SAND2011-4444C

I. Renewable Energy Challenges: the Role of Systems Analysis
II. System Analysis of Algae-based Biofuel Manufacturing
III. Design of Advanced Heat-transfer fluids for CSP

June 28, 2011

Amy Sun, PhD

Chemical & Biological Systems

Sandia National Laboratories

(505)284-5861 acsun@sandia.gov

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National Nuclear Security Administration

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Schedule

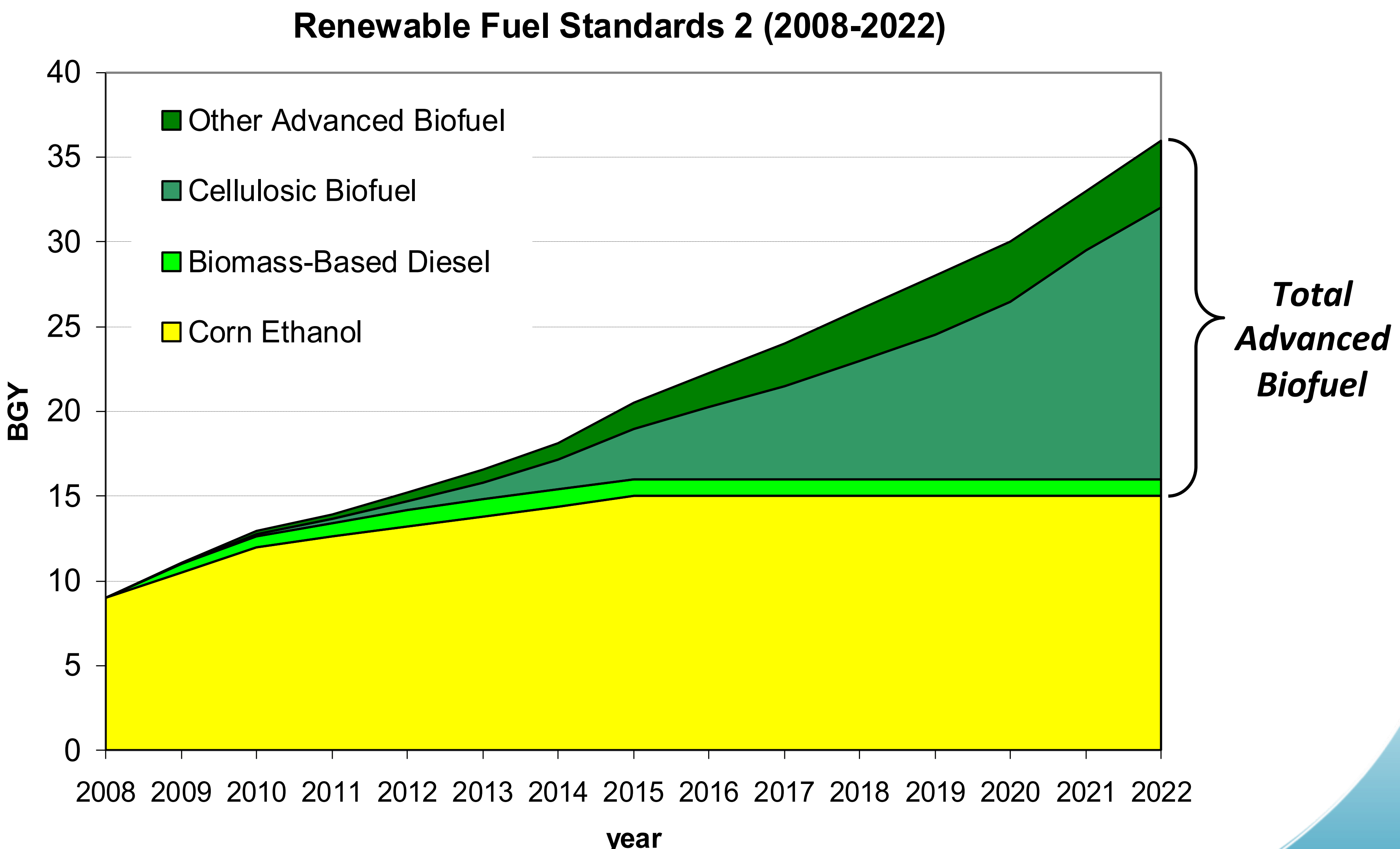
- Sandia Introduction (~15 min)
- Renewable Energy Challenges:
  the Role of Systems Analysis (~45)
- Exercise/Break (30 min)
- System Analysis of Algae-based Biofuel Manufacturing (~30 min)
- Break (10-15 min)
- Design of Advanced Heat-transfer fluids for CSP (~30 min)

Sandia Introduction

I. Renewable Energy Challenges: the Role of Systems Analysis

II. System Analysis of Algae-based Biofuel Manufacturing

III. Design of Advanced Heat-transfer fluids for CSP


Renewable Fuel Standards 2 (2008-2022)
40
35
30
25
20
15
10
5
0
BGY
Other Advanced Biofuel
Cellulosic Biofuel
Biomass-Based Diesel
Corn Ethanol
2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020 2021 2022
year
Total Advanced Biofuel

“Renewable Fuel” requires Lifecycle Greenhouse Gas (GHG) Reduction

Fuel Type	Lifecycle GHG Savings
Corn Ethanol (new plants)	20%
Advanced biofuel	50%
Biomass-based diesel	50%
Cellulosic biofuel	60%

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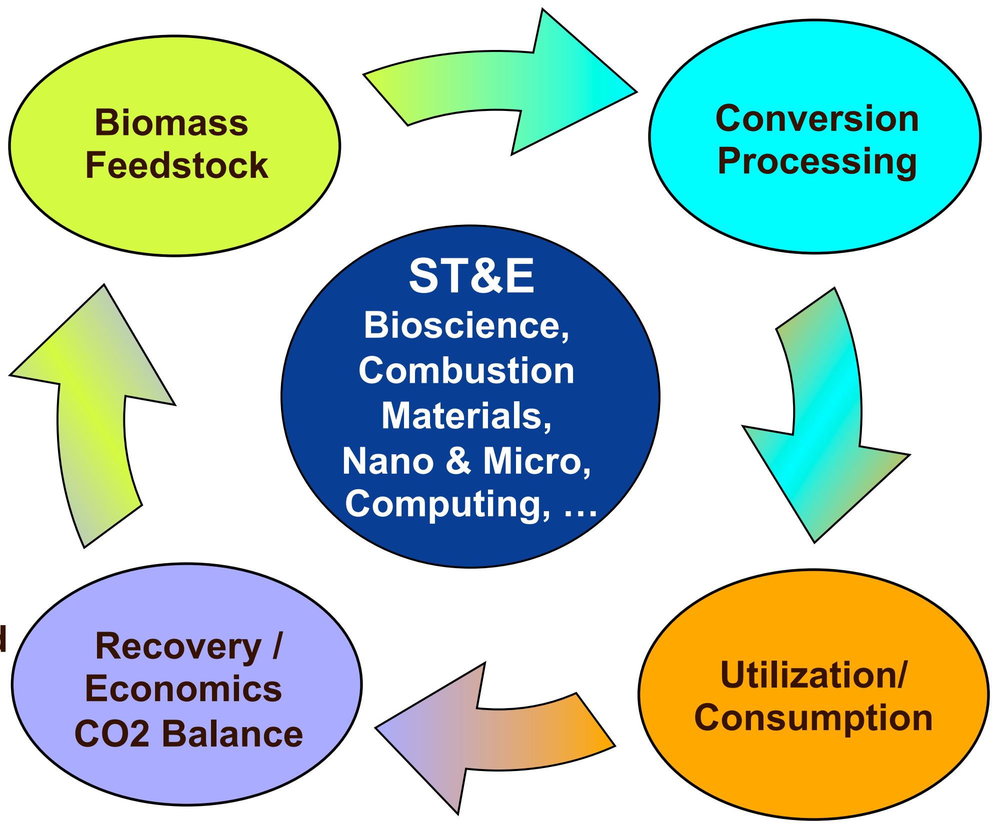
Sandia's Biofuels Strategy:
A Systems Approach

Challenges
- Biomass
  - Production
  - Optimization
  - Pretreatment
  - Scale-up
- Sustainability
  - Water usage

Increase Yield



Challenges
- Biomass processing
  - Catalysis
  - Thermochemical
  - Biochemical
  - Scale-up
  - Microbial communities

Challenges
- Carbon Implications
  e.g. Co-siting with Coal-fired generators
- Biomass production
  e.g. Transportation costs & Water availability

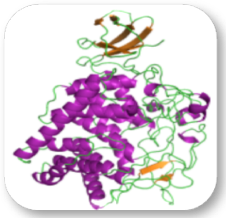
Challenges
- Engine design
- Fuel Distribution
- Fuel Storage
- Materials Compatibility
- US Infrastructure Implications (Systems)

Our program is focused on two primary sources of biomass: cellulose & algae

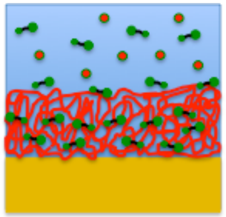
Lignocellulosic Biofuels: Current Projects

- DOE Joint BioEnergy Institute

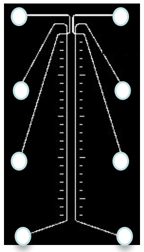
Ionic Liquid Pretreatment (Seema Singh, Brad Holmes)



Optimized Enymes (Ken Sale)



Enzyme-Substrate Interactions (Mike Kent)

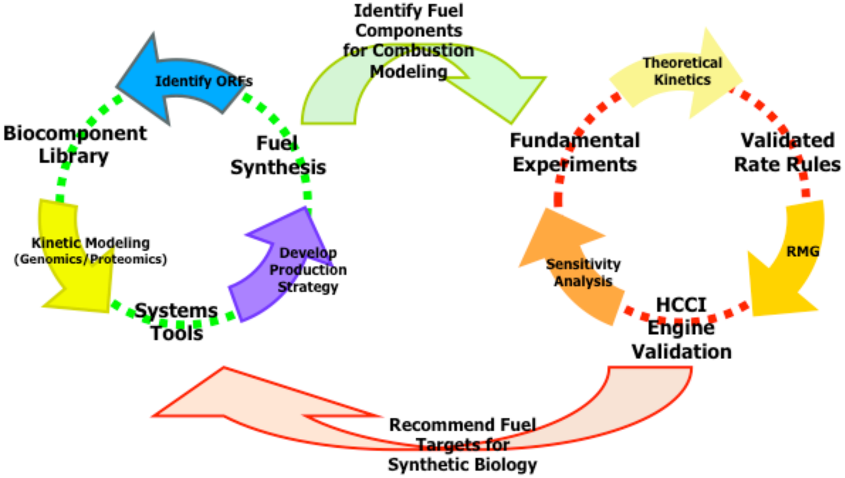


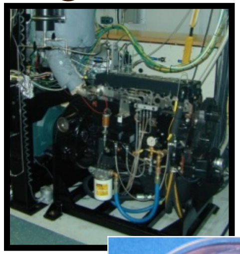
Microfluidic Assays (Anup Singh)

Robotics (Masood Hadi)

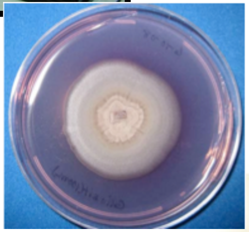
Parts Registry (Tim Ham)

- Tailoring next-generation biofuels and engines





HCCI Engine

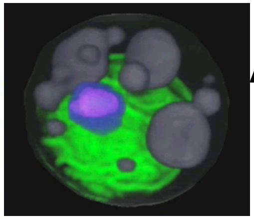


Endophytic Fungi

NextGen LDRD (PI: Craig Taatjes, Co-PI: Masood Hadi)

Algal Biofuels:
Current Projects

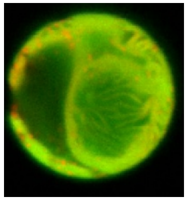
- Understanding and manipulating lipid production



Algae to oilgae (Seema Singh)

