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Emission factor estimation in regional air quality studies of residential natural gas fuel interchangeability

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HIGHLIGHTS

- A statistical inference method is developed for natural gas burner emissions data.
- The method is built to compensate for the typically small sample size.
- The method integrates multiple measures of quantified goodness of fit.
- The method provides a means to evaluate and report confidence of the result.
- Estimates are developed for changes in emissions as functions of Wobbe Number.

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ABSTRACT

Natural gas is a ubiquitous fuel, obtained from a variety of source deposits that present an inherent variation in composition. As newer sources of natural gas become available (such as Liquefied Natural Gas and shale gas) the compositional variation is expected to increase, which can affect emissions during combustion in appliances, including criteria pollutants. Unfortunately, experimental observations of the effect of natural gas composition on combustion products are sparse due to the wide range of burner designs and high cost of experimentation. The current work develops a rigorous methodology for statistical inference on available data that accounts for the limited nature of experimental observations. The goal is to overcome data size and quality limitations and provide best estimates of emission response to fuel composition change by identifying a continuous probability distribution with a high likelihood of representing the data and high correlation to the experimental observations. Quantitative measures of agreement between the data and a set of candidate distributions form the basis of the evaluation. In addition, qualitative assessment of the reliability of distribution identification is derived from a quantitative rating system for desired features of the data set and chosen distribution. Finally, this methodology is applied to sample data from the Lawrence Berkeley National Laboratory to develop a comprehensive and self-consistent set of emission factor estimates applicable to investigations of modeling the effect of natural gas interchangeability on urban air quality. By following the developed process, representative distributions, ranges of estimates, and evaluations of the estimate reliability are obtained for changes in CO, NO_x, NO_2, and HCHO emissions as a function of change in fuel Wobbe Number for six classifications of residential appliances.

1. Introduction

Simulation of air quality impacts in urban airsheds is a widely-used and valuable tool in understanding the impacts of human activity on the atmosphere. Modeling studies inform the research community of likely causes and physical bases of observed atmospheric phenomena and are relied upon by regulatory agencies for guidance in developing new legislation. Studies developing baseline emissions profiles to account for modern levels of human industry, transportation, and other activity have been a crucial scientific tool for regulating agencies to determine emission reduction goals. Furthermore, modeling builds cases for understanding why emission reductions need to be implemented. It is also of interest to understand and anticipate what the effects will be of scenarios that consider changes to baseline emissions. New industry utilizing well-known equipment, phasing in and out of fuel sources, and new industry utilizing newly-developed technology are typical scenarios of interest to regulatory agencies wishing to understand the potential impacts before they become egregious and difficult to curtail.

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Investigating the regional impact of emissions changes involves three major components that must be synthesized to provide a meaningful and appropriately framed prediction, as shown in Fig. 1. The first is the definition of the air quality model itself, including physical models, solution methodology, and baseline emissions. The second is the development of scenario test cases to capture the emissions perturbations that reflect the researcher's objectives. The final input parameter establishes, via measurement or estimation, the emissions factors for the known energy conversion devices in the region, especially as they are affected by the defined perturbation. In investigations of fuel interchangeability, the perturbation is a change in the composition of the fuel.

The current work focuses on the last of these three aspects. In an ideal case, an investigator has detailed knowledge of all energy conversion devices in the region, including (averaged or representative) emission rates for all species of interest. For example, the sum of all home hot water heaters' CO emissions within each node of the simulation domain could be specified. In reality, especially for devices within the residential sector, estimates must be made based on assumptions of the type and number of burners. The bases for the estimates include demographic and land use information as well as available representative emissions rates. Without knowledge of the exact make, model, and operating condition of each device in each home, estimates based on demographic information provide a means to utilize the best data available. However, quantifying emissions factors specific to each burner technology is often difficult, especially for cases that consider off-design operation.

There is therefore a need to develop a methodology for defining technology-dependent estimates of emission sensitivity from limited experimental data. The current work investigates the particular case of natural gas interchangeability, and estimates the changes in emission factors as the composition of the regional natural gas supply is altered. Important to the methodology is an adherence to two major goals in statistical inference: (1) Identification of a model distribution for the data with substantial probability of being a proper representative, and (2) the model and data correlate well. The method is applied to analyze data for residential burners, which will be critical to understand within the South Coast Air Basin of California, where forecasted introduction of new gas sources will alter the composition of residential natural gas [1,2].

