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Darwinian computer models 'evolve' fuel additives

WEST LAFAYETTE, Ind. -- Chemical engineers at Purdue University have developed and demonstrated how a computerized system that mimics evolution can discover new gasoline additives for better engine performance.

The engineers developed "genetic" algorithms -- or computer instructions -- that adapt Charles Darwin's evolutionary model to combine and recombine chemical components until the "fittest" fuel additives emerge. Each additive is made of three sections: a head, linker and tail. But there are about 20 distinct kinds of heads, linkers and tails that can be combined differently to make a nearly endless variety of compounds.

"Based on the combinations, they can have completely different properties," says [Venkat Venkatasubramanian](#), a professor of chemical engineering. The numerous combinations can be likened to biological diversity: the genetic blueprints for all life forms are made of the same four chemical building blocks of DNA, and only subtle variations in gene sequences spell the difference between monkeys and humans.

Rather than trying to study the properties of every possible compound, the evolutionary method naturally selects the best-performing additives.

"We randomly create hundreds of molecules from these heads and tails at the beginning," Venkatasubramanian says. The system can then predict how well the molecules will work by evaluating their structures.

Only the best candidates are kept, and they continue to breed. Their head, linker and tail sections are recombined, and so on, until a final "generation" of highest-performing additives is reached.

Fuel additives are needed to reduce deposits, left over from the combustion of gasoline, that build up on engine valves. The deposits eventually affect the performance of the valves, hindering engine efficiency. Additives latch onto waste material, preventing it from settling on the surfaces of valves.

The work was detailed in a poster presentation Wednesday, July 21, during the Fifth International Conference on [Foundations of Computer-Aided Process Design](#) in Breckenridge, Colo. The paper was written by Venkatasubramanian, graduate students Anantha Sundaram and Prasenjeet Ghosh, chemical engineering Professor James M. Caruthers, all from Purdue, and chemist Daniel T. Daly from Lubrizol Corp. in Wickliffe, Ohio, which funded the research.

Genetic algorithms are not limited to the design of gasoline additives. They have been used in other applications and might become a major force in the design of future drugs, plastics and other products, Venkatasubramanian says.

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