A Compact TD-NMR System for the Estimation of Jet Fuel DCN Using Interpretable Machine Learning

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Compact-NMR

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ARTS-Lab

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Background

Nuclear magnetic resonance (NMR):

- Atomic nuclei with a nonzero (magnetic) dipole moment will align with an external magnetic field
- An oscillating magnetic field applied perpendicular to the external field can then "tip" the nuclei
- The "relaxation" of the nuclei back to equilibrium can be measured as an induced voltage using a pickup coil
- The relaxation behavior of a sample gives insight into its molecular structure

Derived cetane number (DCN):

- The DCN is a common metric that summarizes fuel ignition characteristics
- Traditionally, the DCN of jet fuels are determined using ASTM standards involving sophisticated instrumentation
- New research has focused on alternative approaches, including the use of NMR and IR spectroscopy

Objectives:

- Demonstrate the viability of TD-NMR for fuel analysis
- Estimate DCN from raw T_2 relaxation data

Datasets

- Both hydrocarbon and jet fuel datasets generated for analysis
- All samples probed 3 times, and averaging performed for data augmentation

Tab. 1 Hydrocarbon and jet fuels samples used for dataset generation.

hydrocarbons		jet fuels		
name	DCN	name	POSF	DCN
toluene	6.0	Gevo-ATJ	10151	15.5
1,3,5-trimethylbenzene	8.0	JP-8/Gevo-ATJ	10153	30.5
iso-cetane	14.2	Sasol IPK	7629	31.3
iso-octane	18.9	Shell CPK	13690	37.2
n-propylbenzene	19.5	JP-8/IPK	7718	40.0
methylcyclohexane	22.5	JP-5	10289	40.9
n-butocyclohexane	47.8	Jet-A	4658	47.1
n-heptane	56.0	JP-8	6169	47.3
n-octane	64.4	JP-8	10264	49.6
n-decane	66.4	Jet-A	10325	50.0
n-hexadecane	73.5	JP-8/HRJ Tallow	7719	53.3
n-dodecane	100.3	HRJ Tallow	6308	58.1
–	–	Shell SPK	5729	58.4
–	–	S-8	4734	58.7
–	–	HRJ Camelina	7720	58.9

System Validation

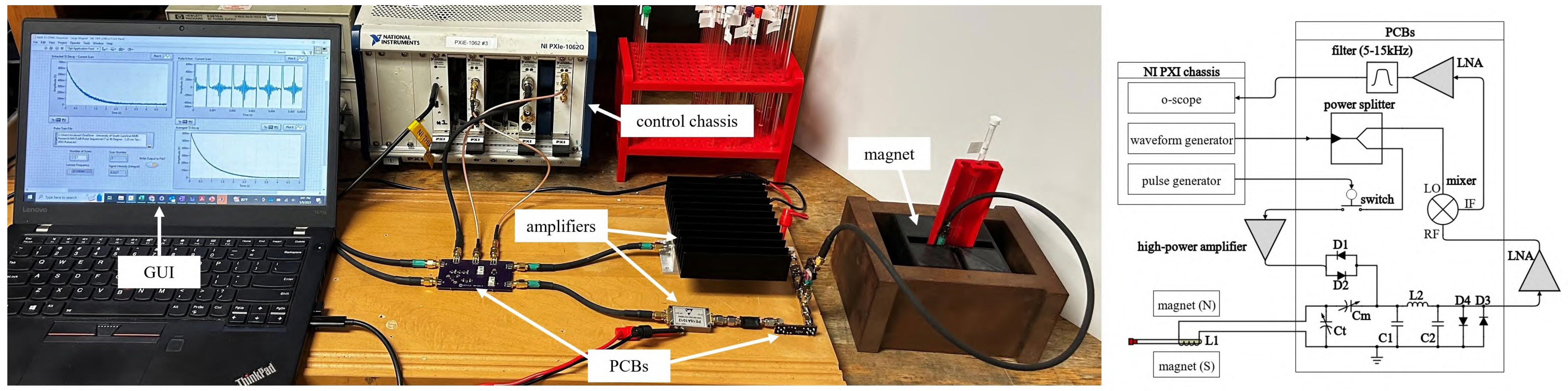

Fig. 1 ARTS-Lab compact TD-NMR system. (a) The desktop setup with key components/subsystems annotated. (b) The system schematic distinguishing external and PCB-mounted components.

