Yale GRADUATE SCHOOL OF ARTS AND SCIENCES

Sooting Tendencies of Phenolic Hydrocarbons

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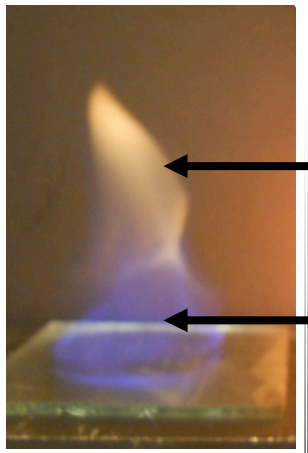
March 23, 2020

Soot and Chemistry

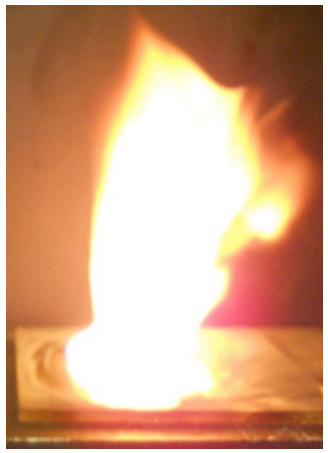
Reaction Pathways for Ethanol and Benzene.



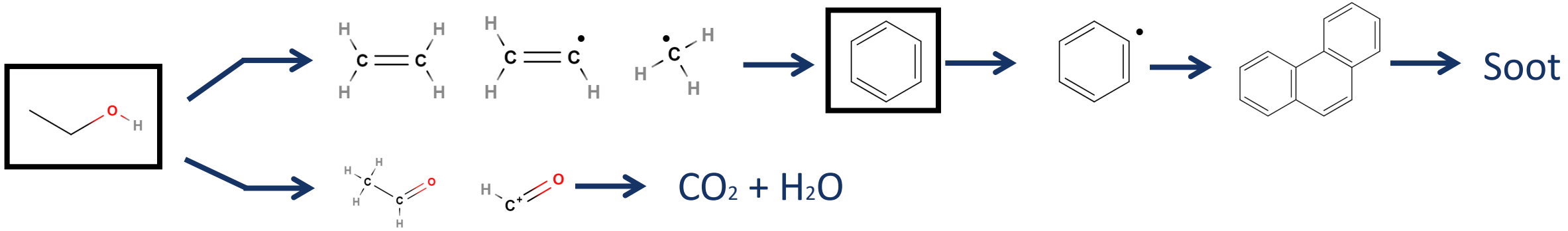
Soot's black body Radiation

Chemiluminescence

Ethanol



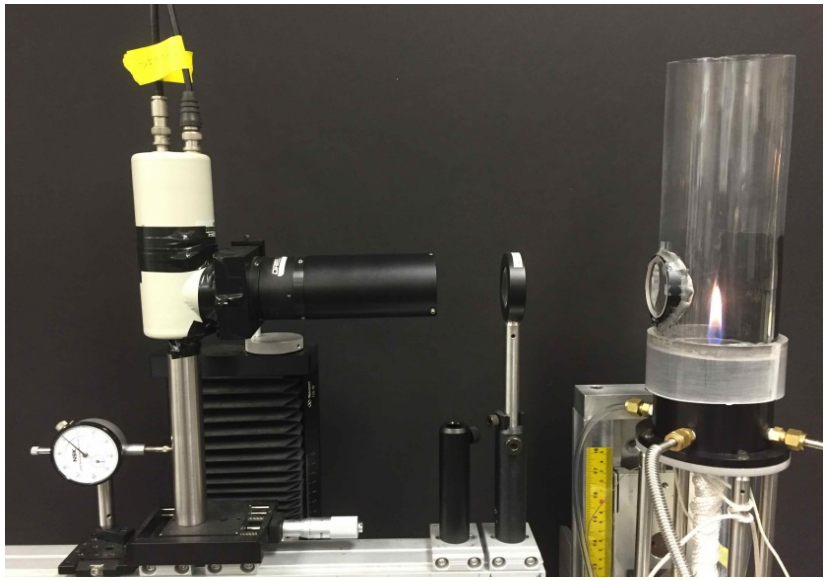
Benzene

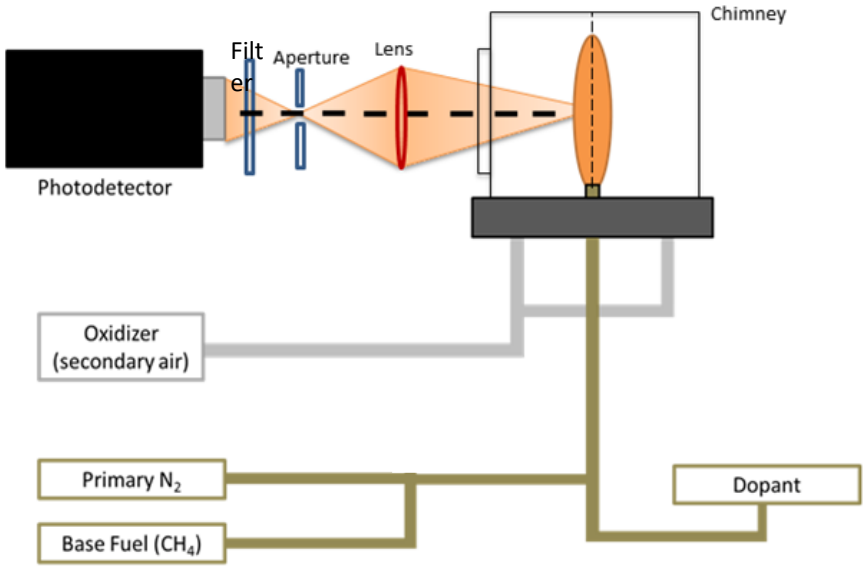


What is Yield Sooting Index?

Yield Sooting Index (YSI) characterizes the influence of molecular structure on soot formation rates in combustion devices.

