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COMPACT TIME DOMAIN NMR DESIGN FOR THE DETERMINATION OF HYDROGEN CONTENT IN GAS TURBINE FUELS

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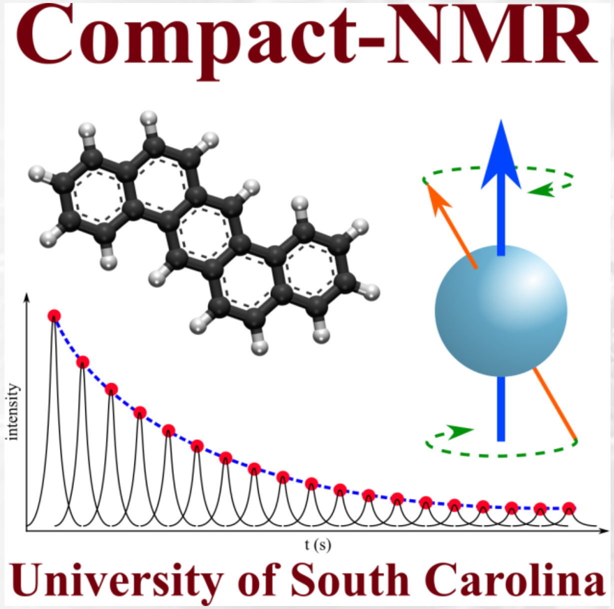
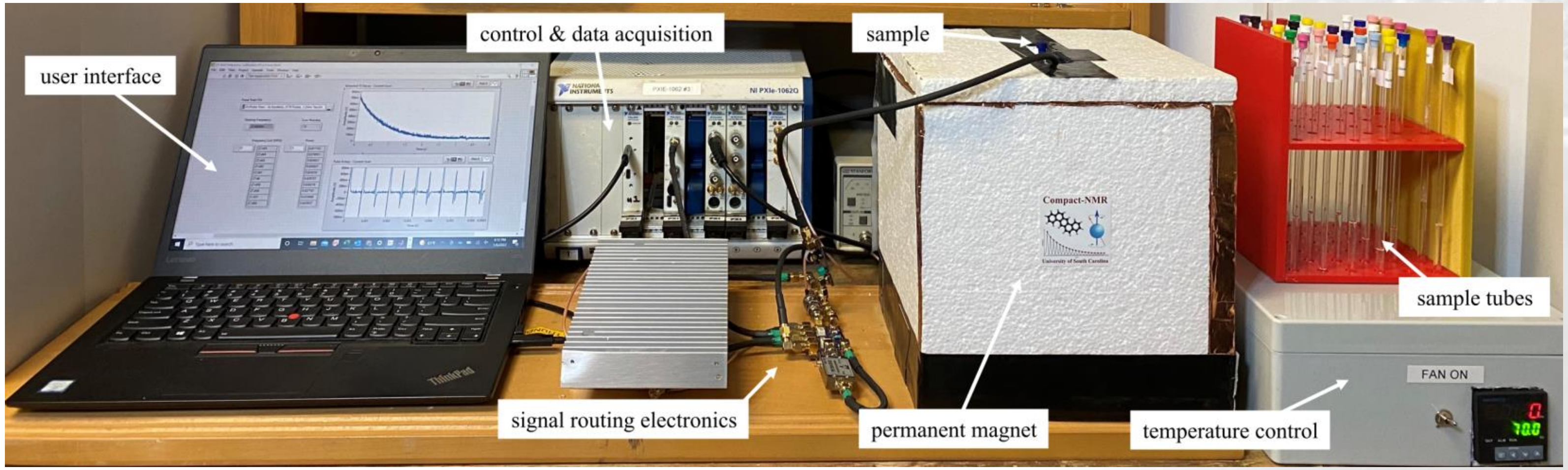
Introduction

- Nuclear magnetic resonance (NMR) is a well-known method for analyzing petroleum fuels
- Hydrogen content is a vital parameter of petroleum distillates
- A compact, low-resolution device could be used for rapid in-situ measurements
- This lab-built TD-NMR device can:
  - Determine hydrogen density for any sample
  - Achieve 0.7% error for hydrogen content in gas turbine fuels



