Computational chemistry shows the way to safer biofuels

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Replacing gasoline and diesel with plant-based bio fuels is crucial to curb climate change. But there are several ways to transform crops to fuel, and some of the methods result in bio fuels that are harmful to health as well as nature.

Now a study from the University of Copenhagen shows that it is possible to predict just how toxic the fuel will become without producing a single drop. This promises cheaper, faster and above all safer development of alternatives to fossil fuel.

Solvejg Jorgensen is a computational chemist at the Department of Chemistry in Copenhagen. Accounts of her new computational prediction tool are published in acclaimed scientific periodical The Journal of Physical Chemistry *A*.

Among other things the calculations of the computer chemist show that bio fuels produced by the wrong synthesis path will decompose to compounds such as health hazardous smog, carcinogenic particles and toxic formaldehyde. Previously an assessment of the environmental impact of a given method of production could not be carried out until the fuel had actually been made. Now Jorgensen has shown that various production methods can be tested on the computer. This will almost certainly result in cheaper and safer development of bio fuels.

"There is an almost infinite number of different ways to get to these fuels. We can show the least hazardous avenues to follow and we can do

that with a series of calculations that take only days", explains Jorgensen.

Chemically bio fuel is composed of extremely large molecules. As they degrade during combustion and afterwards in the atmosphere they peel of several different compounds. This was no big surprise. That some compounds are more toxic than others did not come as a revelation either but Jorgensen was astonished to learn from her calculations that there is a huge difference in toxicity depending on how the molecules were assembled during production. She was also more than a little pleased that she could calculate very precisely the degradation mechanisms for a bio fuel molecule and do it fast.

"In order to find the best production method a chemist might have to test thousands of different types of synthesis. They just can't wait for a method that takes months to predict the degradation mechanisms", explains Jorgensen who continues: "On the other hand: For a chemist who might spend as much as a year trying to get the synthesis right it would be a disaster if their method leads to a toxic result".

It seems an obvious mission to develop a computational tool that could save thousands of hours in the lab. But Solvejg Jorgensen wasn't really all that interested in bio fuels. What she really wanted to do was to improve existing theoretical models for the degradation of large molecules in the atmosphere.

To this end she needed some physical analysis to compare to her calculations. Colleagues at the Department of Chemistry had just completed the analysis of two bio fuels. One of these would do nicely. But Jorgensen made a mistake. And instead of adding just another piece to a huge puzzle she had laid the foundation for a brand new method.

"I accidentally based my calculations on the wrong molecule, so I had to start over with the right one. This meant I had two different calculations

to compare. These should have been almost identical but they were worlds apart. That's when I knew I was on to something important", says Solvejg Jorgensen, who has utilised her intimate knowledge of the theoretical tool density functional theory and the considerable computing power of the University of Copenhagen.

Provided by University of Copenhagen