WHOSE PARTICLE IS IT?
PARTICLE FORENSICS IN THE MOUNT MAUNGANUI AIRSHED

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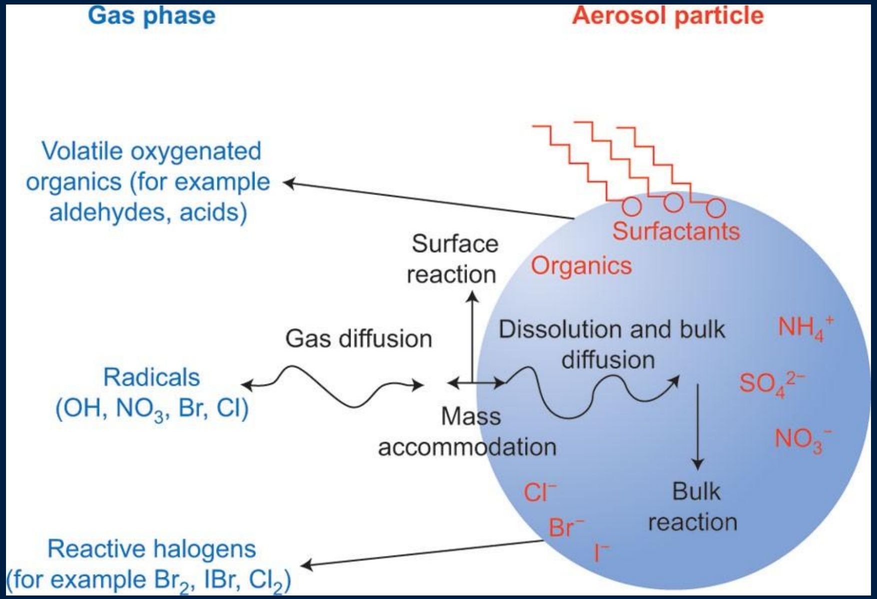
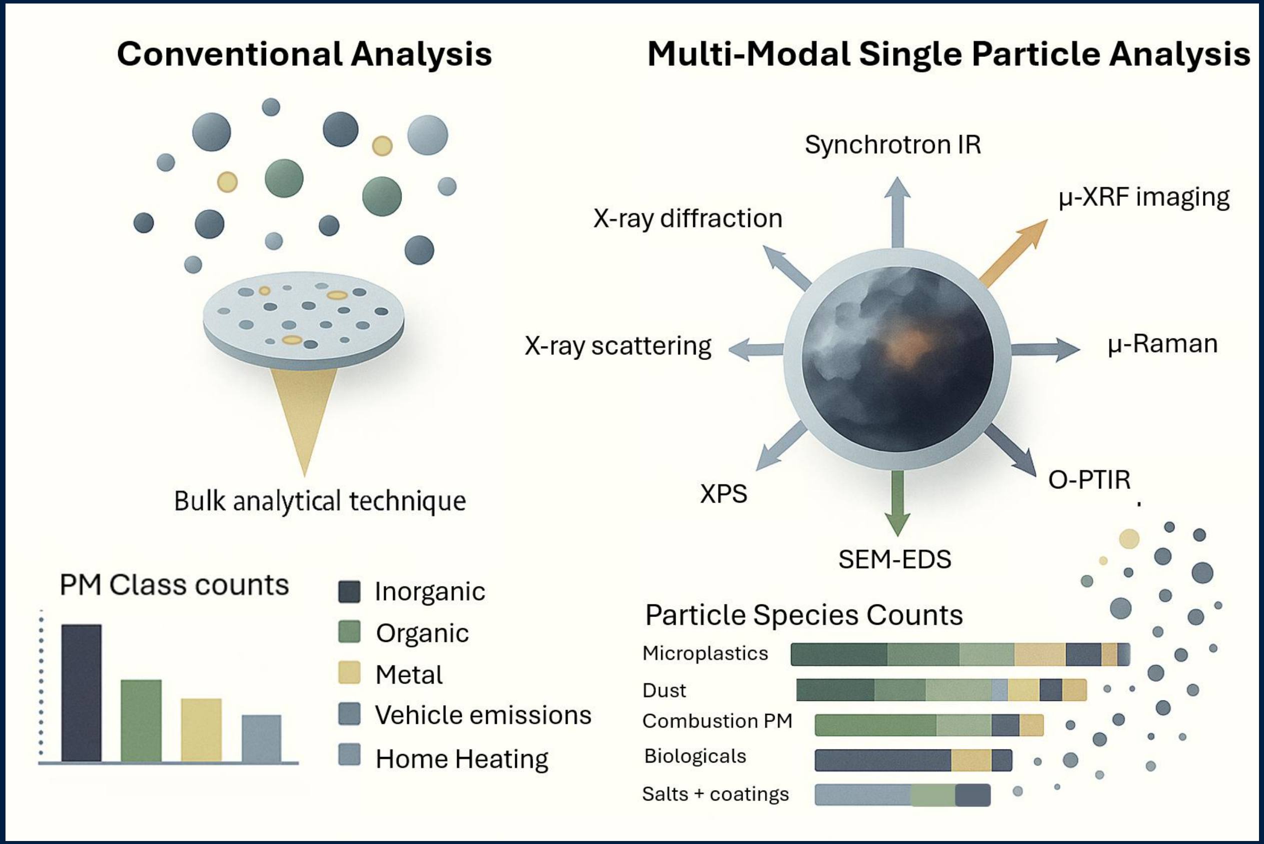
[3] Queensland University of Technology, International Laboratory for Air Quality and Health, Brisbane, Australia
[4] Mote Limited, Level 3, 240 Queen Street, Brisbane, Australia

The Chemistry of the particle matters!





Core Chemistry tells you where it has come from
Surface chemistry tells you where it has been and how it will interact

Mount Maunganui

a coastal industrial zone classified as polluted in 2019

‘Heartbreaking’ reality of Mount Maunganui’s air quality

Alisha Evans, Local Democracy Reporter | Local Democracy Reporting
June 26, 2024 · 3:22pm

Copy Link

Whareroa marae's environmental spokesperson Joel Ngatuere implored council candidates to understand the issues around air quality in Mount Maunganui.

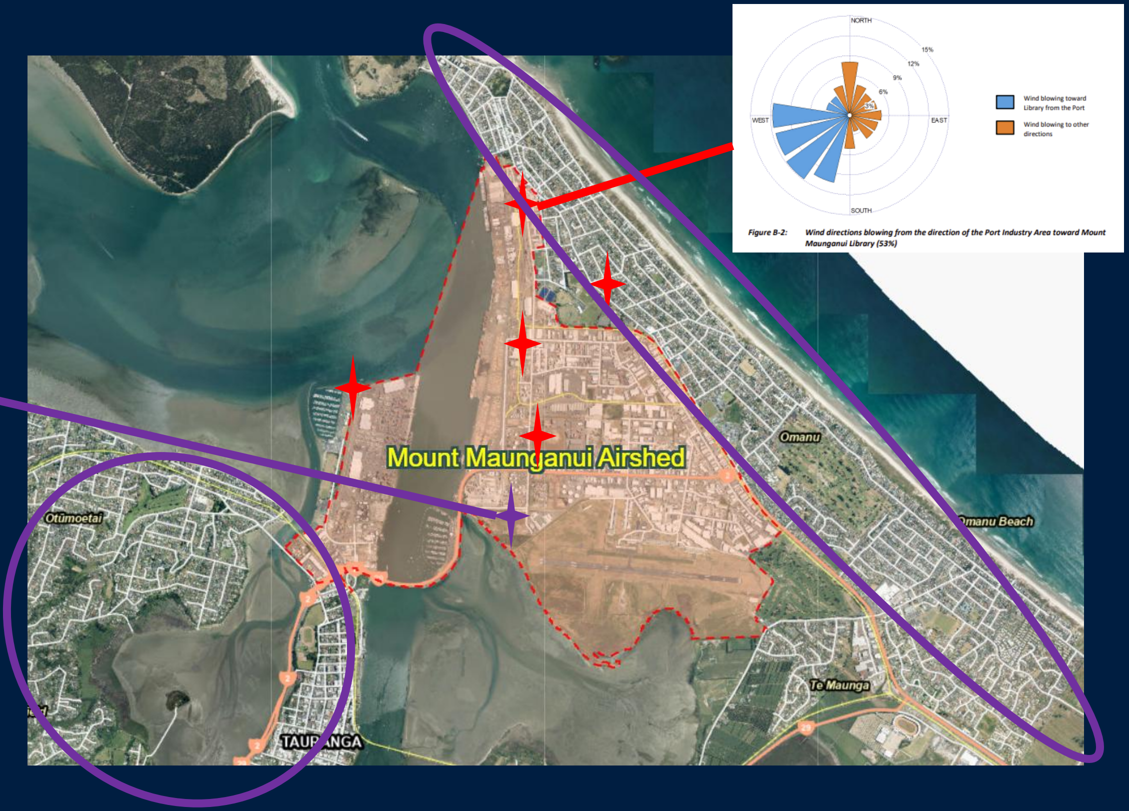


Figure B-2: Wind directions blowing from the direction of the Port Industry Area toward Mount Maunganui Library (53%)

Mount air quality impacting health-review confirms

The review confirmed poor air quality at Mount Maunganui was creating significant health risks and premature deaths. Photo: Supplied.

Social & Health Costs: An estimated $22 million annual economic burden caused by localized air pollution impacts.

