

Destruction and Transformation of Pyrene by Mineral Surfaces during Thermal Desorption

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Thermal Desorption

- Thermal and vacuum wells inserted into soil
- Site covered with a vapor cap
- Soil heated to 100 - 400 °C
 - Thermal Conduction Heating
 - Steam Injection
 - Electrical Resistance Heating
- Contaminants removed by vacuum wells
- Gas collected and treated



Target Average Remediation Temperature

- Chlorinated VOC's
 - BTEX
 - Total Petroleum Hydrocarbons
 - Polycyclic Aromatic Hydrocarbons
 - Pentachlorophenol
 - Dioxins
 - Polychlorinated Biphenyls
- 100 °C
- 150 - 300 °C
- > 300 °C



Removal and Transformation Mechanisms

Evaporation

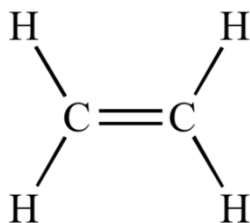
Steam Distillation

Hydrolysis

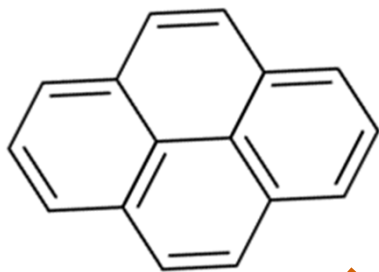
Oxidation/Reduction

Pyrolysis

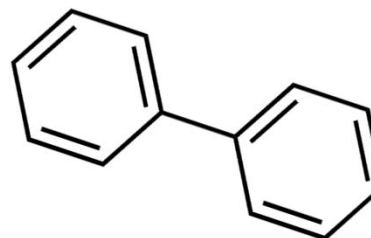
Ethylene



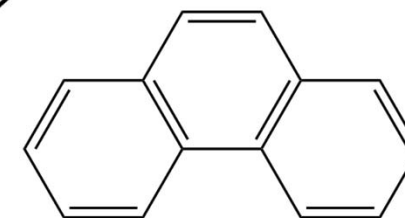
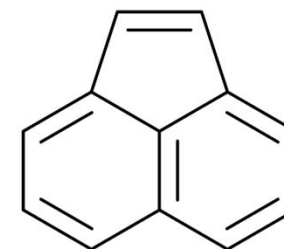
Pyrene