If a chemical compound has a larger YSI number, it will generate more soot in combustion devices.





Test compound	1000 ppm
Methane	40 % by mass
Nitrogen	balance

How we define the YSI?

Line-of-sight spectral radiance

$$LSSR\ Signal = \int dV * B(\lambda, T) * \varepsilon * \eta * f_v$$

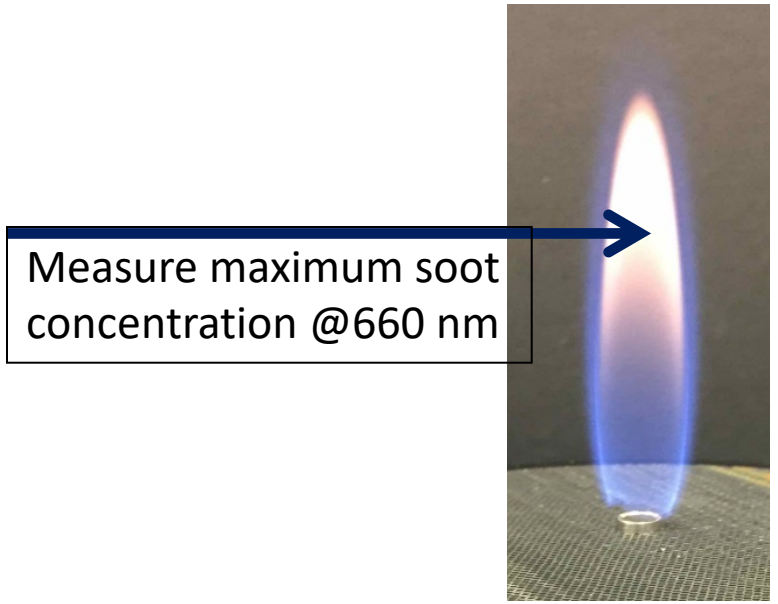
$\boldsymbol{B(\lambda,T)}$- Term describing blackbody radiation from soot particles, depends on wavelength and temperature

$\boldsymbol{dV}$ - Volume element over which the collected signal is integrated

$\boldsymbol{\varepsilon}$ - Emissivity term for soot particles

$\boldsymbol{\eta}$ - Efficiency of the filter and detector

$\boldsymbol{f\_v}$ - Soot volume fraction



Why solid YSI?