Whareroa Marae & Community Impact

- Continuous air quality concerns raised since 2015
- Formal call for a managed retreat of heavy industry in 2020
- Progress stalled by existing industry user rights under the resource management act
- Averages ~500 pollution hotline calls to the regional council annually

Commission chair Anne Tolley said there was a "critical need" to find space for emitting businesses. Bay of Plenty Times Photo / Alex Cairns.

Industrial Land Scarcity: A severe shortage of alternative, appropriately zoned land to facilitate a managed retreat.

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Priority One Tauranga Moana

Mount Maunganui Industry Environmental Accord

signed by 33 businesses in the industrial zone, committing them to take further action to improve their environmental footprint.

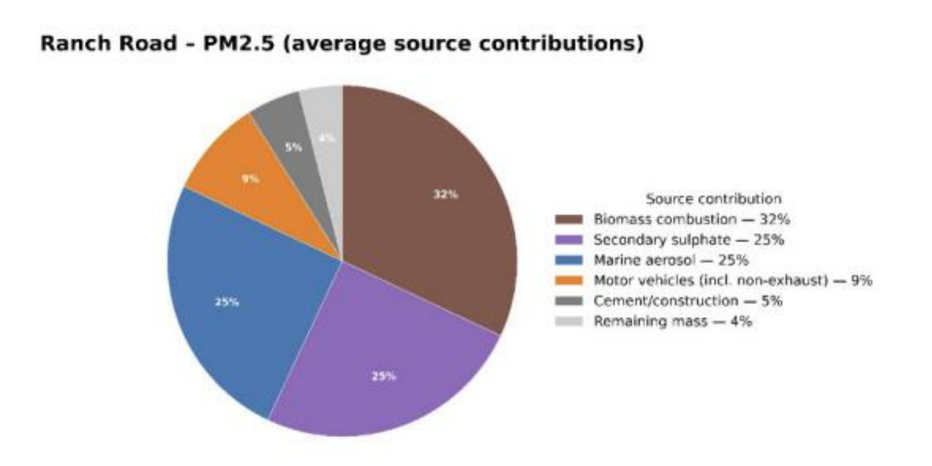
Priority One reports the signatories have committed to 251 actions
- 122 complete
- 120 underway or scheduled.

Community advocates ‘Clear the Air’ point out that these metrics represent voluntary, un-audited self-reporting calling for independently verified reductions in emissions and exposure

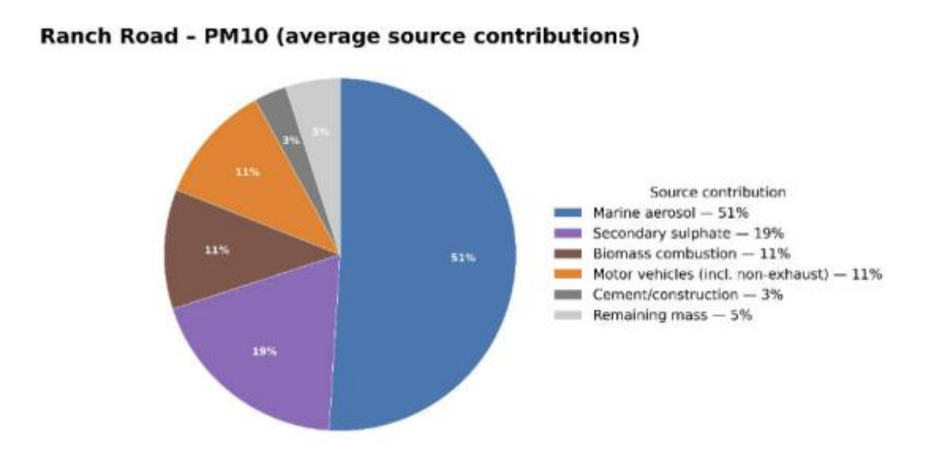
Toi Te Ora Public Health. (2024). *Air Pollution Health Risk Assessment for Mount Maunganui, New Zealand.*
This independent study verified the drop in fine dust and PM10 maximums since 2019

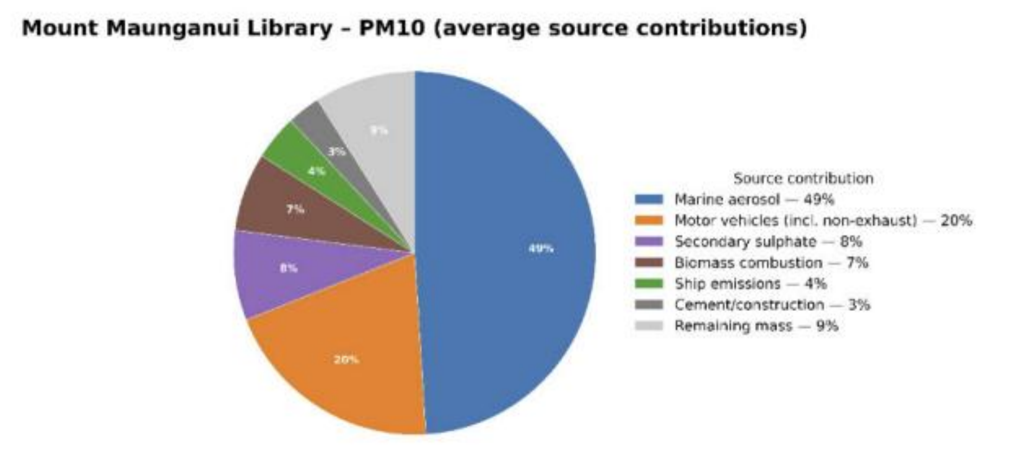
GNS – 2 year long XRF-PMF campaign

Davy, P. K., & Trompetter, W. J. (2023–2025). *Average source mass contributions to PM10 at the Mount Maunganui Library site*



- The airshed-scale mass balance is established
- XRF provides elemental analysis of the whole particle population
- XRF does not provide molecular chemistry (organics) or oxidation state chemistry (inorganics) – models make a lot of assumptions





Broad source factors do not identify individual emitting activities or resolve the particle chemistry

Who is contributing most to the PM population?
Where in the operational processes do they come from?

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Area Sources in Mount Maunganui

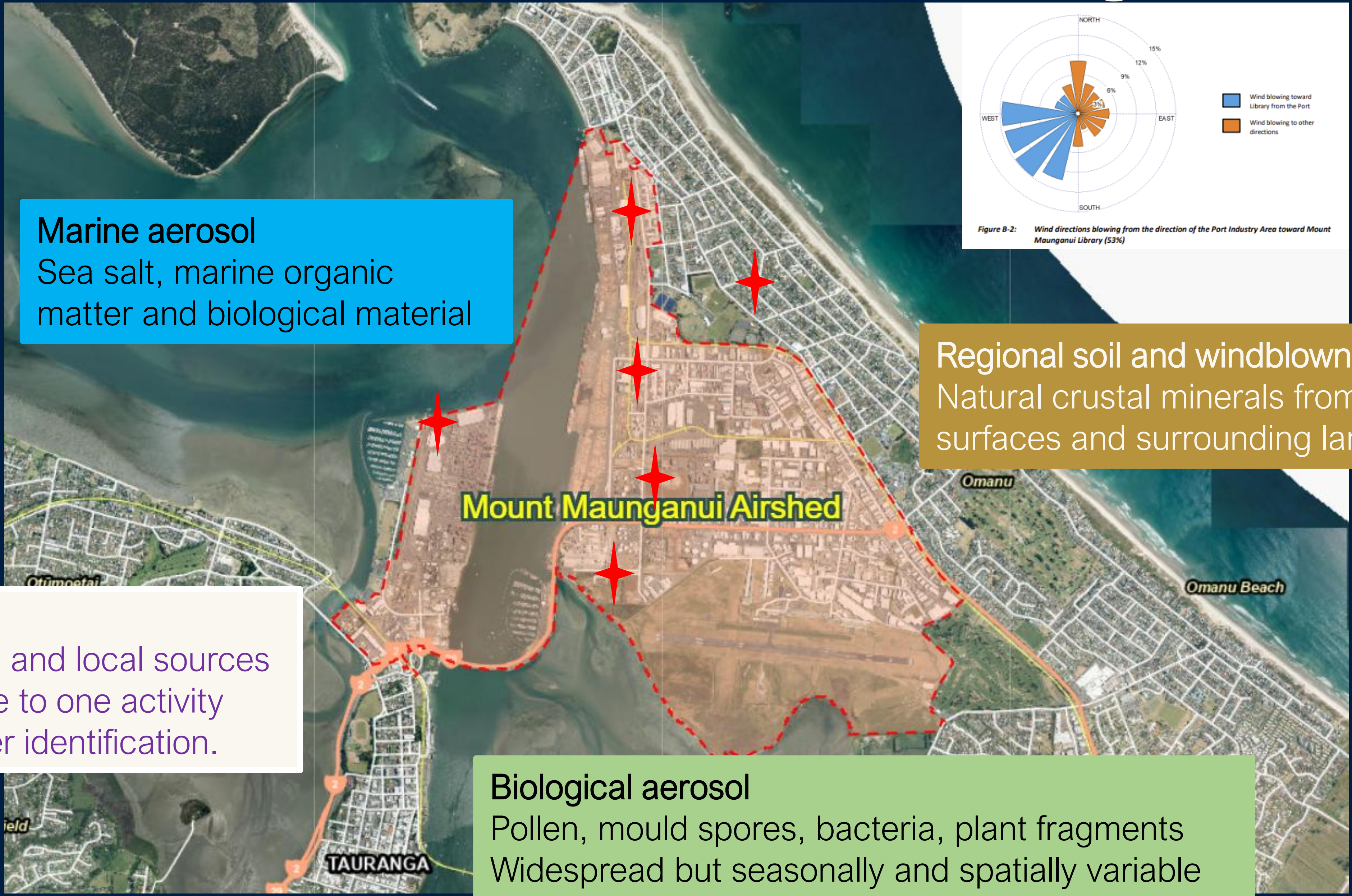

Figure B-2: Wind directions blowing from the direction of the Port Industry Area toward Mount Maunganui Library (53%)

Marine aerosol
Sea salt, marine organic matter and biological material

Regional soil and windblown dust
Natural crustal minerals from exposed surfaces and surrounding land

Microplastics
multiple diffuse and local sources
Not attributable to one activity without polymer identification.

