

A Surrogate Fuel Formulation Approach for Real Transportation Fuels with Application to Multi-Dimensional Engine Simulations

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ABSTRACT

Real transportation fuels, such as gasoline and diesel, are mixtures of thousands of different hydrocarbons. For multidimensional engine applications, numerical simulations of combustion of real fuels with all of the hydrocarbon species included exceeds present computational capabilities. Consequently, surrogate fuel models are normally utilized. A good surrogate fuel model should approximate the essential physical and chemical properties of the real fuel. In this work, we present a novel methodology for the formulation of surrogate fuel models based on local optimization and sensitivity analysis technologies. Within the proposed approach, several important fuel properties are considered. Under the physical properties, we focus on volatility, density, lower heating value (LHV), and viscosity, while the chemical properties relate to the chemical composition, hydrogen to carbon (H/C) ratio, and ignition behavior. An error tolerance is assigned to each property for convergence checking. In addition, a weighting factor is given to each property indicating its individual importance among all properties considered; the overall quality of the surrogate fuel model is controlled by a weighted error tolerance. It is observed that the solver can find an accurate surrogate fuel model for a low-cetane diesel fuel with 11 iterations. Finally, to further check the fidelity of the approach, the proposed surrogate fuel model is validated using a multi-dimensional engine simulation operated under a low temperature combustion (LTC) condition against the available experimental data. The results are also compared with a conventional single component model, viz., n-tetradecane representing physical properties and n-heptane representing chemistry. The results show that the proposed surrogate fuel model can accurately predict the overall combustion process and emissions, simultaneously; while the single component model is unable to predict the combustion process and emissions in the LTC condition for the low cetane diesel fuel.

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INTRODUCTION

The need to develop more efficient and cleaner engines is of increasing importance for today's automotive industry. Although, computational modeling of a wide range of phenomena in internal combustion engines has been a particularly fertile research area over the past 30 years [1], the inclusion of both accurate property models and extensive kinetic information within a combustion code is clearly prohibitive with today's computational resources [2], mainly due to fact that practical transportation fossil fuels, such as diesel, gasoline, kerosene, and so on, consist of complex mixtures of several hundred individual species of different classes. Therefore, a surrogate model approach is generally utilized, which involves choosing a few representative hydrocarbon

species to mimic the characteristics of the target fuel. However, standard rules for the construction of a surrogate model are not yet developed [3].

Generally, single-component or multi-component fuels may be classified, as suggested by Ra and Reitz [4] and Krishnasamy et al. [5, 6], into physical surrogates if they have the same physical properties as the real fuel, or chemical surrogates if they have the same chemical properties as the real fuel. Surrogates which have both the same physical and chemical properties as the commercial fuel are called comprehensive surrogates. Important goals of surrogate models, in terms of physical characteristics, may include volatility parameters, density, viscosity, surface tension, and diffusion coefficients;

important goals of surrogate models related to chemical characteristics may include ignition behavior, molecular structures, adiabatic flame temperature, C/H/O content [2]. Common physical property targets such as density and hydrogen/carbon (H/C) ratio can be readily matched with a single-component surrogate, though doing so obviously does not guarantee a good match to a real transportation fuel's combustion behavior. Other properties of a real fuel such as chemical composition, distillation curve, and molecular transport properties may require many more components to match well.

However, due to the availability of reaction mechanisms, developing multi-component surrogate models that accurately match the physical and chemical properties of real transportation fuels may still be a challenge. Therefore, currently a practical strategy is to develop surrogate models only focusing on certain fuel properties. Based on the goals of surrogate development, different strategies may be used for surrogate selection.

For chemical surrogate model development, a palette of surrogate compounds generally should be determined first, and then the surrogate model searching process is conducted. Recently, Dooley et al. [7] reported a mixture of n-dodecane/iso-octane/1,3,5-trimethylbenzene/n-propylbenzene formulated in a predictive manner to exhibit the same gas phase combustion phenomena of a target Jet-A. Several diesel fuel surrogates containing blends of n-heptane/toluene and n-heptane/toluene/1-hexene were investigated by Luo et al. [8] to study the combustion and emission characteristics of diesel fuel in LTC conditions. Kukkadapu et al. [9] reported a three-component mixture of iso-octane, n-heptane, and toluene and a four-component mixture of iso-octane, n-heptane, toluene, and 2-pentene to study the auto ignition of gasoline in HCCI engines.

