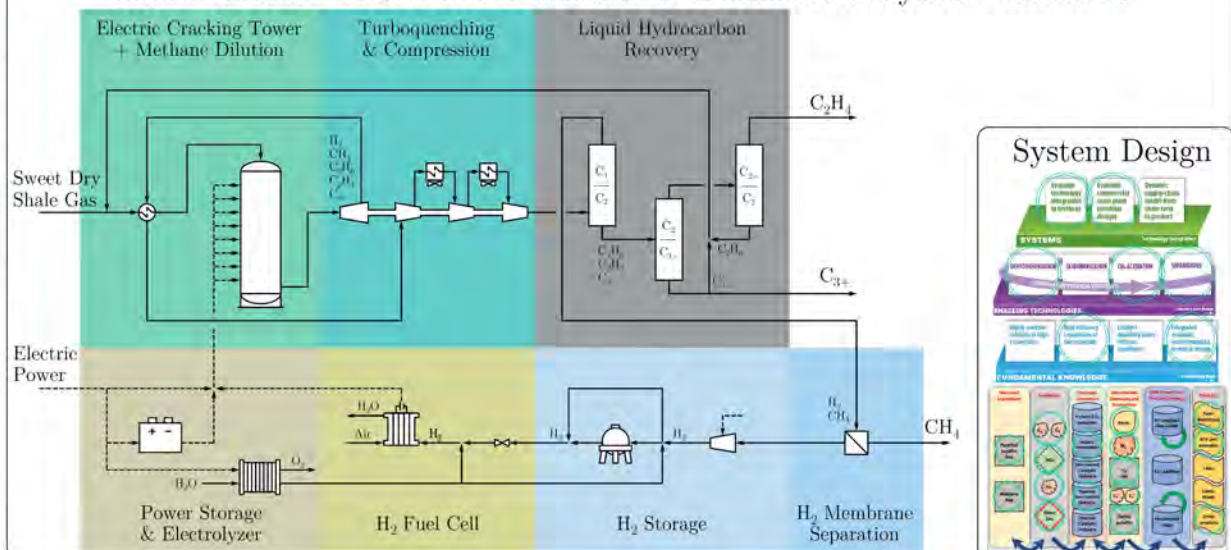


Publications, IP

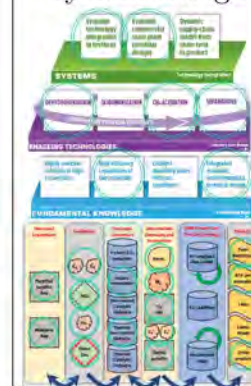
1. Agrawal, Li, US Patent 11,339,104 B2
2. Agrawal, Oladipupo, US Patent 11,267,768 B2
3. Agrawal, Chen, US Patent 11,462,153 B2
4. Agrawal, Chen, US Patent 11,434,184 B2
5. Agrawal, Chen, Oladipupo US Patent 11,578,019 B2
6. Agrawal, Sirolo, Bidia, US Patent 11,603,500 B2
7. Agrawal, Rodriguez, US Proc. Patent Appl. No. 65/347,759
8. Agrawal, R., & Sirolo, J. A. (2023). Decarbonization of chemical process industries via electrification. *The Bridge*, 53(2), 33-40.
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13. Gooty, R.T., Velasco, J.A.C., & Agrawal, R. (2021). Methods to assess numerous distillation schemes for binary mixtures. *Chemical Engineering Research and Design*, 172, 1-20.
14. Chen, Zewei, Yiru Li, Wasim Peter Oladipupo, Edwin Andres Rodriguez Gil, Gary Sawyer, and Rakesh Agrawal. "Alternative Ordering of Process Hierarchy for More Efficient and Cost-Effective Valorization of Shale Resources." *Cell Reports Physical Science* 2 (2021): 100581.
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16. Bidia, Taufik, Yiru Li, Emre Gececi, Jeffrey J. Sirolo, Jeffrey T. Miller, Fabio H. Ribeiro, and Rakesh Agrawal. "Valorization of Shale Gas Condensate to Liquid Hydrocarbons through Catalytic Dehydrogenation and Oligomerization." *Processes* 6, no. 9 (2018): 139.