Biological aerosol
Pollen, mould spores, bacteria, plant fragments
Widespread but seasonally and spatially variable

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Area Sources – Transport and Combustion

Expected PM:

- Exhaust soot - organic carbon
- Heavy fuel oil soot
- Aviation fuel soot
- Brake, tyre, rail and wheel wear
- Resuspended road and yard dust
- Secondary sulfate and nitrate
- Ultra-fine combustion metals

Figure B-2: Wind directions blowing from the direction of the Port Industry Area toward Mount Maunganui Library (53%)

Point Sources

Asphalt production
- Aggregate minerals
- Combustion Soot
- Bitumen Associated organics

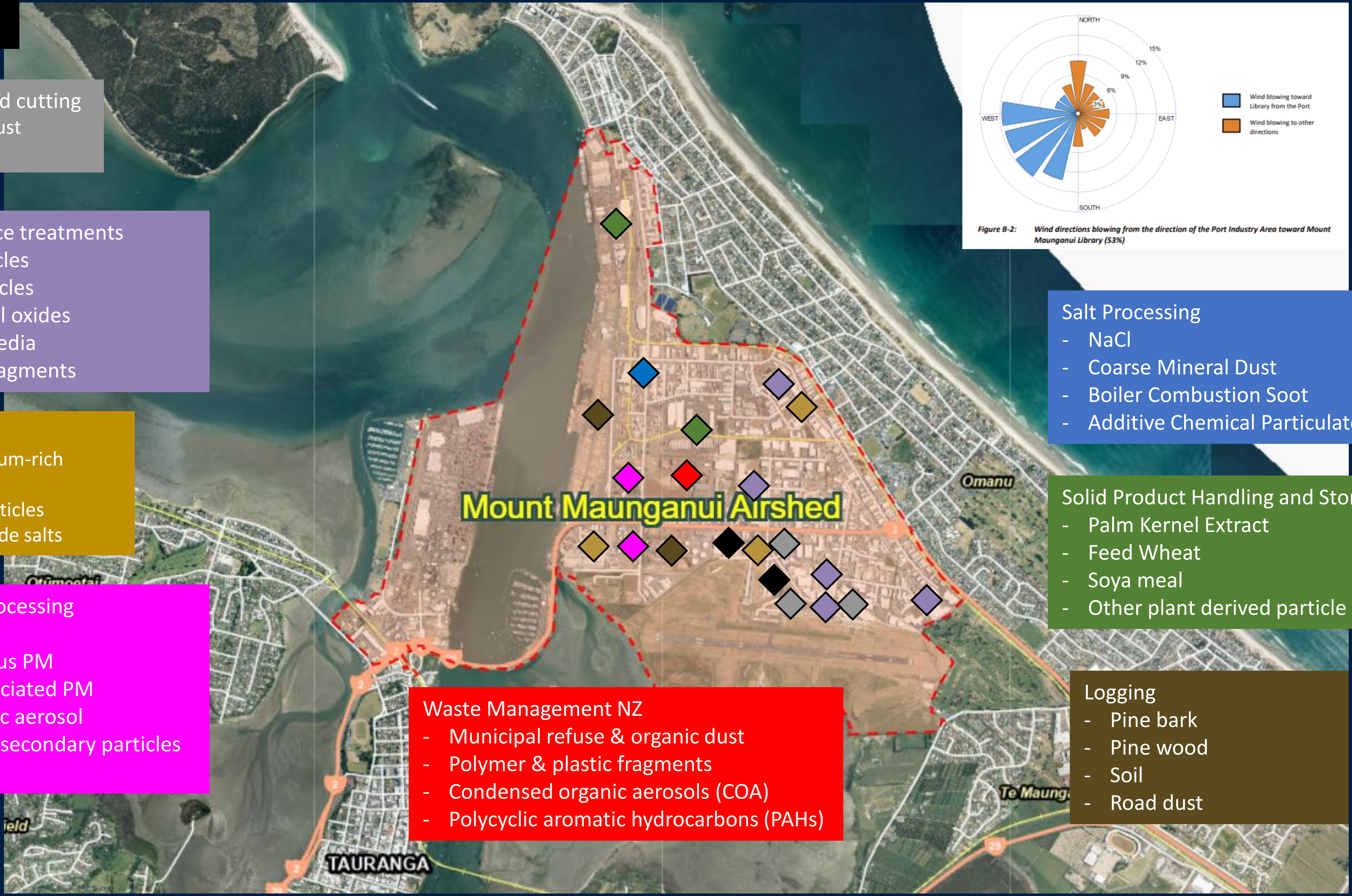
Concrete production and cutting
- Calcium rich mineral dust
- Silicate aggregates

Metalworks and Surface treatments
- Iron-rich steel particles
- Fe–Cr–Ni alloy particles
- Welding-fume metal oxides
- Abrasive blasting media
- Paint and coating fragments

Fertiliser industry
- Phosphate- and calcium-rich fertiliser dust
- Sulphate-bearing particles
- Potassium and chloride salts

Chemical and Resin Processing

- Pine-derived resinous PM
- Synthetic resin-associated PM
- Condensable organic aerosol
- Process-dependent secondary particles



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Salt Processing
- NaCl
- Coarse Mineral Dust
- Boiler Combustion Soot
- Additive Chemical Particulates

Solid Product Handling and Storage
- Palm Kernel Extract
- Feed Wheat
- Soya meal
- Other plant derived particle

Waste Management NZ
- Municipal refuse & organic dust
- Polymer & plastic fragments
- Condensed organic aerosols (COA)
- Polycyclic aromatic hydrocarbons (PAHs)

Logging
- Pine bark
- Pine wood
- Soil
- Road dust

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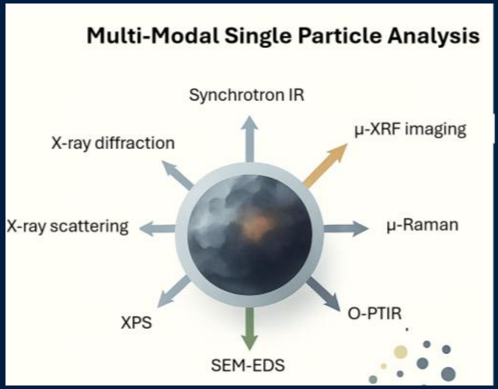
Environmental Samples



Auckland – Coastal Urban
- TSP
- PM10
- Mt Eden (near CBD)
- Kyber Pass (heavy traffic)

Pilot Study – only one or two samples collected over 24 hours in a single location

Clean Marine Air – Coastal clean
- TSP
- PM10
- West Coast onshore winds

Mount Maunganui – Coastal Industrial Zone
- TSP
- PM10
- Three flow rates tested

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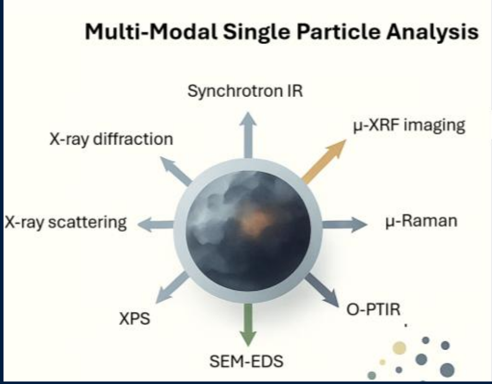
Reference Samples – case study driven

Salts
- Sodium Chloride
- Sodium Sulphate
- Sodium Phosphate
- Sodium nitrate
- Magnesium sulphate
- Magnesium Phosphate
- Magnesium Nitrate
- Potassium Sulphate
- Potassium Nitrate

Combustion Soot
- Heavy Fuel Oil
- Diesel
- Coal
- Pine Wood
- Pallet (treated wood)
- Sparklers (fireworks)

Microplastics
- PET
- PMMA
- PE
- PP
- PLA
- PVC
- Polyurethane
- Polystyrene
- ABS
- Styrene butadiene



Biologicals
- Sea Water
- Pollen
- Mould spores

Animal Feeds
- Palm Kernal Extract
- Poultry Feed

Mineral Dusts:
- Unsealed Road Dust
- Dried River Bed Dust
- Fine Quarry Dust

Vehicle emissions
- Tyre rubber
- Brake dust
- Diesel vehicle exhaust
- Petrol Vehicle Exhaust

Logging Emissions
- Pine Bark
- Debris from debarking row
- Material before logs loading
- Material after log loading
- Material after the sweeper

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Organic PM – Logging Emissions or PKE??

What they share

- Plant-derived, lignocellulosic materials
- Generate fugitive dust during transfer, storage and transport
- Heterogeneous mixtures - not single chemical classes
- Overlapping carbohydrate, C–H and carbonyl IR signatures

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What is Pine dust?