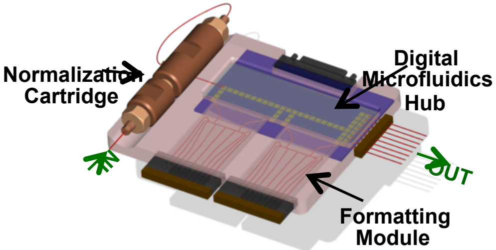
Benchtop to raceway (Jeri Timlin)

Engineering cyanobacteria (Anne Ruffing)



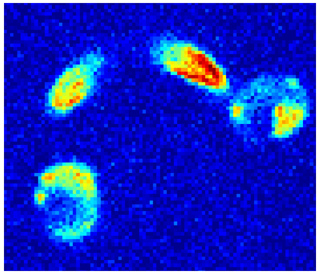
Constitutive Pathways (Patricia Gharagozloo)

- Pond stability

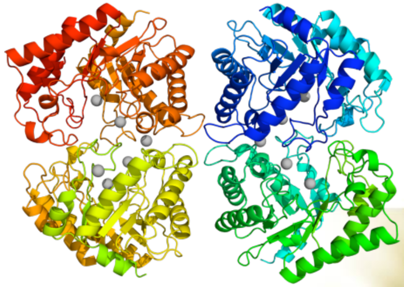


Pond crash forensics (Todd Lane)

- Conversion of algal remnants (DOE SABC)



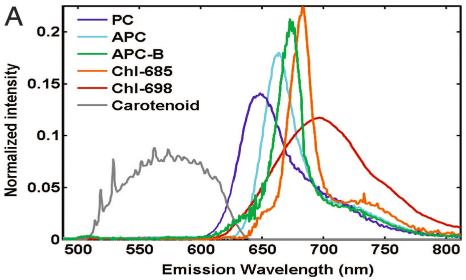
Algae characterization (Howland Jones)



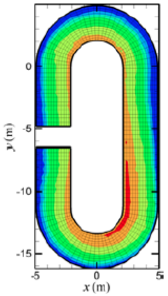
Algal remnant conversion (Masood Hadi, Amy Powell)

Algal Biofuels:
Current Projects

- Integrated biorefinery: Sapphire

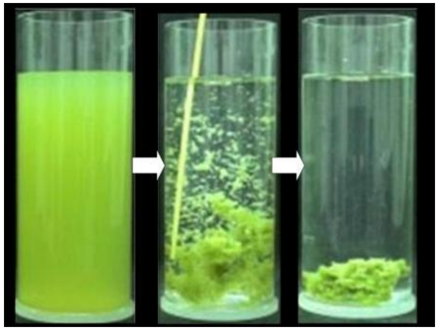


Algae characterization (Jeri TImlin)

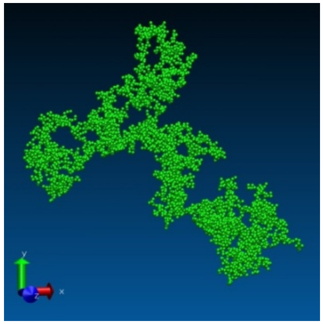


DFT modeling raceways (Scott James)

- Understanding flocculation (John Hewson)



Floc optimization



Floc simulations

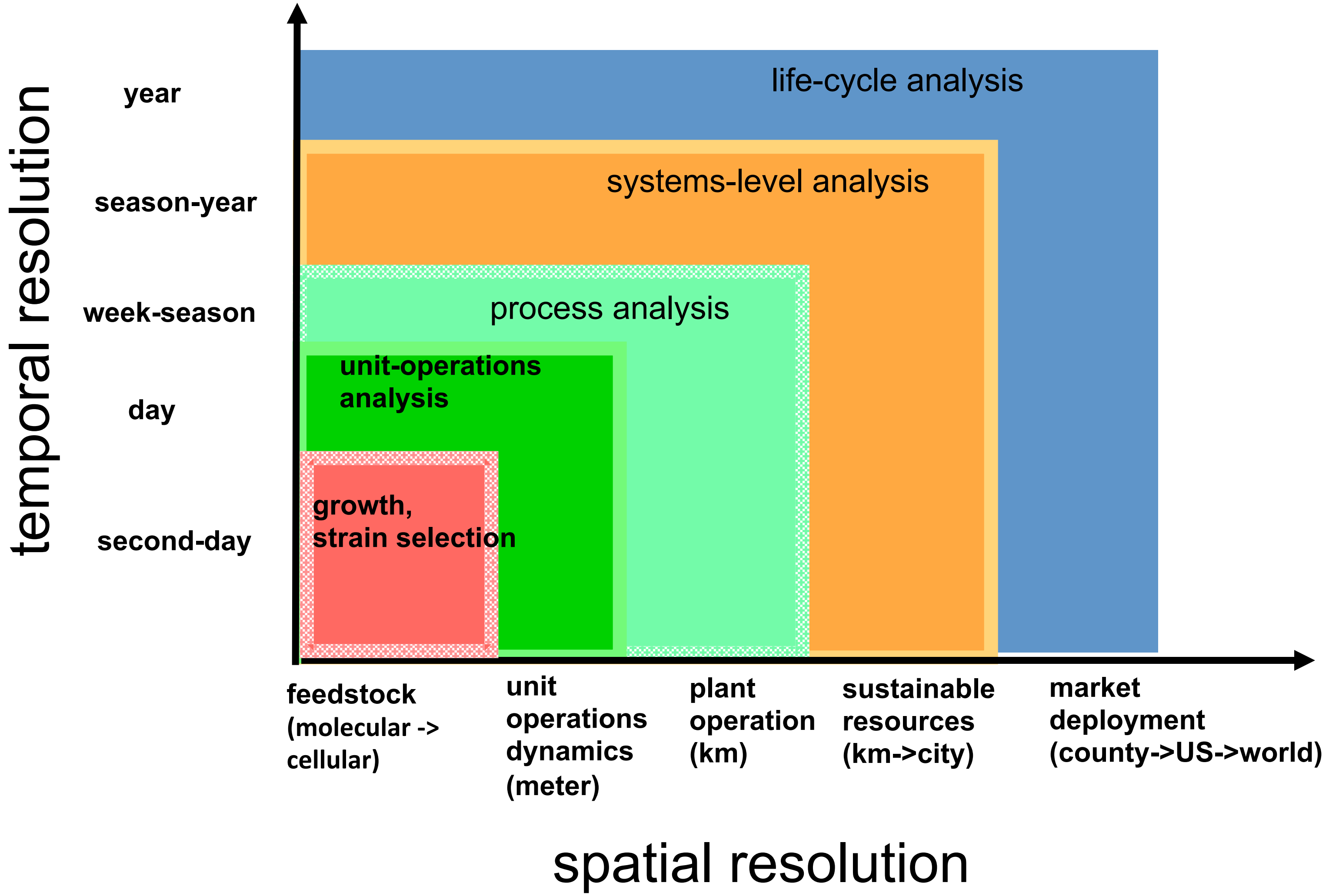
Biofuel Systems Analysis: Current Projects

Technoeconomics

- US-Canada resource assessment using system dynamics.
- US-Israel collaboration on Life Cycle Analysis.
- Tamarisk as a potential feedstock for biofuel/bioenergy.
- Impact of alternative fuel mix to transportation fleet.

Modeling Challenges for Biofuel Life Cycle

- *Each scale informs the global outlook for algae-based biofuel industry*
- *Data are disparate and sparse but required to reduce uncertainties.*



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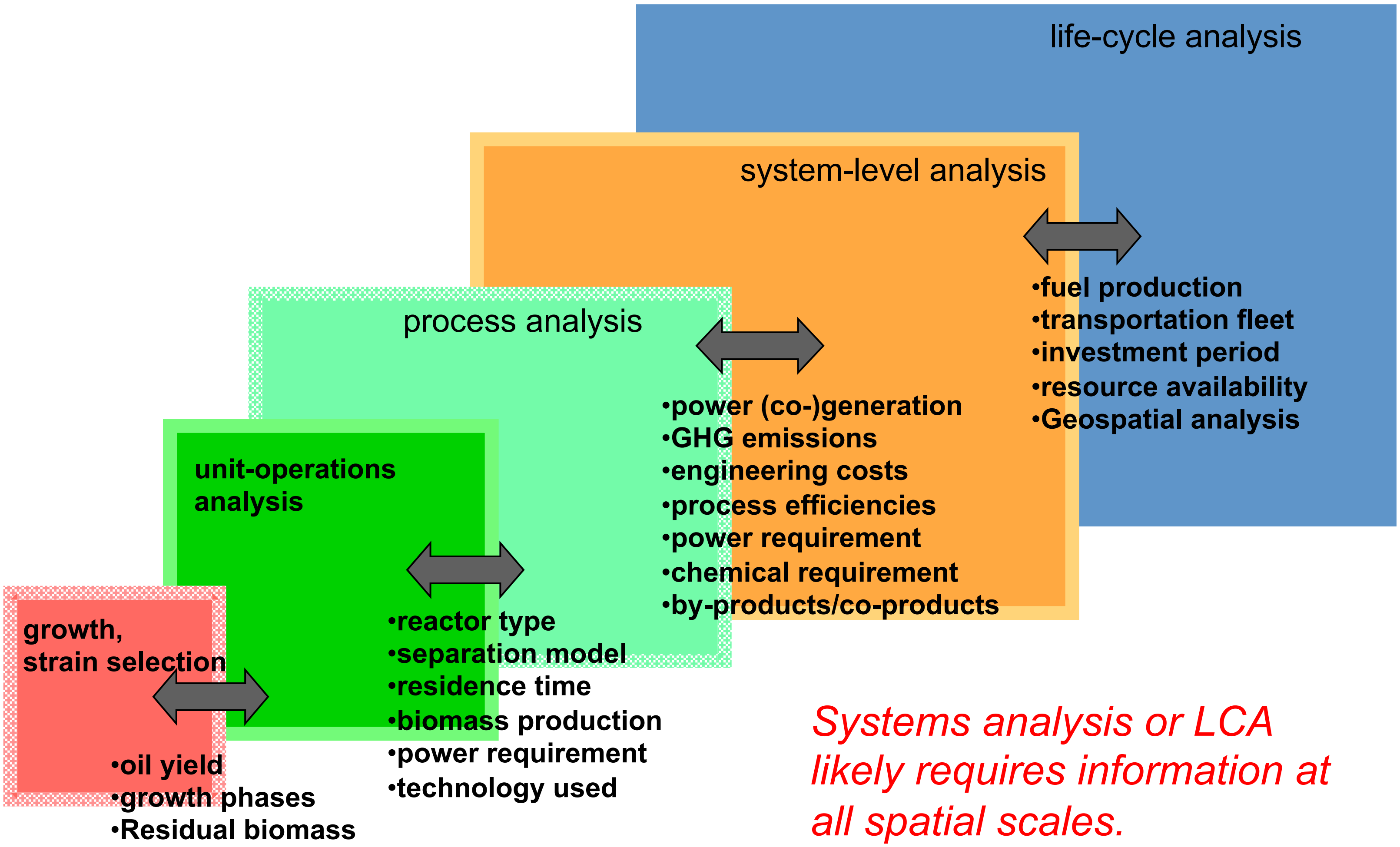
Details Shared by Some or All Levels

