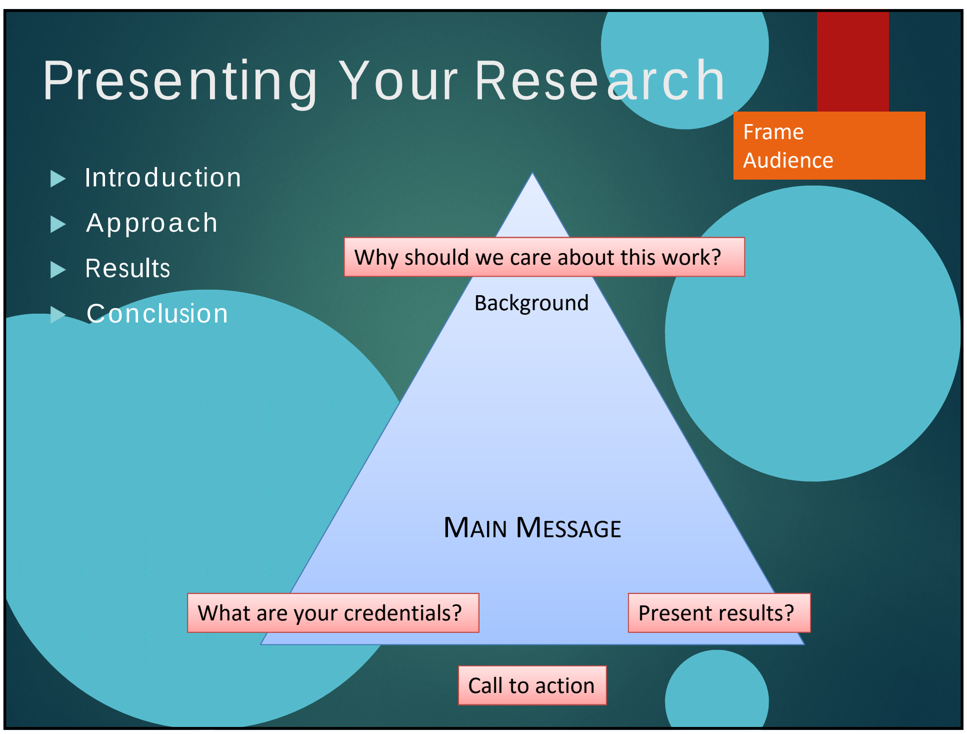

Presenting
YOUR GOALS & RESULTS
Alena Kubatova


Presenting Your Research
Frame Audience
Introduction
Approach
Results
Conclusion
Why should we care about this work?
Background
MAIN MESSAGE
What are your credentials?
Present results?
Call to action

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Fate of polycyclic aromatic hydrocarbons (PAHs) in atmosphere

- Why do we care about PAHs
- Current atmospheric methods used/their limitations
- Analysis of PAHs
- Implication of PAH's Fate

Background

Particulate matter," also known as particle pollution or PM, is a complex mixture of extremely small particles and liquid droplets. Particle pollution is made up of a number of components, including acids (such as nitrates and sulfates), organic chemicals, metals, and soil or dust particles.
The size of particles is directly linked to their potential for causing health problems. EPA is concerned about particles that are 10 micrometers in diameter or smaller because those are the particles that generally pass through the throat and nose and enter the lungs. Once inhaled, these particles can affect the heart and lungs and cause serious health effects. EPA groups particle pollution into two categories:

•"Inhalable coarse particles," such as those found near roadways and dusty industries, are larger than 2.5 micrometers and smaller than 10 micrometers in diameter.

•"Fine particles," such as those found in smoke and haze, are 2.5 micrometers in diameter and smaller. These particles can be directly emitted from sources such as forest fires, or they can form when gases emitted from power plants, industries and automobiles react in the air.

- There is an increasing concern about the occurrence of polycyclic aromatic hydrocarbons (PAHs) in the environment as they are ubiquitous in ambient air and some of them are among the strongest known carcinogens. PAHs and their derivatives are produced by the incomplete combustion of organic material arising, partly, from natural combustion such as forest and volcanic eruption, but with the majority due to anthropogenic emissions.

