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The Role of Process Integration for Greenhouse Gas Mitigation in Industry
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Motivation: Recent Energy Source

Shale Gas Reserves in World

units = trillion cubic feet
Larger circles = technical reserves
Smaller circles = potential reserves
Few facts about Shale Gas in US

Price of Natural Gas   $12.69/MMBtu 6/2008 vs $1.97/MMBtu 4/2012
   Latest: $3.18/MMBtu 4/2017

Price Ethane   $1.38/gal 6/2008 $0.85/gal 11/2012 $0.189/gal 4/2017

Perspectives Article: Jeff Siirola

*The Impact of Shale Gas in the Chemical Industry*


CO₂ emissions  decreased by 12% in last decade, 3% in 2016

U.S. Energy self-sufficiency by 2020
Shale gas not without controversy:
- Water use and water contamination
- Chemicals used in fracking
- Methane emissions
- Disruptions in local communities
Shale Gas in US

Marcellus Shale Gas

Large amount “wet gas”

Horizontal drilling

Hydraulic fracking
In 2035 close to 50% from Shale Gas

Northeast: from 0.3 trillion scft 2009 to 5.8 trillion scft 2035

Goal: Develop Comprehensive Optimization Models for the Design of Supply Chain for Shale Gas Production and Water Management
Strategic Planning of Supply Chain for Shale Gas Production


- **Given:**

  Potential Sites for Well Pads (i)

  Multi-well pads

  Water sources

  Ethane

  Methane

Structure Supply chain?
Water Supply?

3 weeks 4-6 weeks 1-3 months 20-40 years
Site Preparation Drilling Completion Production

Water acquisition Fracturing

Potential Sites for Well Pads (i)

One Quarter

Water sources

Yang et al. (2013)
Junction pipelines and compressors?

Potential Sites for Junction Nodes (j)
Where to install gas processing plants?

• Given are:

Potential Sites for Gas Processing Plants (p)
General Problem Statement: To be Determined

Planning Decisions

- **Site construction:**
  Where and when to construct a well site?

- **Development schedule:**
  Where/when/how many wells to drill?

Design Decisions

- **Gathering network:**
  Where to lay out pipelines?

- **Compressor allocation:**
  Where to install compressors?

Objective is to use optimization models to identify cost-effective development strategies at a tactical level in a reasonable amount of time.
Well Production Profiles

Location Dependent Productivity

MMcf/day

Rapid Decline

months
Optimal Supply Chain Structure

MINLP: 2,343 binary variables, 14,252 constraints, 16,912 continuous variables
Total CPU time= 8.5 hours (<3% optimality gap)

- Processing Plant

Well Pads

236 MMcf/day

Separation Plant
Optimal Supply Chain Structure

- Pipeline Network and Compressors

NPV = $1664.48 million
Optimal Drilling Strategy

Number of Wells Drilled at Every Pad per Period

Water Scarcity

Total Number of Wells Drilled Per Period

- i9
- i8
- i7
- i6
- i5
- i4
- i3
- i2
- i1
Optimal Drilling Strategy

Number of Wells Drilled at Every Pad per Period

Phase 1: Intensive Drilling

Phase 2: Flow Maintenance

Total Number of Wells Drilled Per Period
Optimal Production Profile

- Methane Sales Flow

\[ \text{MMcf/day} = \text{Billon BTU/day} \]
Water management in hydraulic fracturing

1. fracfocus.org
2. Water’s Journey through the shale gas drilling and production processes in the mid Atlantic region.
Water usage in hydraulic fracturing

- 3-5 MM gallons water used to complete a well
  - Accounts for 0.1% of all freshwater withdrawal in the US
- 65-80% water used in fracturing for shale is consumed
  - Accounts for 0.3% of all water consumption in the US
- Water use per unit energy generated is low in comparison to other energy sources

1.3 gal/MMBtu for shale gas
Transportation is a significant factor in well completion cost