- For a general T_2 relaxation curve, initial amplitude ∝ H density

$$\mathrm{SNR} \propto N\,A\,T^{-1}\,B_0^{\frac{3}{2}}\,\gamma_{\mathrm{exc}}\,\gamma_{\mathrm{obs}}^{\frac{3}{2}}\,T_2^*\,n_s^{1/2}$$

- Initial amplitude of 12 hydrocarbon samples (and 8 mixtures) regressed against theoretical H densities

$$\rho_H = \frac{\rho_s N_H}{M_w}$$

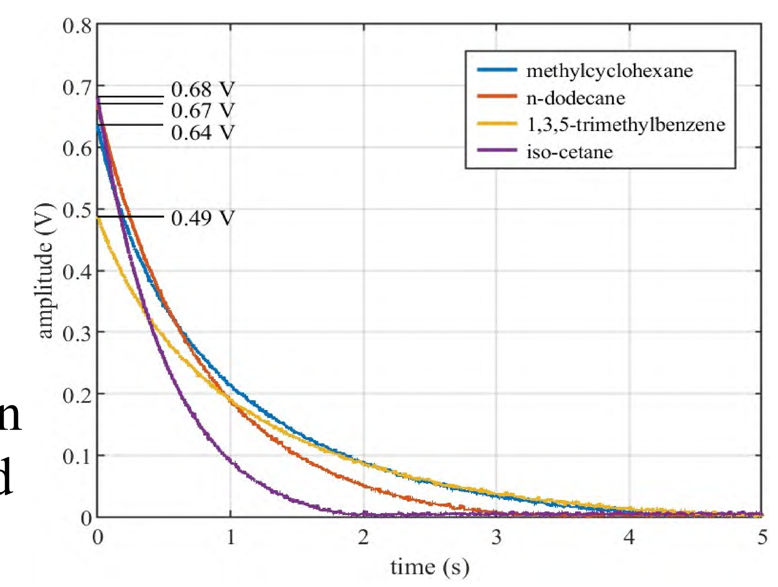

Fig. 2 T_2 relaxation curves of four distinct hydrocarbon samples.

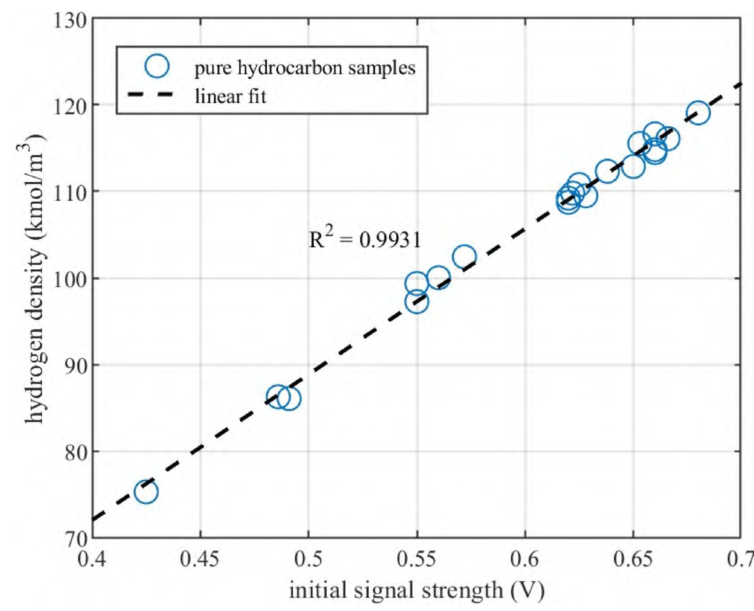

Fig. 3 Hydrogen density vs initial signal amplitude for 12 hydrocarbons and 8 mixtures (1:1 mass ratios).

Regression Analysis

- Random forests elected for DCN regression
- Model inputs comprise 10 features computed from T_2 curves
- Signals truncated after decaying to fraction of their initial strength
- Out-of-bag error and partial dependence → feature importance
- Fitting loops employed to (1) identify optimal fraction of signal for feature computation and (2) tune hyperparameters