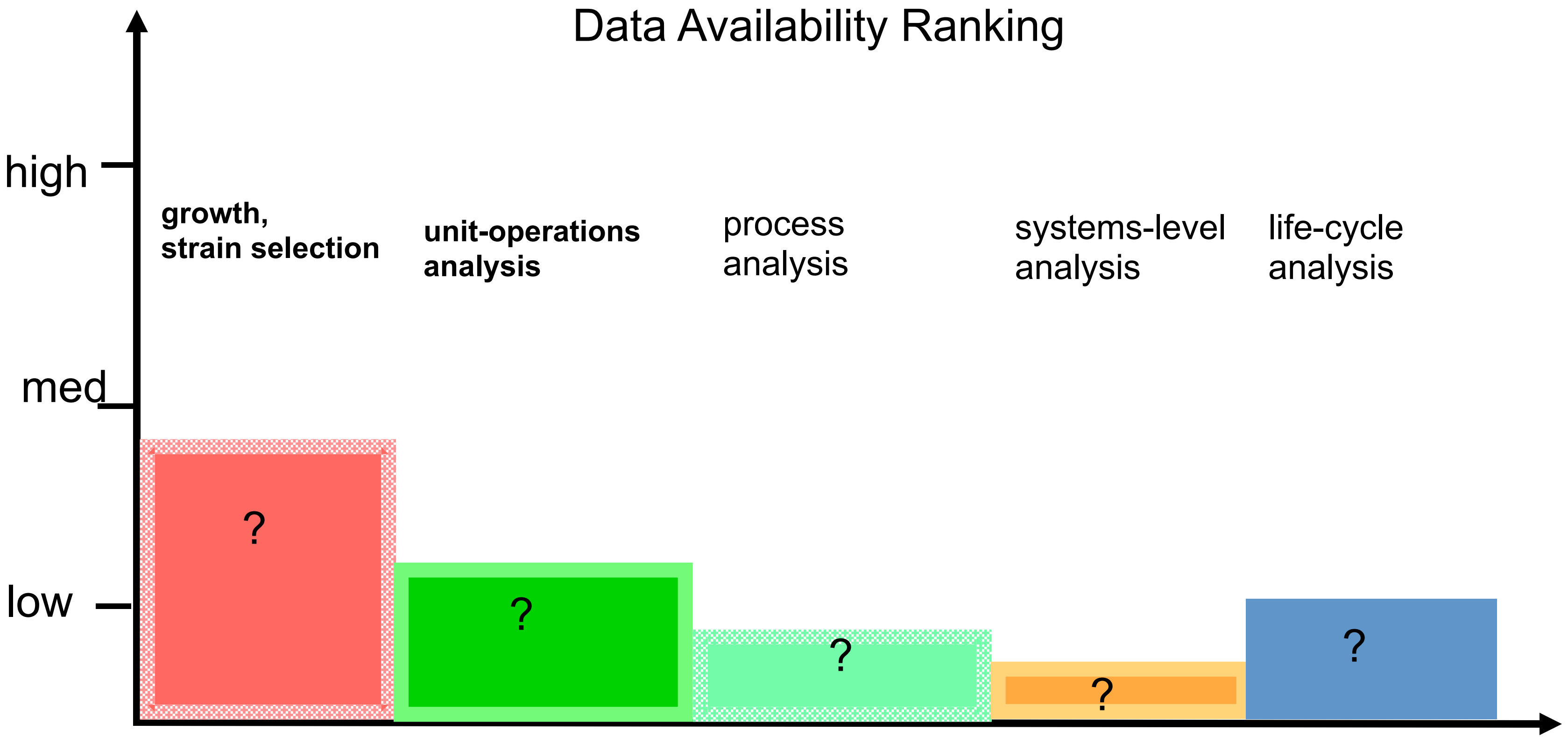
bridging knowledge from disparate sets of data



Systems analysis or LCA likely requires information at all spatial scales.

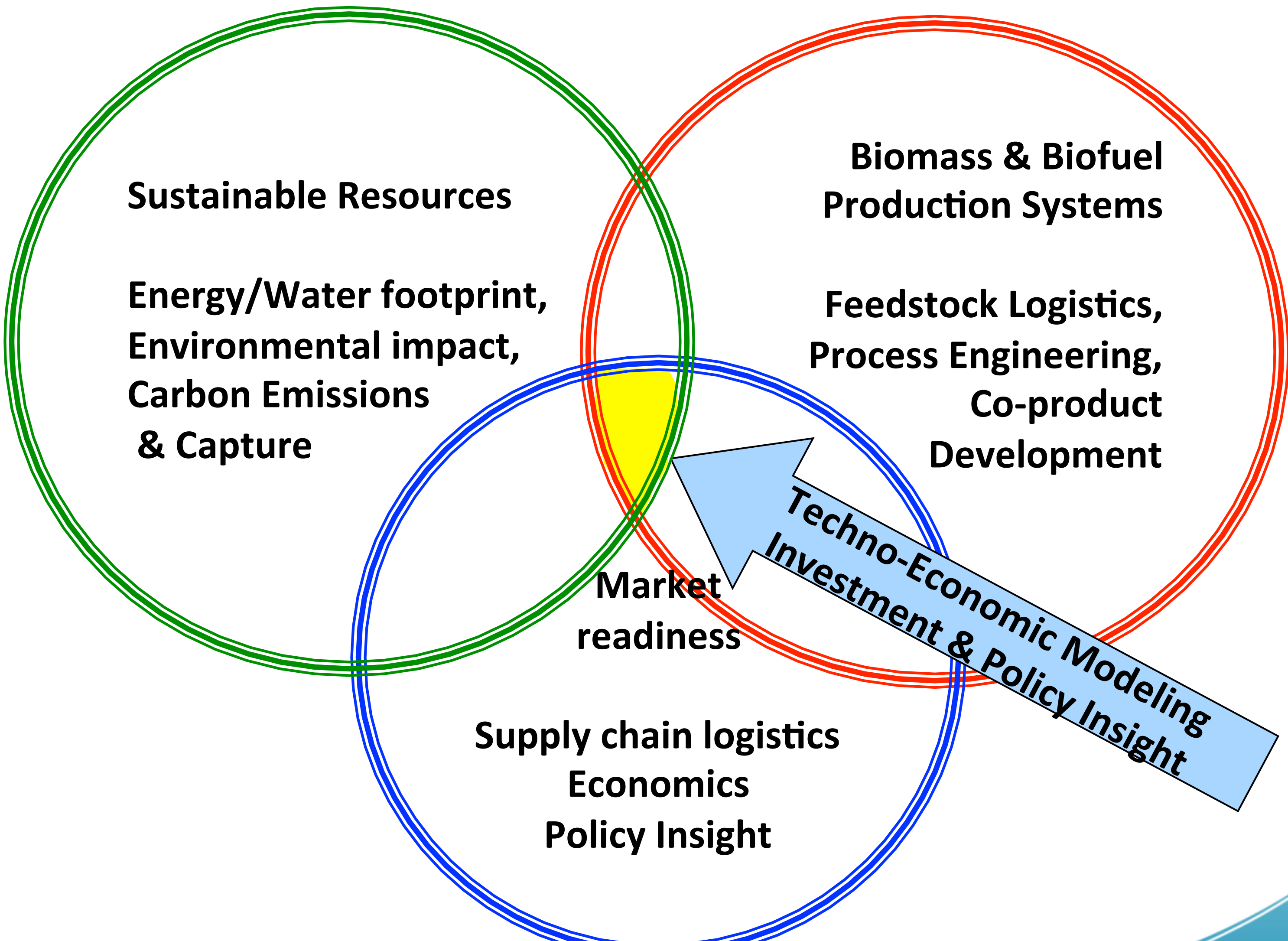
Data Gaps

A priori estimate is essential for soliciting collaborators



What is Techno-Economic Modeling?

Insight obtained by science and economics based simulations of manufacturing processes and/or supply chains



Example Questions addressed by Techno-Economic (TE) Modeling and Analysis

- *Resources*
  "What is the potential for crop/strain X to be a feedstock for bioenergy/biofuel?"
  "What are the necessary steps for biocrude to be refined and distributed?"
- *Environment*
  "Would the new agriculture/cultivation practice be more sustainable than existing practice?"
- *Footprint*
  Carbon/Water/GHG/Land
- *Economics*
  "What are the CAPEX/OPEX associated with this new integrated design?"
- *Policy*
  "What are the possible barriers to large-scale deployment?"
- *Technology*
  "Is technology A superior than technology B?"

Technoeconomic modeling may involve multiple tools/techniques

- ***System-Level Modeling***
  - Life Cycle Analysis
  - System dynamics
  - Integrated Analysis
- ***Engineering Modeling***
  - Back of the envelope
  - Computational Fluid dynamics
  - Mass & energy balance calculations
  - Process GHG footprint assessment
- ***Geographic Information System (GIS) Analysis and Visualization***
  - Land resources (characteristics, availability, etc.)
  - Water resources (fresh, wastewater, other)
  - Solar resource (insolation)
  - Climate/Weather/Temperature Conditions
  - Water evaporation loss
  - CO_2 resources (point source emitters, pipelines)
  - Fuel processing, transport, storage infrastructure
  - Other infrastructure and environmental features
- ***Static CAPEX & OPEX Calculations***
  - Engineering economics
  - Discounted cash flow analysis
  - Financing terms
  - Carbon and co-product credit

Where do we start?

Develop a set of questions to address a topic, a question, or an interest.

Propose a system and boundaries

Seek parameters

Develop causal relations

Develop Insight

List assumptions

Create the model, sub-model(s), spreadsheet, etc.

Conduct Analysis

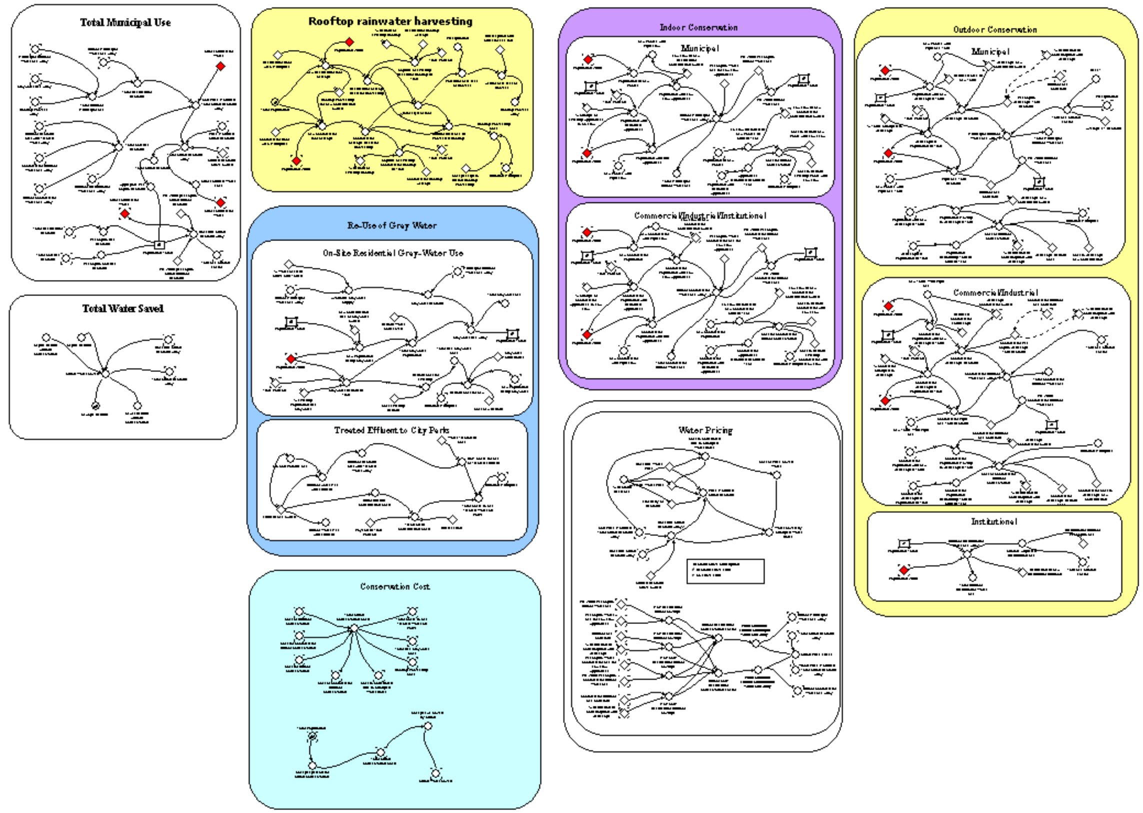
Assess sensitivities

System Dynamics as a methodology for developing causal relations towards an eventual systems model.