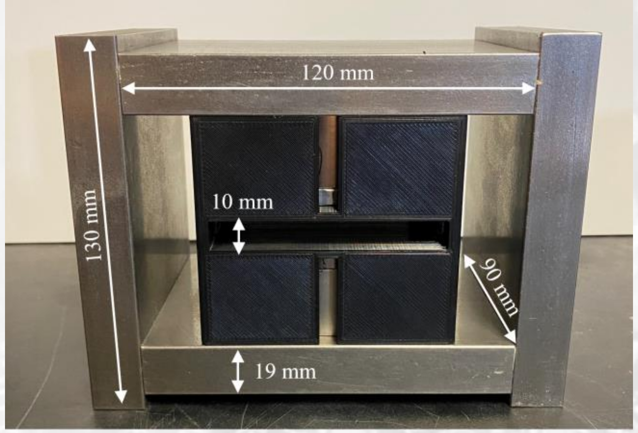
System Design - Overview

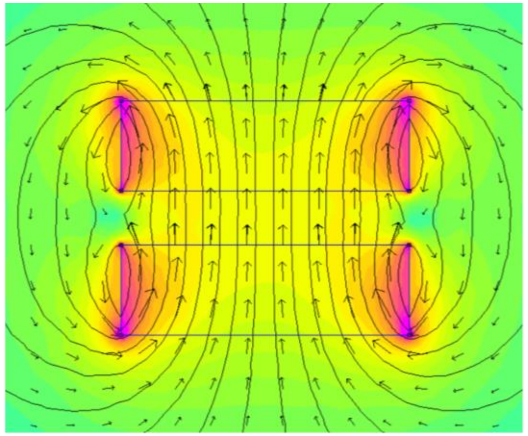
- 0.65 T permanent magnet
- PCB mounted signal routing electronics
- LabVIEW programming and GUI
- NI PXI control chassis



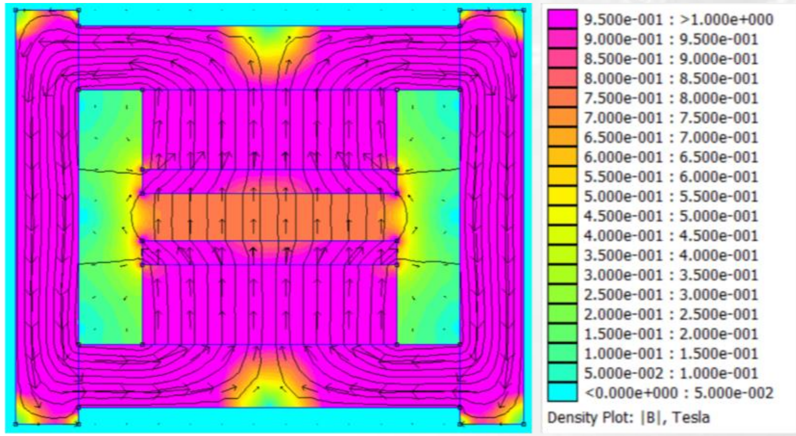
System Design – Permanent Magnet

- Two dipole cylindrical magnets surrounded by a steel yolk
- Static field strength of 0.645 T (27.5 MHz Larmor frequency)
- Placed inside temperature-controlled container
- Finite Element Method Magnetics (FEMM) used for simulation