Atmospheric Particles, Particulate Matter (PM)


Volcanic dust


Forest fires


Sea salt


Fuel Combustion


Transportation

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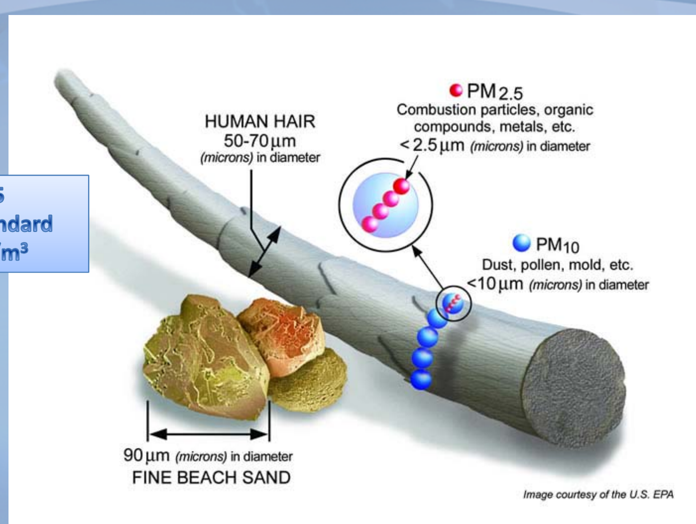
Particulate matter (PM) are tiny particles of solid or liquid suspended in a gas."

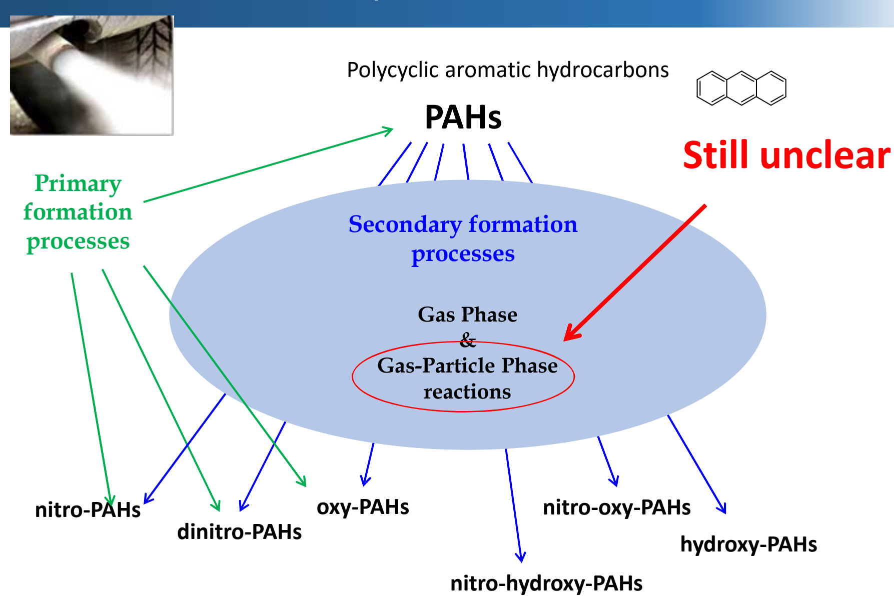
PM2.5 annual standard 12.0 µg/m³



Fate of PAHs in the atmosphere

- High occurrence of PAHs and NitroPAHs in Primary Emissions
- Secondary atmospheric reactions produce additional oxidation product of PAHs
- The information on PAHs derivative is incomplete

