CCSI™
Carbon Capture Simulation Initiative

CCSI Industry Advisory Board (IAB) Program Review Meeting

September 24-25, 2014

Hyatt
Reston, VA

Meeting Focus

- **Review the emerging tools** in the context of the overall CCSI program and objectives,
- **Receive guidance from the tool developers** on specific capabilities and requirements of the tools, and
- **Receive support from tool developers enabling industry partners to utilize the tools** within their own organizations to support carbon capture technology development.

Wednesday, September 24			
Start	**End**	**Topic**	**Room**
8:30	8:45	**Welcome and Day 1 Overview; Meeting Logistics and Safety; Workshop Goals** D. Miller, J. Shinn, M. Syamlal	**Grand Ballroom BC**
8:45	9:30	***Keynote*** Julio Friedmann, Deputy Assistant Secretary for Clean Coal Office of Advanced Fossil Technology Systems US Department of Energy	
9:30	10:00	**Coffee Break**	
10:00	10:30	**Review of Overall CCSI Program** D. Miller	
10:30	12:00	**Comprehensive CCSI Toolset Case Study (1)**	
12:00	12:45	**Working Lunch (collaboration discussion groups)**	
12:45	1:00	**IAB Group Photo**	
1:00	2:45	**Comprehensive CCSI Toolset Case Study (2)**	
2:45	3:00	**Coffee Break**	
3:00	5:30	**Poster/Demo Session (1)** Parallel: Individual discussions with CCSI leadership/T&E progress	**Breakouts**
5:30	6:30	**Reception**	**Ballroom D**
6:30	9:00	**Working Dinner** Speaker: TBD	

NETL · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory

Thursday, September 25				
8:00	9:30	**Poster/Demo Session (2)** Parallel: Individual discussions with CCSI leadership/T&E progress		**Breakouts**
9:30	10:00	**Coffee Break**		**Grand Ballroom BC**
10:00	12:00	**IAB Feedback Session** IAB Members provide feedback to CCSI/DOE Leadership in Grand Ballroom BC	**CCSI Technical Team Discussion** Technical Team Meets in Grand Ballroom A	
12:00	2:30	**Future Directions and Plans for Post-CCSI** Working Lunch • Presentation by CCSI Team • Discussion of Proposed Activities • Wrap up		**Grand Ballroom BC**
2:30	3:00	**Coffee Break**		
3:00	5:00	**Detailed Tool Demonstrations/Tutorials/Discussions** Individual IAB Members and Collaborators interact with simulation tool developers, further test and evaluate tools, plan for testing and evaluation. (schedule times on Wednesday or in advance, if desired)		**Breakouts**

Signup sheet for Thursday afternoon sessions with the Technical Team will be available.