For physical surrogate model development, researchers pay heavy attention to matching the distillation curves of the real fuels [10, 11, 12]. This property is directly related to composition, and is sensitive to even subtle compositional variability. Thus, the volatility is one property with sufficient sensitivity and scope to assess physicochemical authenticity. Indeed, the volatility of a surrogate is actually of critical importance for many of the purposes for which surrogates are intended to serve. Very specific engineering properties, such as relight, combustion and flame characteristics, and fire simulations, require a surrogate with a close match in volatility with the real fuel [13],[14],[15]. The same approach was used by Krishnasamy et al. [5] to develop multi-component surrogate models for the FACE fuels.

Recently, a group at Reaction Design [16] presented an approach that iteratively tests various fuel compositions, within limits, to find an optimized match to the distillation curve, lower heating value, H/C ratio, and RON and MON of the specified gasoline. The number of fuel components considered was limited by the availability of accurate mechanisms, as determined by comprehensive validation studies reported elsewhere. The final composition that satisfied all of the targets within the tolerances specified was considered to be a model fuel specific for a real fuel. Depending on the requirements of the model-fuel application, some targets could be dropped to simplify the resulting model-fuel composition. On the other hand, more criteria such as the Threshold Sooting Index (TSI) could be added as an indicator of sooting propensity in addition to the H/C ratio. An O/C ratio target could also be added for oxygenated fuels. However, there are no details available about the algorithm used for this approach, due to the commercialization of this tool. More recently, Mueller et al. [17] reported a novel approach to formulate surrogate fuels that adequately approximate the compositional, ignition-quality, and volatility characteristics of real-world diesel fuels. In this approach, nuclear magnetic resonance spectroscopy and an advanced distillation curve method were used to characterize fuel composition and volatility, respectively, and the ignition quality was quantified by the derived cetane number.

For current study, the goal is to develop a surrogate fuel formulation approach which can quickly and accurately approximate the essential physical and chemical properties of real transportation fuels based on local optimization and sensitivity analysis technologies. In the next section, we discuss in detail the methodologies used in this paper, starting with a general description of our methodology for formulating the surrogate fuel and ending with discussion of sensitivity analysis methodology.

METHODOLOGY

A good surrogate fuel model should approximate the essential physical and chemical properties of the real fuel. Achieving this target usually requires blending of more than one fuel component. In the current study, normally only comprehensive surrogates, i.e., surrogates with corresponding mechanisms, will be used as candidates. The surrogate fuel formulation approach follows the procedure shown in [Figure 1](#).

Within the proposed approach, several important fuel properties are considered. Under the physical properties, we focus on the following properties:

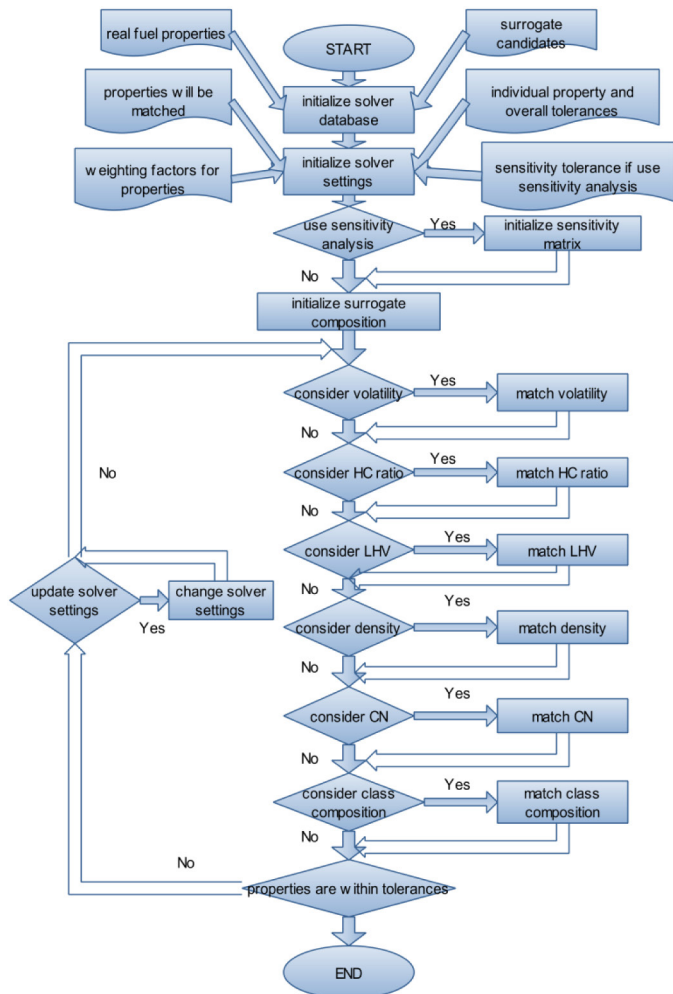


Figure 1. Flowchart of current surrogate fuel formulation approach

Volatility: important for evaporation, cold start, emission, combustion efficiency

Density: important for injection shape, spray development

Lower Heating Value (LHV): important for total energy release, power output

Viscosity: important for spray development

While for the chemical properties, we pay attention to:

Chemical class composition: important to imitate the physical properties and combustion behavior

Hydrogen to Carbon (H/C) ratio: important for local equivalence ratio

Ignition behavior (CN or RON): important for engine speed and operation conditions

An error tolerance is assigned to each property for convergence checking. In addition, a weighting factor is given to each property, indicating its individual importance among all properties considered; the overall quality of the surrogate fuel model is controlled by a weighted error tolerance. The distillation curve is calculated using a discrete multi-component (DMC) model, where the evaporation history of a single drop is simulated [18]. For the current methodology, the local optimization technique is used to match the distillation curve. Sensitivity analysis is used to make sure that approximating one property does not negatively affect the approximations of other properties and thus the overall accuracy of the surrogate model is controlled. If class composition match is required, then it will also be applied during the approximations of other properties. Also, users can approximate a property or a property combination of a fuel that they are interested in.

Approximate Distillation Curve

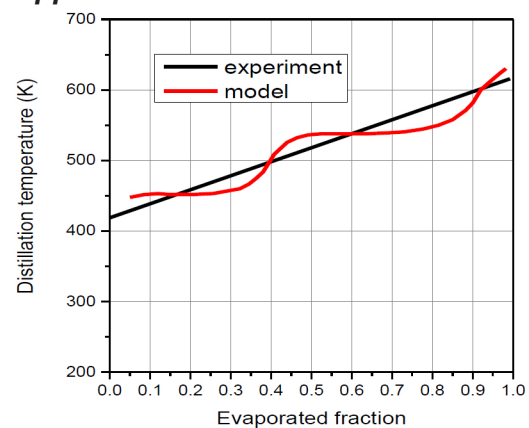


Figure 2. A general situation where the modeled distillation curve deviates from the experimental data

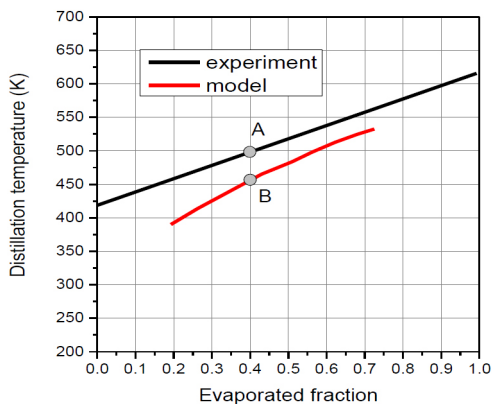
Consider modeling the distillation curve of a real transportation fuel, for example a diesel fuel, using a multi-component surrogate fuel model. Shown in figure 2 is a general situation where the modeled distillation curve deviates from the experimental data. This means that we need to re-distribute the mass among the surrogate fuels. A closer examination of this general situation reveals that we may decompose the general situation into eight situations depending on where we remove the mass from and where we re-distribute the mass to.