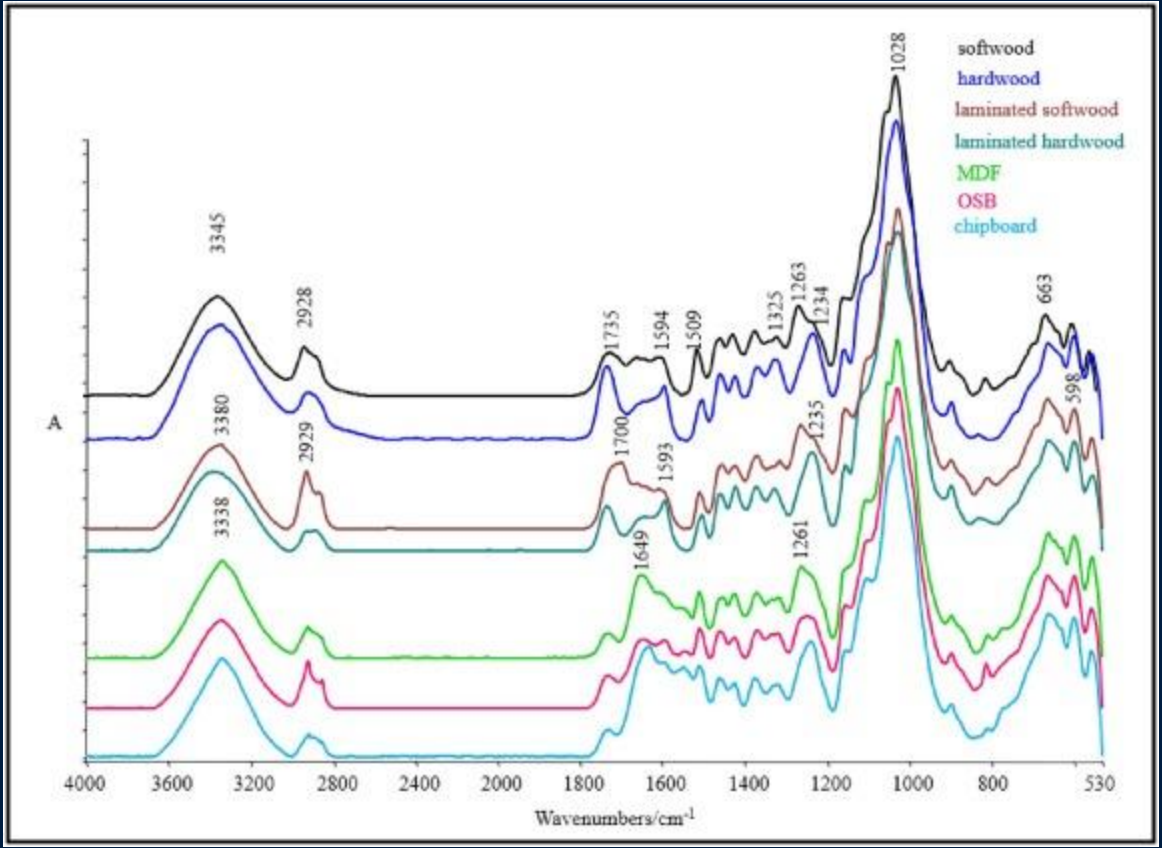
Core diagnostic windows:

- ~1730–1740 cm^{-1} — carbonyl (hemicellulose / oxidation)
- ~1505–1520 cm^{-1} — aromatic lignin
- ~1600 cm^{-1} — aromatic ring vibrations (supporting)
- ~1260–1270 cm^{-1} — guaiacyl lignin (softwood-relevant)
- ~1155–1165 cm^{-1} — polysaccharide C–O–C
- ~1100–1120 cm^{-1} — cellulose/hemicellulose

Known sources of variability

- Species and genetic provenance
- Juvenile vs mature wood
- Earlywood vs latewood
- Geographic and environmental growth conditions
- Post-harvest aging and oxidation
- Milling and dust formation effects
- Particle size, morphology, and surface sensitivity

Bulk IR measurements of woods



What is PKE dust?

Core diagnostic window:

- ~1735–1750 cm^{-1} — ester carbonyl, residual palm-kernel oil
- ~1640–1660 cm^{-1} — amide I; protein, bound-water contribution
- ~1530–1550 cm^{-1} — amide II; protein
- ~1150–1170 cm^{-1} — glycosidic C–O–C; mannan/cellulose
- ~1020–1060 cm^{-1} — carbohydrate C–O; mannan-rich fibre

Known sources of variability

- Palm-kernel provenance
- Palm Kernal processing conditions
- Efficiency of oil extraction and residual lipid content
- Variable protein-to-fibre composition
- Kernel shell and other fibrous material
- Drying, storage, moisture and oxidation
- Particle tissue, size and morphology
- Localised protein-, lipid- and carbohydrate-rich particles

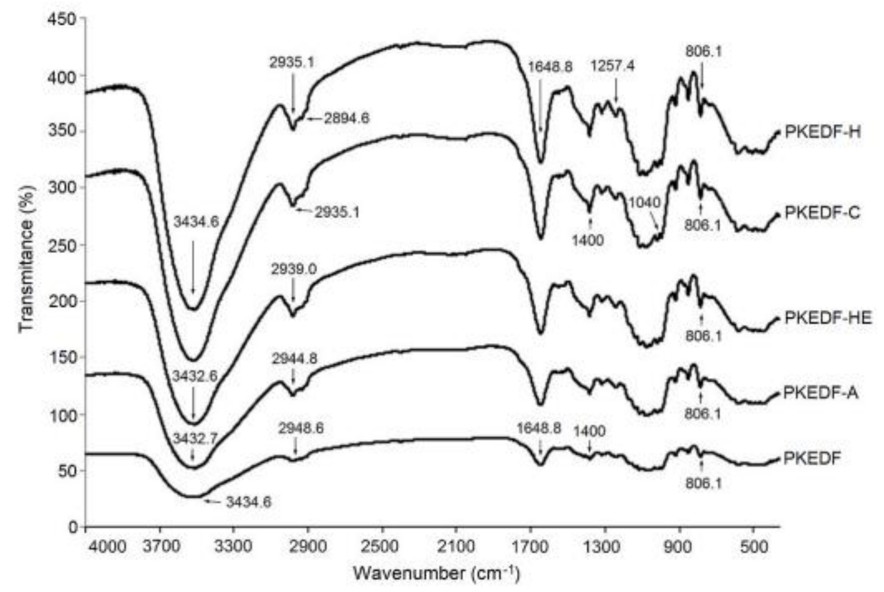
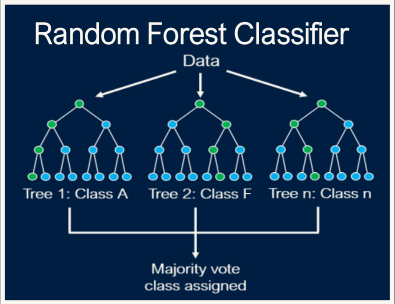


Fig. 2. Fourier-transformed infrared spectroscopy of PKEDF, PKEDF-A, PKEDF-HE, PKEDF-C and PKEDF-H.

Figure shows effects of different solvent treatments for extraction of PKE on FTIR Spectral signatures

Zheng, Y.; Li, Y.; Tian, H. Effects of Carboxymethylation, Acidic Treatment, Hydroxypropylation and Heating Combined with Enzymatic Hydrolysis on Structural and Physicochemical Properties of Palm Kernel Expeller Dietary Fiber. *LWT* **2020**, *133*, 109909.



Particle Classification – Two Source Model

The binary model correctly assigned 82% of pine particles and 70% of PKE particles.

Two-source classification

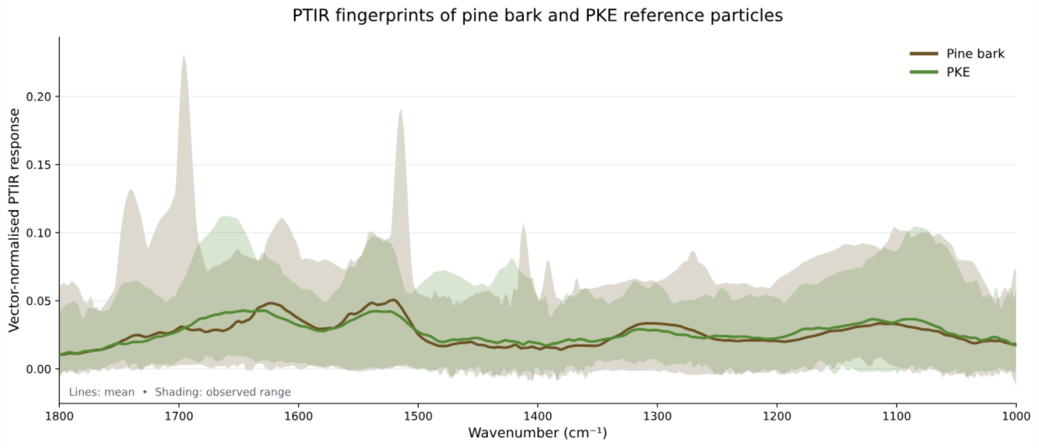
		Predicted: PKE	Predicted: Pine
Actual	PKE	42 (70%)	18
Actual	Pine	21	98 (82%)

78% overall accuracy

76% balanced accuracy

Confused 39 spectra cross classes

- Pine and PKE are partially separable from their PTIR fingerprints.
- A forced binary decision overstates certainty for chemically ambiguous particles.



