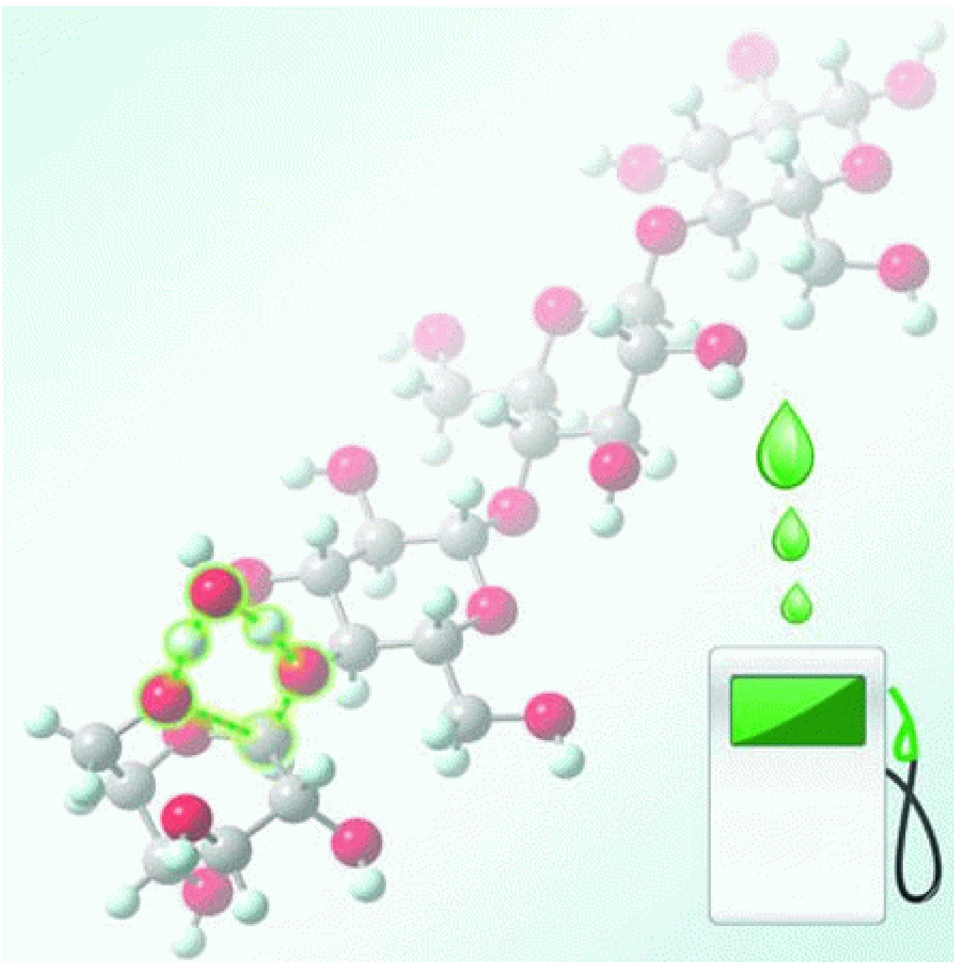
Study offers insight into converting wood to bio-oil