<table>
<thead>
<tr>
<th>Disadvantage</th>
<th>Advantage</th>
</tr>
</thead>
<tbody>
<tr>
<td>4,000 to 6,500 trucks required for a well pad (~90% associated with fracturing)</td>
<td>Flexible operation from well to well</td>
</tr>
<tr>
<td>Road damage (bonding)</td>
<td></td>
</tr>
<tr>
<td>Lack of infrastructure</td>
<td>Lower cost once in place</td>
</tr>
<tr>
<td>Permanent pipeline heavily regulated</td>
<td></td>
</tr>
</tbody>
</table>

SR 29 Continues to Deteriorate (Heavily used by other E&Ps)

Water's Journey through the shale gas drilling and production processes in the mid Atlantic region.
Problem 1: freshwater acquisition

Two types of freshwater sources

- **Uninterruptible** *(long distance; large river)*
  - Supplies freshwater year-round
  - Requires **trucking**

- **Interruptible** *(short distance; creek)*
  - Allows withdrawal if the river flowrate meets minimum requirement
  - Connects to wellpads through **pipelines**

**Objective:** determine the frac schedule that minimizes water transportation cost.
Problem 1: Optimal scheduling of fracturing wells and water acquisition

- **Two-stage stochastic programming model**
- **Given**
  - **Water sources**: historical river flowrate data (R years) (*scenarios*)
  - **Wellpads**: total # of stages
  - **Date restrictions**: drilling completion date, piping connection date, lease termination date
  - # of frac crews available

- **Determine**
  - **Stage 1 Decisions**
    - Wellpad fracturing start date
    - # of stages to frac per day (i.e. frac 2, 3, or 4 stages per day for each wellpad)
    - Starting date of fracturing holiday
  - **Stage 2 Decisions**
    - Volume pumped from interruptible water source

- **Objective**
  - Determine the **fracturing schedule that minimizes expected water transportation cost** (trucks and pipeline).
Discrete-time scheduling model  

STN model (Kondili, Pantelides, Sargent, 1993)

Uninterruptible source

Interruptible source 1

Interruptible source 2

Pad A

Pad J

Pad L

Frac pad s

Frac pad s’

Frac pad s”

Frac crew 1

Frac crew 2

\( V_{rt}^d \) Volume

\( y_{Pr}^d = 1 \)

If pump from the source to impoundment

\( y_{sc}^{dj} = 1 \)

If crew j starts to frac pad s on day d

Truck

Pipeline

\[ d \]

\[ d \rightarrow \text{Transfer} \rightarrow \text{Pad} \]

\[ d \rightarrow \text{Transfer} \rightarrow \text{Pad} \]
Example 1: results

14 well pads
540 time periods
2 impoundments
1 frac crew

SOLUTION

<table>
<thead>
<tr>
<th></th>
<th>Heuristic schedule</th>
<th>MILP schedule⁺</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frac holiday (days)</td>
<td>90</td>
<td>171</td>
</tr>
<tr>
<td>Trucking cost</td>
<td>$5,886,743</td>
<td>$568,827</td>
</tr>
<tr>
<td>Pumping cost</td>
<td>$9,905,219</td>
<td>$12,792,088</td>
</tr>
<tr>
<td>Tot expected cost ($)</td>
<td>$15,791,963</td>
<td>$13,360,915</td>
</tr>
</tbody>
</table>

Trucking cost is reduced by an order of magnitude.