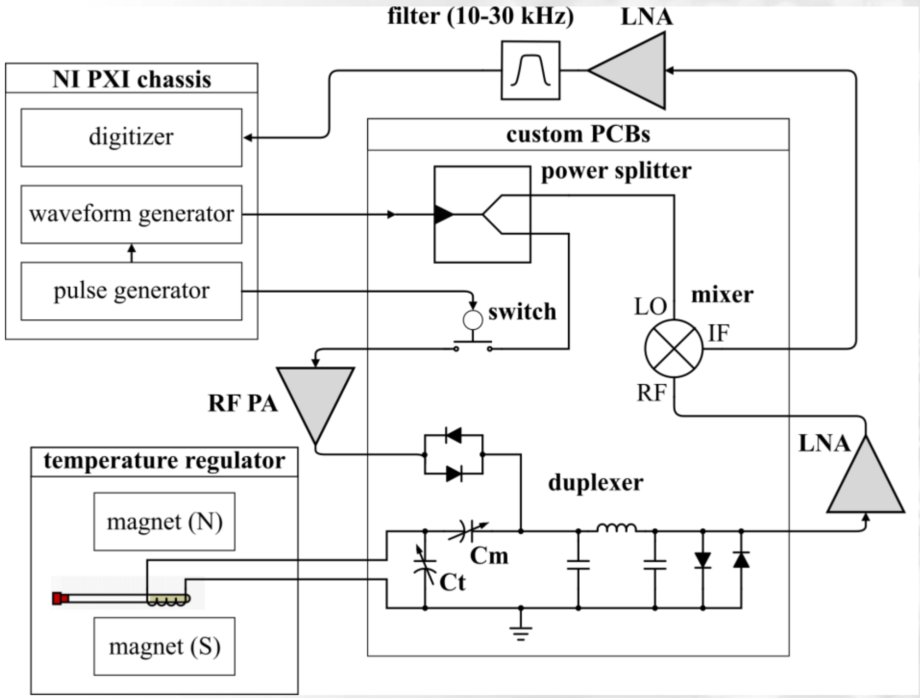
Bare magnets



Magnets with steel yolk & caps

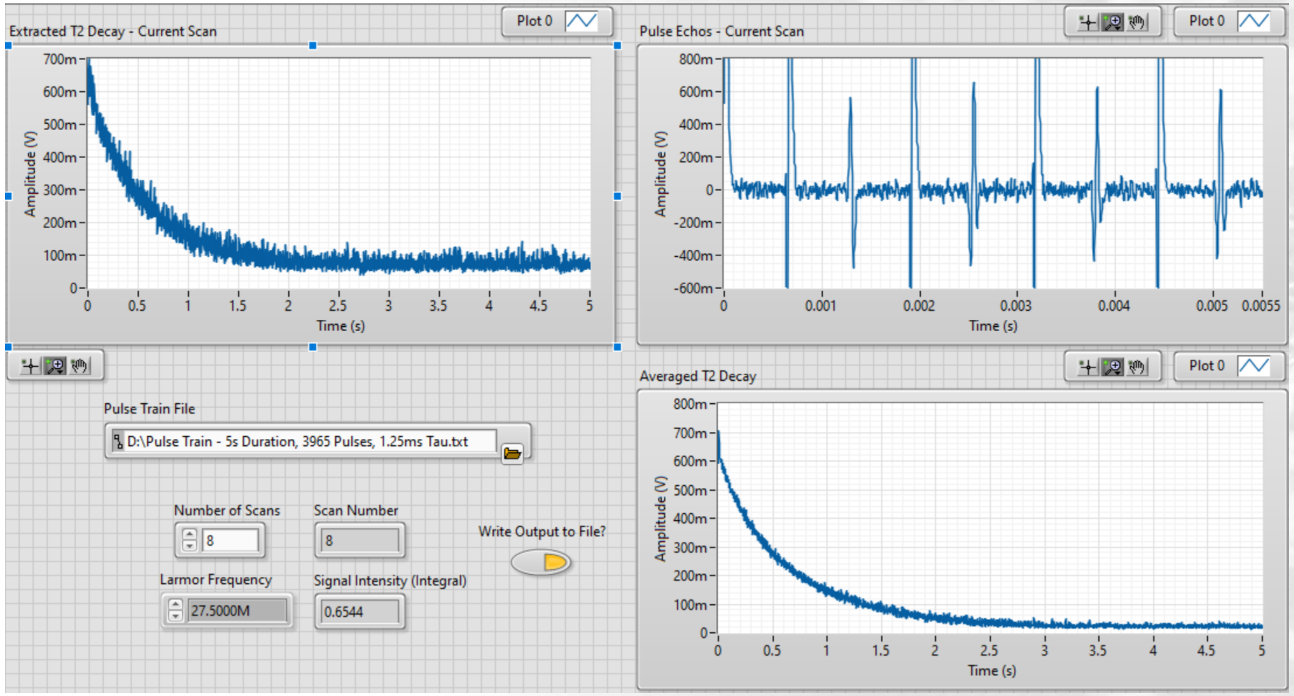
System Design – Signal Routing

- All components mounted on PCBs except for amplifiers
- System is matched to 50 Ω for all ports and cables
- The NMR signal is amplified by 80 dB before being sent to the digitizer