Neither source is represented by a single spectral fingerprint

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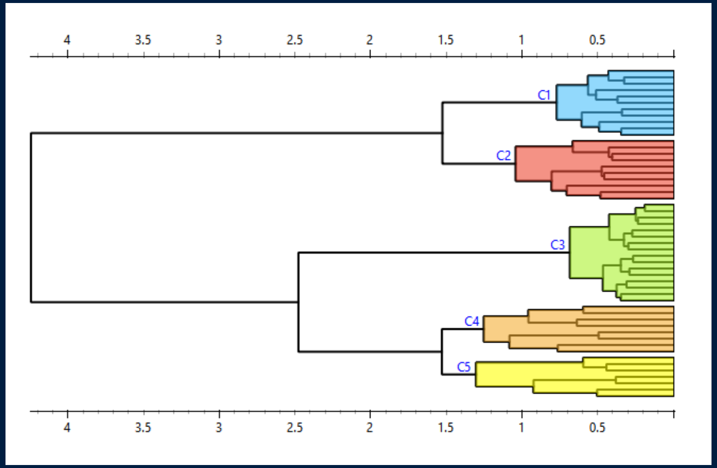
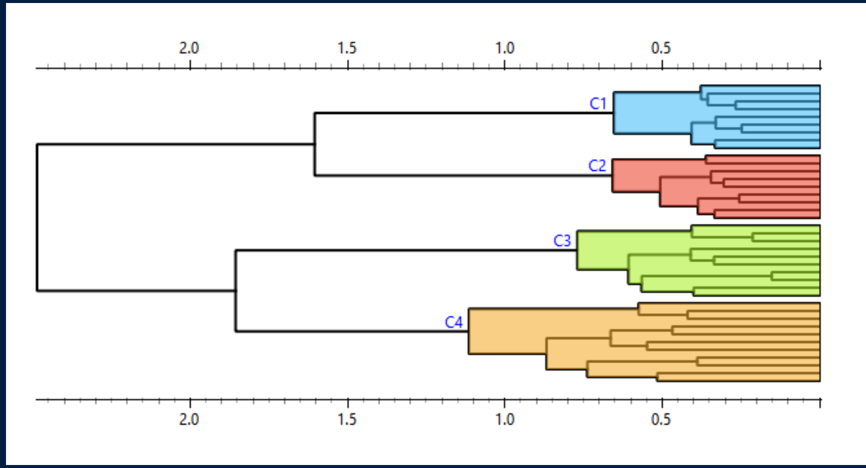
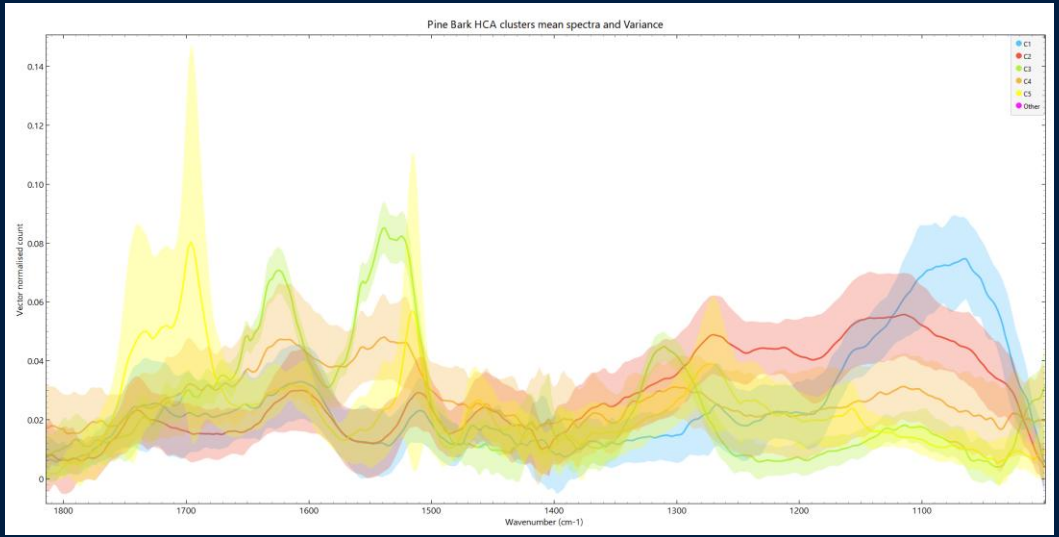
Both Sources are Chemically Heterogenous

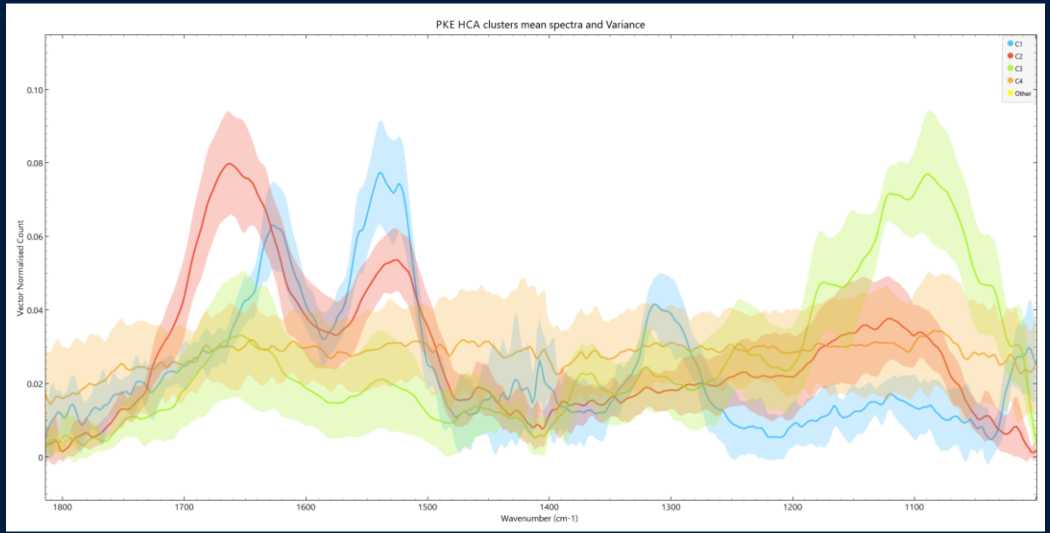
Pine Bark HCA – 5 Sub Groups



PKE HCA – 4 Sub Groups

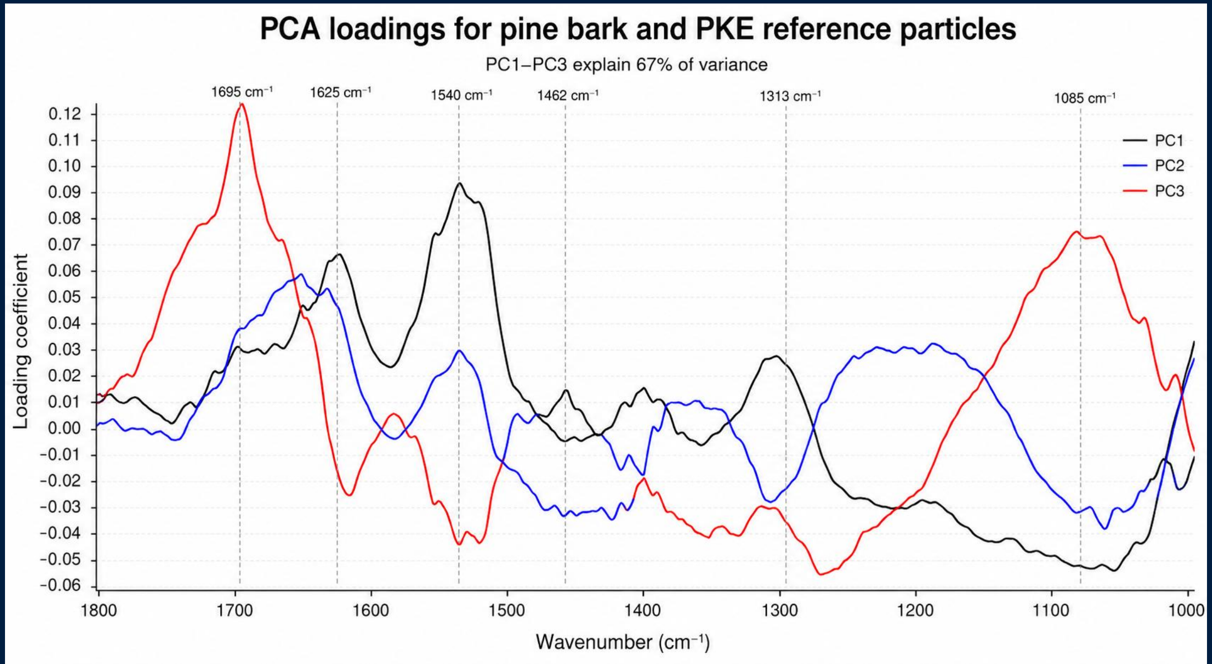






What chemical differences drive the particle groupings?

Principal Components Analysis (PCA) identifies the combinations of spectral features that vary most strongly between individual particles.



PC1 — protein/lignin balance
Differences around 1625, 1540 and 1313 cm^{-1} distinguish particles with stronger protein- or lignin-associated features.

PC2 — carbohydrate structure
Variation across approximately 1200–1085 cm^{-1} reflects differences in cellulose, hemicellulose and other plant carbohydrates.

PC3 — carbonyl and oxidation chemistry
The strong contribution near 1695 cm^{-1} reflects differences in carbonyl-containing material associated with lipids, oxidation and processed plant matter.

The model is not finding one unique pine or PKE marker.
It is separating particles using combinations of protein/lignin balance, carbohydrate structure and carbonyl chemistry.

