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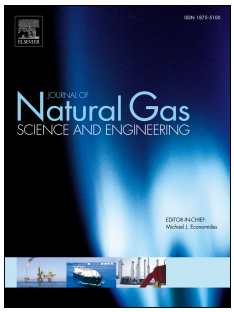

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H.A. Choudhury, S. Intikhab, S. Kalakul, R. Gani, N.O. Elbashir

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Integration of Computational Modeling and Experimental Techniques to Design Fuel Surrogates

H. A. Choudhury[a], S. Intikhab[a], S. Kalakul[b], , R. Gani[b] and N.O. Elbashir[a,c]*

[a]*Chemical Engineering Program and Petroleum Engineering Program, Texas A&M University at Qatar, 23874 Doha, Qatar*
[b]*Department of Chemical and Biochemical Engineering Program, Technical University of Denmark, DK-2800 Lyngby, Denmark*
[a]*TEES Gas & Fuels Research Center, Texas A&M University at Qatar, 23874 Doha, Qatar*

* Corresponding author: Nimir.elbashir@qatar.tamu.edu

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Abstract

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 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 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 target properties of the surrogate blends for example, Reid vapor pressure (*RVP*), dynamic viscosity (η), density (ρ), Research octane number (*RON*) and liquid-liquid miscibility of the surrogate blends) were calculated. In this study, more rigorous property models in a computer aided tool called Virtual Process-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, η 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 VPPD-Lab.