"Low Level Sulfur Detection"

Quantitation of Low-Level Sulfur in Middle Distillate Fuels by ICP-MS Project 105

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ASCENT

Project 105

Low-Level Sulfur Detection

University of Dayton Research Institute

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PM: Ana Gabrielian

Cost Share Partner(s): Airlines, OEMs, Fuel Producers

Objective:

Development of an ICP-MS method capable of quantitating low levels of sulfur in middle distillate fuels—Target concentration range from 10s of parts-per-billion (ppb) to 10s of parts-per-million (ppm)

Project Benefits:

Improved sulfur detection limits over currently available methods supporting SATF candidate fuel testing and approval, advancement of low-sulfur fuel standards, and generation of data supporting research efforts such as CLEEN with partners like NASA and Boeing.

Durability, Performance, Health, and Stealth

Research Approach:

- Measuring sulfur in fuel samples by ICP-MS is especially difficult for several reasons including:
  - Low ionization efficiency for sulfur in an argon plasma
  - High coking potential for fuel samples
  - Significant isobaric interference
- Collision Cell Technology (CCT) is implemented to react sulfur ions with oxygen gas to form sulfur oxide ions which can be detected in a less-crowded mass channel (m/z = 48)
- Using ASTM D8110-25 as a guide for developing an ASTM-Approvable ICP-MS method.

Major Accomplishments (to date):

Draft method established with good performance across a variety of fuels in the 100s of ppb to low-ppm range.

Future Work / Schedule:

- Refine method, finalize performance statistics, conduct multi-lab robustness study, apply method to broader range of SATF/SBC fuels
- Incorporate non-interfering internal standard
- Publish as official UDRI Method

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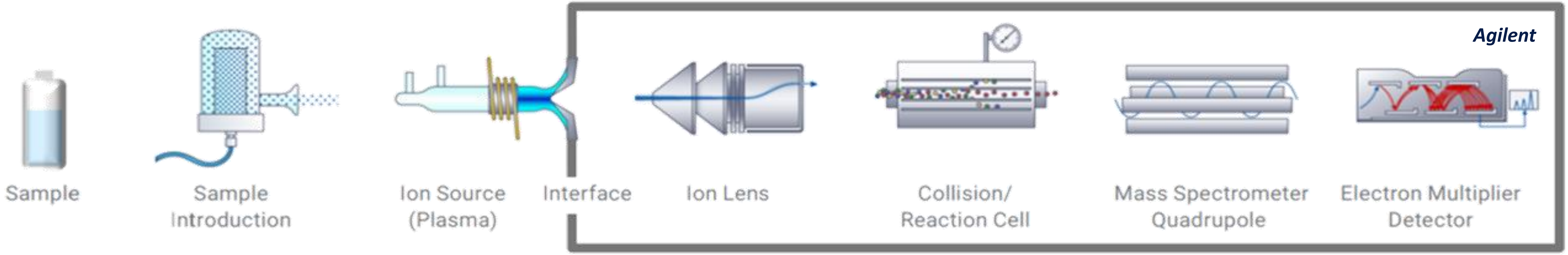
Introduction – why are we doing this?

- Reduced sulfur content in jet fuel supports durability, performance, health, and stealth.
- Legacy Sulfur Test Methods and Specifications only reach a few ppm (mg/kg).
- Existing ICP methods don't measure sulfur.
- Think of this as a research tool.

Method Number	Lower Limit [S]	Measurement	Use Case (Sulfur)
D5453	1 mg/kg	UV Fluorescence	D1655, D7566
D2622	3 mg/kg	Wavelength Dispersive X-Ray Fluorescence (XRF)	D1655, D7566
D4294	16 mg/kg	Energy Dispersive XRF	D1655, D7566
D1266	100 (5*) mg/kg	Lamp	Withdrawn 2025
IP 336	300 mg/kg	Energy Dispersive XRF	D1655, D7566
D7111	N/A	ICP-Atomic Emission Spectroscopy	N/A – Metals
D8110	N/A	ICP-Mass Spec	N/A – Metals

