Researchers design new molecules that boost fuel efficiency

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Pictured in front of Trinity College Dublin's campanile in Front Square are team members, Dr Andrew Ure, Research Fellow, School of Physics; Associate

Professor, Stephen Dooley, School of Physics; Dr Juan Valverde, Business Development Manager, Trinity Research & Innovation. Not present is Dr Manik Ghosh, Research Fellow, School of Physics (now NUI, Galway). Credit: Trinity College Dublin

Researchers from Trinity and TOTAL have designed, synthesized and tested new additives that increase fuel efficiency.

Led by Professor Stephen Dooley in Trinity's School of Physics, the Trinity researchers undertook the project as a result of an open competition by TOTAL, where their proposal welcomed several applications from research teams across the globe.

The research was funded by TOTAL Marketing Services and supported by MaREI, the Science Foundation Ireland Research Center for Energy, Climate and Marine.

The scientific work carried out by Trinity was focused on determining systematically what makes some molecular structures better octane boosters that others. By modifying these structures and adding molecular components as if they were LEGO pieces, the researchers were able to calculate if a given structure met the theoretical principles to become an efficient octane booster.

Global transport continues to rely on internal combustion engines

In the wake of recent emissions scandals, current market research indicates that internal combustion engine sales peaked in 2018 and that from now on sales of electric cars will slowly overtake cars running on fossil fuels. In recent years, many car manufacturers have announced

ambitious plans to electrify their offer—mostly by hybridisation with internal combustion engines.

However, there are still some technological and affordability risks to this transition. The reality is that over 90% of new car sales are still based on internal combustion engines as the main power train. Although electrification is taking place it is unlikely to make significant impacts on emissions over the coming decade.

In addition, there are other transportation modes, such as aviation or maritime, where electrification is simply not an option now. However, we can still make a difference by using additives within ubiquitous, affordable liquid fuels. Fuel additives may become particularly important if applied to biofuels, which already have low greenhouse gas potential.

Professor Stephen Dooley, principal investigator in energy science at Trinity, says, "We risk missing important emissions targets if we do not explore further solutions which may allow vehicles to become more efficient and less environmentally harmful. Considering that liquid fuels are used for almost all vehicle transportation worldwide, even small improvements in efficiencies will have significant global impacts, especially in poorer countries where electric mobility is not an option.

"Particularly, this last point is important if we are serious about CO_2 mitigation and climate justice. Additives of this type, and the methods we developed in discovering them, will be important tools as we transition to the large-scale use of low CO_2 biofuels."

Fuel additives

Fuel additives are used extensively to improve the technical properties of fuels, allowing them to be environmentally safe and perform well in the

engine. Typical additives range from simple dyes, to distinguish different types of fuels, to antioxidants to prevent degradation, and to octane boosters to make them more efficient.

Of these, octane-boosting additives are the most sought after as they allow the vehicle to go further on the same volume of petrol (gasoline) by better controlling how the engine burns the fuel.

Although octane boosters are used extensively there is currently no complete understanding on their molecular mechanism of action. Innovation in this space tends to be identified by blind trial and error, rather than systematic scientific study.

Most of the technical challenges require multidisciplinary research competencies. For example, the team at Trinity included technical specialists in Molecular Thermodynamics, Synthetic Chemistry, Nuclear Magnetic Resonance and Machine Learning and Mathematical Modeling.

The Trinity team (Professor Stephen Dooley, Dr. Andrew Ure, Dr. Manik Ghosh, Dr. John O Brien), adapted pre-existing theories of chemical reaction kinetics and molecular thermodynamics for use with more modern machine learning techniques, making use of the super-computing facilities of the Irish Center for High End Computing (ICHEC).

This allowed them to identify many potential additives, but only those which the theory calculations suggested had the best attributes were chosen for the risky and difficult experimental studies.

Dr. Denis Lançon, TOTAL coordinator for collaborative research with universities, said, "The research outputs that have arisen from this collaboration have been excellent. The results are relevant to a number

of existing business units in the company and there has already been discussion on how to integrate this knowledge across different functions. The Trinity team engaged very proactively with our research personnel and managed to deliver an ambitious research plan on time."

Dr. Juan Valverde, business development and innovation management in Trinity Research & Innovation, says, "Trinity can support companies interested in transitioning to a lower carbon economy. Through engagement with Trinity, industry partners can benefit from globally renowned academic expertise, cutting-edge intellectual property and world class infrastructure. In exchange, our academics are exposed to real life industry-challenges that motivate and inspire their work and ideas."

Provided by Trinity College Dublin