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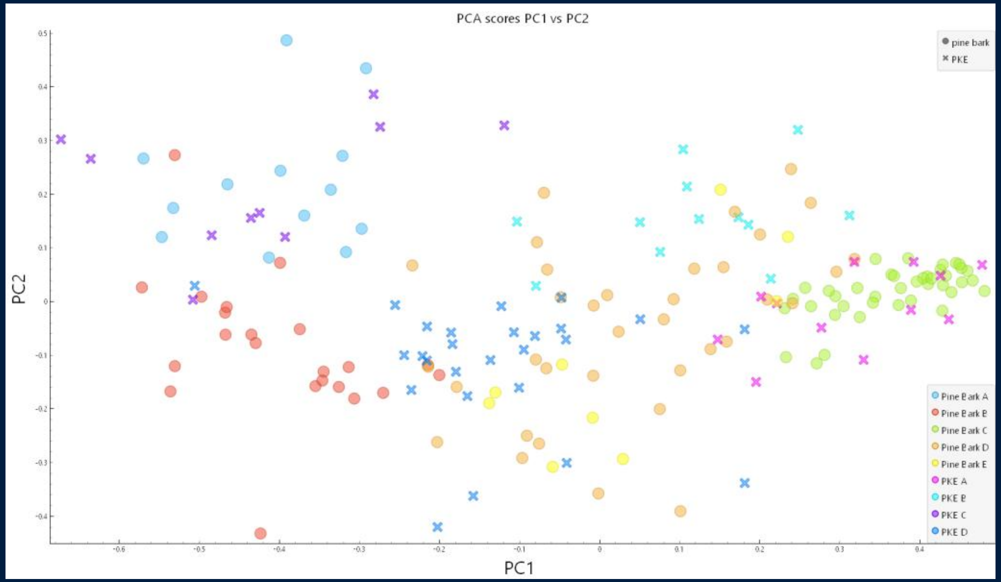
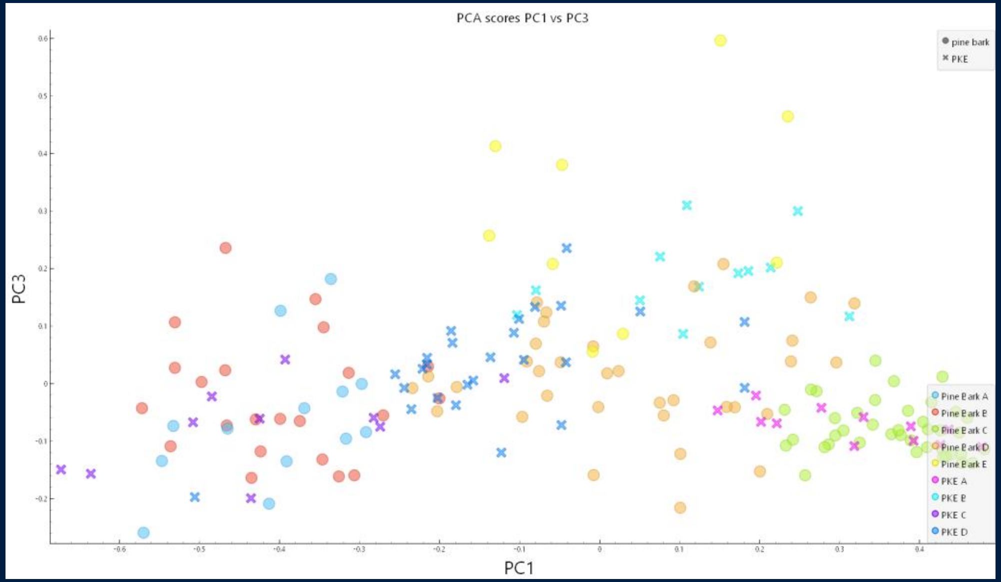
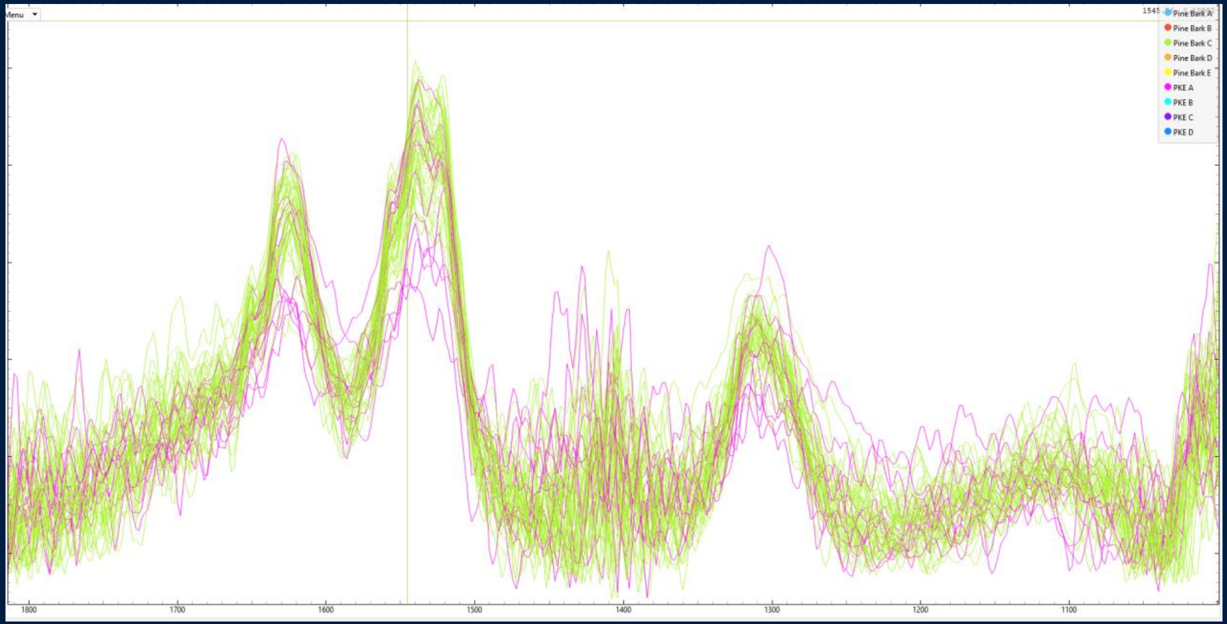
Principal Components Analysis of Subgroups





PCA Scores agree with the binary confusion matrix

- Some subgroups of Pine Bark and PKE overlap in PCA Scores
- Pine Bark C and PKE A overlap particularly strongly in both scores plots



Clear plant-derived chemistry but lack sufficient source-specific information to distinguish pine from PKE.

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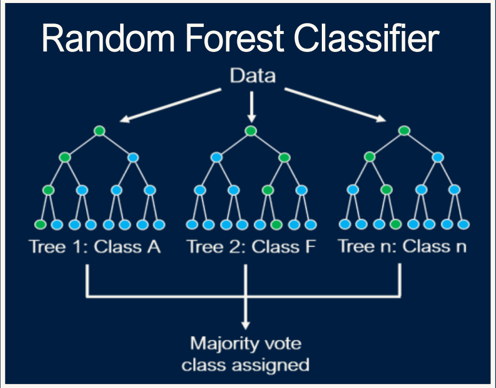
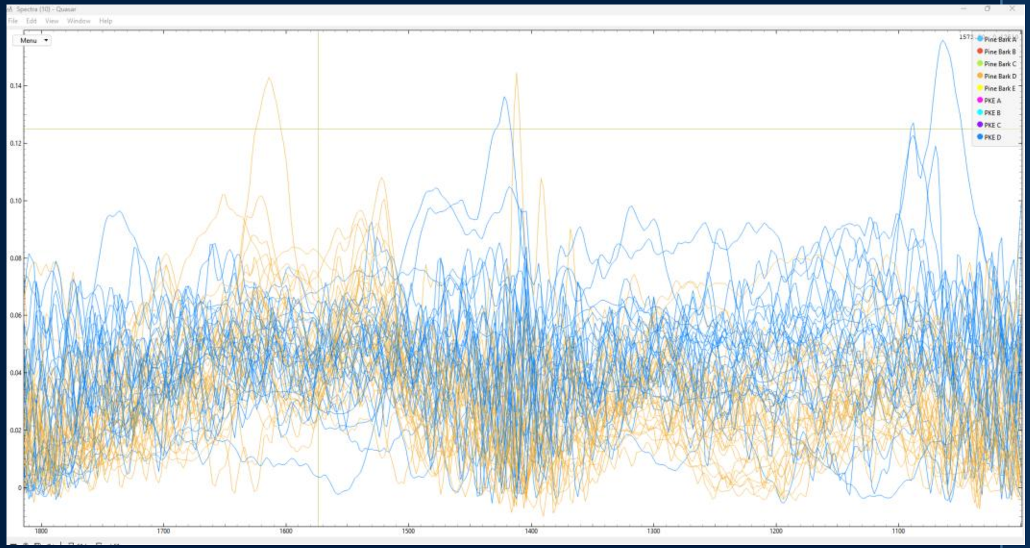


Classification by Subgroup



Removed from future training models

Nine-subgroup classification

Predicted

Actual	Pine Bark A	Pine Bark B	Pine Bark C	Pine Bark D	Pine Bark E	PKE A	PKE B	PKE C	PKE D	∑
Pine Bark A	9	0	0	0	0	0	0	4	0	13
Pine Bark B	1	18	0	0	0	0	0	1	2	22
Pine Bark C	0	0	40	0	0	0	0	0	0	40
Pine Bark D	0	1	3	17	1	1	1	0	11	35
Pine Bark E	0	0	0	1	7	0	1	0	0	9
PKE A	0	0	7	3	0	2	0	0	0	12
PKE B	0	0	0	1	0	0	11	0	0	12
PKE C	2	1	0	0	0	0	1	6	0	10
PKE D	0	1	0	4	1	0	0	2	18	26
∑	12	21	50	26	9	3	14	13	31	179

Best recognised

Pine C 100% • PKE B 92% • Pine B 82%

Main source-crossing confusion

Pine D ⟷ PKE D

72%
subgroup accuracy

68%
balanced accuracy

41
particles crossed sources

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Subgrouping explains the uncertainty but does not completely resolve source attribution.