- **SD is a formal framework for managing multiple interacting subsystems, each of which vary in time**

- **Distinguishing features:**
  - ***feedback***
  - ***time delays***
  - ***coupling between subsystem components***

- **Tools:**
  - ***Vensim***
  - ***PowerSim***
  - ***Stella***

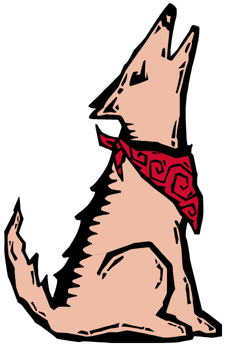


System Dynamics: Rabbits and Coyotes

“Stocks” , “capacitance”, “inventory”, etc.

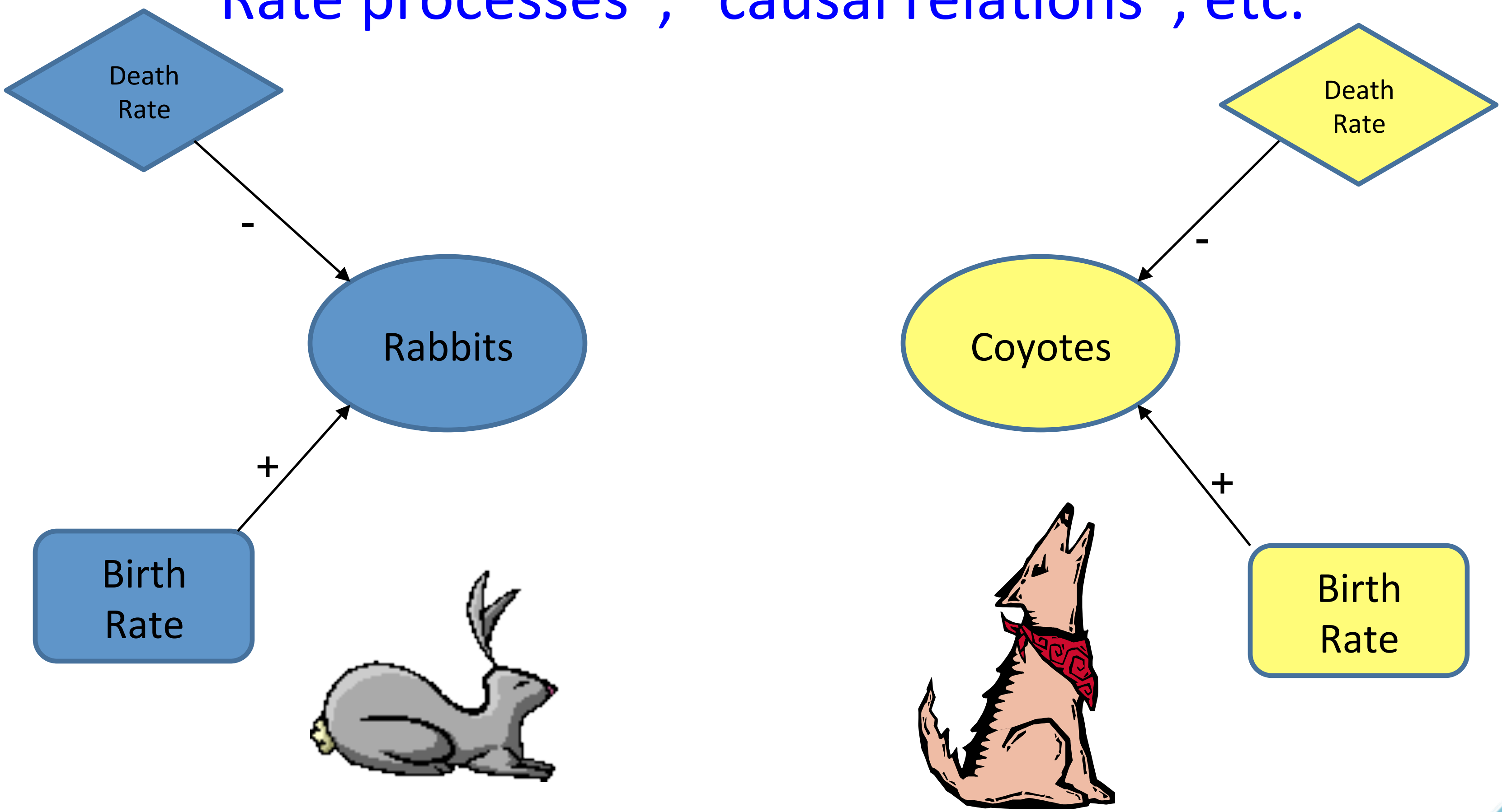
Rabbits

Coyotes



System Dynamics: Rabbits and Coyotes

"Rate processes", "causal relations", etc.



System Dynamics: Rabbits and Coyotes

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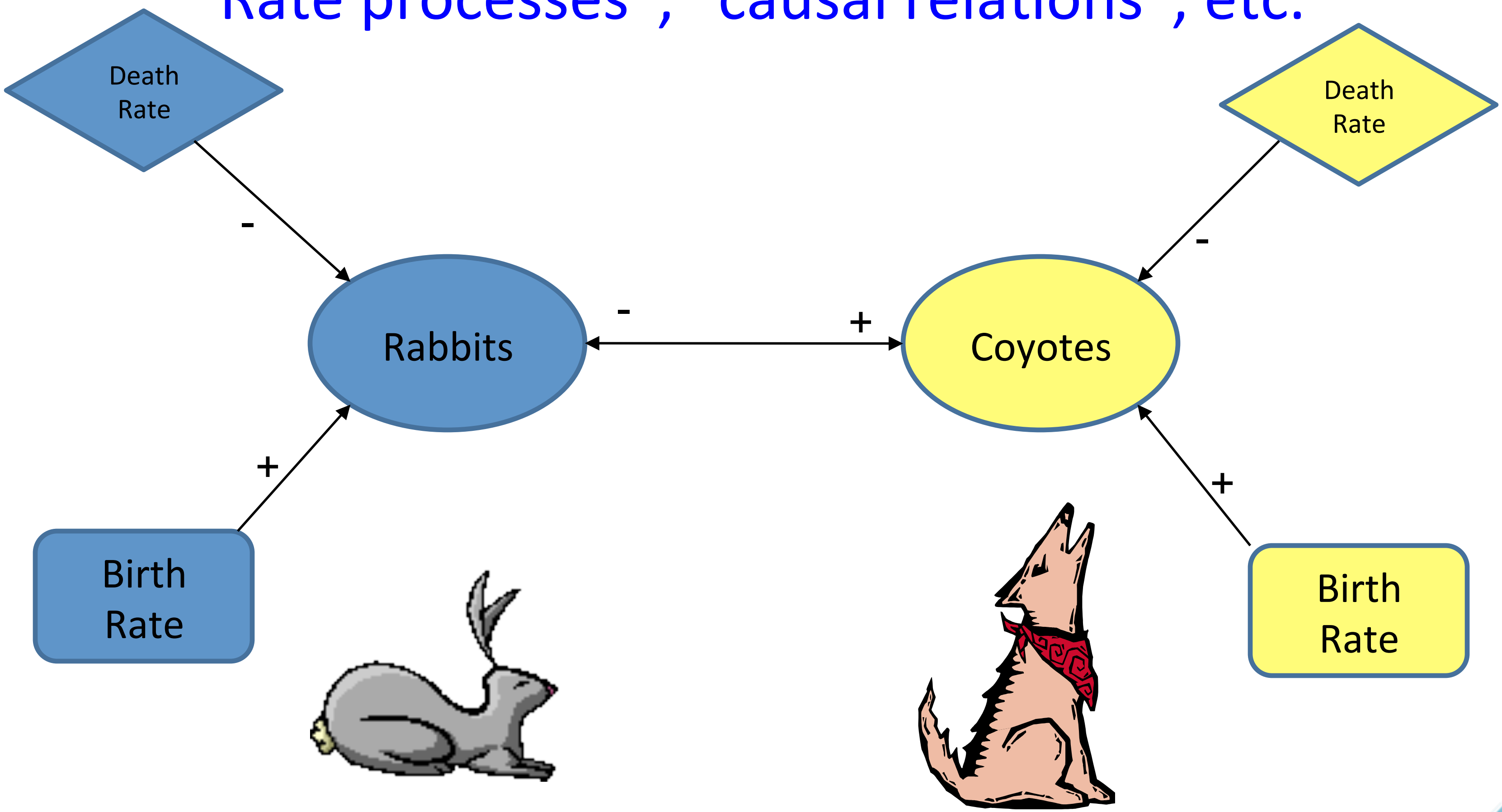
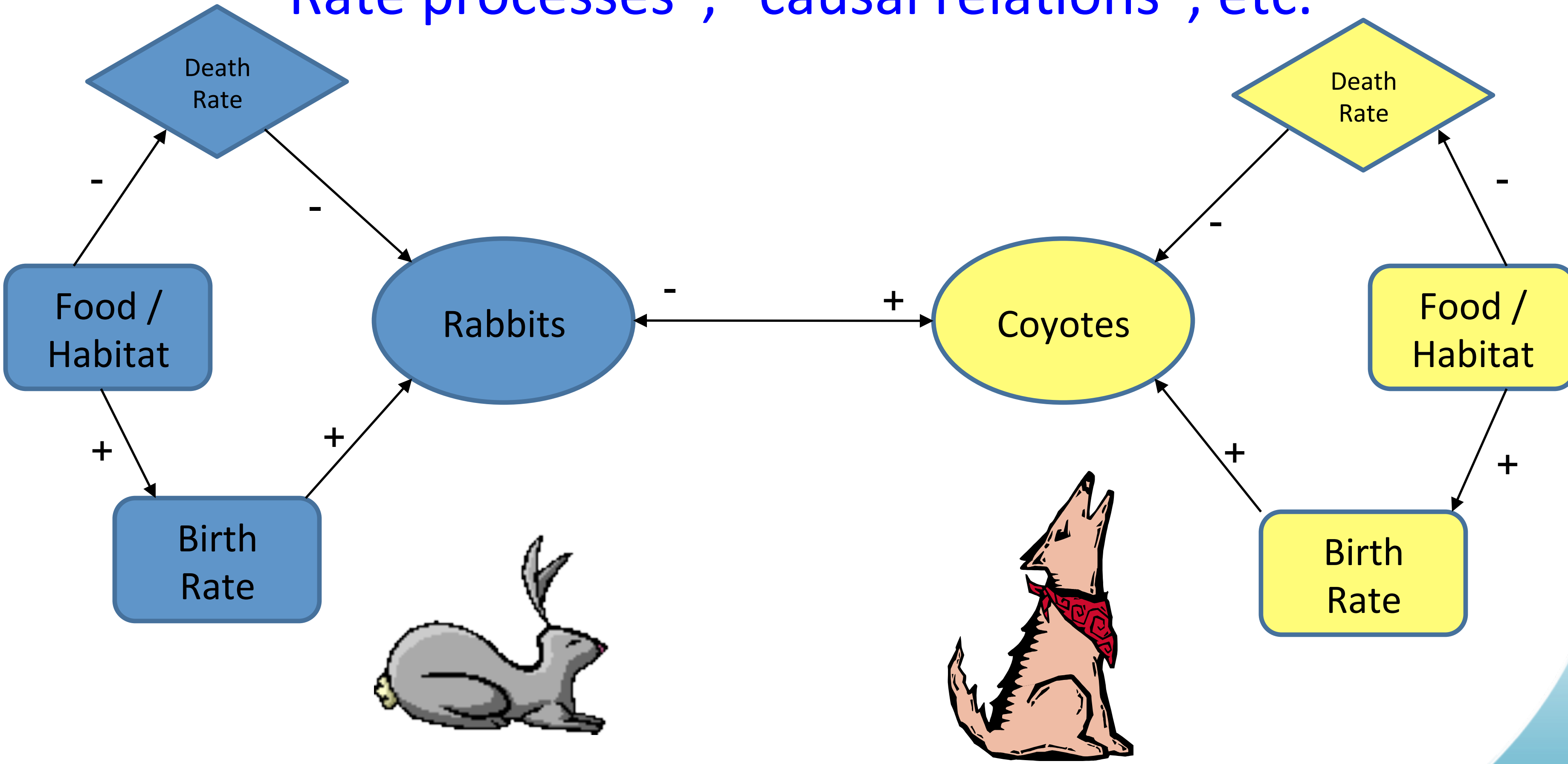