Objective:

Measure the sooting tendencies of lignin-derived phenols, compare them to the aromatic hydrocarbons that are found in current fuels.

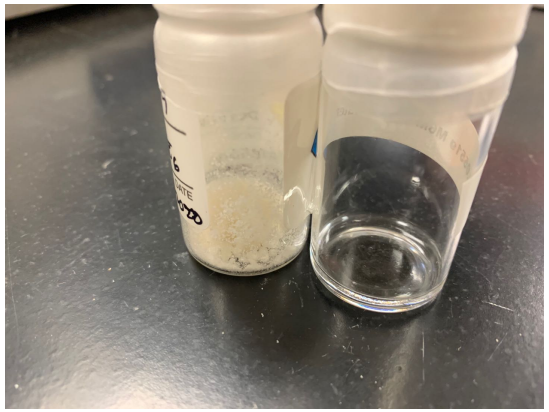
Challenge:

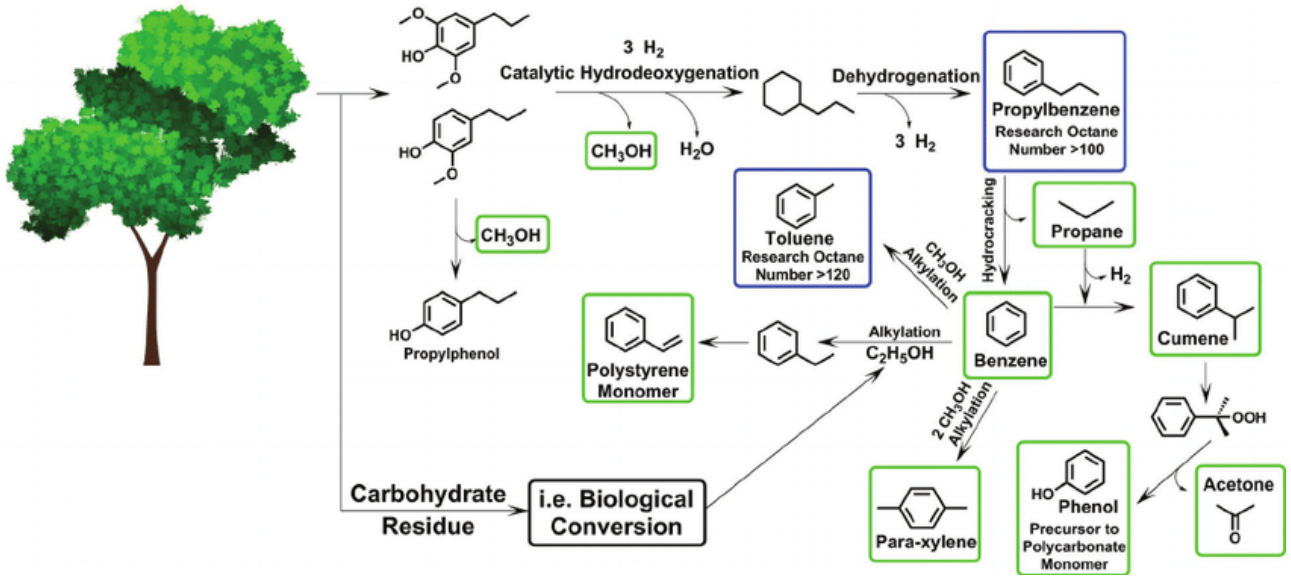
Many lignin-derived phenols are solid at room temperature and our normal approach cannot deal with solid chemical compound.

Solution:

We developed a solid YSI approach to solve it.

