BioEnergy Science Center: a DOE Bioenergy Research Center

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Stabilization of CO₂ concentrations means fundamental change to the global energy system.

Source: Jae Edmonds

**History and Reference Case**

**Stabilization of CO₂ at 550 ppm**

Global Primary Energy 1850-2100 (Exajoules)

- Oil
- Natural Gas
- Coal
- Biomass Energy
- Non-Biomass Renewable Energy
- Oil + CCS
- Natural Gas + CCS
- Coal + CCS
- Nuclear Energy
- End-use Energy

Preindustrial 280ppm
Concern relating to threat of climate change

Concern over future availability of oil and gas

Technology options for transportation

- Supply side options
- Demand side options

- CTL
- Heavy Oil
- GTL
- Ultra Deep Water
- Arctic
- Enhanced Recovery
- Capture and storage (C&S)
- C&S
- CNG
- Hybrids
- Biofuels
- Vehicle efficiency (e.g., lightweighting)
- Diesel-ization
- H₂ for transport

Source: Steve Koonin, BP
Decreasing U.S. petroleum consumption

Congress: The “30 by 30” goal

- Replace 30% of gas and diesel consumption with biofuels by 2030
- Requires approximately 1B dry tons of biomass for 60B gal using current technology
- “Billion Ton Study” – there is enough biomass in the US

State of the Union 2007: The “20 in 10” goal

- Decrease consumption by 20% in 10 years
- Grow production of renewable fuels to 35B gal/year by 2017

Upper limit of corn ethanol is around 18 billion gal per year (National Corn Growers Association)

With capacity being built we will reach this limit within two years

We must add cellulosic biofuels in order to meet our national goals
Potential biomass resource and refinery capacity in 2030
Forest residues (all), crop residues, switchgrass

Data do not include pulp & paper assets in the Southeast
The Southeast and Midwest will be the sources for US biomass
Billion-ton follow-up

- Developed new fine-scaled estimates of potential switchgrass productivity
  - Extend to woody crops (with USDA Forest Service)

Multiplicative model estimates yield as the product of estimated maximum yield, $Y_{max}$ and the fractional reduction due to each limiting variable, temperature ($T$) and precipitation ($P$)

$$Yield = Y_{max} \frac{Y(T)}{Y_{max}(T)} \frac{Y(P)}{Y_{max}(P)}$$

Source: Bob Perlack et al, ORNL Bioenergy Resource & Engineering Systems
Combining National Land Cover Data with the Cropland Data Layer

Source: Tris West et al, ORNL Ecosystem Simulation Science
Conversion routes to biofuels

Many feedstocks, many conversion options, many products, different economics, energy balances

ORNL leads one of three DOE Bioenergy Research Centers

- Funded for $125M over 5 years
  - Awarded June 26
- Start September 07
- Interface with Tennessee Biofuels Initiative
- Two other centers at
  - U Wisconsin
    - www.wisconsinbioenergy.com
  - LBNL
    - jbei.lbl.gov

http://www.bioenergycenter.org
The BESC team has been assembled to overcome biomass recalcitrance

Joint Institute for Biological Sciences

Alternative Fuels User Facility

Complex Carbohydrate Research Center

- Oak Ridge National Laboratory
- University of Georgia
- University of Tennessee
- National Renewable Energy Laboratory
- Georgia Tech
- Samuel Roberts Noble Foundation
- Dartmouth
- ArborGen
- Verenium (formerly Diversa)
- Mascoma
- Individuals from U California-Riverside, Cornell, Washington State, U Minnesota, NCSU, Brookhaven National Laboratory, Virginia Tech
Overcoming recalcitrance is the single coherent overarching theme for the BESC

The fundamental science of biomass recalcitrance is poorly understood

- A large-scale, integrated, interdisciplinary approach is needed to overcome this problem
  - Current research efforts are limited in scope
  - BESC will launch a broad and comprehensive attack on a scale well beyond any efforts to date

- Without advances, a cellulosic biofuels industry is unlikely to emerge
- Knowledge gained will benefit other biofuels and biofeedstocks
BESC will revolutionize how biomass is processed within five years.
# BESC has well-defined objectives

<table>
<thead>
<tr>
<th>Revolutionize the processing of biomass within 5 years</th>
<th>Apply a systems biology approach and new higher-throughput pipelines</th>
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<tbody>
<tr>
<td>• Improve overall yields</td>
<td>• Reduce recalcitrance by targeted modification of plant cell wall composition and structures</td>
</tr>
<tr>
<td>• Simplify operations through consolidated bioprocessing (CBP)</td>
<td>• Develop and understand single microbes or microbial consortia and their enzymes to enable CBP for low-cost cellulose hydrolysis and fermentation</td>
</tr>
<tr>
<td>• Decrease (or eliminate) the need for costly chemical pretreatment</td>
<td>• Provide a synergistic combination of modified plants and CBP for even more cost-effective biofuel production</td>
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</table>
Three linked scientific focus areas will enable BESC to understand and overcome biomass recalcitrance.