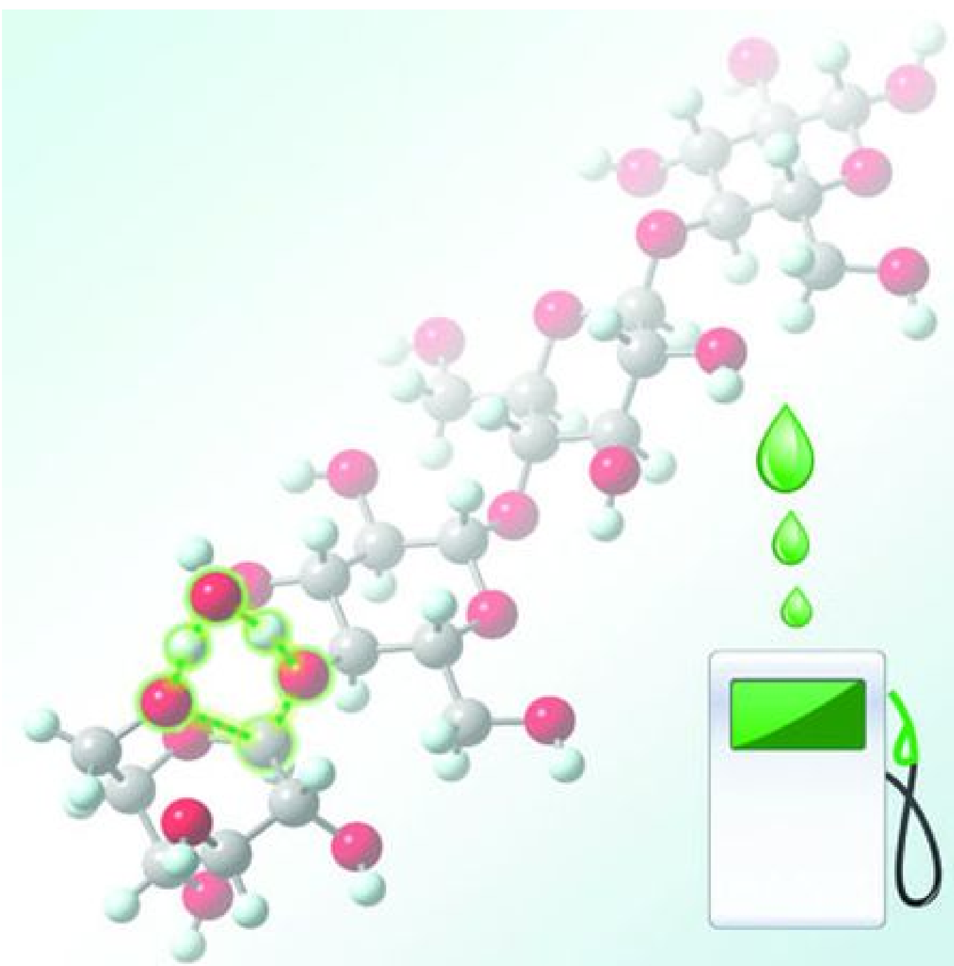
December 14 2012, by Mick Kulikowski



A paper that offers insight into converting wood to useful bio-oils appears as the cover article in the Journal of Physical Chemistry A.

(Phys.org)—New research from North Carolina State University provides molecular-level insights into how cellulose – the most common organic compound on Earth and the main structural component of plant cell walls – breaks down in wood to create "bio-oils" which can be refined into any number of useful products, including liquid transportation fuels to power a car or an airplane.

Using a supercomputer that can perform functions thousands of times faster than a standard desktop computer, NC State chemical and biomolecular engineer Dr. Phillip Westmoreland and doctoral student Vikram Seshadri calculate what's occurring at the molecular level when wood is rapidly heated to high temperatures in the absence of oxygen, a decomposition process known as pyrolysis.



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The results, which could help spur more effective and efficient ways of converting farmed and waste wood into useful bio-oils, appear in a feature article on the cover of the Dec. 13 print edition of the Journal of Physical Chemistry *A*.

Much of the energy that can be extracted from wood exists in the cellulose found in cell walls. Cellulose is a stiff, rodlike substance consisting of chains of a specific type of a simple sugar called glucose. The paper describes a mechanism for how glucose decomposes when heated. The mechanism is somewhat surprising, Westmoreland says, because it reveals how water molecules and even the glucose itself can trigger this decomposition.

"The calculations in the paper show that although the decomposition products and rates differ in glucose and cellulose, the various elementary steps appear to be the same, but altered in their relative importance to each other," Westmoreland says.

Knowing the specifics of the decomposition process will allow researchers to make predictions about the ease of extracting energy from different types of wood from various soil types.

The researchers are now conducting experiments to verify their calculations.

More information: Concerted Reactions and Mechanism of Glucose Pyrolysis and Implications for Cellulose Kinetics

Authors: Vikram Seshadri and Phillip Westmoreland, North Carolina State University

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Abstract: Concerted reactions are proposed to be keys to understanding thermal decomposition of glucose in the absence of ionic chemistry, including molecular catalysis by ROH molecules such as H2O, other glucose molecules, and most of the intermediates and products. Concerted transition states, elementary-reaction pathways, and rate coefficients are computed for pyrolysis of ?-D-glucose (?-Dglucopyranose), the monomer of cellulose, and for related molecules, giving an improved and elementary-reaction interpretation of the reaction network proposed by Sanders et al. (J. Anal. Appl. Pyrolysis, 2003, 66, 29?50). Reactions for ring-opening and formation, ring contraction, retro-aldol condensation, keto?enol tautomerization, and dehydration are included. The dehydration reactions are focused on bicyclic ring formations that lead to levoglucosan and 1,6-?-D-anhydrousglucofuranose. The bimolecular ROH-assisted reactions are found to have lower activation energy compared to the unimolecular reactions. The same dehydration reaction to levoglucosan should occur for cellulose going to cellosan (e.g., cellotriosan) plus a shortened cellulose chain, a hypothesis supported by the very similar activation energies computed when alternate groups were substituted at the C1 glycosidic oxygen. The principles of Sanders et al. that distinguish D-glucose, D-fructose, sucrose, and cellulose pyrolysis prove useful in providing qualitative insights into cellulose pyrolysis.

Provided by North Carolina State University