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Logging Debris Samples
positive control for pine dust, negative control for PKE

Logging Emissions
- Pine Bark
- Debris from debarking row
- Material before logs loading
- Material after log loading
- Material after the sweeper

Mineral Dusts:
- Unsealed Road Dust
- Dried River Bed Dust
- Fine Quarry Dust

Expected outcome:
- No classification of PKE
- Debarking debris: highest proportion of pine-like spectra.
- Ground sweepings before and after log loading: lower pine-like proportion and more rejected spectra After mechanical sweeping: predominantly rejected, expect more mineral-like spectra.

Limitations
- Mineral samples are not from the same region (Canterbury)
- Samples were measured at a different facility and had previously been exposed to synchrotron radiation

Solutions:
- Prepare fresh samples of logging debris and test model performance
- Prepare high purity mineral samples using local sources

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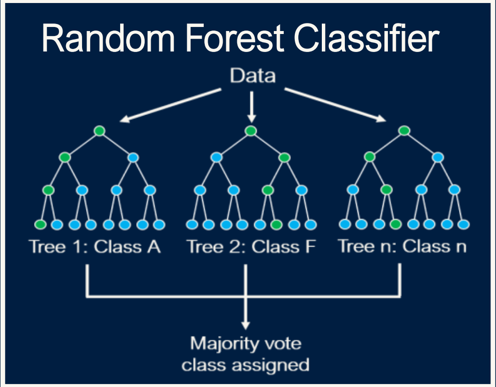


Recognising ambiguity improves the model

- Adding mineral references ambiguous plant, low-signal and mixed organic–mineral classes reduced forced source assignments.
- Remaining errors were concentrated among low-signal, mixed and ambiguous spectra.
- These output classes represent evidence quality as well as predicted chemistry.

10- Class Uncertainty aware model

Actual ↓ Predicted →	Pine A	Pine B	Ambiguous plant	Low signal	Pine E	PKE B	PKE C	Mineral A	Mineral B	Mixed organic–mineral	Σ
Pine A	**7**	0	0	1	0	0	2	0	3	0	**13**
Pine B	1	**19**	0	1	0	0	0	0	1	0	**22**
Ambiguous plant	0	0	**49**	3	0	0	0	0	0	0	**52**
Low signal	0	1	5	**43**	3	1	1	0	1	6	**61**
Pine E	0	0	0	1	**7**	1	0	0	0	0	**9**
PKE B	0	0	0	1	0	**11**	0	0	0	0	**12**
PKE C	1	2	0	0	0	1	**4**	0	2	0	**10**
Mineral A	0	0	0	0	0	0	0	**7**	0	0	**7**
Mineral B	4	1	0	2	0	0	1	1	**8**	1	**18**
Mixed organic–mineral	0	0	0	4	0	0	0	0	0	**77**	**81**
Σ	**13**	**23**	**54**	**56**	**10**	**14**	**8**	**8**	**15**	**84**	**285**

Best recognised

Mixed 95% • Ambiguous plant 94% • PKE B 92%

Remaining overlap

Low signal ↔ mixed / ambiguous

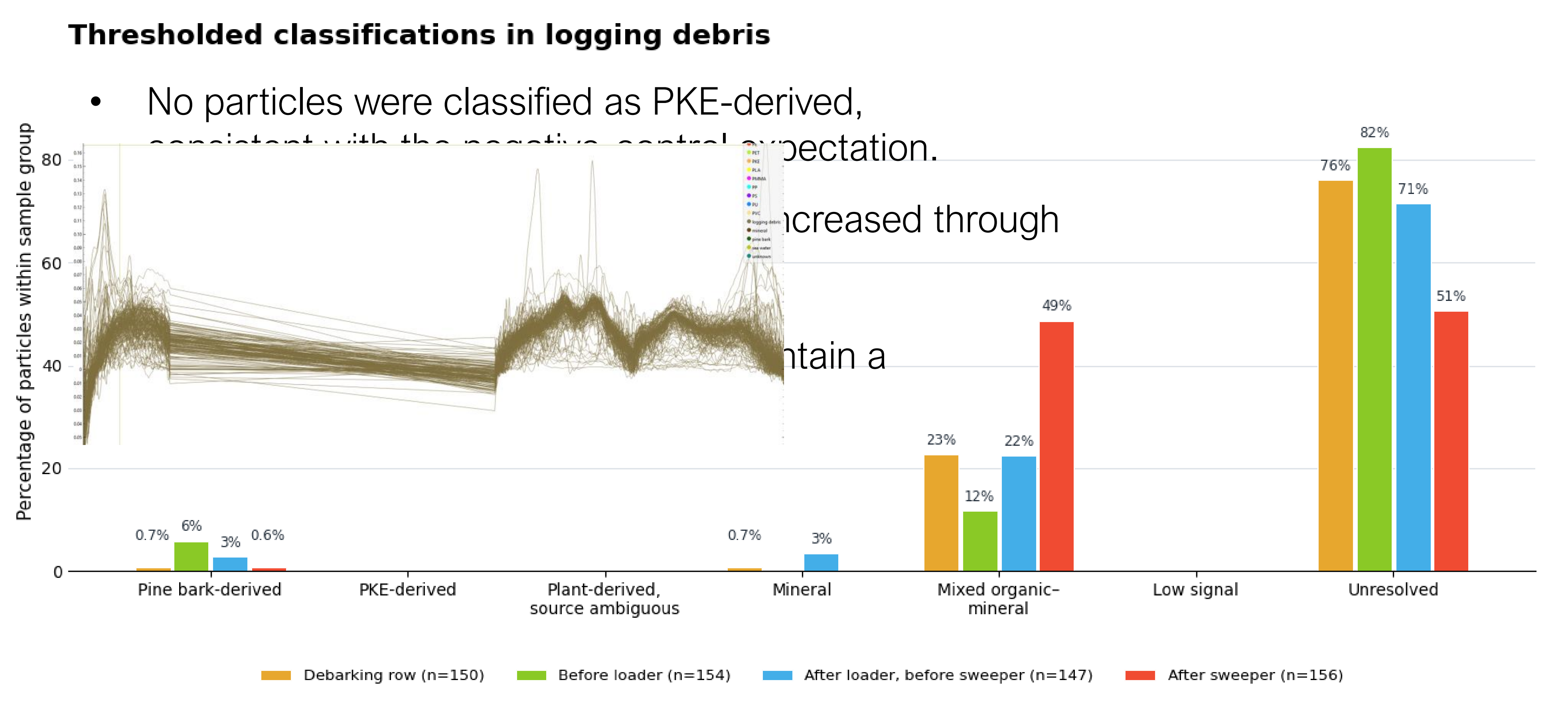
81%
overall accuracy

75%
balanced accuracy

94%
ambiguous plant recall

Logging Debris Samples

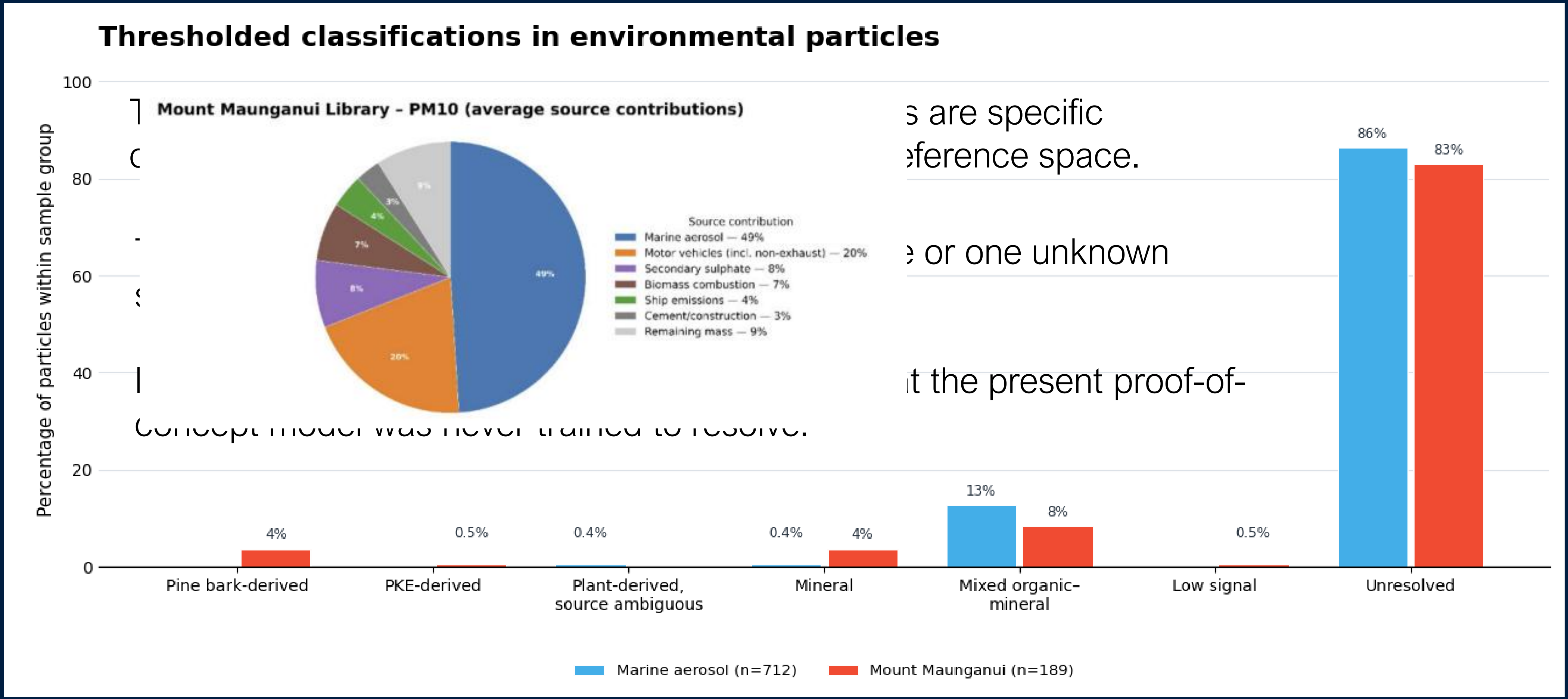
Classification captures increasing mineral contribution through the sweeping process