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{N}}$$

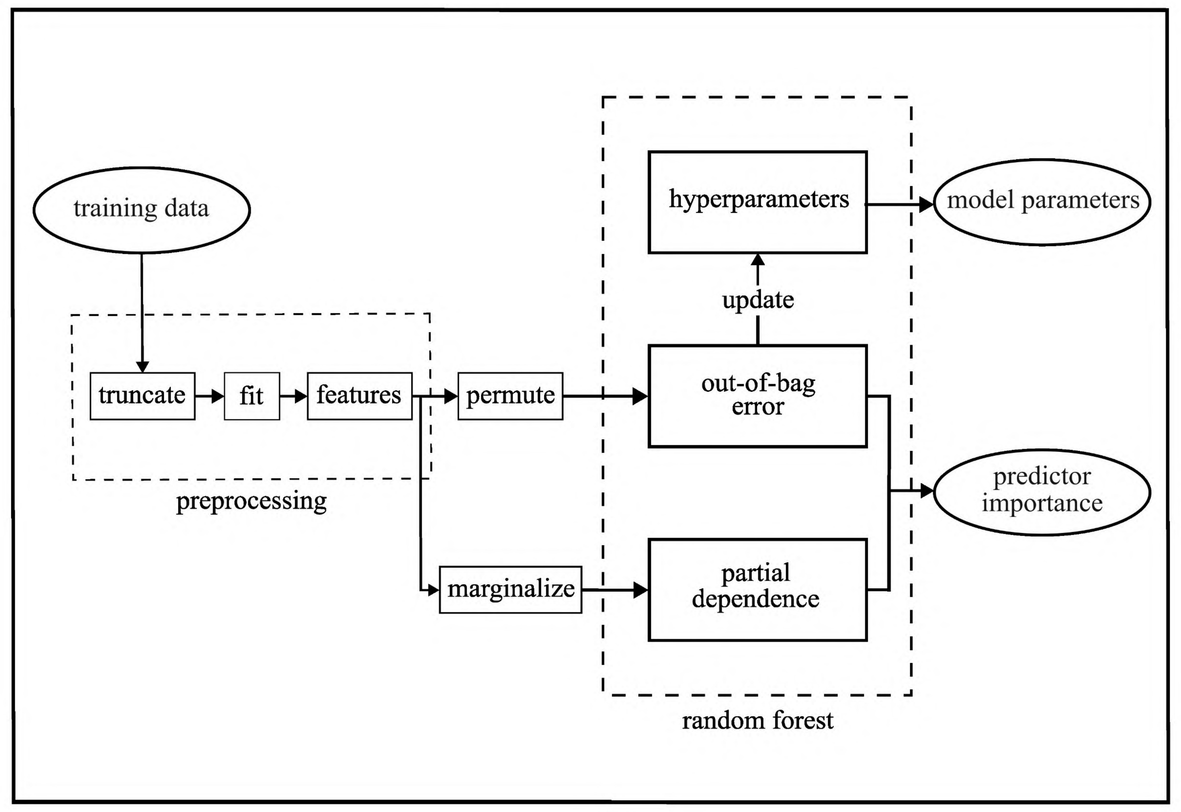

Fig. 4 Random forest training workflow for hyperparameter tuning and feature importance estimations.