CISTAR 2023 Process for Modular and Decarbonized Ethylene Production



System Design



T4P10 - POSTER #6



T4P10
Poster #: 06



Multi-dimensional modeling of inductively-heated Steam Methane Reforming (SMR) reactor

Yufei Zhao, Chengtian Cui, Cornelius M. Masuku
Davidson School of Chemical Engineering, Purdue University



GOALS

- Substitute energy supply for alkane reforming by combustion of fossil fuel with renewable electricity;
- Develop 1st principle dynamic heterogenous model of electrified SMR (E-SMR) reactor;
- Characterize the performance and evaluate potential for industry use

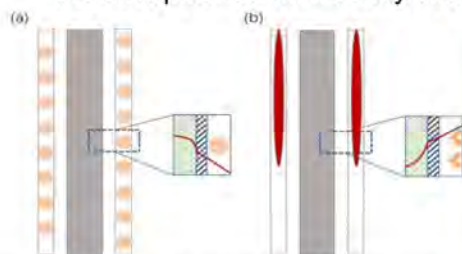


Fig 1. (a) E-SMR tube by induction heating. (b) Conventional SMR reactor tube (reproduced from S.T.Wismann et al.)

MAIN FINDINGS

Induction heat:

$$P_{Ind} = P_{ED} + P_{Hys}$$

$$P_{ED} = \frac{2\pi^2 \mu^2 Z^2 B_0^2 f^2 \cos(\omega t)^2}{5\rho}$$

$$P_{Hys} = A_{Hys} f \rho_{cat}$$

SMR model:

Mass conservation

$$\frac{\partial C_i}{\partial t} + \nabla \cdot (-D_i \nabla C_i + C_i \mathbf{u}) = S_j$$

Energy conservation

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (-\lambda \nabla T + \rho \mathbf{u} E) = Q_j$$

OUTCOMES

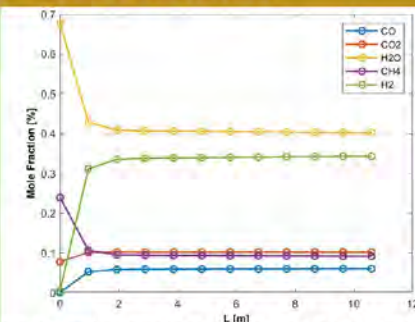


Fig 2. Mole fraction of components under Inlet P=21.59bar, Inlet U=1.6237m/s; Isothermal(1000K).

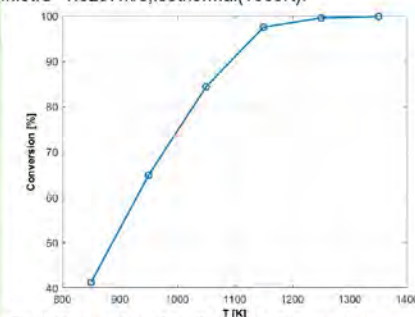


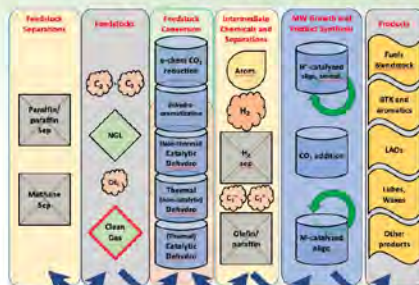
Fig 3. Conversion of methane w.r.t temperature

IP & INNOVATION

- Catalyst used as both conductive and electromagnetically inductive object is directly heated up by renewable electricity



SYSTEM DESIGN & BENCHMARKS



- Conventional SMR reactor

CO ₂ emission/H ₂	kg/kg	12.5473
CO ₂ emission/total	%	1.6898
Energy Efficiency	%	62.07

IMPACT & FUTURE

- Impact**
 - ✓ Contribute to the decarbonization and electrification of conventional hydrogen production
- Future**
 - Validate the consistency of E-SMR model with published experiments

T4P12 - POSTER #8



T4P12
Poster #: 8



Shale gas field development under production profile uncertainty

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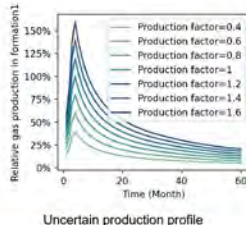
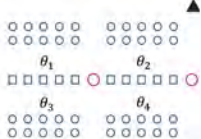
GOALS

Given an undeveloped shale gas field, the goal is to Identify the **most profitable**

- gas development strategies
- pipe installation strategies

Assumption

- The field is divided into **different sections**.
- Each section has **5 candidate wells**.
- There are **2 formations** across this field.
- Limited resources**: number of rigs, pipeline capacity and budget.
- Uncertain** production factor.