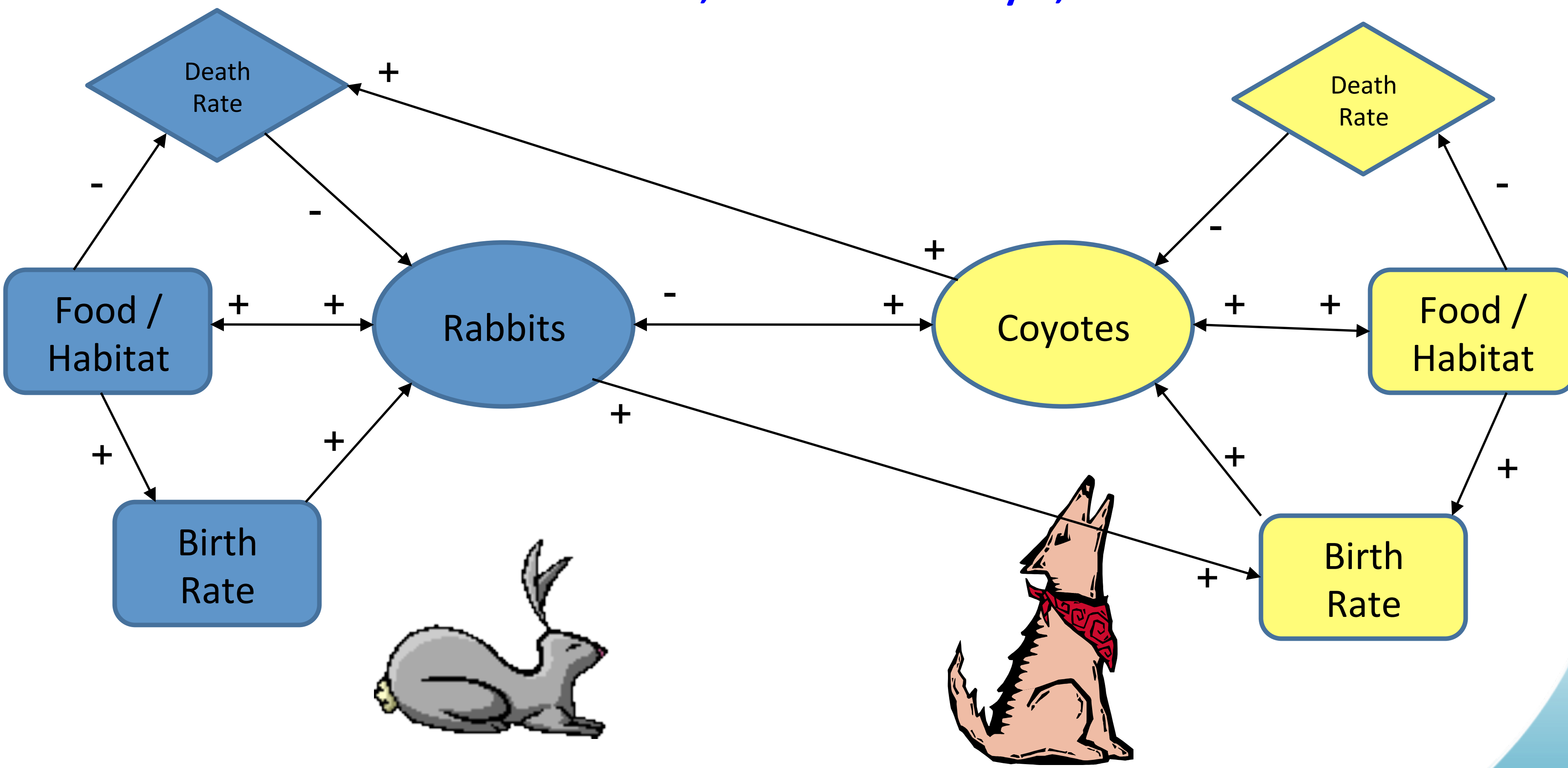
System Dynamics: Rabbits and Coyotes

“Rate processes”, “causal relations”, etc.



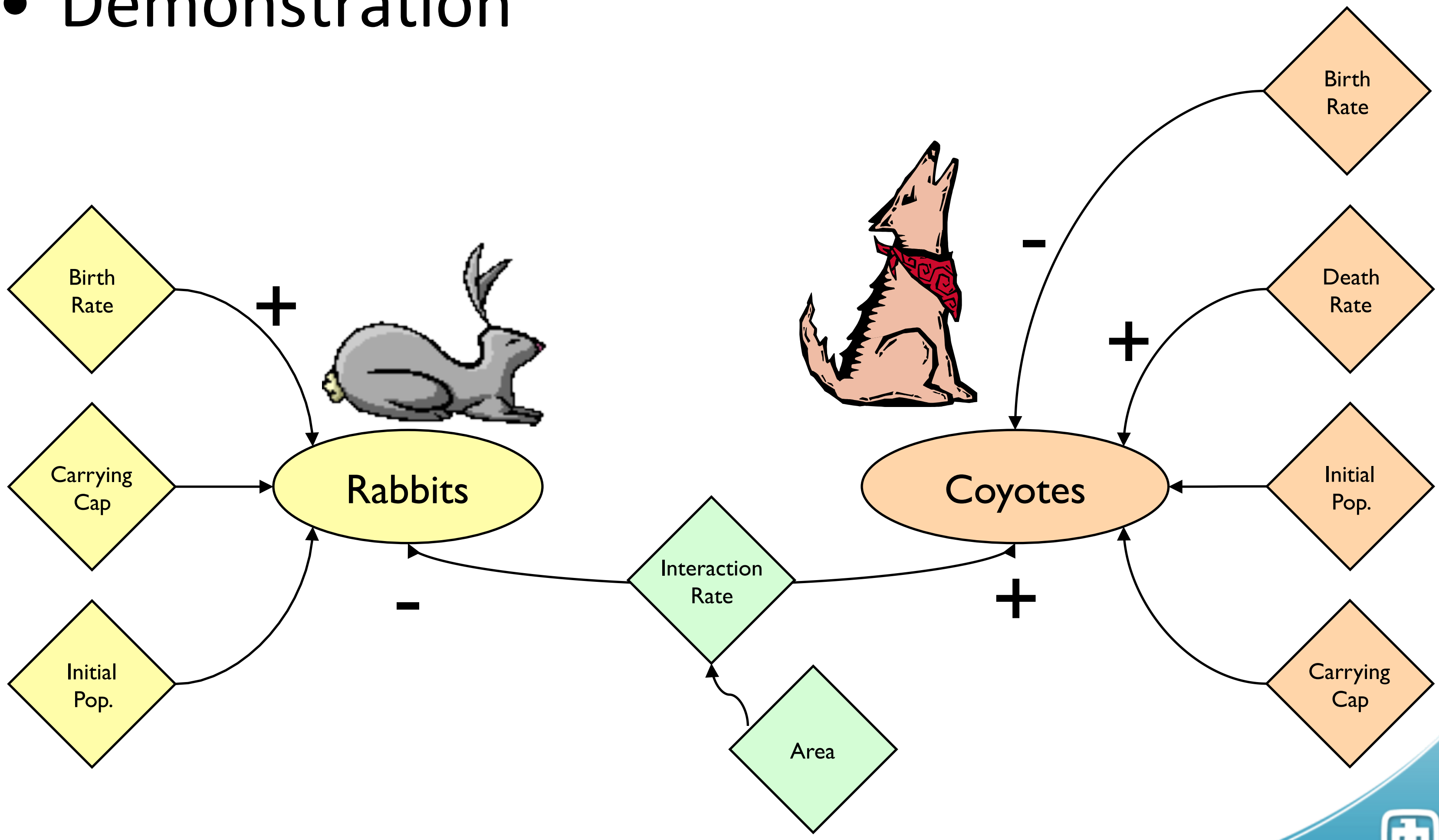
System Dynamics: Rabbits and Coyotes

“feedback”, “time delay”, etc.

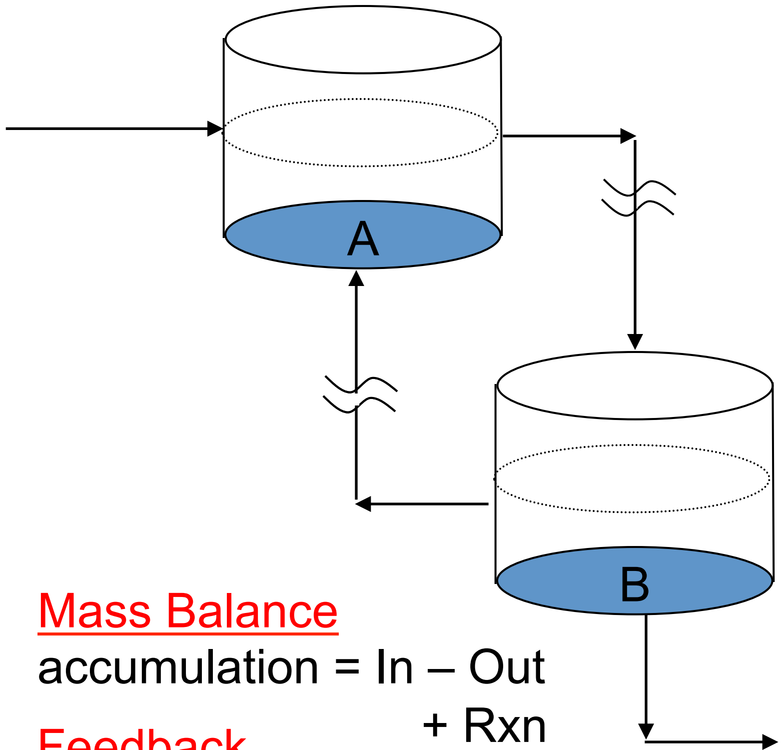


PowerSim Model: Rabbits and Coyotes

- Demonstration



System Dynamics is transient dynamics.



Mass Balance
accumulation = In – Out + Rxn

Feedback
accum.= In–Out+Rxn+Recycle

Delay $In_B = Out_A(t+\Delta t)$
$Recycle_A = Recycle_B\ (t+Dt)$

	Chemical Engineering	System Analysis (Energy)
Transient Dynamics	**Continuity, Mass Balance, Thermodynamics, Fluid Mechanics, Feedback**	**Continuity, Feedback, Delay**
Disturbance, Forcing functions, Exogenous variables	**Rxn Kinetics, Start-up/Shut-down, Raw Material**	**Climate change, conflict, growth, infrastructure**
Likely Sphere of Influence	**Technical**	**Mixed Regulatory, Political, and Entrepreneurial bodies**
Time scale	**sec-day**	**years**
Rate Quantity	**kg/hr**	**MWatt**

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The 90-Billion Gallon Biofuel Deployment Study

Todd West, Ph.D.

