Docket #: S19-133

Streamlined method for estimating hydrocarbon fuel properties using a compact, economical Fourier Transformation Infrared-based (FTIR) analyzer

Stanford researchers have developed a streamlined method for simultaneously estimating a broad range of hydrocarbon fuel physical and chemical properties for a wide range of fuels. These properties are estimated with vapor-phase mid-infrared spectra (measured using a commercially-accessible FTIR spectrometer) and machine learning models.
This invention could be used to provide fast, accurate, and economical estimations of hydrocarbon fuels' properties with small amount of sample during the early stage of alternative fuel development. It has the potential to expedite the process of alternative fuel certification, which is one major hurdle for market acceleration of the global alternative fuel and hybrid vehicle industry.

Stage of Research

- **Proof-of-concept**
- The team demonstrated that mid-infrared spectra together with regularized linear models trained with a dataset consisting of 64 hydrocarbon fuels can accurately estimate 15 physical and chemical properties
- Ongoing research to extend wavelength range and to analyze more parameters

Applications

- **This compact and economical FTIR based analyzer can:**

    - Make estimations on fuel properties
    - Perform classification on fuel types
    - Infer scientific information
- Estimations can be used as an **early-screening tool** by reducing false positives

Advantages

- **Promotes alternative hydrocarbon fuels** which causes less emission and more sustainability
- **Analyzes broad range of fuel properties for a wide range of fuels.** Currently 15 properties and 64 different fuels
- **Requires small amount of fuel sample**
- **Physical and chemical properties analyzed include:** total number of carbon and hydrogen per average molecule, molecular weight, hydrogen to carbon ratio, initial boiling point, density, surface tension, net heat of combustion, C2H4 yield, flashpoint, lean blowout, derived cetane number, ignition delay time, kinematic viscosity, total cycloparaffin weight percentage
- **Fast and accurate estimation process** (linear combinations of absorption cross sections)
- **Easy to use** in practice
- **Can streamline the process of alternative fuel certification**, which can help accelerate the global alternative fuel and hybrid vehicle market
- **Large market size** for alternative fuels - $614 billion by 2022, 3% of U.S. GDP in 2017

Publications

- Wang, Yu, Yiming Ding, Wei Wei, Yi Cao, David F. Davidson, and Ronald K. Hanson. "On estimating physical and chemical properties of hydrocarbon fuels using mid-infrared FTIR spectra and regularized linear models." Fuel 255 (2019): 115715.

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