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Integration of computational modeling and experimental techniques to design fuel surrogates

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1	Integration of Computational Modeling and Experimental Techniques to Design Fuel
2	Surrogates
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16	Keywords: Fuel surrogates, Gasoline blend, , GC-DHA, Additives, Alternative Fuel, GTL
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19 20	
21	Abstract
22 23	Conventional gasoline comprises of a large number of hydrocarbons that makes it difficult to utilize in a model for prediction of its properties. Modeling is needed for a better understanding of the fuel flow and
24 25	combustion behavior that are essential to enhance fuel quality and improve engine performance. A simplified alternative is to develop surrogate fuels that have fewer compounds and emulate certain
26 27	important desired physical properties of the target fuels. Six gasoline blends were formulated through a computer aided model based technique "Mixed Integer Non-Linear Programming" (MINLP). Different
28 29	target properties of the surrogate blends for example, Reid vapor pressure (<i>RVP</i>), dynamic viscosity (η), density (α). Research octane number (<i>RON</i>) and liquid-liquid miscibility of the surrogate blends) were
30	calculated. In this study, more rigorous property models in a computer aided tool called Virtual Process-
31 32	Product Design Laboratory (VPPD-Lab) are applied onto the defined compositions of the surrogate gasoline. The aim is to primarily verify the defined composition of gasoline by means of VPPD-Lab. ρ . n
33 34 35	and RVP are calculated with more accuracy and constraints such as distillation curve and flash point on the blend design are also considered. A post-design experiment-based verification step is proposed to further improve and fine-tune the "best" selected gasoline blends following the computation work. Here,

advanced experimental techniques are used to measure the *RVP*, ρ , η , *RON* and distillation temperatures. The experimental results are compared with the model predictions as well as the extended calculations in

38 VPPD-Lab.

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