MAIN FINDINGS

Multistage Stochastic Programming Model and Custom Solution Algorithm

Objective

Maximize Project's
Net Present Value

Key Decisions

When and which
wells to be developed

Key Constraints

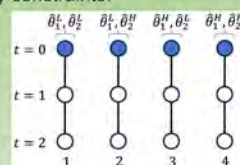
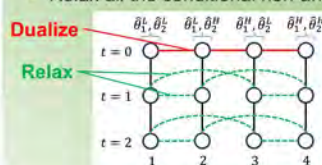
- Well development constraint
- Rig allocation constraint
- Pipeline capacity constraint
- Cash flow constraint
- Initial/Conditional non-anticipativity

Uncertainty

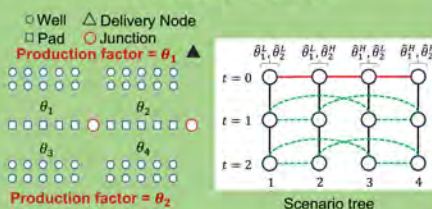
- Type 2 endogenous uncertainty**: production profile revealed when a well is drilled.
- Independent** uncertain production factor for each section (θ_1 and θ_2).
- Two realizations** (high and low) for each uncertain parameter \rightarrow 4 scenarios.

Lagrangian Decomposition (LD)

- Dualize all the initial non-anticipativity constraints.
- Relax all the conditional non-anticipativity constraints.



Illustrative Example



QR Code for Reference Paper



OUTCOMES

Assume the expected production profile follows
Section 2 = Section 3 > Section 4 > Section 1

Case study 1

All sections are at the **same level of uncertainty**.

Fixed variance	Budget [Cost per well]	# of wells developed in period t_i			
		Section 1	Section 2	Section 3	Section 4
0.25	Unlimited	1	1	1	1
	20	1	1	1	1
	15	1	1	1	1
	10	0	2	1	1
Fixed Budget Unlimited	Variance (Unit = 1)	Section 1	Section 2	Section 3	Section 4
	0.01	0	2	2	0
	0.04	0	2	1	1
	0.09	0	2	1	1
	0.16	1	1	1	1

Case study 2

Sections are at **different level of uncertainty**.

Fixed Budget Unlimited	Sections 1,4 Variance	Sections 2,3 Variance	# of wells developed in period t_i			
			Section 1	Section 2	Section 3	Section 4
0.01	0.01	0.04	0	3	1	0
	0.01	0.25	0	2	1	1
	0.01	0.49	1	1	1	1

- Reduce the **risk** of developing low production wells by planning the **proper development sequence** of candidate wells.

IP & INNOVATION

- Propose a **multistage stochastic model** to address the shale gas field development under production profile uncertainty.
- Apply the **Lagrangian decomposition** method to solve this problem.
- Provide **development insights** through case studies with different setting of uncertainties.

SYSTEM DESIGN & BENCHMARKS

20 wells & 10 pads example. (16 scenarios)

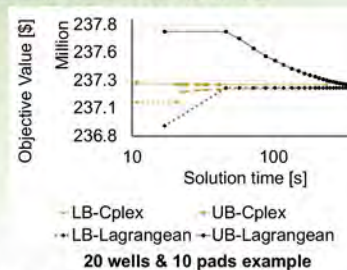
- LD finds the same optimal solution **7 times faster** than CPLEX.

Model	# of binary variables	# of continuous variables	# of constraints
Stochastic model	25,152	35,713	135,617
Scenario problem	1,440	2,233	2,759

30 wells & 20 pads example (64 scenarios)

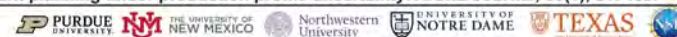
- This example **cannot be directly solved by CPLEX** within 10 hours.
- LD can provide a solution within 1% gap in **10 iterations**.

Model	# of binary variables	# of continuous variables	# of constraints
Stochastic model	197,760	269,569	1,438,273
Scenario problem	2,880	4,213	5,119



Reference: Peng, Z., Li, C., Grossmann, I. E., Kwon, K., Ko, S., Shin, J., & Feng, Y. (2022). Shale gas field development planning under production profile uncertainty. *AIChE Journal*, 68(1), e17439.