Local Optimization

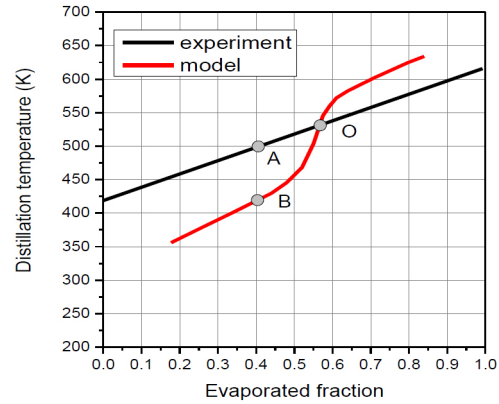
Figure 3 is a schematic diagram that shows the four situations where the distillation temperature (corresponding to point B) is under-predicted compared with the experimental distillation temperature (corresponding to point A) at a specific evaporated fraction (equal to 0.4). Consider the four situations to see where to remove the mass and where to re-distribute the mass to, and how the local optimization algorithm is designed. In Figure 3 (a), the whole modeled distillation curve is below the experimental distillation curve, which indicates that too much mass is assigned to surrogate components with lower distillation temperatures. At the experimental point where the

evaporated fraction equals to 0.4, we can see that modeled distillation temperature is about 450 K (corresponding to point B). Thus, we remove mass from the surrogate components whose distillation temperatures are below 450 K, and re-distribute the obtained mass to surrogate components whose distillation temperatures are above 450 K. In Figure 3 (b), compared with Figure 3 (a), the modeled distillation curve intersects with the experimental distillation curve above the distillation temperature corresponding to point A. Similar operations can be done, except that the obtained mass should only be re-distributed to surrogate components whose distillation temperatures are above the modeled distillation temperature about 425 K and below or equal to the distillation temperature corresponds to intersection O, which is about 525 K in this case. This is because the distillation temperatures are already over predicted at evaporation fraction locations above 0.55 (corresponding to intersection O). Adding more mass to surrogate components whose distillation temperatures are above 525 K will cause the distillation temperature to be even more over predicted.

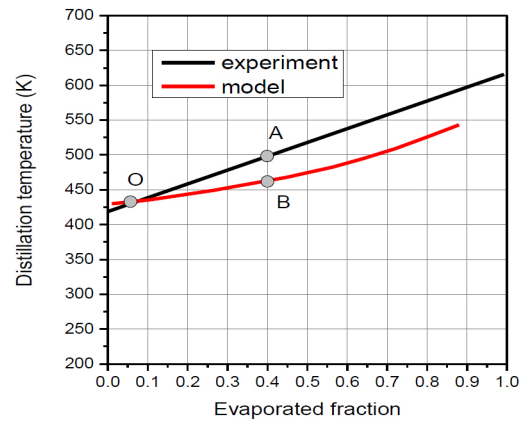
In Figure 3 (c), the modeled distillation curve intersects with the experimental distillation curve below the distillation temperature corresponding to point A, compared with Figure 3 (a). Again, similar operations can be done, except that we only remove mass from the surrogate components whose distillation temperatures are below the modeled distillation temperature about 450 K and above the distillation temperature corresponding to intersection O, which is about 425 K in this case. In the situation of Figure 3 (d), the modeled distillation curve intersects with the experimental distillation curve below and above the distillation temperature corresponding to point A, compared with Figure 3 (a). The mass of the surrogate components, whose distillation temperatures are below 460 K and above the distillation temperature corresponding to intersection P, which is about 425 K in this specific case, should be removed and re-distributed to the surrogate components whose distillation temperatures are above 460 K and below or equal to the distillation temperature corresponding to intersection O, which is about 550 K in this specific case.



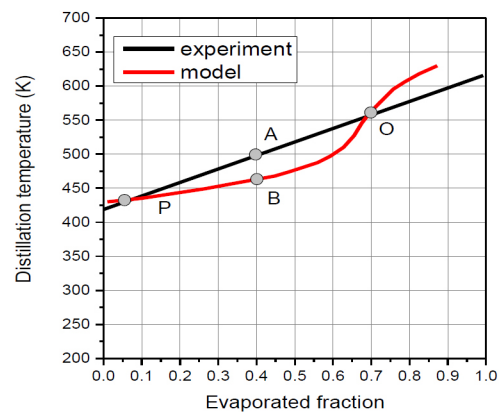
(a)



(b)



(c)



(d)

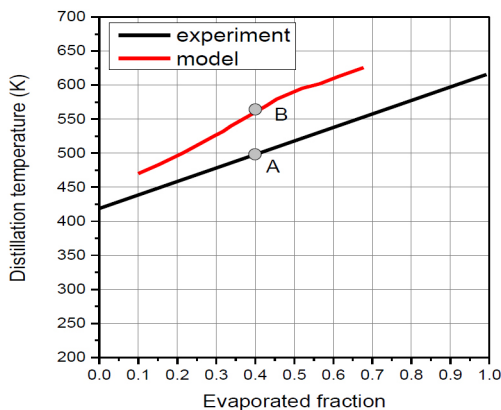
Figure 3. Schematic diagram when distillation temperature (corresponding to point B) is under-predicted compared with experimental distillation temperature (corresponding to point A) at a specific evaporated fraction

Figure 4 is a schematic diagram that shows another four situations where the distillation temperature (corresponding to point B) is over-predicted compared with the experimental distillation temperature (corresponding to point A) at a specific evaporated fraction (equal to 0.4).