- 14,010 $\rightarrow$ 1,350 truck trips.
- CO₂ emissions from trucking reduced from 630 $\rightarrow$ 60 metric tons

Computational Results

<table>
<thead>
<tr>
<th># of binary var</th>
<th>36,745</th>
</tr>
</thead>
<tbody>
<tr>
<td># of continuous var</td>
<td>150,277</td>
</tr>
<tr>
<td># of constraints</td>
<td>41,610</td>
</tr>
<tr>
<td>CPU time (s)</td>
<td>1722</td>
</tr>
<tr>
<td>Gap (%)</td>
<td>4.2</td>
</tr>
</tbody>
</table>

Problem solved with GAMS 24.0/cplex 12.5 on an Intel 2.93 GHz Core i7 CPU with 4GB memory.
Average daily impoundment storage comparison

Heuristic schedule

MILP schedule
Impaired Water Management: Reuse & Recycle

Drouven, Grossmann (2017)

Limited treatment and use of advanced friction reducer

Savings freshwater: 328,000,000 liters
Planning of electric power Infrastructures

Motivation

Electricity mix gradually shifts to lower-carbon options

World net electricity generation by fuel, 2012-40 (trillion kWh)*

World net electricity generation from renewable power by fuel, 2012-40 (trillion kWh)*

High variability in the renewables capacity factor

- Increasing contribution of intermittent renewable power generation in the grid makes it important to include operational details at the hourly (or sub-hourly) level in long term planning models to capture their variability.
Problem Statement

Given a region with:

A set of **existing** and **potential generators** with the respective

- generation technology *

  if existing:
  - nuclear: steam turbine
  - coal: steam turbine
  - natural gas:
    - steam turbine,
    - gas-fired combustion turbine,
    - and combined cycle
  - solar: photo-voltaic
  - wind turbines

  if potential:
  - nuclear: steam turbine
  - coal: IGCC w/ or w/o carbon capture
  - natural gas:
    - gas-fired combustion turbine,
    - combined cycle w/ or w/o carbon capture
  - solar:
    - photo-voltaic
    - concentrated solar panel
  - wind turbines

- location, if applicable
- nameplate capacity
- age and expected lifetime
- CO₂ emission
- operating costs
- investment cost, if applicable
- operating data
  - if thermal: ramping rates, operating limits, spinning and quick-start maximum reserve
  - If renewable: capacity factor

* Assume no hydropower
Problem Statement

Given:
- Projected load demand over the time-horizon at each location
- Distance between locations
- Transmission loss per mile

Find:
- When, where, which type and in how many generators to invest
- When to retire the generators
- Whether or not to extend their lifetime
- Power flow between locations
- Detailed operating schedule

in order to minimize the overall operating, investment, and environmental costs
Modeling Strategies
To tackle the multi-scale aspect and reduce the size of the model

- **Time scale approach:**
  - 1 representative cycle per season (e.g., a day or a week) with hourly level information

- **Region and cluster representation**
  - Area represented by a few zones
  - Potential locations are the midpoint in each zone
  - Clustering of generators*

- **Transmission representation**
  - Flow in each line is determined by the energy balance between each region $r$.
  - This approximation ignores *Kirchhoff’s Circuit Law*

*Palmintier, B.S., Webster, M.D., Heterogeneous unit clustering for efficient operational flexibility modeling, 2014*
MILP Model

Summary of constraints:

• **Energy balance:** ensures that the sum of instantaneous power generated at region \( r \) plus the net power flow being sent to this region equal the load demand plus a slack for curtailment.

• **Capacity factor:** limits the generation of renewable generators to be equal to a given fraction of the capacity in each hour.

• **Unit commitment constraints:** compute the startup and shutdown, operating limits and ramping rates for thermal generators.

• **Operating reserve constraints:** determine the maximum contribution per thermal generator for spinning and quick-start reserves, and the minimum total operating reserves.

• **Investment constraints:** ensure that the planning reserve and renewable energy contribution requirements are satisfied, and limit the yearly installation per generation type.

• **Constraints of number of generators:** define the number of generators that are operational, built, retired, and have their life extended at each time period \( t \).