Two working hypotheses

1. Missing stem-wood reference chemistry in the model
2. Synchrotron-associated alteration of organic particles.

Environmental Samples
Mount Maunganui and Clean Marine Air



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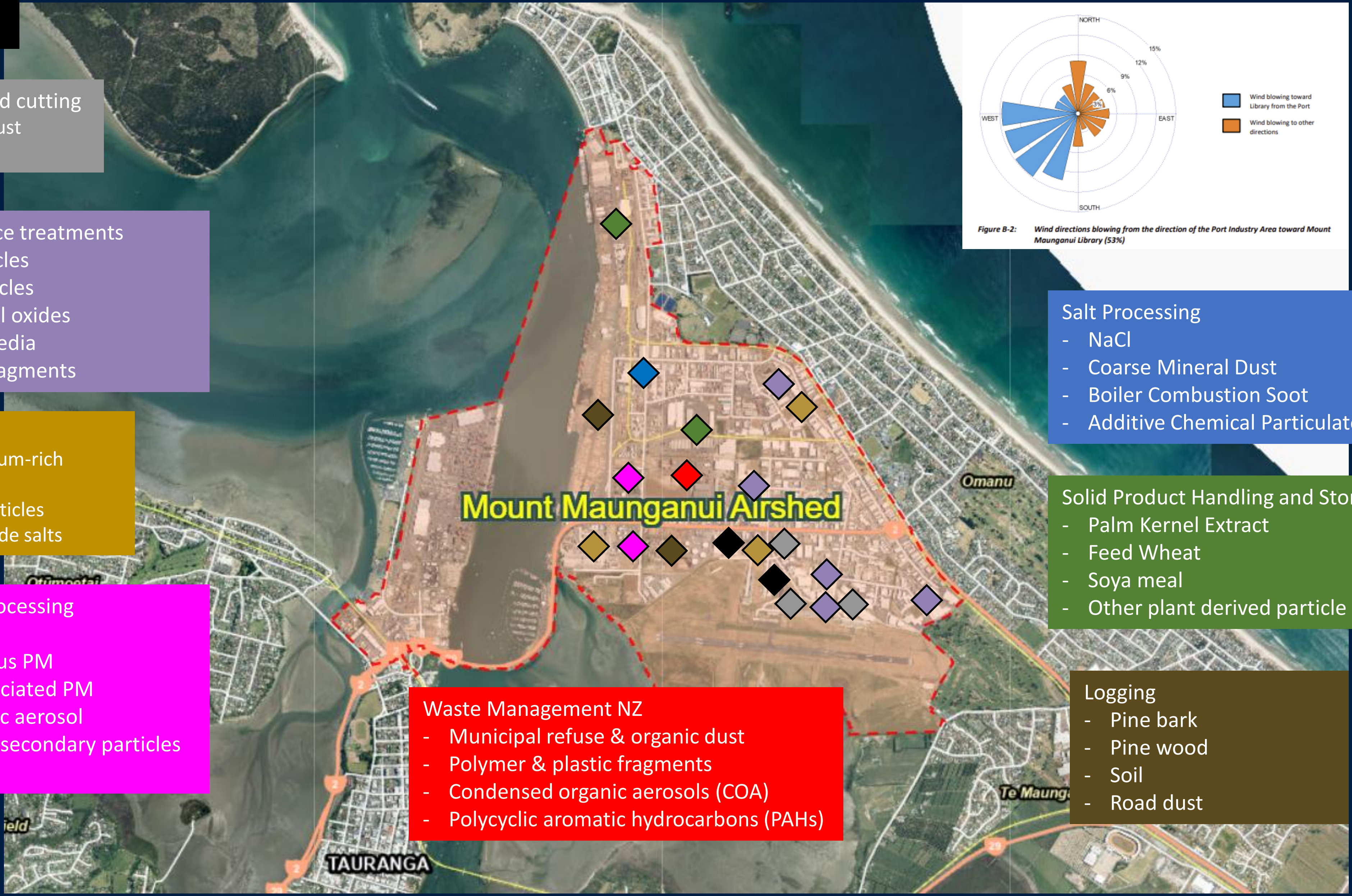

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Conclusions

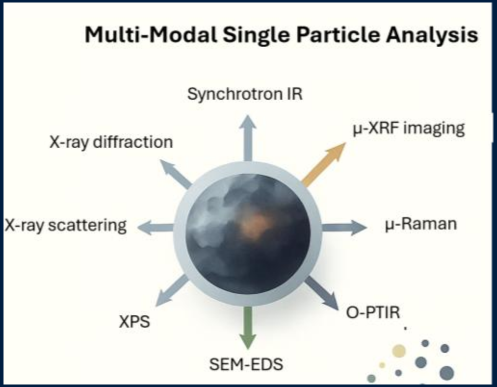
- The logging controls recovered the expected increase in mineral-associated particles through the loading and sweeping sequence.

- Mount Maunganui contained candidate pine-bark-like and mineral-like signals, but most particles remain outside the current reference space.

- The present model is a proof of concept - not yet a complete quantitative description of the particles in airshed.
  - We have spent 2 years developing reliable single particle measurements across the range of particle types in complex industrial environments

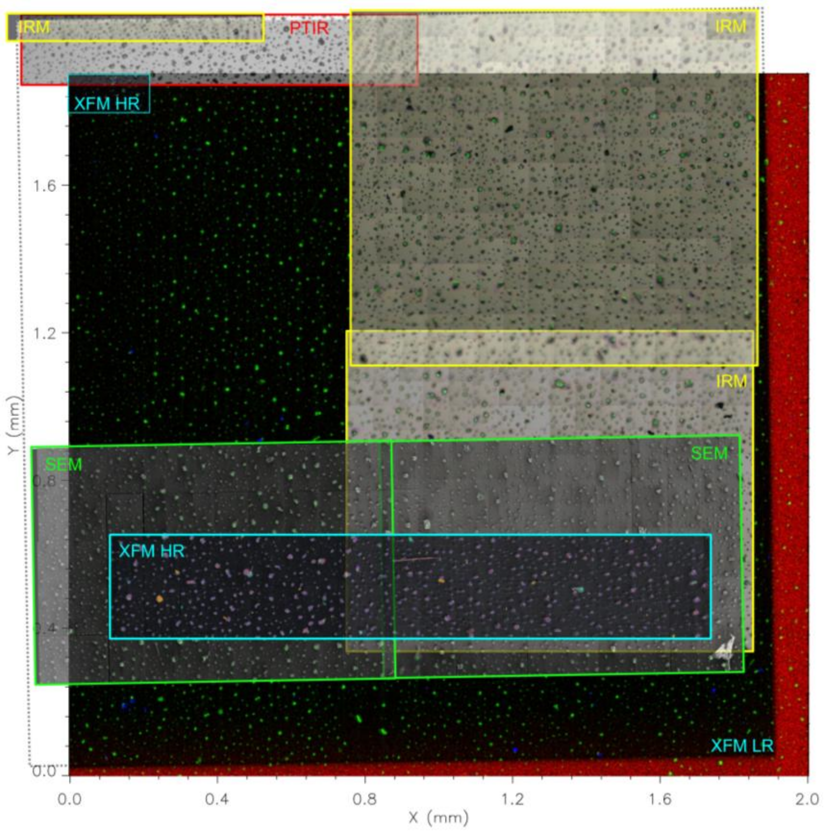
  - We have developed preliminary models for the different techniques and reference particle types that are very promising for particle-by-particle source attribution in environmental samples.

Reliable attribution requires wider range source references and multiple, independent lines of particle-level evidence.



Multimodal Fusion – Future Frontier

- Define diagnostic features from each mode: molecular bands and ratios, elemental composition, morphology, size and spatial associations.
- Co-register features at the individual-particle level and combine them into a shared particle-by-feature matrix.
- Build multimodal reference definitions that capture both characteristic source features and within-source variability.
- Test environmental particles against the combined reference space, retaining uncertainty when evidence is incomplete or conflicting.
- Apply validated classifications to environmental samples across space and time to identify emission patterns and evaluate mitigation.



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MOTE MEASUREMENT | NETWORKS

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