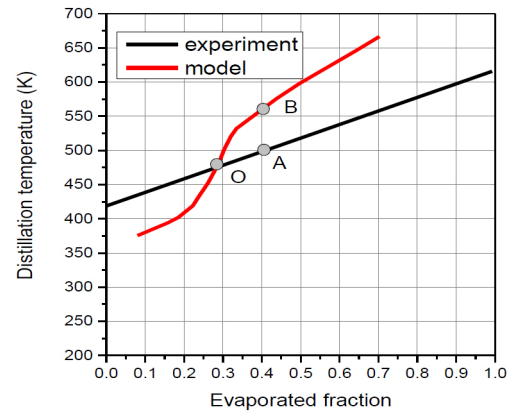
In Figure 4 (a), the whole modeled distillation curve is above the experimental distillation curve, which indicates that too much mass is assigned to surrogate components with higher distillation temperatures. At the experimental point where the evaporated fraction equals to 0.4, we can see that modeled distillation temperature is about 560 K (corresponding to point B). Therefore, we should remove the mass from the surrogate components whose distillation temperatures are above 560 K, and then re-distribute the obtained mass to surrogate components whose distillation temperatures are below 560 K. Similar analyses can be applied to other situations of Figures 4 (b), (c), (d).

With the understanding of where we should remove the mass from and where we should re-distribute the mass to, we still need to know how to calculate the amount of mass that needs to be removed or added for each surrogate component, based on the distillation temperature deviation at each experimental point or each evaporated fraction location.

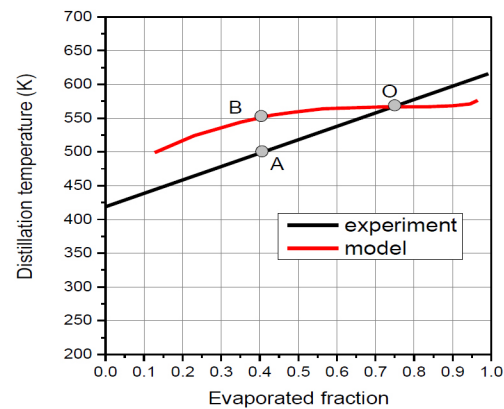
To make it clear, consider the situation in Figure 3 (b) as a specific example. In this case, we will remove the mass from the surrogate components whose distillation temperatures are below the modeled distillation temperature about 425 K; the obtained mass will be re-distributed to surrogate components whose distillation temperatures are above 425 K and below or equal to the distillation temperature corresponds to intersection O, which is about 525 K in this specific case. Physically, we know that the mass deduction of the surrogate component (call it surrogate C) whose distillation temperature is closest to 425 K has dominant effect in changing the shape of the modeled distillation curve at evaporation fraction 0.4. For the current study, we first define the mass reduction amount for surrogate C, which will be the reference for the mass reduction amounts of other surrogate components whose mass will be removed.



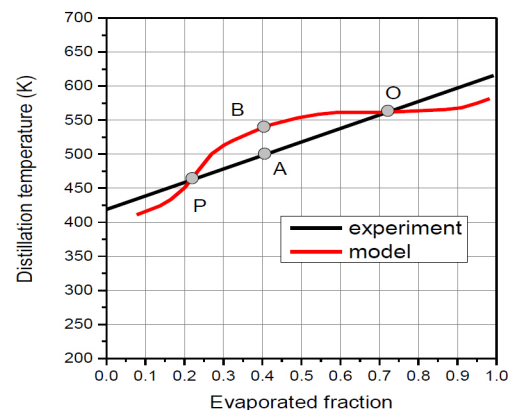
(a)



(b)



(c)



(d)

Figure 4. Schematic diagram when distillation temperature (corresponding to point B) is over predicted compared with experimental distillation temperature (corresponding to point A) at a specific evaporated fraction