Sandia National Laboratories
Livermore, California

Sandia National Laboratories

Joint project conducted by GM and Sandia National Laboratories is a true supply-chain approach to future large-scale biofuels

Feedstock → Storage and Transport → Conversion → Distribution

A number of organizations provided direct input and reference materials for Sandia-GM study*

Feedstock → Storage and Transport → Conversion → Distribution

ceres — the energy crop company™

USDA

POET™

coskata

MASCOMA

Union Pacific

Kinder Morgan

Mendel Biotechnology

Purdue University Agricultural Economics

Oak Ridge National Laboratory — Managed by UT-Battelle for the Department of Energy

INL Idaho National Laboratory

NREL National Renewable Energy Laboratory — Innovation for Our Energy Future

Bio — Biotechnology Industry Organization

Argonne National Laboratory

*Views expressed in this presentation are those of the study authors and do not necessarily reflect the views of organizations listed here

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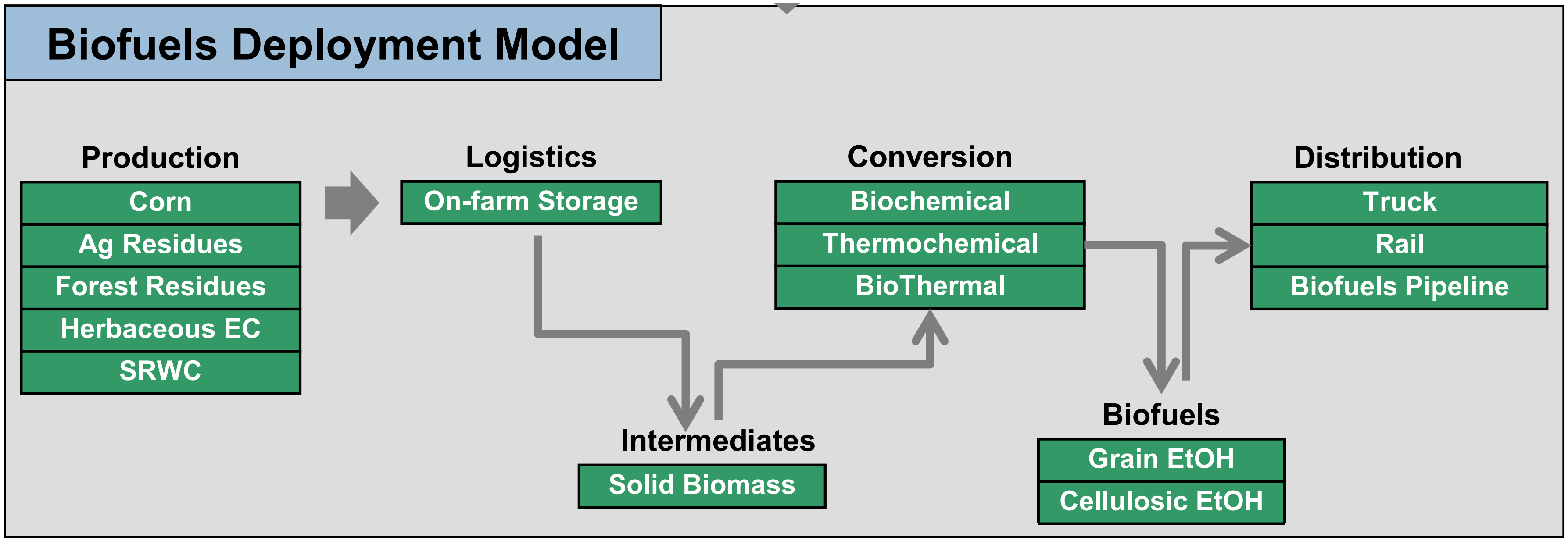
What questions did we seek to answer?

1. What must happen to grow ethanol production to 90B gal by 2030?
2. What is required for cellulosic ethanol to be cost competitive with gasoline?
3. What are the greenhouse gas, energy, and water footprints associated with this level of ethanol production?
4. What risks could impact cellulosic ethanol's production and competitiveness goals and how can we mitigate these?

Sandia built a ‘Seed to Station’ system dynamics model to explore the feasibility of large-scale ethanol



Model scope:

- Timeframe considered: 2006 to 2030
- State-level granularity

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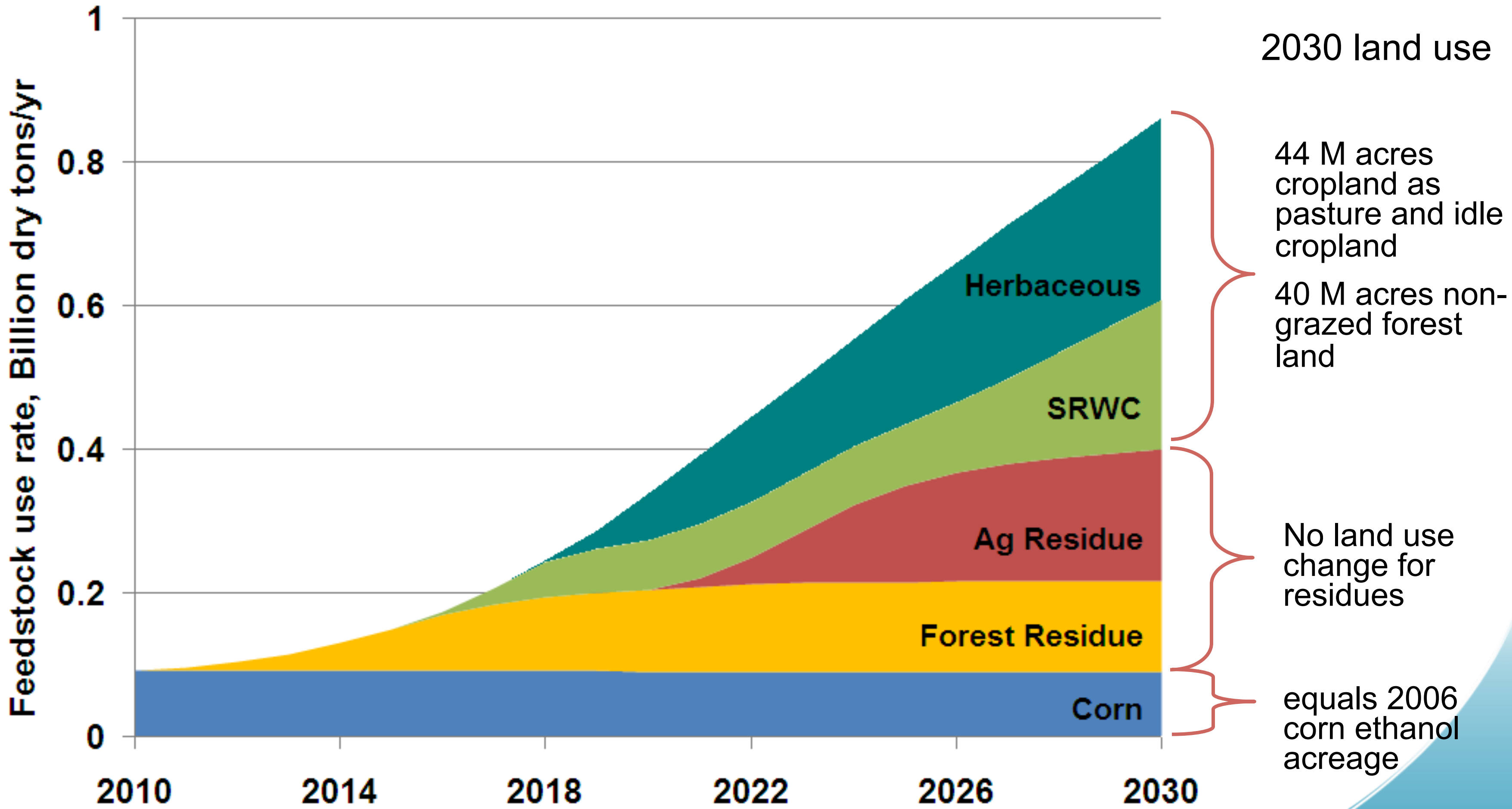
Biomass for 90 billion gallons of ethanol can be produced largely without reducing current active cropland

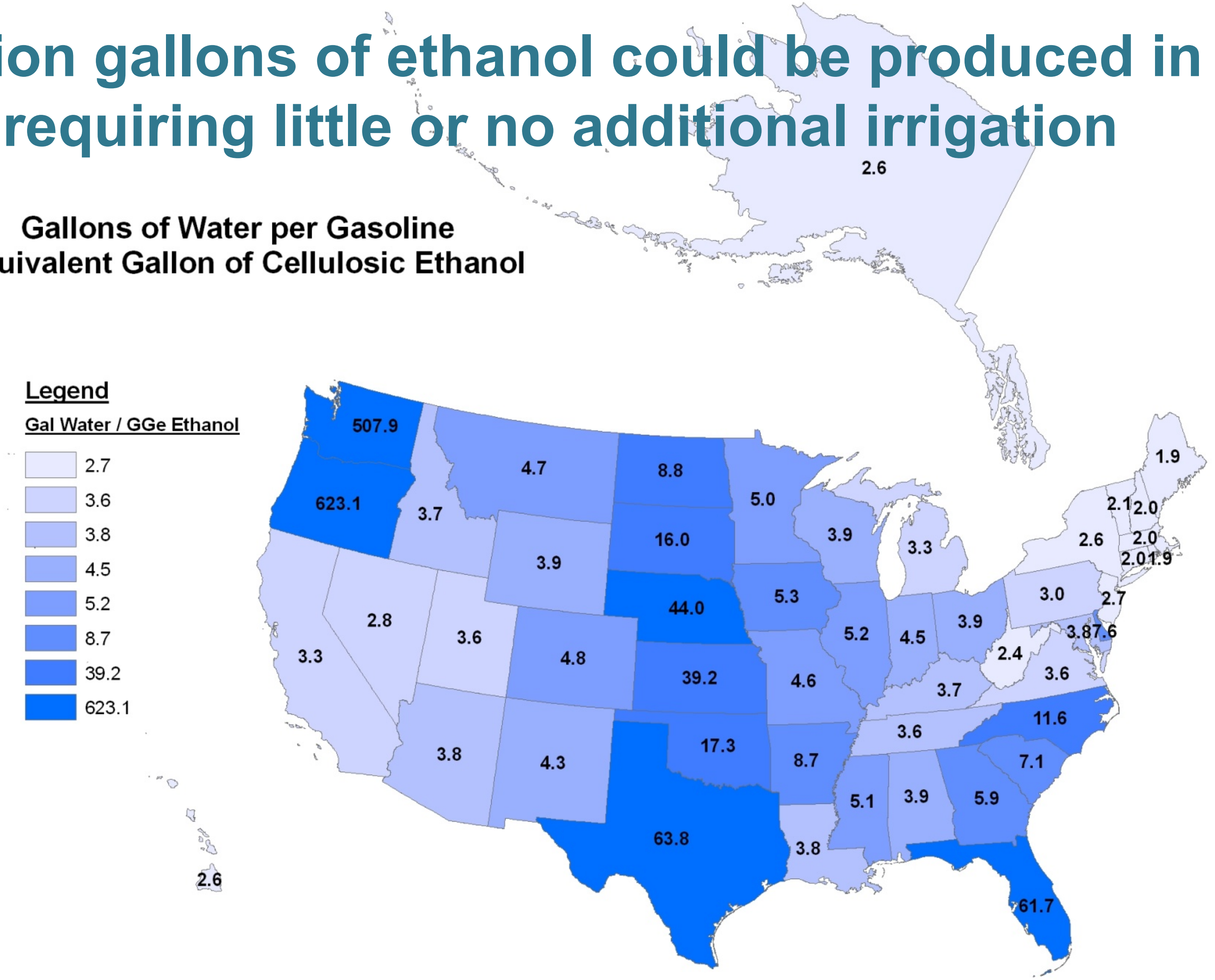


What is required for cellulosic ethanol to be cost competitive with gasoline?

- Cellulosic biofuels can compete with oil at $90/bbl assuming:
  - Average conversion yield of 95 gallons per dry ton of biomass
  - Average conversion plant capital expenditure of $3.60 per installed gallon of nameplate capacity
  - Average delivered feedstock cost of $52 per dry ton

- Sensitivity analyses varying these assumptions individually gave potential cost-competiveness with oil priced at $70/bbl to $120/bbl

50 Billion gallons of ethanol could be produced in states requiring little or no additional irrigation



Additional ethanol could be produced in low-irrigation areas of high water use states.

*Gasoline production uses 3-7 gallons (typically brackish) water per gallon gasoline.

Tamarisk as a Potential Feedstock for Biofuel/Bioenergy

June 20, 2011

Amy Sun & Kirsten Norman

Sun & K. Norman, “Use of Tamarisk as a Potential Feedstock for Biofuel Production,” SAND2011-0354.