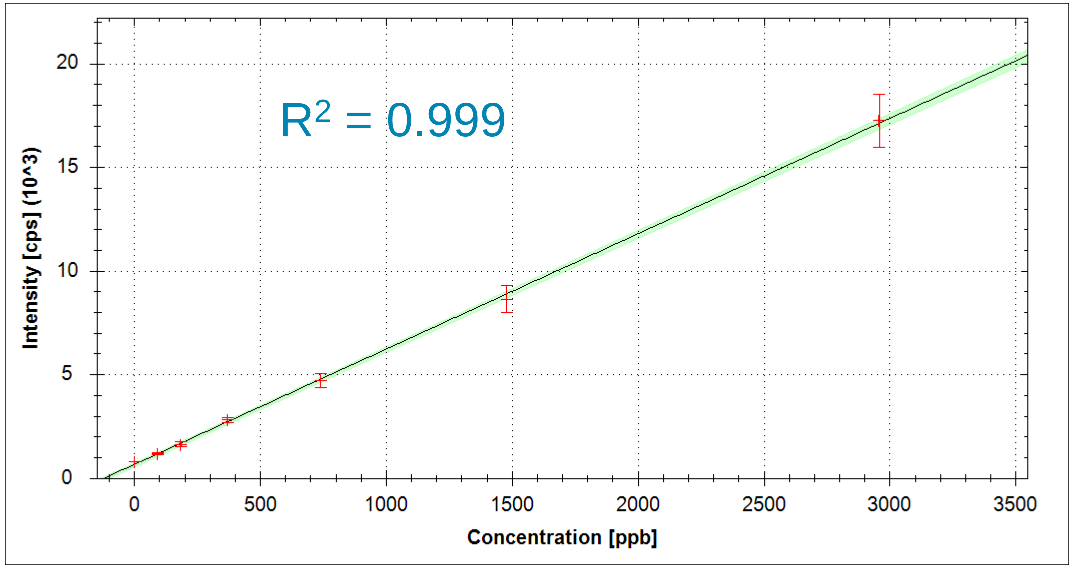
Introduction: Technique Overview



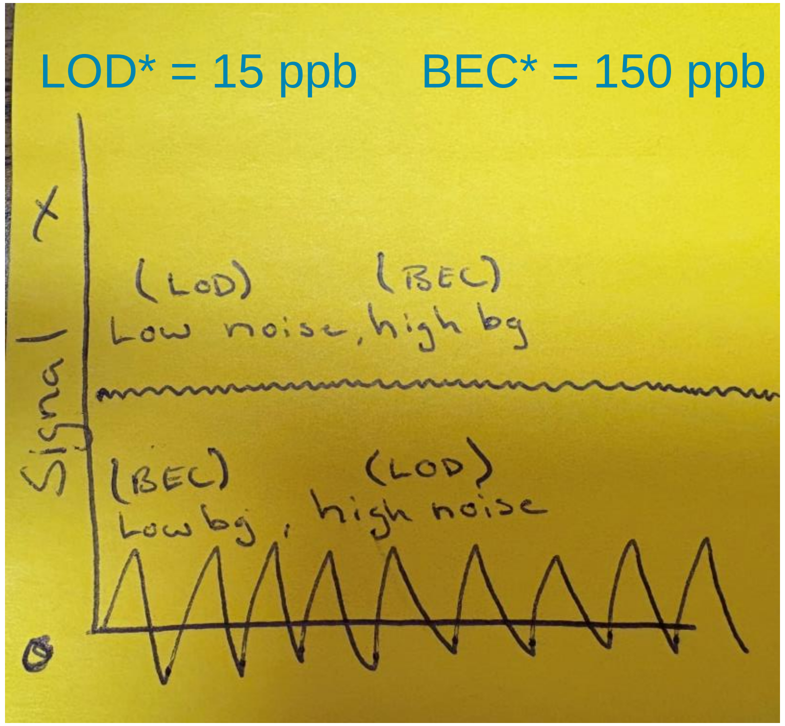
- Sulfur has high ionization energy (10.4 eV)
  - Only ~10% ionized in “standard plasma”
- Sulfur is light and inefficiently transported by ion optics.
- High-Carbon Matrix (Jet Fuel) requires addition of $^{16}O_2$ (m/z = 32)
  - $^{16}O_2$ = Isobaric Interference with ^{32}S
- $^{32}S^{16}O^{+}$ (m/z = 48) easy to make
  - Not obscured by $^{16}O_2$
  - ^{36}Ar + ^{12}C (m/z 48) *may* interfere