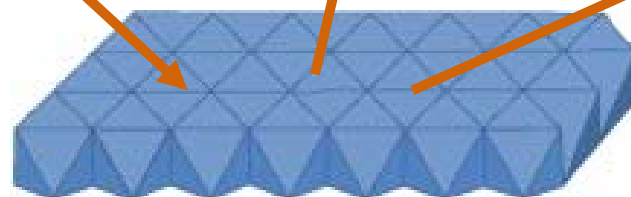
Biphenyl



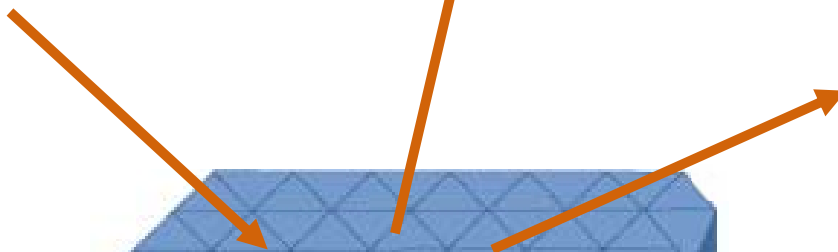
Acenaphthylene

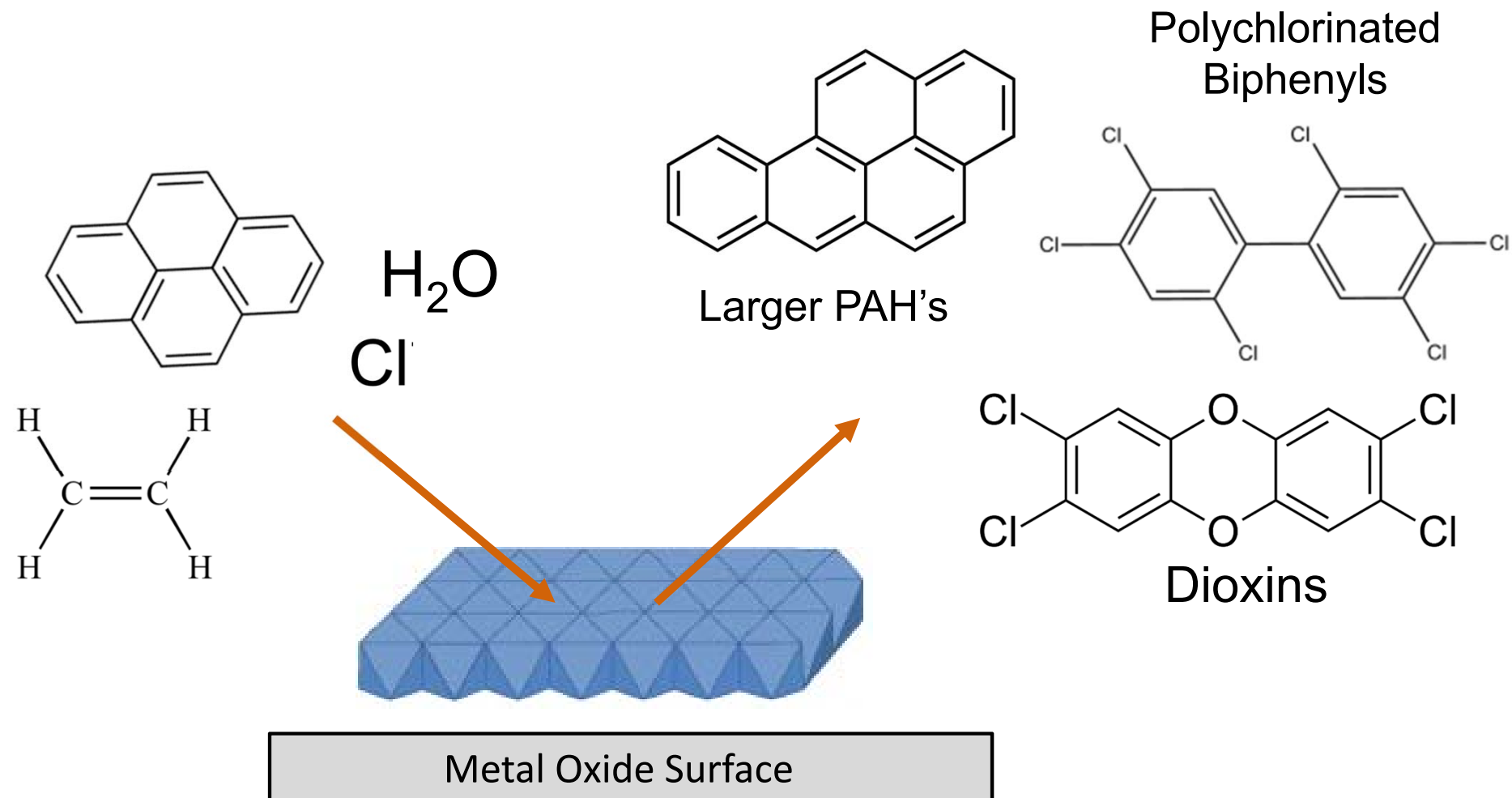


Phenanthrene



Metal Oxide Surface





Objectives

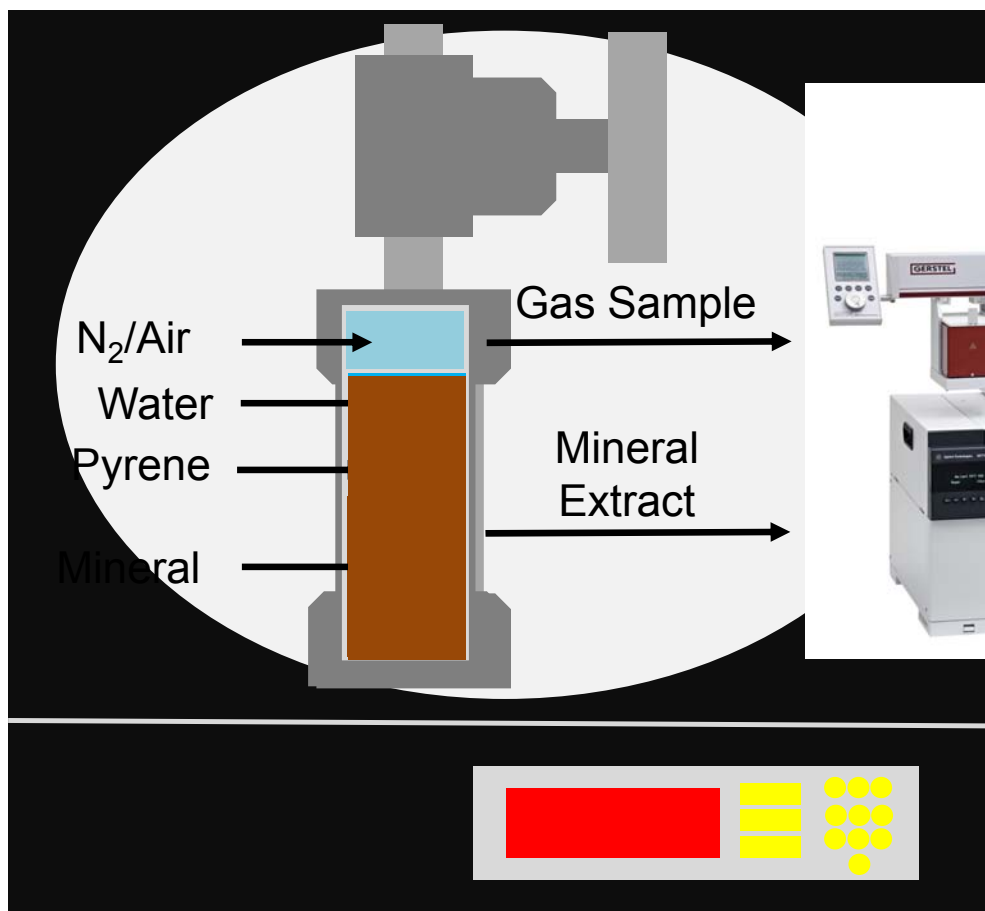
- 1) *Determine the relative importance of transformation by mineral surfaces at various temperatures*
- 2) *Identify trends in solution properties and mineral composition on transformation*
- 3) *Evaluate by-product formation in natural composite soil*
- 4) *Identify conditions that maximize contaminant degradation while minimizing toxic by-product formation*