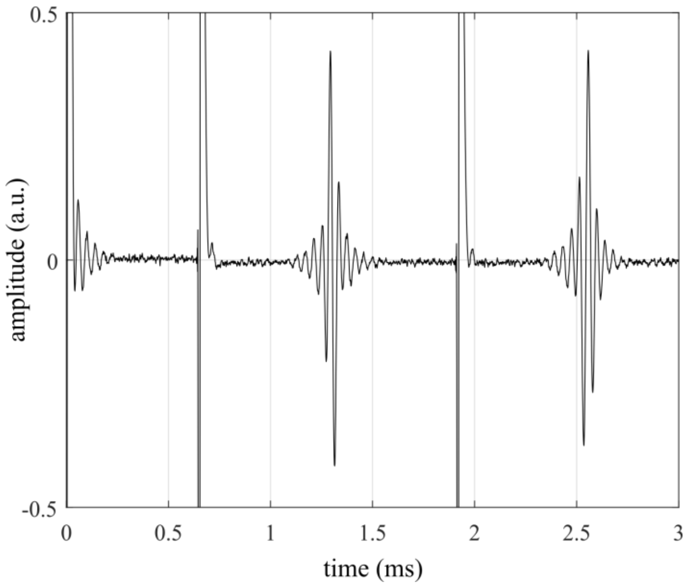
System Design – Control & Data Acquisition

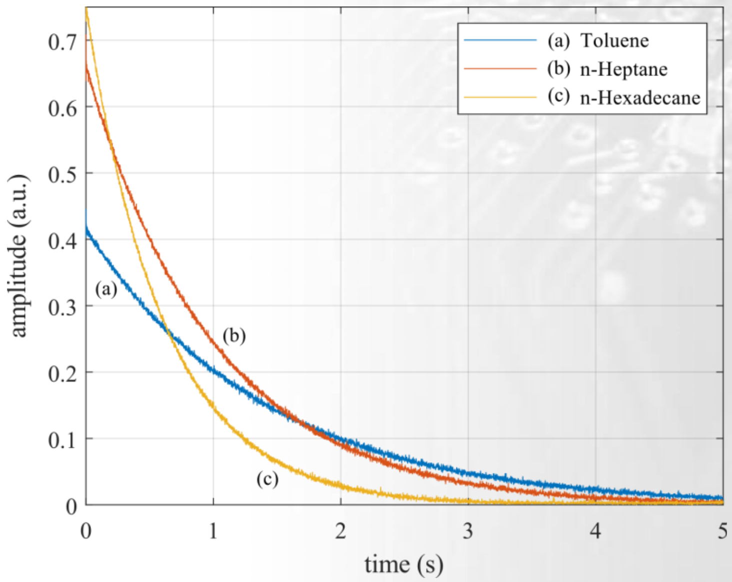
- NI PXI chassis
  - Arbitrary waveform generator
  - Pulse generator
  - 16 to 24-bit digitizer
- LabVIEW GUI displays the current scan and the averaged scans
- Collects decay data over a 5 second period
- 16 scans take 4 minutes



Results & Discussion

- A CMPG sequence with 3965 total pulse echoes (2 shown below) were used to construct T2 decay curves
- An array of pure hydrocarbons (3 shown below) was tested to establish a basis
- Initial signal amplitude is directly proportional to hydrogen density





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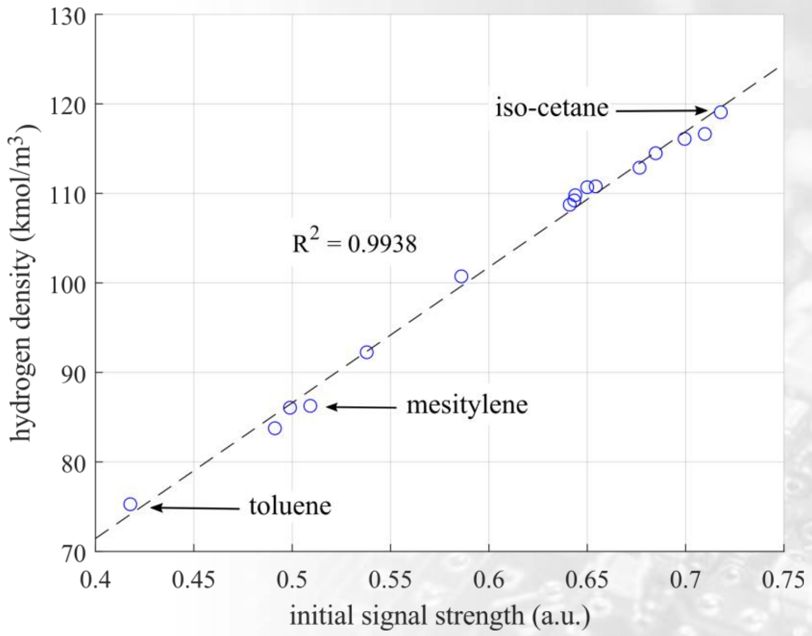
Results & Discussion