Following a brief review of the current state of natural gas interchangeability measures in Section 2, Section 3 presents the analysis methodology. Section 3.1 introduces the source data and demonstrates the need for a rigorous model distribution selection process. Section 3.2 presents the model distribution selection process, 3.3 discusses the method of estimating emission factor changes once a model distribution is chosen, and 3.4 provides an overview of the reliability rating method. Section 4 presents sample results from the distribution selection process, indicates the selected distributions for all data sets along with their reliability scores, and provides in-depth analysis of the cases determined to be non-normal. Additionally, Section 4 provides the final estimates of emission factor changes and provides a comparison to sample daily emissions estimates in the South Coast Air Basin of California.

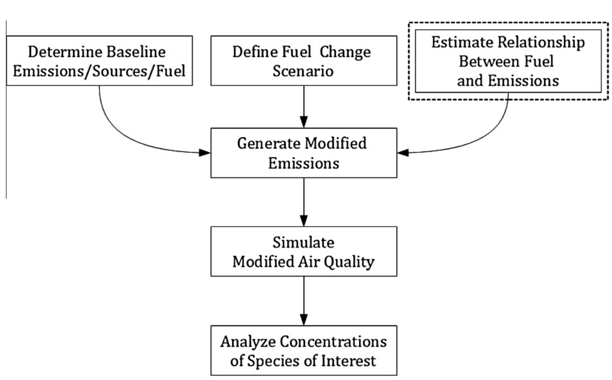

Fig. 1. Workflow in simulating regional air quality changes due to local changes in natural gas supply. Dashed box indicates the portion of the process that is the focus of the current work.

2. Background

As defined by the Gas Interchangeability Task Group, gas interchangeability is "the ability to substitute one gaseous fuel for another in a combustion application without materially changing operational safety, efficiency, performance or materially increasing air pollutant emissions" [3]. It is particularly important to note that interchangeability is not based on the fuel properties alone, but explicitly on the in-operation performance and behavior of the fuel in installed devices. Thus, interchangeability indices and standards are also based on testing appliances after manufacturing and installation. Definitions created in such a manner allow for assurance that the interchangeability limits apply to a wide range of end-use scenarios and configurations. Historically, the focus of interchangeability tests has been devoted largely to residential appliances, due to the fact that residential consumers account for a large percentage of total US natural gas consumers [4–9].

Changes in the natural gas composition delivered to residential devices can affect the safe operation, reliability, and ultimate lifespan of their incorporated burners. Altering the chemical makeup of the fuel can result in off-design operation. Stability issues such as flashback and blowout may cause reduced reliability or potentially hazardous operation [4–10]. Reshaping of the flame itself may occur as a result of changes in heat content and fluid properties. As a result, unexpected impingement with the burner's solid walls and quenching of the flame accelerate wear and degradation and alter emissions levels. Of particular concern are products of incomplete combustion, such as carbon monoxide, which directly cause human health concerns and device reliability issues [4–9]. Additionally, the amount of entrained or forced air may be insufficient and result in higher flame temperatures which lead to soot (a constituent of total particulate matter) [4–10]. Finally, NO_x formation is governed by complex thermally-controlled reactions and can thus be affected by fuel composition. NO_2 is of particular concern due to its role as a tropospheric ozone-forming photochemical oxidant and respiratory irritant.

Empirical evaluation of flame and emissions changes is difficult and often specific to individual burner design. In addition, issues of reliability often require extensive and long-term testing that can be logistically challenging and costly [6]. To avoid these difficulties, qualitative measures are used in the field to indicate proper performance. For example, yellow tipping (when the tip of the flame shifts in visible color from blue to yellow due to a change in temperature) indicates both CO and soot production [4–9]. Although ubiquitous in the field, this solution has limited utility for research requiring detailed emissions information.

Thus, a number of researchers have developed methods to address properly the subtleties and details of interchangeability [11–13]. However, the data still have significant limitations. The most pressing of these shortcomings is data size and breadth, since there have not been many comprehensive studies to date. Additionally, the definition of the interchangeability inherently refers to burner designs and appliance performance in operation according to design and tuning specifications. Thus, fundamental and theoretical studies cannot be applied directly as strict predictors of interchangeability. Therefore a need exists to develop methods of predicting emission changes due to natural gas composition that are based on limited experimental data sets and to provide