The Computerworld Honors Program

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Final Copy of Case Study

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STATUS:
Laureate

Organization:
Reaction Design

Organization URL:
www.reactiondesign.com

Project Name:
Model Fuels Consortium

What social/humanitarian issue was the project designed to address? What specific metrics did you use to measure the project's success?

This project addresses the global reduction of harmful greenhouse gasses and soot particulates emitted by combustion engines. Medical science points to the small soot particles that are found in combustion engine exhausts as a key health threat that may be responsible for everything from asthma to certain types of cancer. A 2011 report prepared by the American Lung Association cites that as many as 37,500 premature deaths could be prevented annually by reducing soot emitted by diesel engines; however, new engine designs typically require several multi-year cycles of building and testing prototype units. That said, recent advancements made in the capability and performance of computers have enabled engine designers and fuel engineers to use software simulation to "build and test" in a virtual environment, which could drastically reduce the time it takes to bring cleaner engines to market. But, to realize this benefit, designers need accurate and predictive models of both current and future fuels. In 2005, Reaction Design launched the Model Fuels Consortium (MFC) to address increasing industry and government interest in lowering greenhouse gas and toxic pollutant emissions. It is comprised of global automotive manufacturers and energy producers who work collaboratively to develop accurate fuel models that can predict the amount of pollutant emissions, which are a result of the combustion process in engines. With these models, developers are able to quantitatively predict the effects of various engine design modifications and exhaust after-treatment techniques on the amount and size of particulate emissions in a virtual environment, which has enabled them to more rapidly develop environmentally conscious engine designs. Specific metrics that were used during the project included quantitative accuracy of the software models versus experimental data and computation time required to complete the simulations.

Please describe the technologies used and how those technologies were deployed in an innovative way. Also, please include any technical or other challenges that were overcome for the successful implementation of the project.

Scientists have been developing computer models of the combustion process for over two decades. These models have gained varying degrees of use in industry, but have been limited by two key factors: accuracy and speed of computation. To tackle the issue of accuracy, we needed not only the expertise to build models in software, but also sufficient data to validate that the models accurately emulated what would happen in the real world. The MFC is the first project of its kind that brings together the engine design community and the fuel providers. Only with the participation of both the suppliers and the users of the fuels were we able to create and validate models using actual performance data, rather than academic or theoretical examples. In the process of creating the models, however, we had to overcome the aversion of competitors to share information for the greater advancement of the industry as a whole, not to mention the technical challenges associated with making the models useful in a practical design timeframe. Combustion is a complex chemical process that is affected by many factors. Consequently, the software models are mathematically intensive and can require significant compute resources. The technical innovation came in the way that we pieced together data from a variety of sources and used it to create models that performed accurately over the entire range of interesting operating conditions. Moreover, we faced a key technical challenge in the development of a fundamental model for how soot is formed in the combustion process. Understanding the fundamental chemistry of soot formation was a critical piece of developing a computational alternative to experimental testing, and it required the creation of specific experiments that we ran in a unique laboratory environment at the University of Southern California.

Please list the specific humanitarian benefits the project has yielded so far.

Member companies of the MFC have been using the work products from the project since 2006. Engines using our work are in the process of being designed and introduced. While the benefits are hard to measure in absolute terms, we estimate that the use of the software and models to create cleaner engines will enable the reduction of pollutant emissions on the order of tens of thousands of tons annually when compared to current levels.

Please provide the best example of how the project has benefited a specific individual, enterprise or organization. Feel free to include personal quotes from individuals who have directly benefited from the work.

"Fuel producers must consider a widening product range, from cleaner, high-performance petroleum blends to alternative fuels that vary in quality," said Alipio Ferreira Pinto, Jr., Downstream R&D GM at Petrobras. "The MFC helps us make good decisions by creating accurate and industry-validated computer models of complex fuels." "Developing energy-efficient and low-emission combustors has become a key requirement for industrial turbines," stated Lou Cerone, GE Energy VP, Energy Technology. "Modeling and simulation are critical elements in the cost-effective design of next-generation combustors that need to be cleaner burning, while capable of using a wide variety of fuels." "Increasing fuel efficiency and reducing emissions have become the driving forces in the automobile industry," stated Axel Winkler, head of the CFD division at Volkswagen Group Powertrain Research. "The accomplishments of the first phase of the MFC caused us to broaden our tool landscape and strategies we were putting in place for research. At first, we were skeptical that Reaction Design's MFC would provide a meaningful completion to our technical road map, but once we had the opportunity to evaluate extensively the comprehensive solutions being developed by the group, it was clear to us that MFC was worth the investment. We view our membership as a valuable resource in our ongoing efforts to develop highly efficient and innovative engine designs." "Automakers face a number of compliance issues to meet strict environmental regulations that add to the complexity of engine design and lengthen the design process," said Charles Westbrook, senior scientist at LLNL and chief technical advisor to the MFC. "MFC members recognize the importance of science-based soot modeling, because it can predict behavior, meaning we can test new designs on a computer rather than a physical prototype. This can shave days, weeks or months from a design cycle."