<table>
<thead>
<tr>
<th>Continuous variables:</th>
<th>Integer variables:</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Power output at sub-period ( s )</td>
<td>• no. of generators installed at period ( t )</td>
</tr>
<tr>
<td>• Curtailment generation slack at ( s )</td>
<td>• no. of generators built at ( t )</td>
</tr>
<tr>
<td>• Power flow between regions at ( s )</td>
<td>• no. of generators retired at ( t )</td>
</tr>
<tr>
<td>• Deficit from renewable quota at ( t )</td>
<td>• no. of generators with life extended at ( t )</td>
</tr>
<tr>
<td>• Spinning reserve at ( s )</td>
<td>• no. of generators ON at sub-period ( s )</td>
</tr>
<tr>
<td>• Quick-start reserve at ( s )</td>
<td>• no. of generators starting up at ( s )</td>
</tr>
<tr>
<td></td>
<td>• no. of generators shutting down at ( s )</td>
</tr>
</tbody>
</table>
MILP Model

Objective function:

Minimization of the net present cost over the planning horizon comprising:

- Variable operating cost
- Fixed operating cost
- Startup costs
- Cost of investments in new generators
- Cost to extend the life of generators that achieved their expected lifetime
- Fuel consumption
- Carbon tax for CO₂ emission
- Penalty for not meeting the minimum renewable annual energy production requirement

Even with the approximations adopted, this is still a very large MILP model. In order to allow longer representative cycles per season, we propose a decomposition algorithm based on Nested Benders Decomposition*.

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* Birge, J.R., Decomposition and Partitioning Methods for Multistage Stochastic Linear Programs, 1985
* Pereira, M.V.F., Pinto, L.M.V.G, Multi-stage stochastic optimization applied to energy planning, 1991
* Sun & Ahmed, Nested Decomposition of Multistage Stochastic Integer Programs with Binary State Variables, 2016
Case Study: ERCOT (Texas)

- **30 year** time horizon (1st year is 2015)
- Data from **ERCOT database**
- Cost information from NREL (Annual Technology Baseline (ATB) Spreadsheet 2016)
- All costs in **2015 USD**
- Regions:
  - Northeast (midpoint: Dallas)
  - West (midpoint: Glasscock County)
  - Coastal (midpoint: Houston)
  - South (midpoint: San Antonio)
  - Panhandle (midpoint: Amarillo)
- Fuel price data from EIA Annual Energy Outlook 2016 - Reference case
- No imposed carbon tax
- No renewable generation quota requirement
- Maximum transmission line capacity
Results

• 1 representative week per season

Total cost: $198.0 billions

Full-space MILP Model
Integer variables: 2,901,964
Continuous variables: 4,136,547
Equations: 8,476,641
Solver: CPLEX
optcr: 1%
CPU Time: Out of memory!
Decomposition: 7 hrs

61-fold increase in PV-solar capacity
31% increase in natural gas combined-cycle capacity
6% decrease in wind capacity
30% decrease in natural gas steam turbine
06-421

Design Project

Design of Aromatics Plant from Shale Gas

Ignacio Grossmann
Jeffrey Siirola
Marcellus deposit might contain more than 400 trillion cubic feet of natural gas!!

241 trillion cubic feet recoverable gas ⇒ 10 years of total US consumption natural gas

Mostly wet gas 10-15% condensates ⇒ ethane cracker in Pittsburgh by Shell!
Design Project:

Preliminary design and cost estimation of Aromatics Plant from Shale Gas

Plant to produce aromatics 500 Mlbs/yr*

Aromatics: Benzene, Toluene, Xylenes (ortho, para, meta)

Plant location: Monaca (next to Shell’s projected cracker)

Feedstocks: methane (1 atm, 60F; 95% methane, 2.5% ethane)?
Price methane: $3.50/MBtu

Price Benzene: $1,400/tonne
Price Toluene: $1,300/tonne
Price Xylenes: $1,200/tonne (higher price if separated into o, m, p)

* M=mega/million
Which chemical route: methane, ethane or ethylene feedstocks?