Show me the Data!

- Developed ICP-MS method to detect S as SO
- 6 Cal Standards (100 – 3000 ppb)
- Good precision (repeatability)
- Accuracy & Robustness testing underway

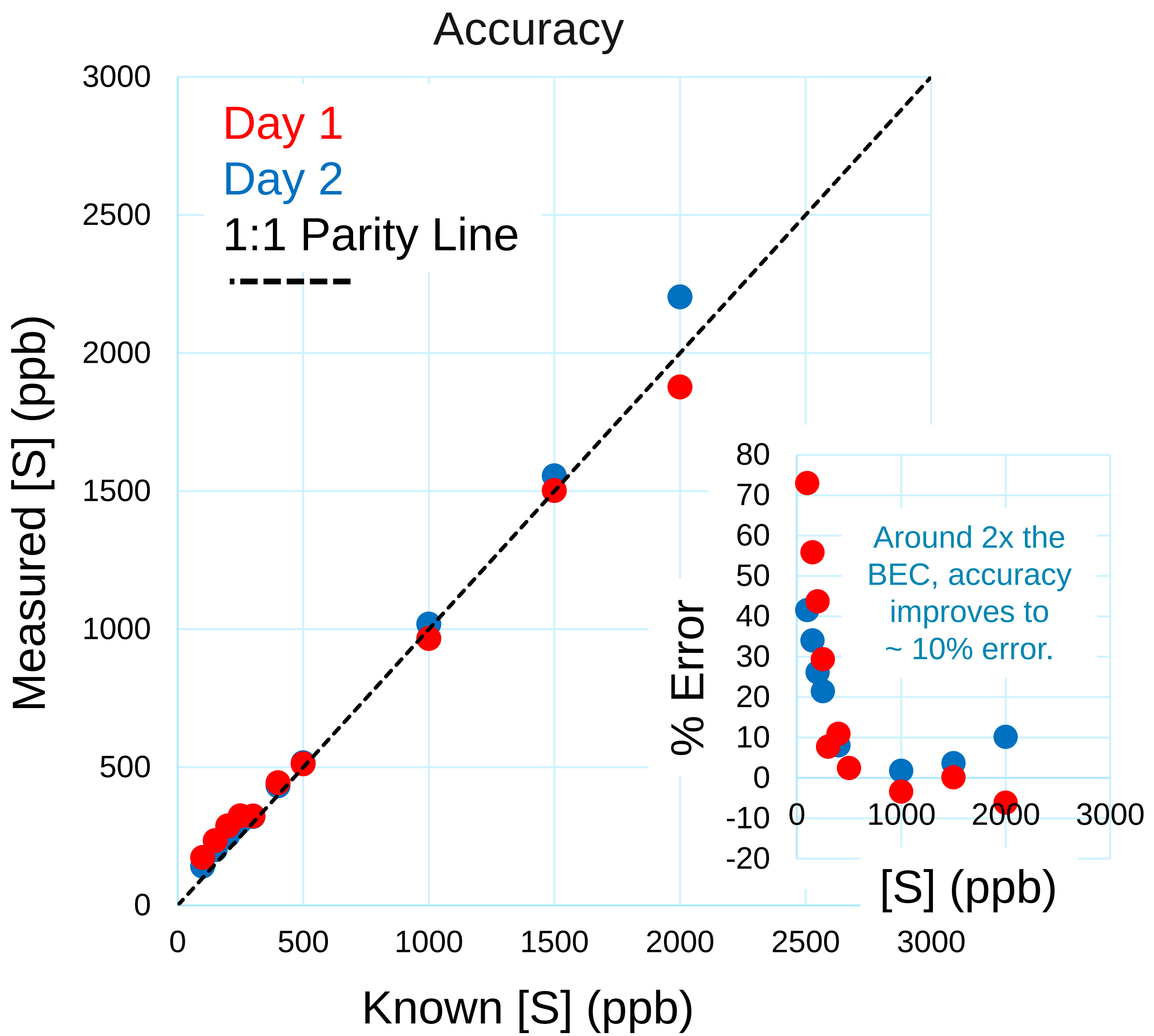


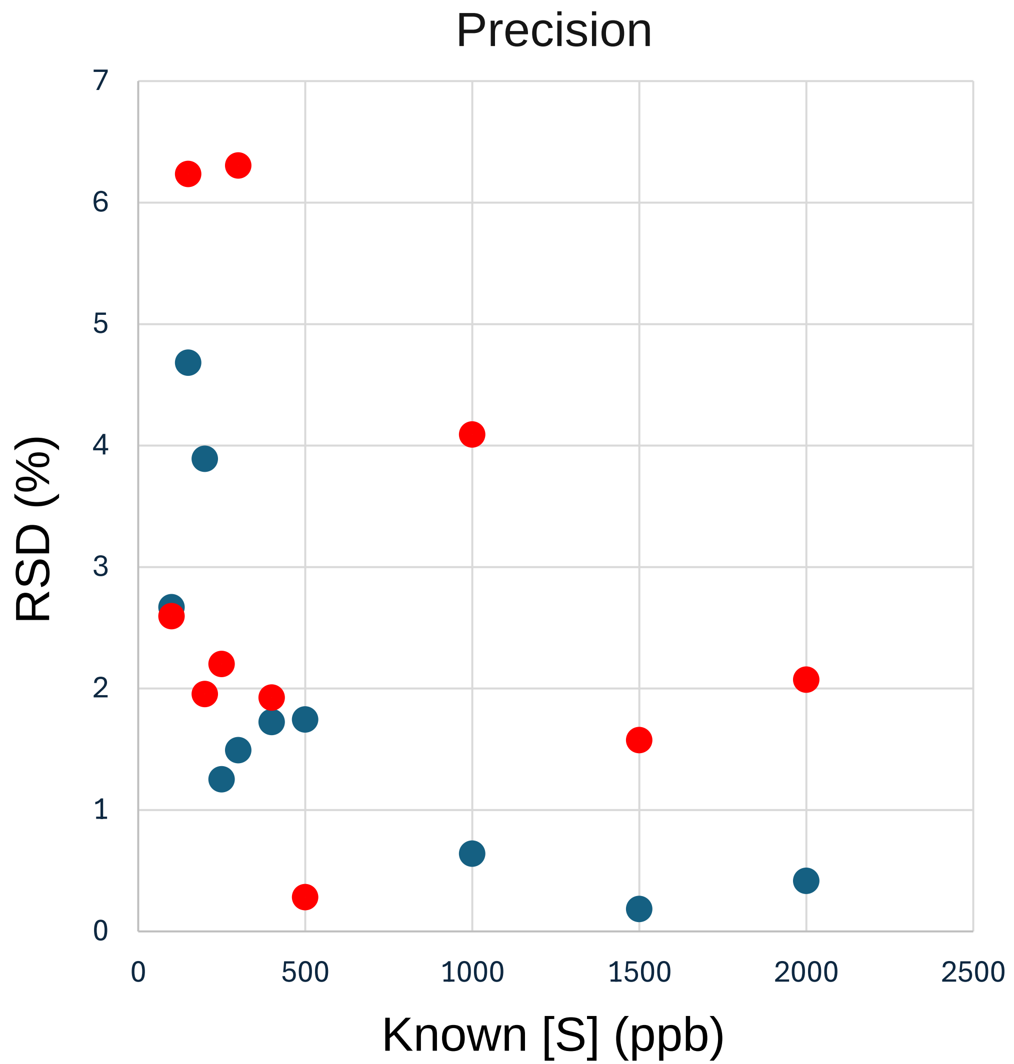
Calibration standards are made by diluting a Specpure 5000 µg/g Sulfur (Dibutyl Sulfide) standard in Kerosene.



