Objective 1.1 Science and Technology Results Provide Meaningful Impact on the Field – High Impact Publications

**Biofuels SFA**

- HPC simulation of lignin aggregation on cellulose shows stronger binding to crystalline regions

**Objective:**

- Use of simulations to analyze the interaction of lignin and cellulose at the molecular level to understand mechanism of lignin in recalcitrance. Petascale computer simulations of lignin with cellulose molecules were run on the ORNL Jaguar supercomputer under INCITE award.

**New Science:**

- Lignin was found to strongly associate with itself and cellulose.
- Non-crystalline regions of cellulose were observed to have a lower tendency to associate with lignin than crystalline regions due to higher hydration.

**Significance:**

- The results suggest that the recalcitrance of crystalline cellulose to hydrolysis arises not only from the inaccessibility of inner fibers but also due to the promotion of lignin adhesion.

HPC simulation of lignin aggregation on cellulose shows stronger binding to crystalline regions

**Background:**

- Lignin aggregation on cellulose is a major barrier to viable biofuel production.

**Approach:**

- Petascale computer simulations of lignin with cellulose molecules were run on ORNL’s Jaguar supercomputer under INCITE award.
- Two types of cellulose models were simulated: crystalline and non-crystalline.

**Objective:**

- Use of simulations to analyze the interaction of lignin and cellulose at the molecular level to understand mechanism of lignin in recalcitrance.

**Results:**

- Lignin was found to strongly associate with itself and cellulose.
- Non-crystalline regions of cellulose were observed to have a lower tendency to associate with lignin than crystalline regions.
- This was found to arise from more favorable hydration of the non-crystalline regions.

**Significance:**

- The results suggest that the recalcitrance of crystalline cellulose to hydrolysis arises not only from the inaccessibility of inner fibers but also due to the promotion of lignin adhesion.

Citation: B. Lindner, L. Petridis, R. Schulz, J.C. Smith. “Solvent-Driven Preferential Association of Lignin with Regions of Crystalline Cellulose in Multimillion Atom Molecular Dynamics Simulation”. *Biomacromolecules* (in revision, 2013). Contact: smithjc@ornl.gov