Development of an on-site threshold detection tool for hydrocarbon contamination in soils

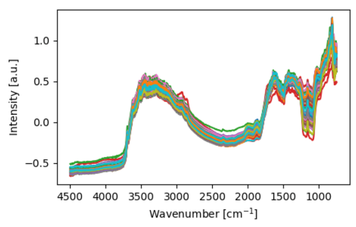
Deeksha Beniwal (deeksha.beniwal@ziltek.com),
Radha Krishnan Nachimuthu, Chaya Smith, Georgios Tsiminis, and Sean Manning
(Ziltek Pty Ltd, Edwardstown, SA, Australia)

Motivation

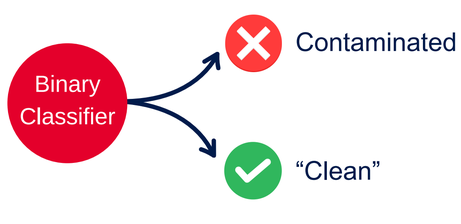
- Rapid on-site assessment is needed for efficient remediation.
- Traditional lab tests are expensive, slow, and resource-intensive.
- **RemScan Rapid Scan**: a new assessment tool for quickly identifying hydrocarbon contamination in soils.
- Target: 1,000 ppm regulatory standard for clean soils.
- Faster project completion and reduced remobilisation efforts.

Operational Principle

Contaminated Soil



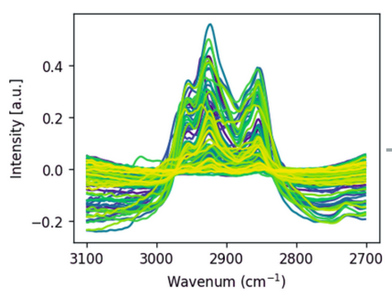
Mid-Infrared Spectra



Threshold = 1,000 ppm / 0.1%

Methodology

- **Training dataset:** 17,836 calibration samples with known contamination levels:
  - Samples > 1,000 ppm = 8,750
  - Samples < 1,000 ppm = 9,086
- **Validation dataset:** 6,880 field samples collected from commercial remediation projects
  - Samples > 1,000 ppm = 3,485
  - Samples < 1,000 ppm = 3,398
- Trained multiple classifiers and tested various pre-treatments and spectral windows.
- Evaluated model performance using three metrics: accuracy, macro F1 score, and Matthew's correlation coefficient.
- Identified interfering signals, including calcium carbonate and soil organic carbon (>10%) [1, 2].



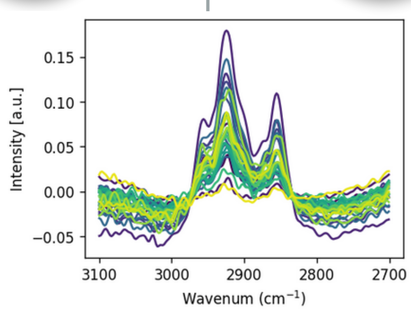
Training Spectra

	filename	tph	class_id
0	7832_13_01-29Jan14-1577_0000 (2)	100000	0
1	7832_13_01-29Jan14-1577_0001	100000	0
2	7832_13_01-29Jan14-1577_0002	100000	0
...	...	...	...
997	17738_12_09-03Feb14-1577_0003	1000	1
998	17738_12_09-03Feb14-1577_0004	1000	1
999	17738_12_10-03Feb14-1577_0000	781	1