Solid and its solution:



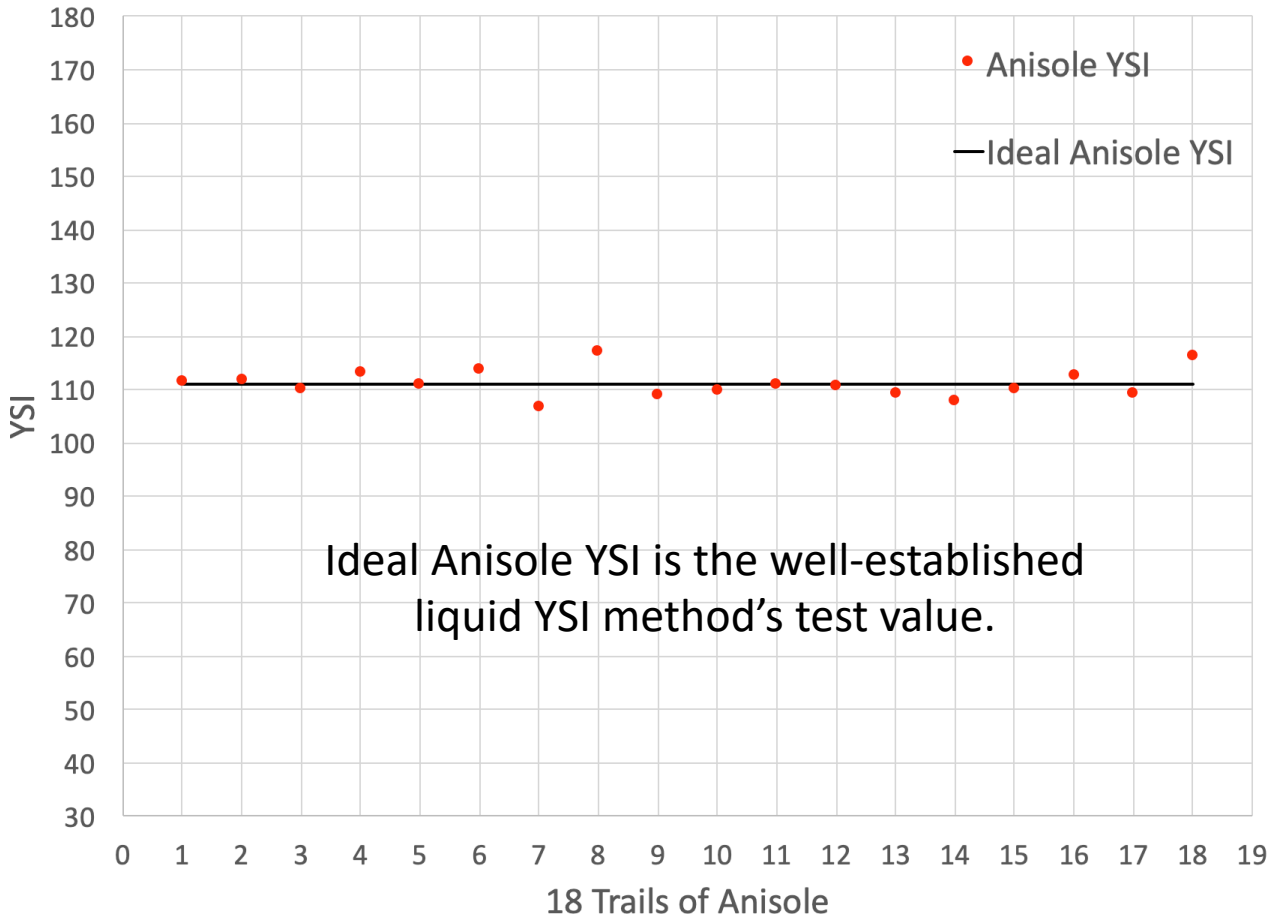


A synergistic biorefinery based on catalytic conversion of lignin prior to cellulose starting from lignocellulosic biomass - Scientific Figure on ResearchGate.

Solid YSI Method and Validation

Solid YSI Measurement Method:

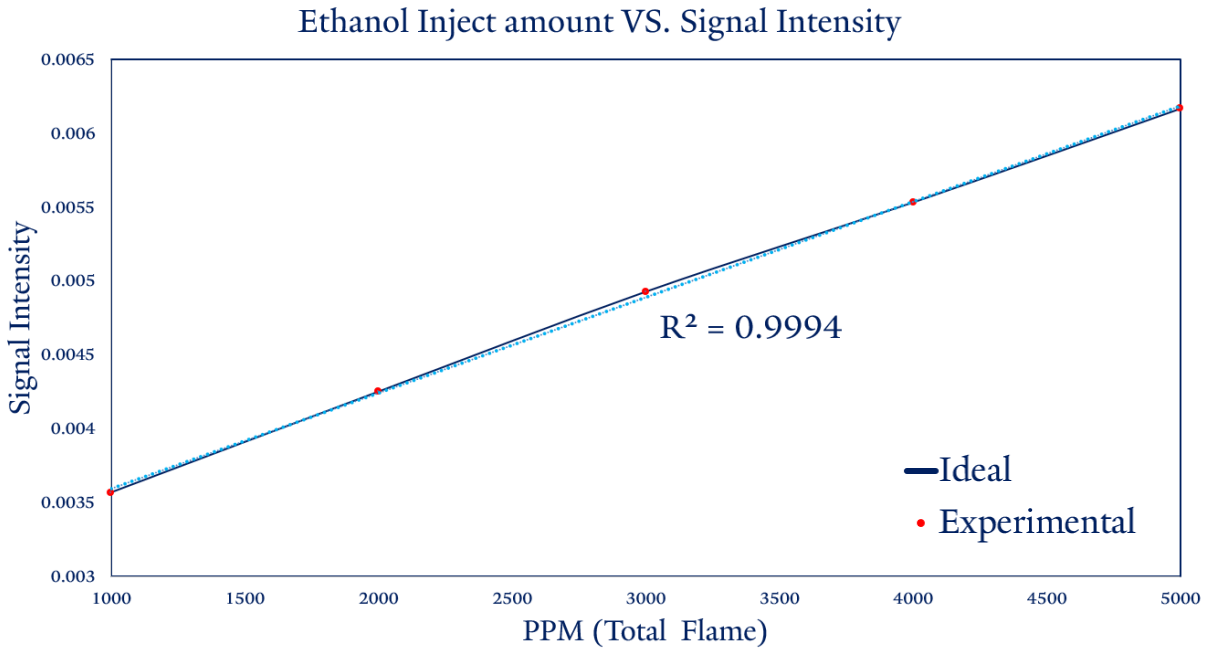
1. Make a 1:4(dope: ethanol) ratio mixture.
2. Measure density of this mixture, which is essential for the calculation of dope concentration in flame.
3. Test the mixture in flame with 5000 ppm.



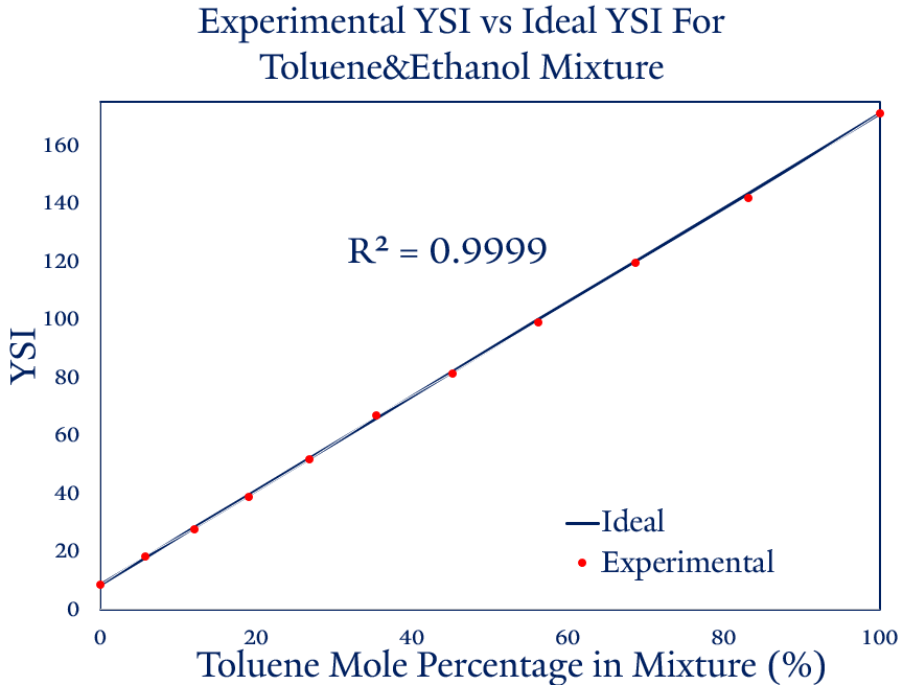
18 Anisole Trails Mean YSI: 111.23
Ideal Anisole YSI: 111.0

Experimental Data Support

Radicals' contribution to YSI does not interact with each other.