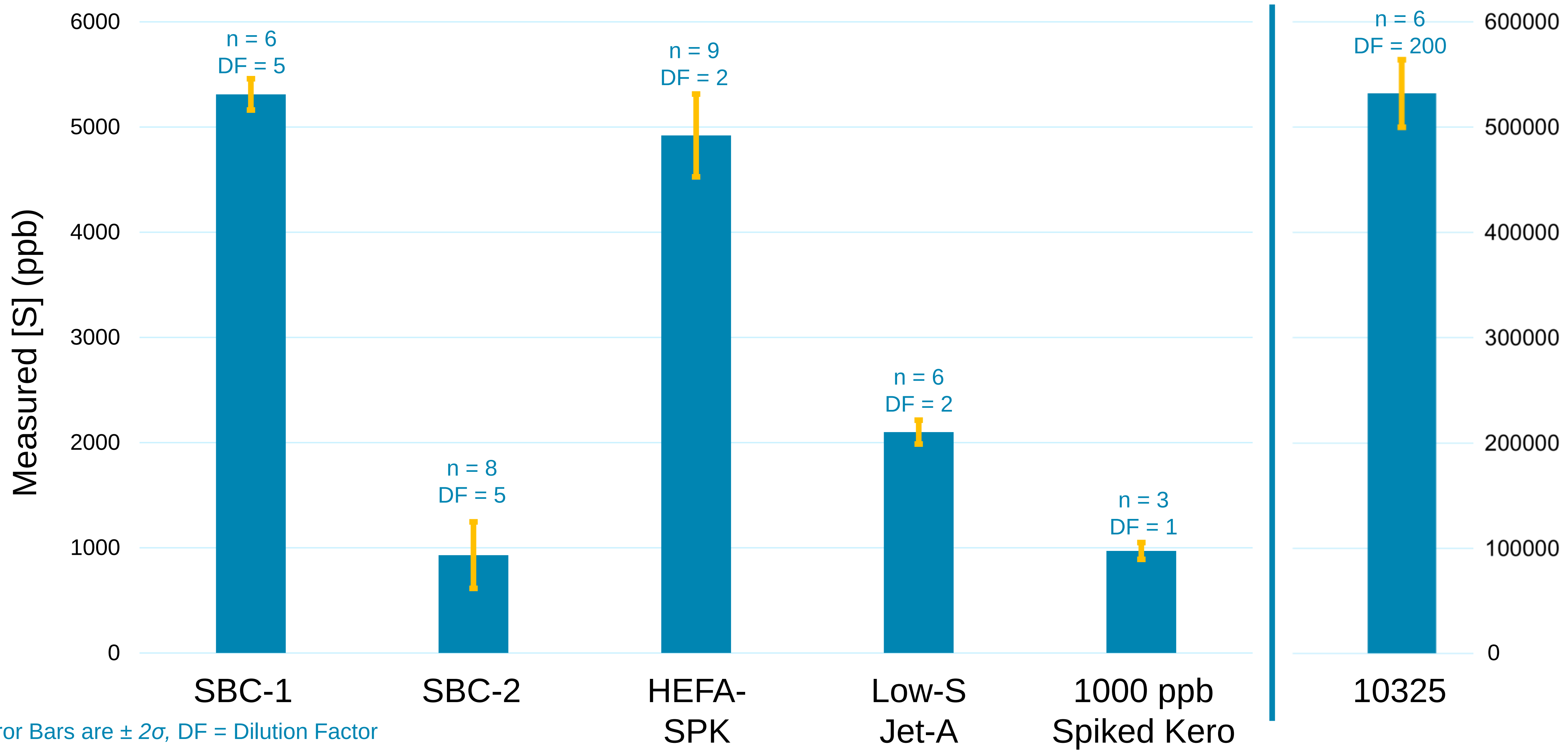
*Calculated by instrument software package