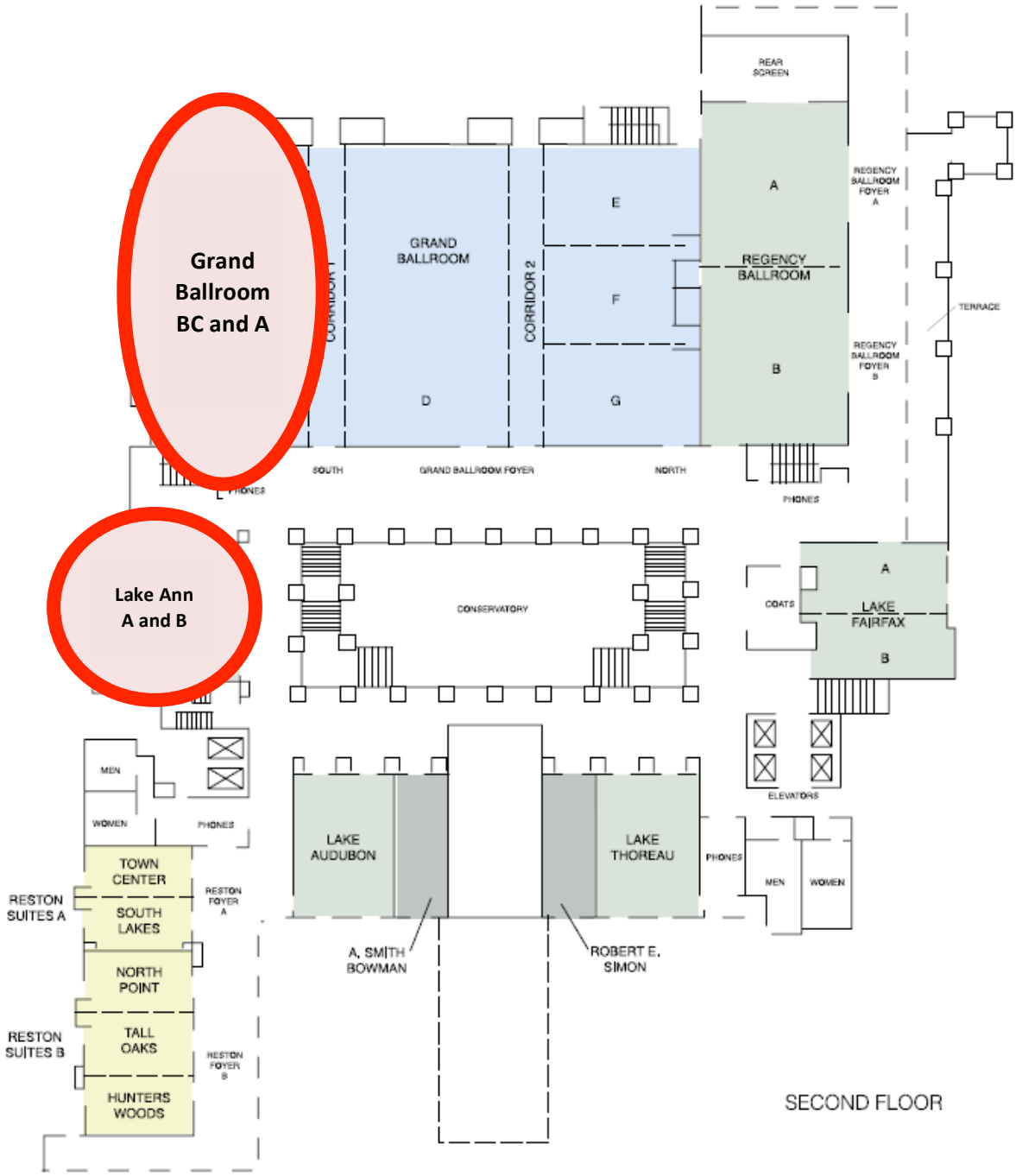
Poster/Discussion/Demo Sessions

Presenter(s) in parentheses

1. **Process Systems Engineering**
   Grand Ballroom A
   1.1. FOQUS Workflow (Eslick, Leek, Boverhof)
      1.1.1. FOQUS: Simulation-Based Optimization (Eslick, Chen)
      1.1.2. FOQUS: Quantification of Uncertainty (Tong, Ou, Ng)
      1.1.3. ALAMO: Automatic Learning of Algebraic Models for Optimization (Sahinidis, Wilson)
      1.1.4. iREVEAL: CFD to Surrogate Process Models (K. Agarwal)
      1.1.5. Data Management Framework: Provenance Tracking & Integration (Epperly, Cheah)
   1.2. Oxycombustion System Optimization (Eason, Ma)
      1.2.1. Model details (Dowling)
   1.3. Dynamic Reduced Model Builder (Ma)
   1.4. Advanced Process Control Framework (Mahapatra)
   1.5. Software Engineering/Release Management (Calafiura, Beattie)

2. **Multi-scale models**
   Lake Ann A
   2.1. Solid Sorbent Carbon Capture Models and Compression System (Bhattacharyya, Omell , Yu, Chen)
   2.2. MEA Model Evaluation and Comparison with Validation Data (Morgan, Chinen, Tong)
   2.3. Solvent Model Development and Calibration with 2MPZ (Bhat, Sherman, Ajayi)
   2.4. Solid Sorbent Models and Discrepancy Approach to Scale-Up (Mebane, Bhat, Li)

3. **Particle and Device Scale Models**
   Lake Ann B
   3.1. 1MW bubbling fluidized bed adsorber with quantified predictive confidence (Sun, Lai, Storlie, J. Xu, Pan, Dietiker, Li)
   3.2. High resolution filtered models for hydrodynamics and heat transfer considering horizontal tubes (Sundaresan, Ryan, Lane)
   3.3. Particle attrition and coal pulverization models (Okhuysen, W. Xu)
   3.4. Wetted wall CFD model for high viscosity solvent (J. Xu, Freeman, Zheng)
   3.5. Filtered solvent model with OpenFOAM (Carney, Singh, Sundaresan, Ali)
   3.6. A General Framework for Hierarchical Model Calibration (Storlie)


Grand Ballroom BC and A
Lake Ann A and B
REAR SCREEN
GRAND BALLROOM
CORRIDOR 2
E
F
G
D
A
REGENCY BALLROOM
B
REGENCY BALLROOM FOYER A
REGENCY BALLROOM FOYER B
TERRACE
SOUTH
GRAND BALLROOM FOYER
NORTH
PHONES
CONSERVATORY
COATS
LAKE FAIRFAX
ELEVATORS
MEN
WOMEN
TOWN CENTER
SOUTH LAKES
NORTH POINT
TALL OAKS
HUNTERS WOODS
RESTON SUITES A
RESTON SUITES B
RESTON FOYER A
RESTON FOYER B
LAKE AUDUBON
LAKE THOREAU
A. SMITH BOWMAN
ROBERT E. SIMON
SECOND FLOOR