K. Norman & A. Sun, “Technoeconomic evaluations of Tamarisk as a Potential Feedstock for Biofuel Production.” In preparation for Environmental Science & Technology.

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Tamarisk (saltcedar) is the 3rd most abundant invasive species in Western United States

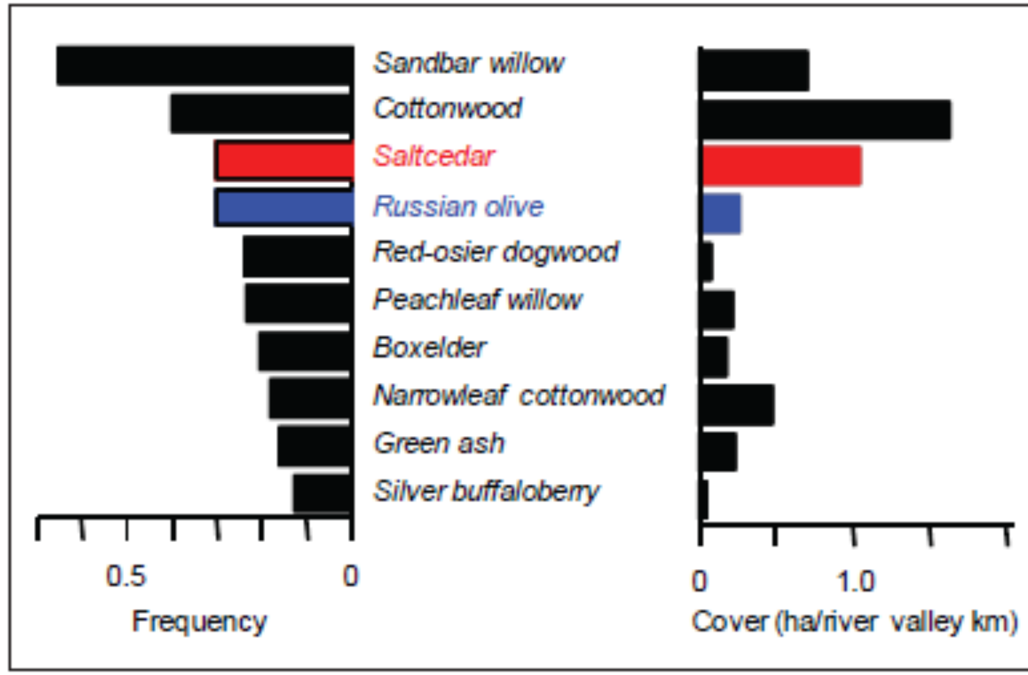


Figure 4. Frequency of occurrence and normalized vegetation cover of *T. ramosissima* and *E. angstifolia* compared to native trees on Western U.S. rivers, from a survey of woody riparian vegetation at 475 randomly chosen stream-gaging stations reported in Friedman and others (2005). Modified from figure 1 in Friedman and others (2005), which contains the scientific (Latin) names of the plants.

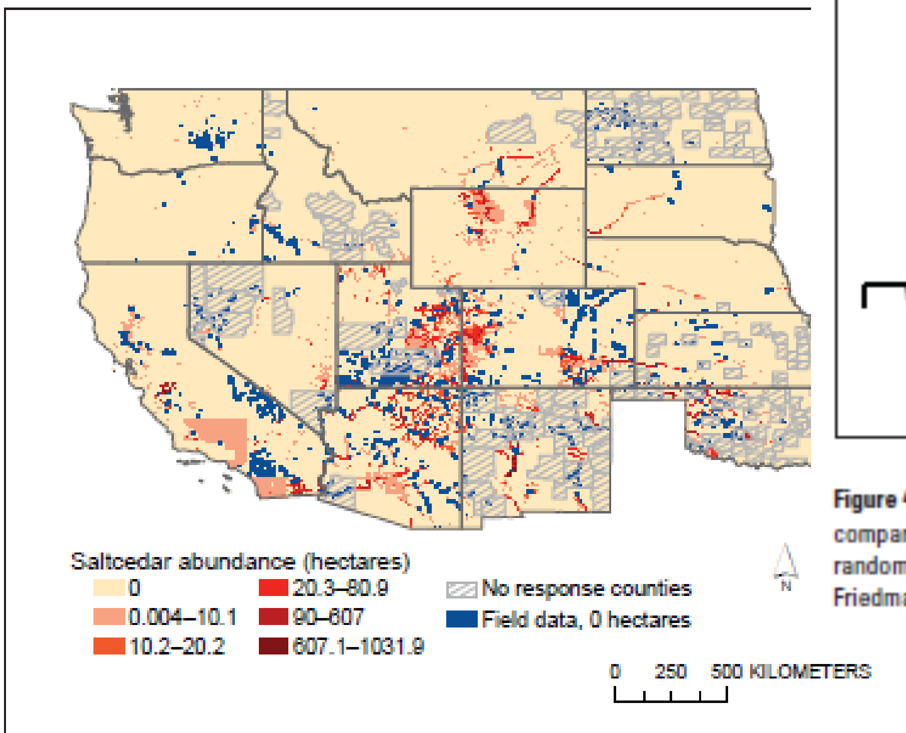


Figure 3. Quarter-quadrangle estimates of saltcedar area surveyed at the county level in 2004. Quarter quadrangles from where field data reported saltcedar but where the area estimates were zero are highlighted in blue. Data set produced by the Western Weed Coordinating Committee with funding from the Center for Invasive Plant Management. 1 hectare = 2.47 acres.

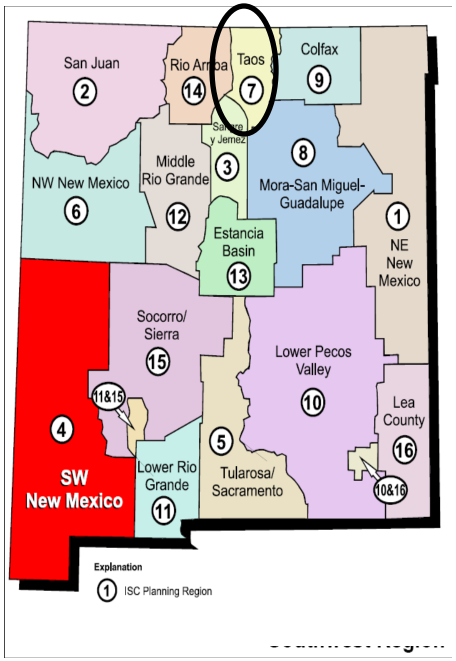
Source: USGS SIR2009-5247

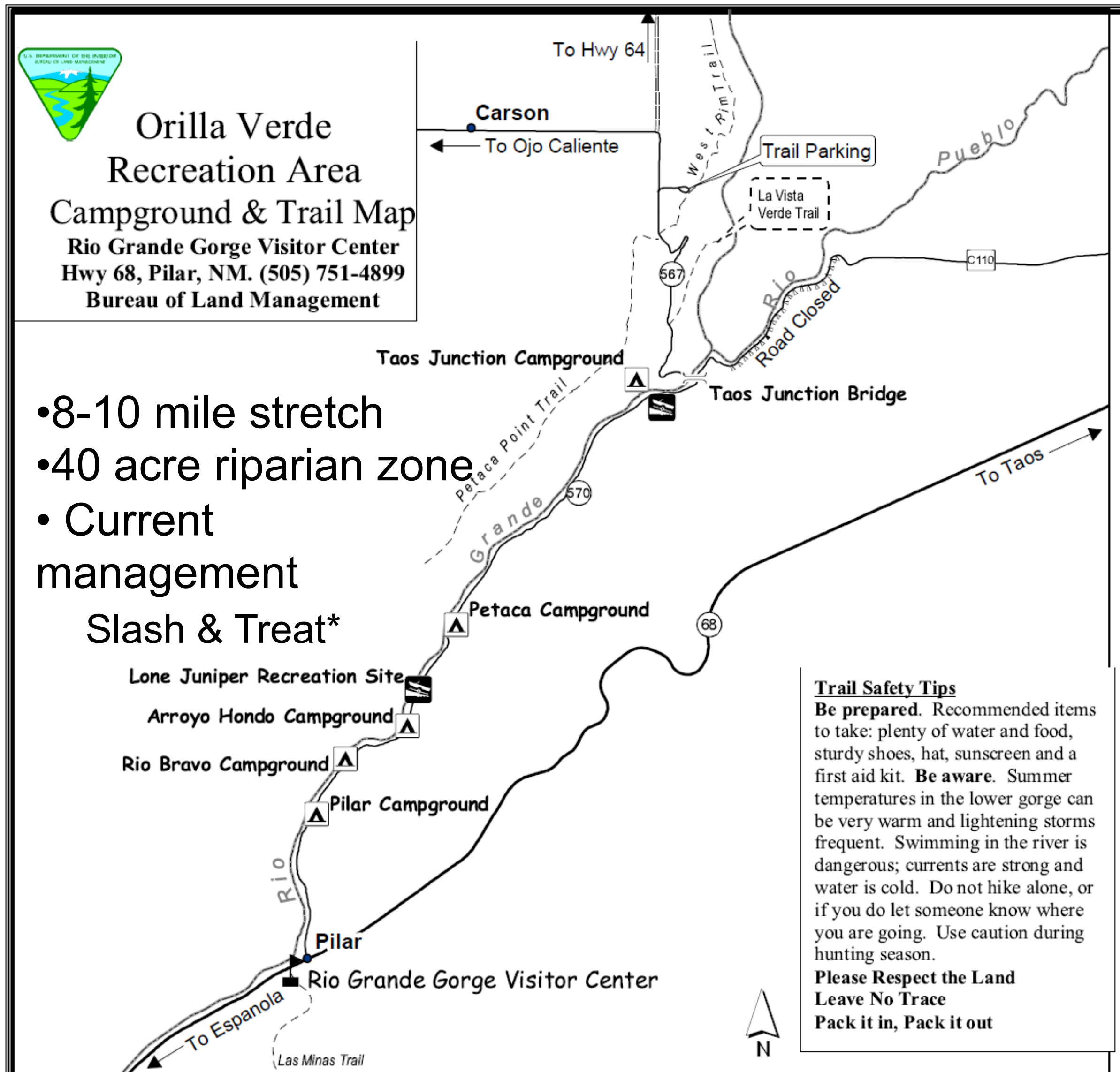
Tamarisk (saltcedar) along riparian regions

Blooming Saltcedar

Riparian vegetation: Cottonwood (dark green), Willow (light green)

NM Small Business Assistance with RiverBrink, LLC.





- 8-10 mile stretch
- 40 acre riparian zone
- Current management
  - Slash & Treat*

*Bureau of Reclamation: 2009 Monitoring Report for Treatment of Saltcedar (*Tamarix spp.) and Other Invasive Nonnative Vegetation – Orilla Verde*

Relevant questions

- Would saltcedar be a suitable feedstock for small-scale biofuel production?
- What are the possible technical pathways for converting saltcedar into biofuels?
- What are the water and energy footprints?
- What is the cost of producing biofuels from saltcedar?

Life Cycle Analysis – options for saltcedar

Harvest

Mechanical removal
- Excavator
- Cut at base using chainsaw.
- Pull out roots using plow.
- Use lopper to remove branches

Refinement on site
- Chipper
- Hammer mill
- Pelletizer

Storage
- Warehouse on-site
- Store at refinery

Schedule (12 hr/day)
- Year round
- Off-season (winter, spring)

Transport

Mobile unit
On-site mobile refinery. No transport.

Nearest Municipality
Haul by truck to plant to Taos.

River transport
Load onto a boat to Pilar.

Rail cart
Rail cart to centralized biorefinery in Bernalillo.