Sulfur Calibration – Spike Test



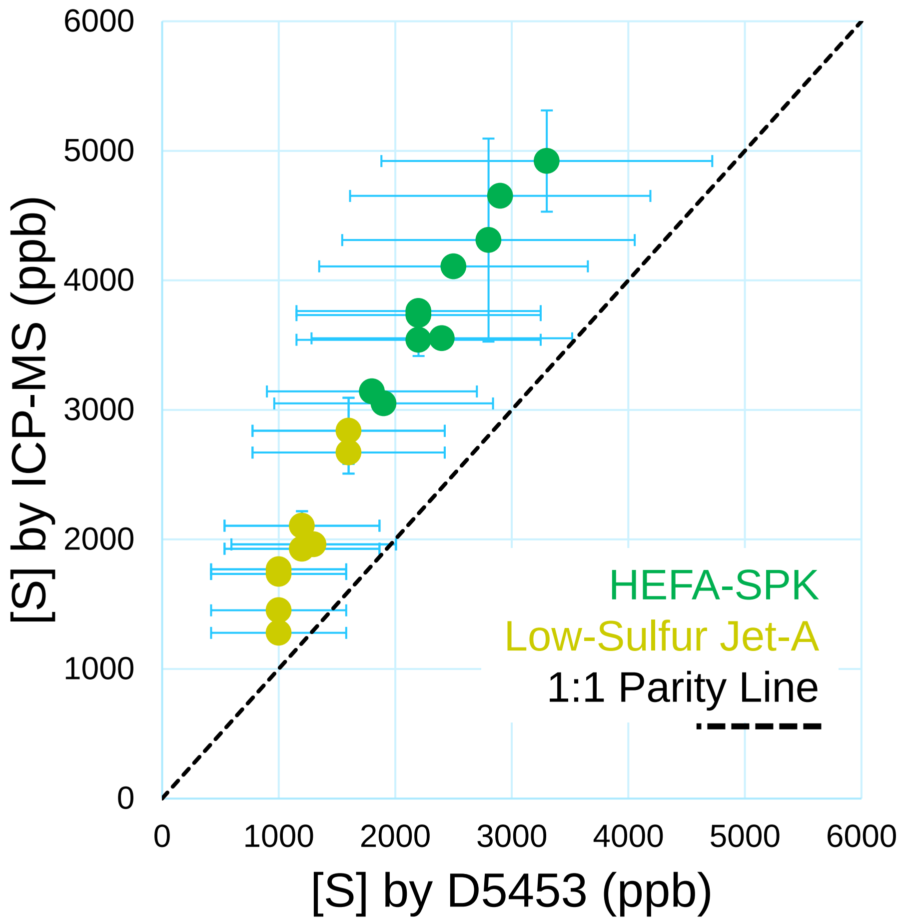


Application Across a Range of Test Fuels



*Error Bars are ± 2σ, DF = Dilution Factor

EcoDemonstrator Test Case



- HEFA-SPK and Jet-A data points are all the same fuel with aliquots taken from different sampling locations.
- Fuels with D5453 data presented as 1000 ppb [S] were reported as <1000 ppb, i.e., below the quant limit.
- ICP-MS appears to consistently over-report compared to D5453.
- ICP-MS appears to differentiate between points that would not be differentiable based on D5453 Reproducibility data.

Y values are ± *2σ* | X values are ± R (Reproducibility), DF = 2

Summary: Method Highlights and Next Steps

- Calibrated Range = 100 – 3000 ppb
- Limit of Detection = 15 ppb
- Limit of Quantitation = 300 ppb

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- How did we do?
- Do you have any fuel we can test?
- Would you like to try this at your place?

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Participants

- UDRI Fuel Science Group Members:
  Amanda Arts, Willie Steinecker, & Zach West (PI)

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