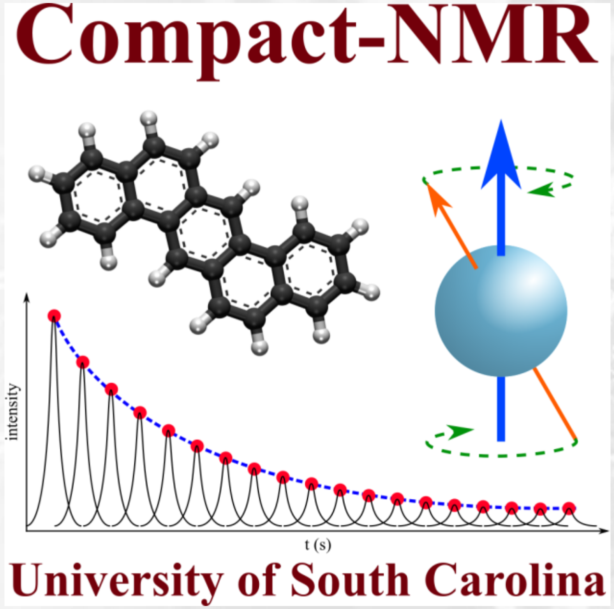
- A linear function was created using the data from the pure hydrocarbons
- This can be used to estimate hydrogen density in any sample
- Hydrogen content (mass %) is the ratio of hydrogen density to mass density
- Hydrogen content was estimated in 6 different gas turbine fuels with a maximum error of 0.7%



fuel	known ¹H content	measured ¹H content	% error
JP-8	14.4	14.5	0.7
Jet-A	14.2	14.1	0.7
JP-5	13.4	13.4	0.0
Shell CPK	14.1	14.0	0.7
Shell SPK	15.5	15.6	0.6
Gevo-ATJ	15.3	15.4	0.6

Conclusion

- A simple, compact NMR instrument was developed for the characterization of petroleum distillates
- Demonstrates a high repeatability between tests
- Can accurately determine hydrogen content in jet fuels, which is an important combustion property
- Tests are quick, non-destructive, and require no special sample preparation
- Future work will be dedicated to scaling down the size and performing multi-exponential decay analysis