Fate of PAHs in the Atmosphere



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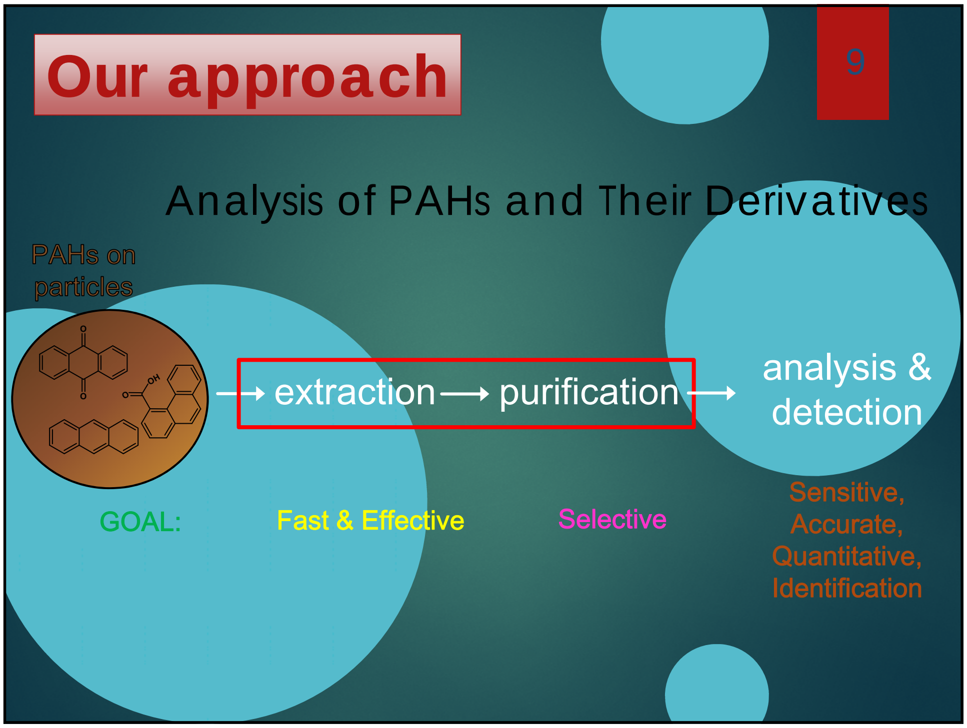
Our approach
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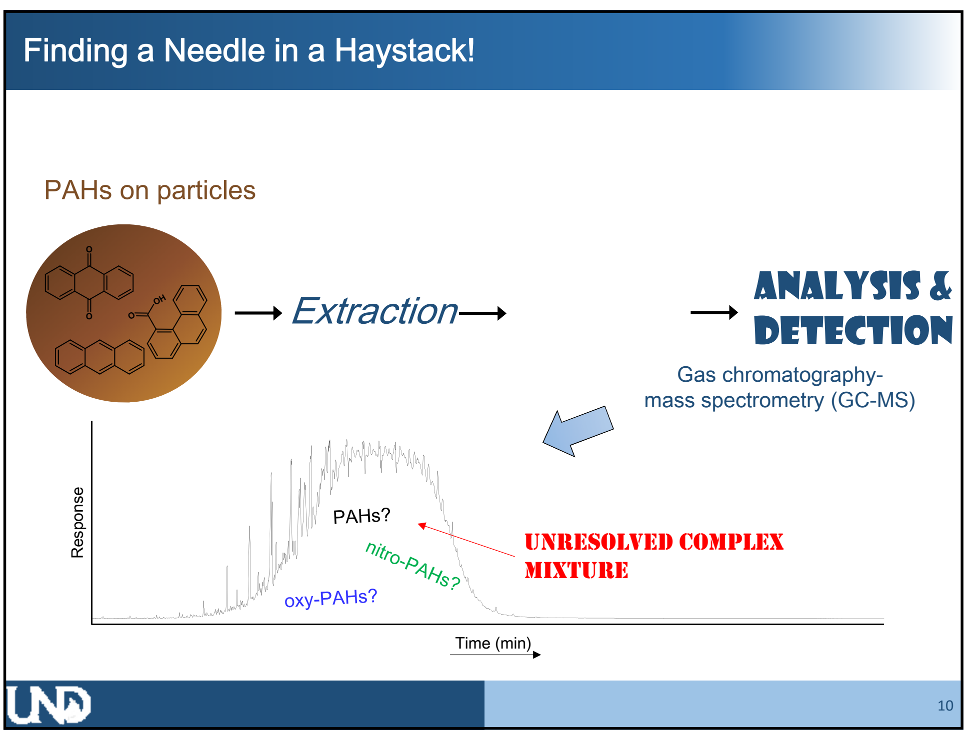
Analysis of PAHs and Their Derivatives
PAHs on particles
extraction
purification
analysis & detection
GOAL:
Fast & Effective
Selective
Sensitive, Accurate, Quantitative, Identification