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T7P3 - POSTER #9



T7P3
Poster #: 9



Distributed manufacturing for electrified chemical processes in a microgrid

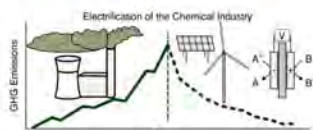
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Background

- Chemical industries: **major source of greenhouse gas emissions.**
- Solution : **Electrification of the chemical industry.**

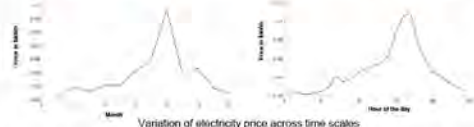


Electrification of the chemical industry

- Electrification helps **decarbonize** the chemical industry and move from fossil fuels to more **renewable energy sources.**

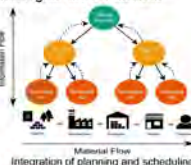


Variation of renewable resources in their output across different locations and time scales



Variation of electricity price across time scales

- To deal with the spatial and temporal variations due to renewable resources and prices, electrification requires incorporating energy management into decision-making at all levels ranging from **supply chain planning** to **scheduling**.
- To make the best use of resources, we need optimization models which include both lower and higher-level decisions.



Integration of planning and scheduling



Microgrid



Distributed chemical manufacturing (DCHEM)

Objective

The objective of this research is to **design a network to facilitate DCHEM for electrified chemical processes** with the power demand satisfied by renewable sources as well as power from an external source coordinated by a microgrid by using an MILP (Mixed Integer Linear Programming) model

Optimization Model

- Objective: **Maximize profit (annual)**



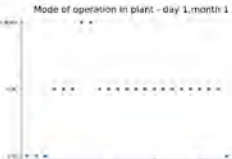
Representation of region



Investment decisions



Monthly decisions

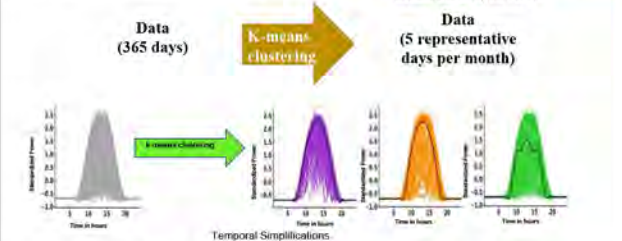


Mode of operation in plant - day 1, month 1

Constraints on investment decisions
Constraints on monthly decisions
Constraints enforcing physical feasibility of hourly variables
Mode Transition, stoichiometric, power equation constraints



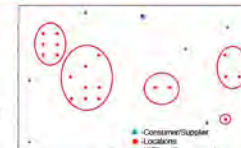
Decisions taken by the model



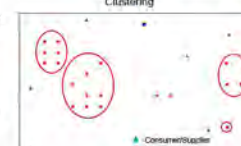
- Issue: Model has **millions of variables and constraints** for a moderate number of locations even after temporal simplifications. It is very difficult to solve the model without any algorithm

Algorithm

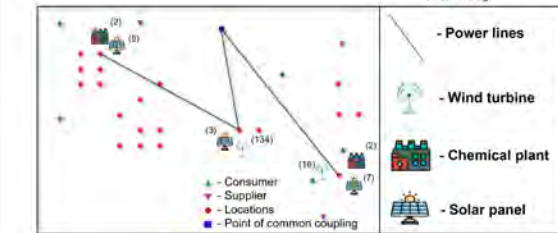
- Step 1: Cluster the locations based on coordinates
- Step 2: Solve the aggregated problem relaxing the operating variables
- Step 3: Disaggregate each cluster keeping the other clusters and their investment decisions fixed
- Step 4: Solve an IP to match transmission lines between clusters obtained from previous step
- Step 5: Fix the investment decisions unrelax the operating decisions and solve for them



Clustering



Disaggregation



Solution

Upper bound (\$)	19.50 M
Total Profit from proposed algorithm (\$)	18.94 M
Time for aggregation (h)	7.14
Time for disaggregation (h)	0.35
Time for solving operation decisions (h)	0.03
Solver	Gurobi 10.0
Hardware Type	AMD EPYC 7643 2.3GHz, 48C/96T, 1 TB

References

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