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Formulation of optimal surrogate descriptions of fuels considering sensitivities to experimental uncertainties

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ABSTRACT

Transportation fuels consist of a large number of species that belong to different families of compounds. Surrogate fuel representations have been formulated to better understand their fundamental chemical composition and to emulate combustion properties. These descriptions are formulated using experiments or through computations, which has thus led to the existence of two different notions of surrogates. There is further distinction of concepts through the use of physical and chemical surrogates, which are designed to emulate those specific properties. Although several surrogate design methodologies have been proposed in literature, they do not incorporate information on experimental uncertainty. By addressing this issue, it is shown that this information is crucial for the reliable construction of surrogates through computations. To incorporate physical fuel properties, a consistent approach through the use of the recent ASTM D2887 distillation curve standard is discussed. Then, a formal computational procedure is presented that incorporates information of experimental uncertainties into the surrogate description. It is shown that surrogates then describe a feasible region and are hence not unique. Both physical and chemical properties are utilized as combustion property targets (CPTs) and consistency with experimental formulations is demonstrated for JP-8 and Jet-A (POSF 4658) surrogates. In addition, the use of convex optimization puts existing concepts for surrogate representation on a more rigorous basis and several conclusions are drawn, particularly on the importance of specific CPTs and weighting factors of regression-based approaches. Also, the effect of using simplified models for the evaluation of CPTs on the final surrogate composition is shown by considering the example of linear blending rules for ignition delay. Finally, the surrogate representation problem is connected to multi-parametric optimization and bounds on surrogate compositions are calculated as a function of the experimental uncertainty along with comparisons against experimental results.

1. Introduction

Transportation fuels consist of a large number of compounds that affect physical and chemical properties of the mixture. To simplify the complexity, these fuels are often represented by a surrogate description [1], which involves choosing a certain set of compounds, usually present in the original fuel, called *palette* compounds, to closely emulate certain properties of the present fuel. The significant challenge is, however, to determine the specific composition that best emulates relevant properties of interest while keeping the number of compounds small to reduce modeling complexity. The accepted quantities of interest are commonly referred to as combustion property targets (CPTs) [2]. These include both physical and chemical properties, namely density, viscosity, hydrogen-to-carbon ratio, aromaticity and cetane index [3]. Several surrogate studies have pursued these criteria based on empirical correlations or experimental testing [3,4]. Pitz et al. [5,6] reviewed efforts for gasoline and diesel fuels on surrogate formulations, kinetic model development, and experimental validation. Due to compositional variability of original fuels, it is important to choose combustion properties that capture the fuel description while being easy to measure and insensitive to procedural uncertainties. Dooley et al. [7] provided a list of CPTs in an aim to further develop a generic methodology for gas-phase combustion kinetic phenomena. Colket et al. [8] formulated a roadmap for the construction of jet fuel surrogates along with introducing and considering multiple surrogates for a particular fuel, depending on the CPTs.

Currently, two different paradigms of surrogates exist in the literature, namely experimental and computational surrogates. The

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Nomenclature

β	recovered mass fraction
ϵ'_j	relative error threshold for jth CPT
ϵ_j	absolute error threshold for jth CPT
γ_j	sensitivity coefficient
λ_j	dual variable for constraint j
$\mathcal{E}$	ellipsoid
θ_i	threshold sooting index of compound i
$\mathbf{A}$	polyhedron matrix in composition space
$\mathbf{a}_i$	ith row in constraint matrix
$\mathbf{B}$	ellipsoid transformation matrix
$\mathbf{b}$	polyhedron right-hand side in composition space
$\mathbf{l}$	lower bound of hypercuboid
$\mathbf{m}$	molecular weight
$\mathbf{Q}$	ellipsoid quadratic transformation, $\mathbf{Q} = \mathbf{B}\mathbf{B}^T$
$\mathbf{u}$	upper bound of hypercuboid
$\mathbf{v}$	constraint perturbation
$\mathbf{w}$	general point in composition space
$\mathbf{x}$	mole fraction
c_i	number of carbon atoms in species i
d_i	derived cetane number of compound i
f	objective function
F_j	constraint function for jth CPT
h_i	number of hydrogen atoms in species i
N_{nl}	number of nonlinear CPTs
N_s	number of species/compounds in palette
p^*	optimal objective when constraints perturbed by $\mathbf{v}$
p_0	ambient pressure
R	Chebyshev radius
S_j	feasible region for jth CPT
T_0	ambient temperature
t_j	target value for jth CPT
DCN	derived cetane number
+	positive entries
−	negative entries
AA	axis-aligned
DC	distillation curve
HC	H/C ratio
IDT	ignition delay time
in	inner hypercuboid
MV	maximum-volume
MW	molecular weight
TSI	threshold sooting index