Finding a Needle in a Haystack!
PAHs on particles
Extraction
ANALYSIS & DETECTION
Gas chromatography-mass spectrometry (GC-MS)
Response
PAHs?
nitro-PAHs?
oxy-PAHs?
UNRESOLVED COMPLEX MIXTURE
Time (min)
UND
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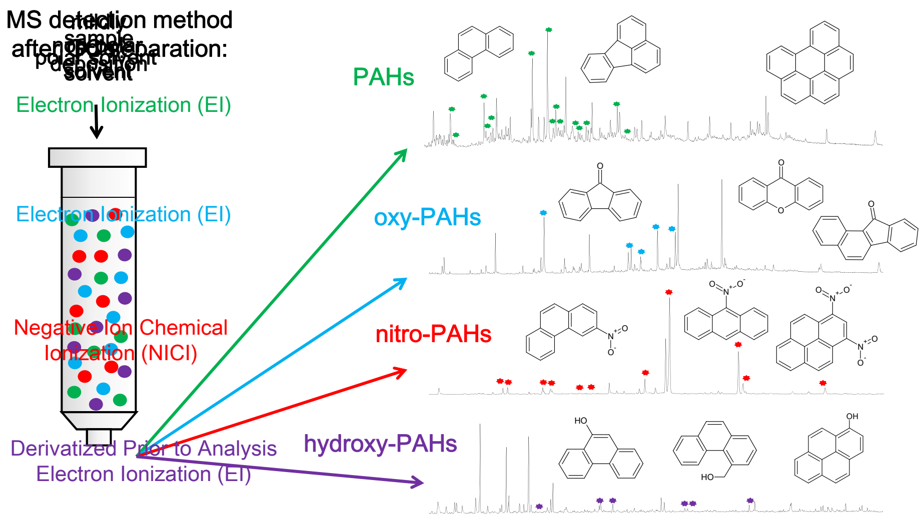
Using Solid Phase Extraction (SPE)

Isolating PAHs and PAH Derivatives From One Another



Cochran et al. *Anal. Chim. Acta* **2012**, *740*, 93–103.

Products observed for the reaction with O_3 upon trimethylsilylation and GC/MS analysis

Reaction Products		MW	ID	EI-MS ions
OH-3-ring-PAH	$C_{14}H_{10}O$	194/266	tentative	266(100), 251(20), 191(15)
di-OH-3-ring PAH	$C_{14}H_{10}O_2$	210/354	tentative	354(100), 73(50)
9-hydroxyphenanthrene	$C_{14}H_{10}O$	194/266	standard	266(100), 251(20), 191(15)
4-hydroxyphenanthrene-5-carboxaldehyde	$C_{15}H_{10}O_2$	222/294	tentative	293(50), 205(100), 176(25)
4-phenanthrenic acid	$C_{15}H_{10}O_2$	222/294	standard	294(75), 279(65), 205(100)
diOH derivative of 4-ring PAH	$C_{16}H_{12}O_2$	236/380	tentative	380(30), 290(40), 202(30)
diOH derivative of 4-ring PAH	$C_{16}H_{12}O_2$	236/380	tentative	380(30), 290(60), 202(20)
OH-4-ring PAH	$C_{16}H_{10}O$	218/290	standard	290(100), 275(50), 259(55)
OH-4-ring PAH	$C_{16}H_{10}O$	218/290	tentative	290(100), 275(50), 259(55)
OH-4-ring PAH	$C_{16}H_{10}O$	218/290	tentative	290(100), 275(50), 259(55)
1-hydroxypyrene	$C_{16}H_{10}O$	218/290	standard	290(100), 275(30), 259(20)
phenanthrene-4-carboxaldehyde-5-carboxylic acid	$C_{16}H_{10}O_3$	250/322	standard	322(15), 294(50), 205(30), 189(100)
diOH-4-ring PAH	$C_{16}H_{10}O_2$	234/378	tentative	378(100), 73(30)
diOH-4-ring PAH	$C_{16}H_{10}O_2$	234/378	tentative	378(100), 73(30)

Conclusions

From Method Development to Simulating Atmospheric Reactions

Method Development

Extraction	Developed an extraction method to simultaneously and efficiently extracts PAHs and a wide range of PAH derivatives from different PM matrices.
Sample Preparation	Optimized SPE to fractionate PAHs and classes of PAH derivatives from one another in order to increase the sensitivity in the detection and quantification.
Analysis & Identification	Established APCI as a tool to identify PAH oxidation products that do not have standards readily available.

Simulate PAH Oxidation & Heterogeneous Processes

Identification of Products	Identified products formed from the oxidation of PAHs with different gas conditions in a small flow reactor, closing the mass balance for PAHs and their products during the nitration of 3–4 ring PAHs.
Real-World Kinetics	Designed and constructed a large-scale atmospheric simulation chamber and investigated the PAHs and derivatives formed during the aging of diesel engine exhaust.

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