There are 7 chemical routes (5 from methane): 3 examples

Methane: Steam reforming → Water gas shift → Methanol → Methanol to Aromatics
Methane: Methane to Aromatics
Ethane: Ethane to Aromatics (last year)
Synthesis of Process Flowsheet

Example: Methane to Aromatics

Methane

? 

Hydrogen
Methane
Ethylene
Benzene
Toluene
Xylenes

Aromatics

What units for reaction, separations and heat integration?

Membrane/reactor (Iglesia et al./Berkeley)?

Issue: Life catalyst
Shale Methane Gas to Aromatics
via Methanol to Aromatics

Group 14
Jochen Cremer, Lorenz Fleitmann, James Phua, Xiaobin Wei
Heat Integration – Results and Savings

Savings: 70%

Before H.I.:
- Cooling Duty: 684 MW
- Heating Duty: 415 MW

After H.I.:
- Cooling Duty: 301 MW
- Heating Duty: 32 MW
Economic Evaluation
Process is profitable

- Total Revenue = $447 million
- Net Present Value = $469 million
- Payout time = 2.3 years
- Return on Investment = 24%
Design Project

Propylene from Shale Gas Methane vs. Propane Dehydrogenation

Ignacio Grossmann
Jeffrey Siirola
Acknowledgments

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NETL

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EQT Corporation

Carrizo
Design Project:

Preliminary design and cost estimation of Propylene Plants from Shale Gas Methane and Propane Dehydrogenation

Plant to produce propylene 500,000 tonnes per year

*Plant location: U.S. Gulf Coast (built 2015)*

Purity spec propylene: 99.5% (mole %)

*Price Propylene: $1,330/tonne*

Feedstock 1: **propane** (liquid; 95% propane, 2.5% ethane, 2.5% butane)

*Price propane: $1.30/gal*

Feedstock 2: **methane** (1 atm, 60F; 87-96% methane, 1.8-5.1% ethane, 0.1-1.5% propane)

*Price methane: $3.50/Mbtu*

* M=mega/million
Conclusions

1. Proposed Multiperiod MINLP Model for Shale Gas Production
   a) Structure of supply chain: Plants Natural Gas, Pipelines and Compressors
   b) Operation supply chain: Drilling strategy, Supply of water

2. Branch-Refine-Optimize Algorithm: Large-scale Nonconvex MINLP

3. MINLP model: systematic optimization Shale Gas Production Systems

4. Proposed MILP Scheduling Models for Water management

5. MILP models can reduce transportation costs and freshwater consumption through recycle

Future Work

a) Expand scope and effective solution methods (Drouven, Grossmann, 2014)

b) Handling uncertainties in investment problem: stochastic programming
Example 2: Results reuse/recycle/treatment

<table>
<thead>
<tr>
<th>SOLUTION COMPARISON</th>
<th>Heuristic schedule</th>
<th>MILP schedule</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transportation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Freshwater pumping</td>
<td>9.91</td>
<td>10.79</td>
</tr>
<tr>
<td>Freshwater trucking</td>
<td>9.19</td>
<td>7.22</td>
</tr>
<tr>
<td>Wastewater</td>
<td>0.27</td>
<td>0.37</td>
</tr>
<tr>
<td>Treatment</td>
<td>0.64</td>
<td>0.70</td>
</tr>
<tr>
<td>Disposal</td>
<td>4.93</td>
<td>4.23</td>
</tr>
<tr>
<td>Storage</td>
<td>0.08</td>
<td>0.10</td>
</tr>
<tr>
<td>Total cost (MM$)</td>
<td>25.02</td>
<td>23.41</td>
</tr>
<tr>
<td>Revenue (MM$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gas production</td>
<td>205.29</td>
<td>237.56</td>
</tr>
<tr>
<td>Net Expected Profit (MM$)</td>
<td>180.27</td>
<td>214.15</td>
</tr>
</tbody>
</table>

- 4.19 MG of freshwater saved.
- 15.7% increase in revenue achieved.