former is the more widely adopted approach [7], which uses only experimental procedures to determine CPTs, from which surrogates are then determined. In contrast, the formulation of computational surrogates are a more recent approach and are determined by evaluating CPTs using only simulations. The accuracy of these so-defined computational surrogates in emulating the properties of the fuel dependents on computational models employed, and different modeling approaches can lead to different surrogate specifications; experimental confirmation of these surrogates is therefore necessary to ensure consistency. Reaction Design's *Surrogate Blend Optimizer* utilizes non-linear optimization algorithms to arrive at the surrogate mixture composition. This method was first described in [9] to construct a seven-component fuel blend for modeling gasoline. Several groups [10–12] utilize a computational approach by posing the determination of a surrogate composition as an optimization problem and utilizing both physical and chemical properties as CPTs. Aviation fuel surrogates have been derived using this approach of increasing palette sizes, with upto six-component surrogates being constructed [13]. However, common to all of these methods is the assumption of exact experimental fuel properties and a regression-based objective function that requires a weight for each CPT. This was improved upon more recently by Won et al. [14], by using experimental uncertainties to eliminate certain candidate mixtures formed as a result of discretization of the composition space. Each mixture is verified whether it indeed satisfies the constraints to the specified experimental thresholds, and is used to further narrow down the search space through a global search. Thus, there is a requirement for methods that incorporate and propagate experimental uncertainties to the final surrogate composition in a computationally efficient manner. This paper addresses this issue by providing a rigorous mathematical formulation for the surrogate representation problem along with methods to incorporate information on experimental uncertainty into the final surrogate description, which is shown to be necessary for reliable computational predictions.

Physical property emulation is another subject that requires more investigation in the area of surrogate representation. Violi et al. [3] matched volatility of fuels along with other chemical properties relevant for ignition using experimental techniques. Certain computational approaches for physical property emulation include matching only evaporation [15,16] and distillation characteristics [17–19]. Ahmed et al. [11] utilized a computational approach for constructing surrogate compositions by including both physical and chemical properties. However, the use of experimental distillation curves based on the ASTM D86 standard [20] and advanced distillation curve methodology (ADC) [21], as the descriptor of physical fuel characteristics is questionable due to experimental uncertainties of this approach. Recent advancements in the distillation standard [22] are shown in this paper to offer a solution which is consistent with a computational approach and to provide a viable characterization for distillation.

This paper primarily aims to quantify the effect of experimental uncertainty in the surrogate composition. The use of tools from optimization theory imparts rigor and helps quantifying bounds on compositions as a function of uncertainties. Certain experimental surrogate mixtures are utilized for benchmarks and provide a connection between the computational and experimental surrogate approaches.

Table 1 summarizes the palettes of various jet fuel surrogates used in this paper. The compounds present in these palettes are specifically chosen to be representative of different classes of organic compounds [2], which include n-paraffins, iso-paraffins, cycloparaffins and aromatic compounds. This variation also offers a suitable benchmark for CPT evaluations since a purely computational approach is adopted in this paper. Both 4- and 5-compound surrogates are used to highlight the palette size independence of the approach that will be developed in this paper. Note that the surrogate in Violi et al. [3] differs from both Stanford A and B mixtures [23] only in composition. However, the procedure described is shown to capture the necessary details and distinguish them even when the differences are not immediate. The surrogate due to Dooley et al. [7] relies on higher aromatics and serves as an important benchmark for both the chemical mechanism [24] and physical property evaluations, which is performed based on the group contribution method [25]. This surrogate also represents a different fuel (Jet-A POSF 4658) and is utilized to demonstrate that the procedure developed in the present work is independent of the underlying fuel description.

The remainder of this paper is outlined as follows. The method used to incorporate physical properties and experimental uncertainties is described in detail in Section 2. First, a consistent approach to using distillation curves as a CPT is presented. Subsequently, the incorporation of experimental uncertainties in computational approaches to surrogate representations is discussed. The presented methodology is applied to the construction