Yield Sooting Index (YSI) Primer and Bibliography

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1 Purpose

Yield Sooting Index (YSI) characterizes the intrinsic chemical propensity of a pure compound or a fuel mixture to produce soot in a combustion environment. This property strongly affects the fuel-to-fuel variations in particulate emissions from engines, powerplants, and other combustion devices. Thus YSI data is valuable for predicting the emissions benefits (or drawbacks) of proposed fuels.

While chemical sooting propensity always impacts the potential range of particulate emissions, other fuel properties—such as volatility and cetane number—may be important as well for particular devices. These other properties can be combined with chemical sooting propensity into "emission indices" to predict the relative emissions from different fuels in a specific device. For example, the Particulate Mass Index (PMI) of Aikawa et al. estimates the soot emissions from Gasoline Direct-Injection (GDI) engines based on chemical sooting propensity—as measured by Double Bond Equivalent (DBE)—and volatility—as measured by vapor pressure—of the fuel's components [1].

2 Definition

YSI is measured by sequentially doping the fuel of a methane/air coflow nonpremixed flame with equal concentrations of the test fuel and with two index compounds. The dopant concentration is chosen to be sufficiently small that the dopants do not change the flame size and shape, temperature distributions, etc. The index compounds are usually *n*-heptane and toluene, but other choices may be more appropriate for a given situation; e.g., benzene and phenanthrene for aromatic test compounds with multiple rings.

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The maximum soot concentration $S_{\max}$ is measured in each of the three flames, then the YSI of the test fuel is calculated from equation (1), where A and B are constants chosen so that the YSI's calculated for the two index compounds have the correct values from the database.

$$\text{YSI} = A \times S_{\max} + B \tag{1}$$

$S_{\max}$ is typically defined as either the maximum soot volume fraction at any point in the flame, the maximum radially-integrated soot volume fraction at any height in the flame, or the maximum line-of-sight luminosity at any height in the flame.

3 Volume 2 versus Volume 1

Volume 1 of this database contained two mutually-incompatible sub-databases. The first was a "low-scale" database for compounds with low sooting tendency (primarily alkanes, cycloalkanes, and oxygenates). The second was a "high-scale" database for compounds with high sooting tendency (primarily aromatic hydrocarbons). These two incompatible scales were necessary because the total range of sooting tendencies—from the one-carbon oxygenate methanol to the four-ring aromatics pyrene and fluoranthene—was too large for accurate measurements at both ends with the existing soot measurement techniques.

However, we have subsequently implemented a color-ratio pyrometry diagnostic that is based on consumer digital camera technology and has a much greater dynamic range [2] [3]. With this diagnostic we were able to measure a range of compounds from each database in a single experiment and create a "unified database" that includes all of the compounds in a single scale. Volume 2 presents that database. Details of the procedure are discussed in a paper that is in preparation [4]; this Primer will be updated when that paper has been accepted.

4 YSI-molar versus YSI-mass

The YSI procedure requires doping the base flame with equal concentrations of the test and index compounds, but "equal concentrations" can be defined in different ways. In our earliest work it was defined in terms of mole fraction, e.g., the mole fraction of each dopant in the fuel mixture = 1000 ppm. However, adding a fixed mole fraction requires knowing the molecular weight of the dopant; for pure hydrocarbons this is no problem, but for practical fuel mixtures the molecular weight may not be available. Therefore, when we began studying real fuels we switched to defining the dopant concentration in terms of mass, e.g., the mass fraction of each dopant in the fuel mixture = 0.5 %.

To prevent confusion, we are now referring to these two types of measurements as "YSI-molar" and "YSI-mass". All of the results in this database are YSI-molar.

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6 YSI Bibliography

Tables 1 and 2 list articles and presentations related to YSI from our group and from others.

Table 1: List of YSI measurements from Yale

Ref	Scale	Mode	Test Compounds
[5]	high	YSI_{molar}	one-ring aromatic hydrocarbons
[6]	high	YSI_{molar}	multi-ring aromatic hydrocarbons
[7]	low	YSI_{molar}	oxygenates, alkanes, alkenes, cycloalkanes
[8]	low	YSI_{molar}	unsaturated esters
[4]	unified	YSI_{molar}	oxygenates through multi-ring aromatics
[3], [9]	low	YSI_{mass}	diesel fuels and surrogates

Table 2: List of general YSI literature

Ref	Comments
[10]	numerical simulation of measured YSI's
[11]	predictive QSPR model of measured YSI's

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