Conversion

Liquid Fuels
Thermochemical:
Gasification
Pyrolysis

Biochemical:
Enzymatic
Saccharification
Fermentation

Solid Fuels
Pellets

Other
Wood flour
Syngas

Distribution

Liquid/Gas Fuels
Trucks
Rail transport
Pipeline transport
Pumping station
Blending station

Solid Fuels
Trucking to
Hardware stores
or
Lumber yard

Other
Trucking to
Plastics
or
Bioproducts plants

End Use

Liquid Fuels
Biodiesel

Solid Fuels
Home heating: pellet stove, pellet basket (fireplace, wood stove)

Power plants: coal-fired or Combined Heat and Power (CHP)

Other
Filler in wood-plastic composites. (e.g. Signs)
Construction: deck boards, door/window profiles

Baseline system

Harvest ⟹ **Transport** ⟹ **Conversion**

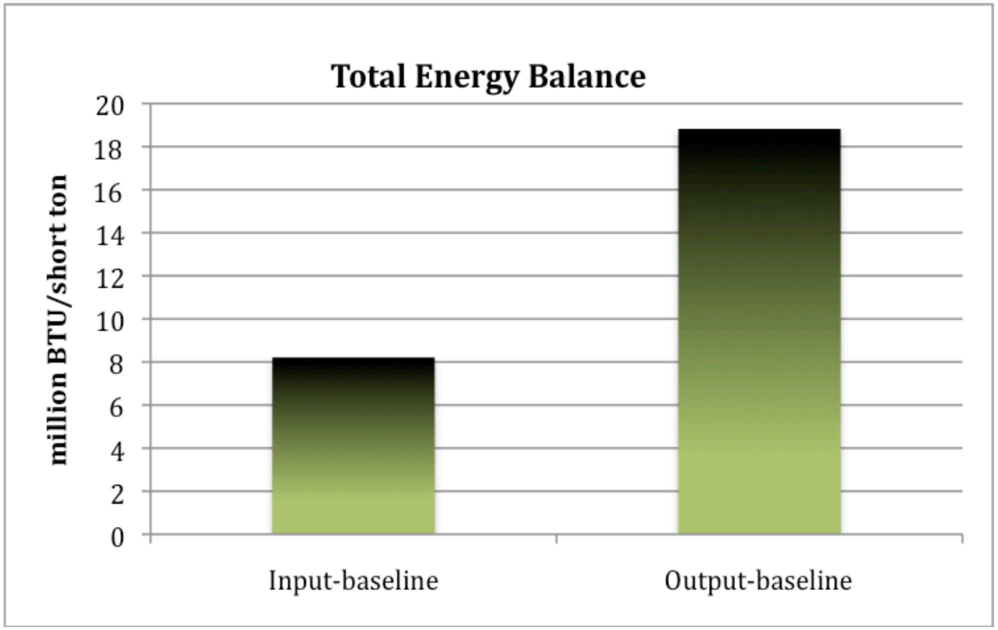
Harvest	Transport	Conversion
<u>Mechanical removal</u> Manual removal using chainsaws. <u>Refinement on-site</u> Chipping and drying. <u>Storage</u> Warehouse on-site.	<u>Conversion On-Site</u> Whole trees transported by truck <1 mile.	<u>Liquid Bio-fuel Production</u> Portable pyrolysis unit, treat bio-crude on-site.

Source: AgriTherm

Table 1. Parameters and assumptions for harvest and transportation steps in a baseline system of saltcedar for biofuel.

Harvest		Transport	
Harvest energy Input	1.96 mmBTU/st	Transport energy Input	0.0352 mmBTU/st
Tamarisk coverage	25%	Number of trucks	1
Total site acreage	40 acres	Hauling Capacity	2 tons/truck
Growth density	106 trees/acre	Gas Mileage	8 miles/gallon
Tree height	9.7 m	Harvest Days	200 days
Crop rotation	6 years	Harvest	0.74 tons/day
Per acre yield	3.71 tons/acre/year	Hauling distance	1 mile round trip
Total yield	148 tons/year		
Chainsaw fuel	15.7 gal/ton		

Overall Energy Balance



Data gaps filled by

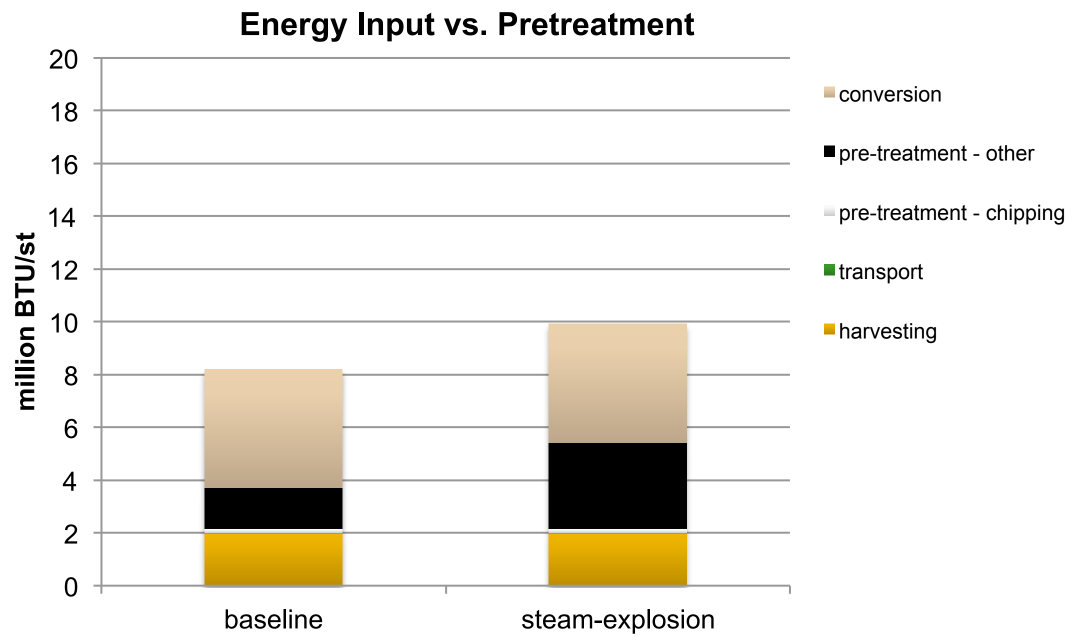
Cellulosic biomass literature.

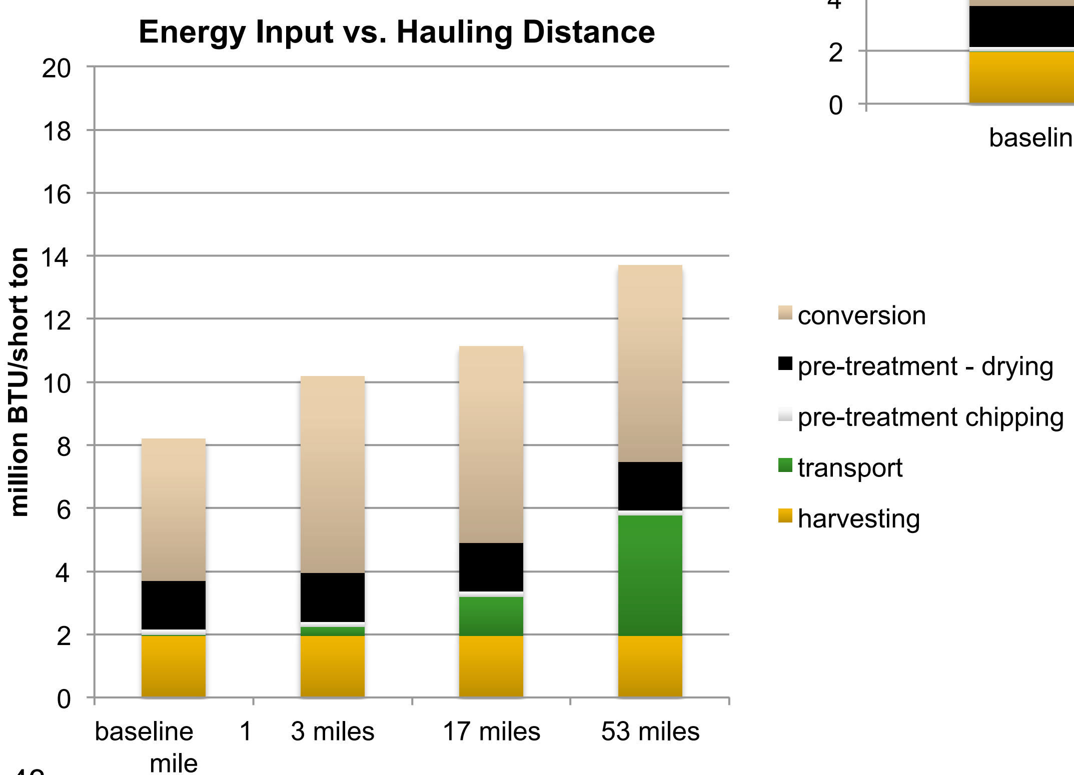
- PNNL-18284 report on fast pyrolysis.
- AgriTherm
- others

Table 2. Overall portable pyrolysis energy balance for saltcedar to biofuel baseline system in mmBTU/st.

Energy Input		Energy Output	
TOTAL	6.65	TOTAL	18.82
Harvest	2.00	Bio-oil	11.50
Transport	0.0352	Bio-char	3.82
Pretreatment	0.155	Bio-gas	3.50
Conversion	3.50		
Post-conversion Treatment	1.00		

Sensitivity Analysis





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Be aware!

- The process of developing your ideas and how you communicate your results is just as important as developing your solutions.
- Keep track of your references.
- Units of Measure!!!!
- Don't get too bogged down into details or circular thinking. Ambiguity is inevitable in most cases. Every method has its limitations (e.g. SD is not the only game in town.)
- It's okay to draw from similar systems studied in the past.
- Be a honest broker. Provide insight to further our understanding and discoveries. A no-go decision is just as important to your stakeholders as a go decision.

Interdependency between systems learning to manufacturing and nano-/micro-/macro- science

- The rate processes that have high sensitivities and/or the high uncertainties need the most help from high-fidelity modeling and experimental validation.
- Bottlenecks in logistics planning are opportunities for new science and exploratory solutions.
- Bottlenecks in rate processes are also opportunities for R&D (e.g. catalytic conversion, drying, etc).
- Improvements in molecular or cellular pathway synthesis have the greatest potential downstream impact.

Exercise/Break

Assignment

- **For the five topics listed below, please choose one topic and develop the following:**
  - ***Develop a set of relevant questions to address the topic.***
  - ***Develop a causal relation diagram by first listing the stocks, rate processes, and constants that you need to develop your systems model.***
  - ***Relate the rate processes and determine whether each relation is positive or negative.***
  - ***Rank each relation in three ways***
    - *Available information*
    - *Your estimate of sensitivities*
    - *Relevance to your questions*

Topic Areas*

Example 1: Oil and gas producers co-produce brackish water during the process of oil and gas production in deep wells. The salinity and mineral content of water makes it unsuitable for agricultural or municipal use, but it may be treated with algae. What is the potential of co-producing algal biofuel and fresh water in existing rural exploratory area?

Example 2: Hydroelectric dams are a source of renewable energy that is available and operating for a century. DOE is interested in transformative technologies or steps that can boost power generation while increasing flexibility for environmental and human needs. Suggest new ideas with supporting TE analysis.

Example 3: A new adhesion substrate that can increase algae lipid growth by 5 folds has been discovered in your laboratory. Conduct a TE analysis to assess the impact of this new technology on deploying algae biofuel to meet 0.1% biodiesel fuel in the U.S.

*Note: these are purely hypothetical examples

Topic Areas* (cont'd)

Example 4: Your have just been informed that EPA has issued a new renewable fuel standard that mandates 10% reduction in NOx emission relative to jetcrude, assess the additional production cost of algae-to-biocrude process required to the meet the new standard.

Example 5: You have conducted a CFD analysis of a newly designed energy storage system that increases the efficiency of a standard residential solar-based power system by 15%, but the storage system adds cost and footprint to the existing PV design. Assess the market potential for its commercialization.

*Note: these are purely hypothetical examples

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Example 2

Conceptual Influence Diagram of Seasonal Forecasting, Basinwide Integrated Hydropower Operation