- **Biomass Formation and Modification**
  - Populus
  - Switchgrass
  - Plant Cell Wall

- **Characterization and Modeling**

- **Biomass Deconstruction and Conversion**
  - Enzymes
  - Microbe

Legend:
- Lignin
- Hemicellulose
- Cellulose
### BESC integrates three key science focus areas

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<th>Characterization and modeling</th>
<th>Biomass deconstruction and conversion</th>
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</table>
| • What gene products control cell wall structure, composition, and recalcitrance?  
  • How will changes in cell wall structure and composition affect plant productivity, pest resistance, and/or sustainability? | • What structural and compositional elements contribute to recalcitrance?  
  • Can new analytical methods, systems biology data, and computational models enable predictive simulation of lignocellulose formation and deconstruction? | • What limits the rate of biomass deconstruction, and how can these limits be overcome by altered biocatalysts?  
  • Will the combination of altered cell walls with better conversion offer a breakthrough? |

**Challenge:**
- Identify genes that control biomass production and cell wall synthesis
- Understand the complexity of plant cell wall structure and its relationship to recalcitrance
- Improve deconstruction rates and understand how microbes and enzymes attack biomass substrates
Computational Biology

- Annotation, DNA sequence analysis, gene finding, regulatory regions, comparative analyses - plants and microbes
- Systems analysis of mRNA and protein expression patterns
- Metabolic and regulatory network reconstruction in plants and microbes
- Image analysis and reconstruction software for 3-D tomography or confocal, cryo-EM
- Protein structure prediction and docking calculation
- Protein complex molecular dynamics
Ultra-scale modeling and simulation of biological systems

Exocellulase on crystalline cellulose based on explicit water model by Brady (Cornell) and provided by Himmel (NREL). The 1,000,000 atom simulation ran for 50 nsec using LAMMPS code on Jaguar 1024 processors by Uberbacher, Agarwal, Locascio, and Ghattyvenkatakrishna (ORNL).
Ultra-scale modeling challenges in BESC

Larger scale (e.g. cellulosomes) - Increase in scale to 10’s of millions of atoms

Millisecound timeframes

Multiscale simulation methods and force fields for systems of 100 million atoms scale – microbial and plant cell wall structures and cellulosomes

New force fields based on neutron dynamical measurements integrated with computational molecular simulation
Data Management and Integration

Laboratory Information Management System for tracking samples, procedures, data, IP, models

Lab instrument / user input interfaces to LIMS for data input and tracking

Systems knowledge base with data and information about key plants and microbes in the Center, metabolic, regulatory and signaling maps, with links to primary genome sequence annotation and underlying experimental data.
BESC – a highly integrated cutting-edge research team

- Biomass Formation and Modification
  UGA, ORNL, UT, Noble Foundation, ArborGen

- Plant Cell Wall Biosynthesis and Gene Identification

- Biomass Modification for Recalcitrance
  - Populus
  - Switchgrass

- Characterization and Modeling
  Ga Tech, NREL, ORNL, UGA, UC-Riverside, UT, Cornell

- Computational Biology and Data Analysis

- Computational Biology
  Chemical analysis, Imaging, Molecular analysis, Biomass sample prep, Pretreatment

- Data Management (IT) Web Portal

- External collaborators and data access

- Biomass Deconstruction and Conversion
  Dartmouth, Diversa, BNL, Cornell, Mascoma, NREL, ORNL, UGA, UT, VaTech

- Biomass-Biocatalyst Interface
  New tools for biomass reaction and recalcitrance, Diversity mining

- Improved Bioconversion with Microbes and Enzymes for Consolidated Bioprocessing

- Biofuel Production Assays
A functional management structure integrates BESC activities and objectives with clear lines of authority.
BESC leverages substantial firm commitments and investments

- **State of Tennessee, through UT:** >$24.6M
  - JIBS construction: $11.6M
  - Research equipment: $3M
  - Joint UT-ORNL research: $10M
  - 3 Governor’s Chairs: $3M–$5M
- **State of Tennessee:** $48M
  - $40M for 5M-gal/year pilot switchgrass-to-ethanol facility, located <40 miles from ORNL, to be operational in 2009
  - $8M in agricultural price supports

- **Georgia Research Alliance:** $6M
  - $3M for equipment,
  - $1.5M for two Eminent Scholar hires (matched by $1.5M from UGa and Georgia Tech)

- **Virginia Tech:** $0.5M in cost share support

- **Oklahoma Bioenergy Center**
  - Update to Governor Henry’s letter
  - >$10M at the Noble Foundation as part of this $40M center with University of Oklahoma and Oklahoma State

**Total:** More than **$90M**
BESC’s distinctive strengths

- One coherent focused theme: Biomass recalcitrance
- Positioned to attack the most important current barrier to the emergence of a cellulosic biofuels industry
- The best team and management for revolutionary advances to overcome recalcitrance
BESC larger context

Science
- Visiting Scientists
- Science Board
- Graduate students
- Post-docs
- BESC S&T core team
- Scientific Impact
- Sun Grant R&D
- Other R&D

Translation and Application
- States support
  Direct - TN, GA, NC, others
- Use-inspired drivers, licensing $$
- IP, tools, processes, platforms
- Technology maturation
- Commercialization
- Pilots
- VC investments
- Industry partnerships
- Benefit to farmers
- Benefit to consumers
- Biofuels industry growth

Science Board

Sun Grant R&D

Other R&D