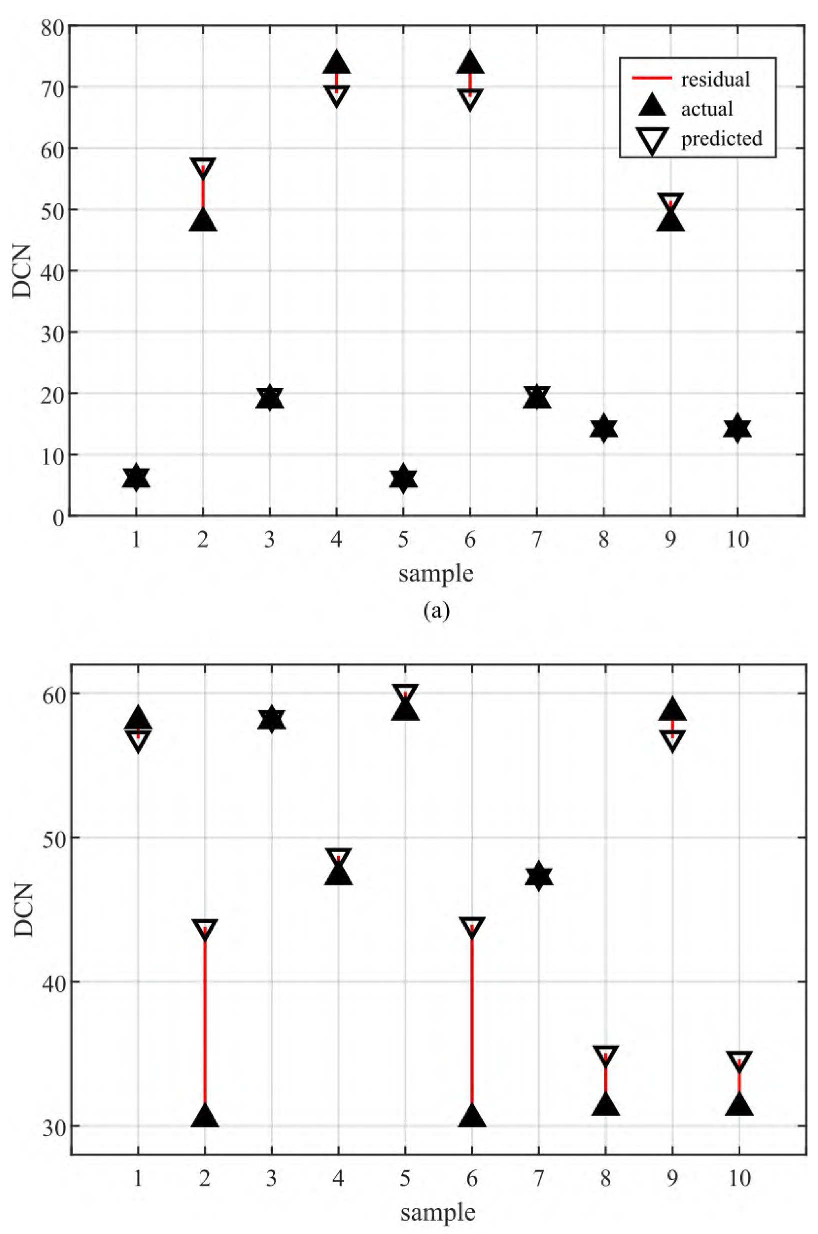

Fig. 5 Model predictions on the validation dataset. (a) Hydrocarbons: RMSE of 3.92. (b) Jet fuels: RMSE of 6.28.

Results

- Model achieved RMSE of just **0.96** predicting on two new jet fuel samples
- Range of optimal truncation: **23% - 25%**
- Enhanced understanding of hydrocarbon/jet fuel feature space

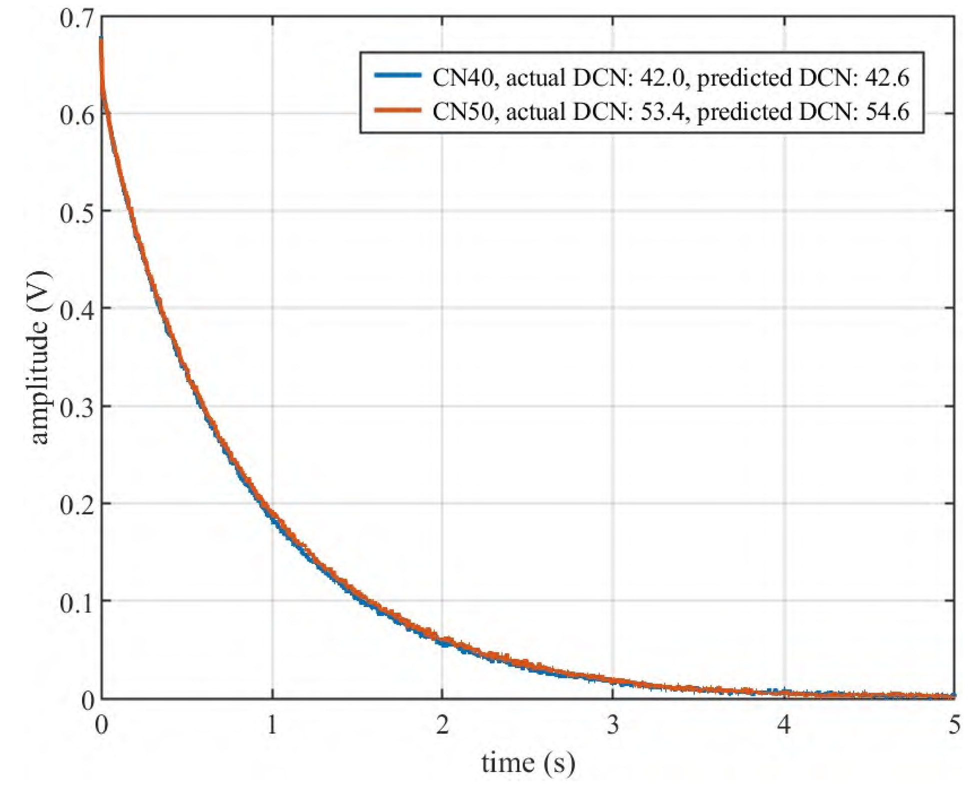

Fig. 6 T_2 relaxation curves of two test fuel samples. The legend details true and model-predicted DCNs.

Conclusions

- This work proposed/validated the use of TD-NMR for fuel-based sensing
- An interpretable approach for estimating DCN from raw T_2 relaxation data was presented
- Future work to focus on the betterment of predictions and the incorporation of a flow-through system

References

[1] J. Martin, A. Downey, W. Janvrin, A. Varillas, Compact-NMR (cNMR), 2023.

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[3] J. Martin, A. Downey, S. H. Won, Compact time domain nmr design for the determination of hydrogen content in gas turbine fuels, InProc: International Design Engineering Technical Conferences and Computers and Information in Engineering Conference, Vol. 86205, American Society of Mechanical Engineers, 2022.

Access the data for yourself!
https://github.com/ARTS-Laboratory/Dataset-hydrocarbon-and-fuel-processing

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