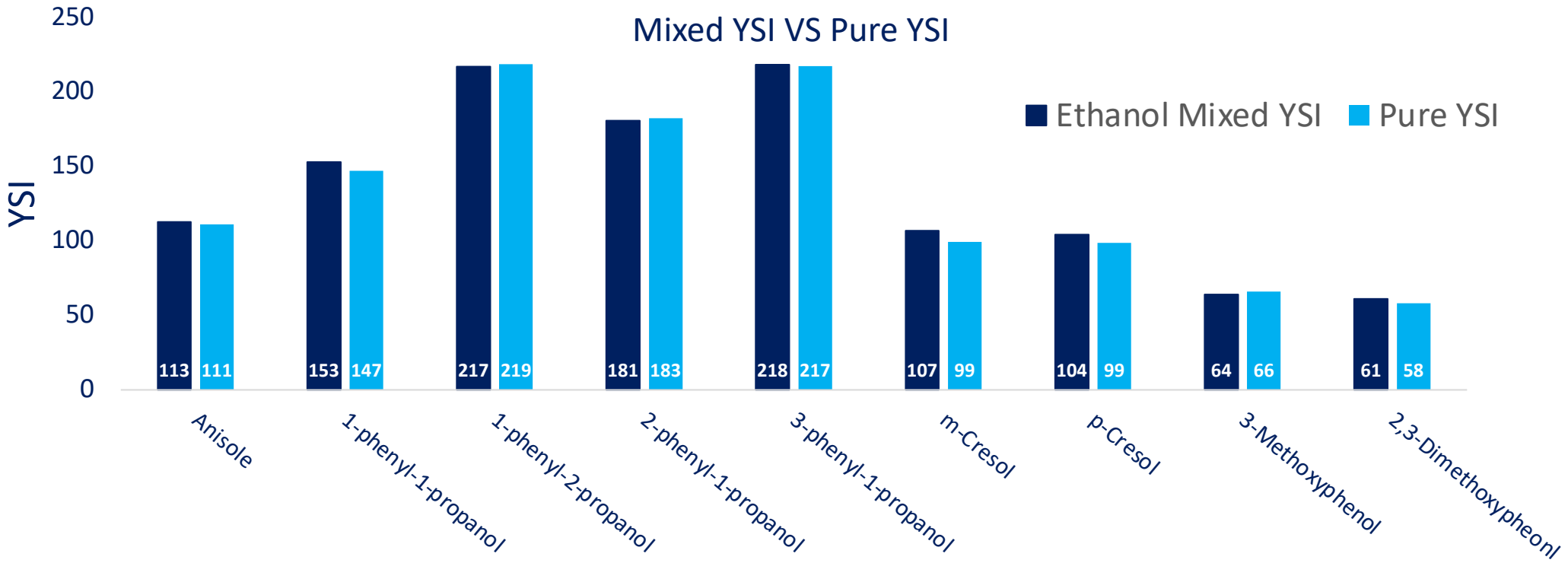
Increase the doping concentration 5 times, YSI still keep a good linearity.



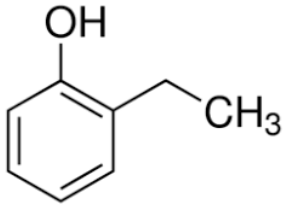
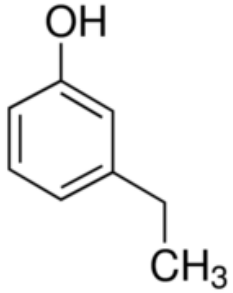
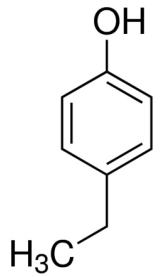
Mix different chemicals at different ratio, YSI still keep a good linearity.

