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NEAR-INFRARED DATA TREATMENTS FOR IMPROVED FUEL PROPERTY PREDICTIONS

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Fuel quality surveillance, a key aspect of fuel acquisition and utilization, represents a significant investment in time, materials and manpower. The United States Naval Research Laboratory has been engaged in a program to develop rapid automated sensor-based fuel quality surveillance technologies. This approach is based upon deriving mathematical relationships between spectroscopic and chromatographic fuel data and measured specification properties. This has led to the development of the Navy Fuel Property Monitor (NFPM), which is capable of providing real-time estimates of a wide range of fuel specification properties for jet and diesel fuels through the proper interpretation of NIR spectral data. In addition, the NFPM has the capability to detect and quantify synthetic Fischer-Tropsch and biofuels alone or when blended with petroleum-derived fuels, and can discriminate between ultralow and high-sulfur diesel fuels. Using a fiber-optic reflectance probe, the NFPM also has the potential to be used as an in-line sensor to provide real-time remote sensing of fuel grade and specification property monitoring for a wide variety of strategic and commercial fuel quality assurance procedures. While chemometric modeling of fuel spectra is not a new concept, in order to realize the full potential of this technique, we have developed novel algorithms to maximize and assess the precision and robustness of the models used to correlate NIR data to the desired fuel properties and to extend this approach to non-petroleum derived fuels. Many of the limitations, discussed at the 2007 IASH Conference, that fuels pose as calibration training samples can be mitigated by the intelligent removal of samples that, while not true outliers, are still not constructively contributing to the correlation of interest. Genetic Algorithms (GA) have been employed to simulate an evolutionary process whereby the most statistically relevant subset of all available samples are selected for during model construction, while still maintaining all samples for validation purposes. Versatility, meanwhile, can be improved by developing improved calibration transfer strategies that provide for the remote deployment of many field instruments using one set of calibration models developed in the laboratory.