TECHNOLOGY ENABLES RESEARCHERS TO SEE MOLECULES IN A NEW LIGHT

An interdisciplinary team of top researchers at the University of Louisiana at Lafayette is exploring a "green" way to use glycerol, a byproduct of biodiesel manufacturing.

Its members are identifying and testing enzymes present in bacteria commonly found in soil. An enzyme is a protein that speeds up chemical processes. These scientists are working to develop enzymes that are able to convert glycerol into compounds with much higher value for the chemical industry.

They are harnessing the power of Zeke, UL Lafayette's supercomputer, to make mind-boggling computations and then convert these data into images that can be examined using virtual reality at the Louisiana Immersive Technologies Enterprise on campus.

LITE is one of only a few public facilities that combine high-speed networks and high-performance computing with 3-D visualization and immersive technologies.

"So this enzyme project is an amazing confluence of brainpower, computer horsepower, computational chemistry and advanced immersive visualization," said Dr. Bradd Clark, dean of the Ray P. Authement College of Sciences at UL Lafayette.

SI FENG

Dr. Dipesh Bhattarai, left, and Si Feng use The Flex, an immersive visualization tool, to get a 3-D look at a glycerol dehydratase protein molecule.

As the volume of biodiesel, an alternative to fossil fuels, has increased dramatically worldwide, the amount of glycerol produced has grown too. For every 10 pounds of biodiesel, about a pound of glycerol is created. So glycerol is abundant and inexpensive but of limited use.

Dr. Rakesh K. Bajpai is a professor of chemical engineering and holds UL Lafayette's endowed chair in bioprocessing. He is also associate director of the Bioprocessing Research Laboratory in the university's College of Engineering.

Using a chemically modified enzyme to convert glycerol would be a "green" alternative to chemical processes that require more energy, Bajpai said. "Using this modified enzyme, we would not be producing anything harmful and we would reduce waste."

Enzyme development is of great interest in Europe and the United States. In 1994, a French group of scientists sequenced the gene of an enzyme that was capable of converting glycerol. Last year, a patent was granted for improvements of the enzyme's properties. When a patent is obtained, future work on that enzyme becomes off limits to other researchers.

Clark said Dr. Wu Xu, an associate professor of biochemistry at UL Lafayette, is working to improve a different type of enzyme, one that is even more efficient than the patented one.

Xu has identified about 25 similar enzymes. However, testing each enzyme using traditional chemistry would be expensive and time consuming. So scientists at UL Lafayette's Center for Advanced Computer Studies are using its supercomputer, Zeke, to come up with calculations and visualizations of enzymes ideal for glycerol conversion.

Bajpai explained that enzymes fit chemical compounds "like a key in a lock." The desired product of the enzyme is obtained when a water molecule is removed from glycerol. "If the glycerol fits exactly, the enzyme can unlock the water molecule. If it doesn't match up precisely, nothing will happen," he said.

Dr. Dipesh Bhattarai and Si Feng, UL Lafayette research scientists, used the computations of Dr. Yen-Shan Liu, a researcher in Dr. Wu's lab, to develop 3-D images of the enzyme with the most potential.

These enzyme molecules are large. That may seem like an oxymoron, but in the overall scheme of tiny particles that make up matter, enzyme molecules are giants.

Some molecules are composed of only a few atoms. The enzymes that the UL Lafayette team is studying are made up of about 15,000 atoms.

The images can be displayed in The Flex, an interactive 3-D immersive space in LITE that has a three-projector curved screen, motion tracking and an immersive sound system. The researchers can add and subtract atoms; the images morph to illustrate the new configurations.

When viewed through special eyeglasses, the images are three-dimensional. "You actually feel like you can touch the molecule. That's the exciting part," Bhattarai said.

When the scientists find the virtual enzyme they want to produce in the laboratory, they will turn to another team member, Dr. Andrei Chistoserdov, an associate professor of biology and microbiology, to genetically modify the bacteria so they will produce desired enzymes.

LITE's technology may be used in another enzyme-related project. Dr. Stephen Dufreche, an assistant professor of chemical engineering, is exploring the use of enzymes to create trinitrotoluene, better known as TNT.

Chemical processes have been used to make the explosive for the past 80 or 90 years. "But with those processes, we make an undesirable byproduct in environmentally unacceptable quantities," Bajpai said. "We think that if we can make it enzymatically, we can make it in an environmentally safe manner."