Method Validation

Experimental Data Support



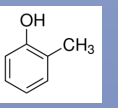
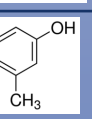
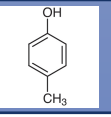
Ethylphenol example

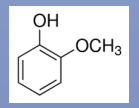
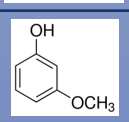
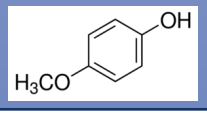
	2-Ethylphenol	3-Ethylphenol	4-Ethylphenol
			
Trial 1:	116.96	125.81	121.94
Trial 2:	117.51	140.69	133.30
Trial 3:	122.34	137.80	132.40
Final YSI result:	Mean **118.94**	Mean **134.77**	Mean **129.21**

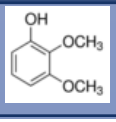
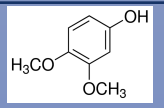
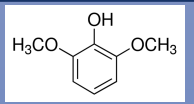
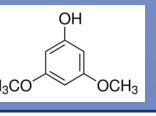
Solid YSI Result Summary

1. Slightly increase oxygen concentration in a molecule can decrease its YSI.

2. Computational study is under planning for this.

Compound	Structure	YSI
m-cresol		107.0
o-cresol		101.9
p-cresol		104.4

Compound	Structure	YSI
2-Methoxyphenol		64.0
3-Methoxyphenol		64.1
4-Methoxyphenol		54.9

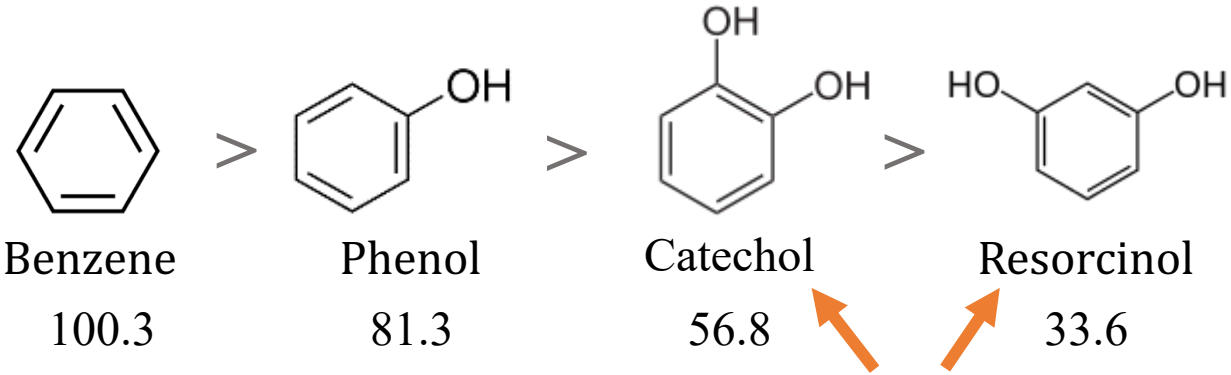
Compound	Structure	YSI
2,3-Dimethoxyphenol		61.3
3,4-Dimethoxyphenol		49.5
2,6-Dimethoxyphenol		63.3
3,5-Dimethoxyphenol		50.8

Something more interesting

Our recent results shows:

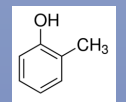
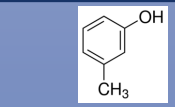
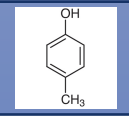
1) increase –OH function group, the YSI will be lower.

2) the position of -OH function groups have high impact on the YSI.



–OH function position have a high impact!

For now, we do not have a deep understanding on why for some compounds, the –OH function groups position matter more than others. We are continue looking insight this question.

Compound	Structure	YSI
m-cresol		107.0
o-cresol		101.9
p-cresol		104.4

–OH function position have a low impact

Acknowledgements

This material is based upon work supported as part of the Co-Optimization of Fuels & Engines (Co-Optima) project sponsored by the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy (EERE) under the Bioenergy Technologies Office (BETO) and Vehicle Technologies Office (VTO) Program Award Number DE-EE0007983.