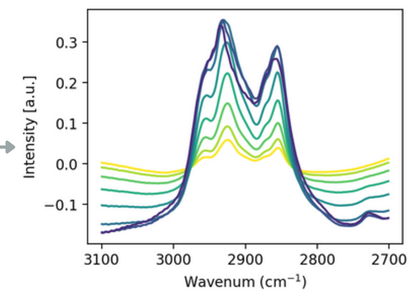
Reference Information

Training Model

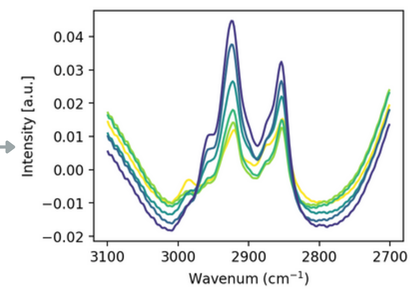
Prediction



Validation Spectra

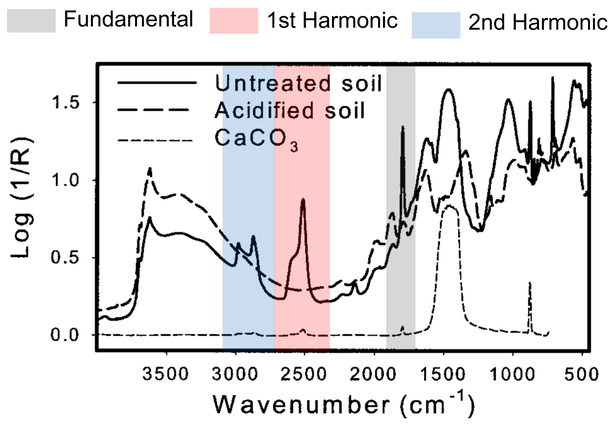


Contaminated: TPH > 1,000 ppm

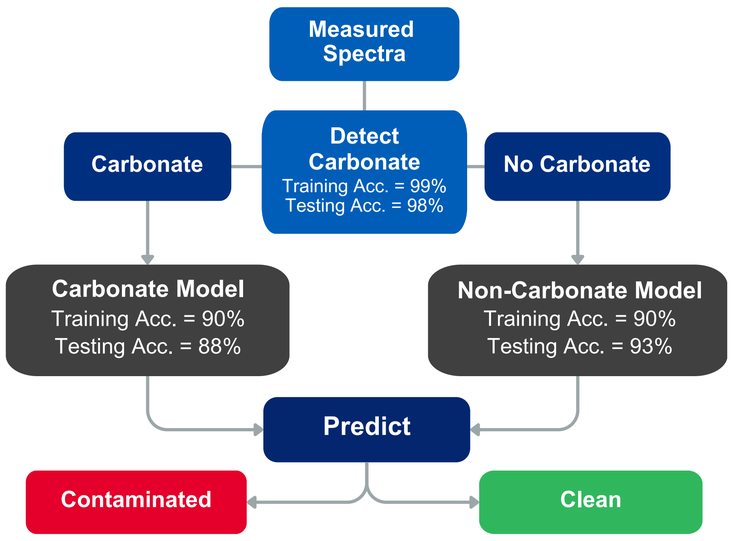


Clean: TPH < 1,000 ppm

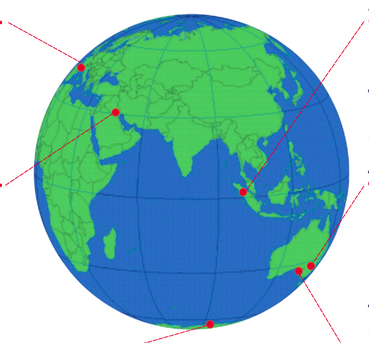
Model Workflow



Comparison of mid- and near-infrared spectra of highly calcareous soil before and after acid treatment for carbonate removal, highlighting three vibrational modes. The $CaCO_3$ spectrum is included for reference. Image from Ref. [2].



Case Studies



France
Sample count: 897
Accuracy: 88%

Kuwait
Sample count: 354
Accuracy: 93%

Antarctica
Sample count: 737
Accuracy: 91%

Indonesia
Sample count: 2,038
Accuracy: 95%

Victoria
Sample count: 538
Accuracy: 100%

Adelaide
Sample count: 32
Accuracy: 100%

Example Application

- Decommissioned petrol stations require clean-up.
- Typical backfill soils include dolomite and sand.
- Clean soil samples were collected from suppliers.
- Samples were spiked with known levels of diesel.
- **RemScan Rapid** was used to assess sample contamination.

Dolomite

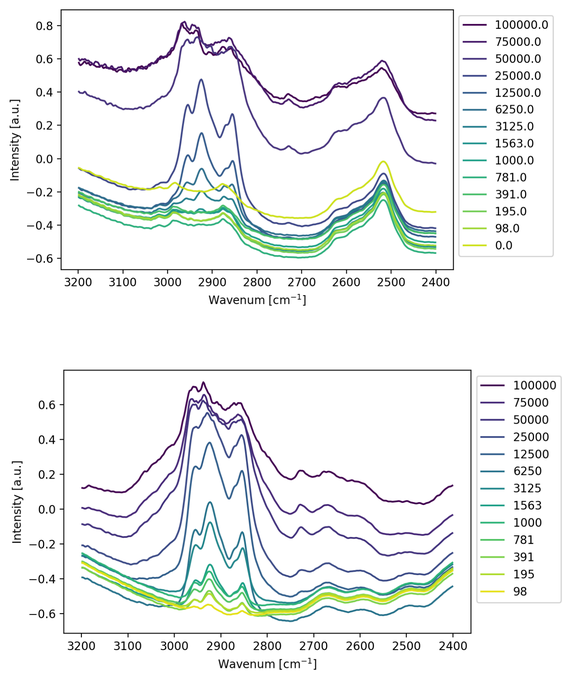
Sample count: 180
- Class A: 90 (>1,000 ppm)
- Class B: 90 (<1,000 ppm)

Model: Carbonate
Accuracy: 92%

Sand

Sample count: 150
- Class A: 90 (>1,000 ppm)
- Class B: 60 (<1,000 ppm)

Model: Non-Carbonate
Accuracy: 100%



Mid-infrared spectra for Dolomite (top) and Sand (bottom) samples, spiked with a known level of diesel. The TPH concentration (in mg/kg) is indicated in the legend.

Conclusions

- Developed a binary classifier for the rapid assessment of hydrocarbon-contaminated soils.
- Identified potential interfering signals, including calcium carbonate and soil organic carbon (>10%).
- Implemented a robust method for handling carbonate signatures.
- Assessed classifier performance using historical customer data.
- Results are promising, with a prediction accuracy of around 90%.
- Future work will include:
  - Refinement of training data,
  - Further refinement of the model structure for edge cases,
  - Testing lighter hydrocarbons (e.g., petrol).

References

1. Le Guillou, F., et al. 2015. How does grinding affect the mid-infrared spectra of soil and their multivariate calibrations to texture and organic carbon? Soil Research, 53(8), pp.913-921.
2. McCarty, G.W., et al. 2002. Mid-infrared and near-infrared diffuse reflectance spectroscopy for soil carbon measurement. Soil Science Society of America Journal, 66(2), pp.640-646.