References

- Nikolskaya, E., and Hiltunen, Y., 2020. “Time-domain nmr in characterization of liquid fuels: A mini-review”. Energy & Fuels, 34(7), pp. 7929–7934.
- P. McIntosh, L., 2013. CPMG. Springer Berlin Heidelberg, Berlin, Heidelberg, pp. 386–386.
- Barbosa, L. L., Kock, F. V. C., Silva, R. C., Freitas, J. C. C., Lacerda, V., and Castro, E. V. R., 2013. “Application of low-field nmr for the determination of physical properties of petroleum fractions”. Energy & Fuels, 27(2), pp. 673–679.
- Barbosa, L. L., Kock, F. V., Almeida, V. M., Menezes, S. M., and Castro, E. V., 2015. “Low-field nuclear magnetic resonance for petroleum distillate characterization”. Fuel Processing Technology, 138, pp. 202–209.
- Barbosa, L. L., Montes, L. F., Kock, F. V., Morgan, V. G., Souza, A., Song, Y.-Q., and Castro, E. R., 2017. “Relative hydrogen index as a fast method for the simultaneous determination of physicochemical properties of petroleum fractions”. Fuel, 210, pp. 41–48.
- Montes, L. F., Oliveira, E. C., lvaro C. Neto, Menezes, S. M., Castro, E. R., and Barbosa, L. L., 2019. “Low-field nmr: A new alternative to determine the aromatic content of petroleum distillates”. Fuel, 239, pp. 413–420.
- Santos, P. M., Amais, R. S., Colnago, L. A., Rinnan, ., and Monteiro, M. R., 2015. “Time domain-nmr combined with chemometrics analysis: An alternative tool for monitoring diesel fuel quality”. Energy & Fuels, 29(4), pp. 2299–2303.
- da Rocha, G., Colnago, L. A., Moraes, T. B., Zagonel, G. F., de Muniz, G. I. B., Peralta-Zamora, P. G., and Barison, A., 2017. “Determination of biodiesel content in diesel fuelby time-domain nuclear magnetic resonance (td-nmr) spectroscopy”. Energy & Fuels, 31(5), pp. 5120–5125.
- Prestes, R. A., Colnago, L. A., Forato, L. A., Vizzotto, L., Novotny, E. H., and Carrilho, E., 2007. “A rapid and automated low resolution nmr method to analyze oil quality in intact oilseeds”. Analytica Chimica Acta, 596(2), pp. 325–329.
- Won, S. H., Veloo, P. S., Dooley, S., Santner, J., Haas, F. M. ,Ju, Y., and Dryer, F. L., 2016. “Predicting the global combustion behaviors of petroleum-derived and alternative jet fuels by simple fuel property measurements”. Fuel, 168, pp. 34–46.
- ASTM D7171-20 (2020) Standard Test Method for Hydrogen Content of Middle Distillate Petroleum Products by Low-Resolution Pulsed Nuclear Magnetic Resonance Spectroscopy. American Society for Testing Materials: West Conshohocken, PA, 2017.
- Mondal, S., Kumar, R., Bansal, V., and Patel, M. B., 2015. “1h nmr method for the estimation of hydrogen content for all petroleum products”. Journal of Analytical Science and Technology, 6(24).
- Khadim, M. A., Wolny, R. A., Al-Dhuwaihi, A. S., AlHajri, E. A., and Al-Ghamdi, M. A., 2003. “Determination of hydrogen and carbon contents in crude oil and petroleum fractions by nmr spectroscopy”. Arabian Journal for Science and Engineering Section B: Engineering, 28(2A), pp. 147–162. PETROLEUM.
- ASTM D4808-17 (2017) Standard Test Methods for Hydrogen Content of Light Distillates, Middle Distillates, Gas Oils, and Residua by Low-Resolution Nuclear Magnetic Resonance Spectroscopy. American Society for Testing Materials: West Conshohocken, PA, 2017.
- ASTM D3701-17 (2017) Standard Test Method for Hydrogen Content of Aviation Turbine Fuels by Low Resolution Nuclear Magnetic Resonance Spectrometry. American Society for Testing Materials: West Conshohocken, PA, 2020.
- Sahebjavaher, R. S., Walus, K., and Stoeber, B., 2010. “Permanent magnet desktop magnetic resonance imaging system with microfabricated multiturn gradient coils for microflow imaging in capillary tubes”. Review of Scientific Instruments, 81(2), p. 023706.
- Meeker, D., 2010. “Finite element method magnetics”. FEMM, 4(32), p. 162.
- Louis-Joseph, A., and Lesot, P., 2019. “Designing and building a low-cost portable ft-nmr spectrometer in 2019: A modern challenge”. Comptes Rendus Chimie, 22(9), pp. 695–711.
- Claridge, T. D., 2016. “Chapter 3 - practical aspects of high-resolution nmr”. In High-Resolution NMR Techniques in Organic Chemistry (Third Edition), T. D. Claridge, ed., third edition ed. Elsevier, Boston, pp. 61–132.
- Nates, S., Carpenter, D., Dryer, F. L., and Won, S. H. Preferential Vaporization Potential of Jet fuels Evaluated by NMR Spectroscopy.
- Won, S. H., Rock, N., Lim, S. J., Nates, S., Carpenter, D., Emerson, B., Lieuwen, T., Edwards, T., and Dryer, F. L., 2019. “Preferential vaporization impacts on lean blow-out of liquid fueled combustors”. Combustion and Flame, 205, pp. 295–304.
- Carpenter, D., Nates, S., Dryer, F. L., and Won, S. H., 2021. “Evaluating ignition propensity of high cycloparaffinic content alternative jet fuel by a chemical functional group approach”. Combustion and Flame, 223, pp. 243–253.