Materials

Mineral	Formula	Redox Couple	Standard Potential (V)
Birnessite	$\delta\text{-MnO}_2$	$\text{Mn}^{4+}/\text{Mn}^{2+}$	1.23
Magnetite	Fe_3O_4	$\text{Fe}^{3+}/\text{Fe}^{2+}$	0.98
Hematite	Fe_2O_3	$\text{Fe}^{3+}/\text{Fe}^{2+}$	0.73
Quartz	SiO_2	$\text{Si}^{4+}/\text{Si}^{2+}$	-0.86

Experimental Methods



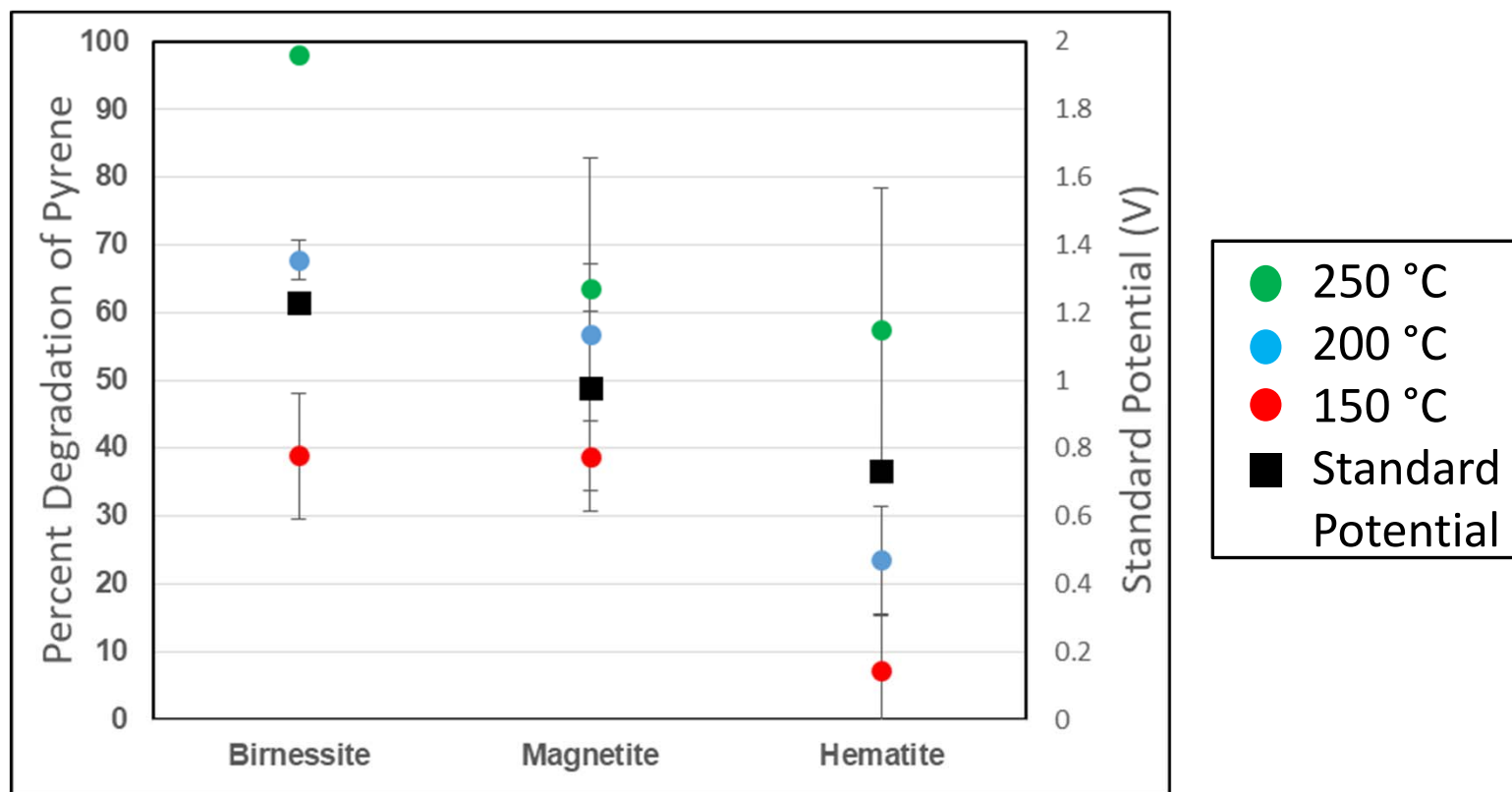
By-Products Detected

(2 hours, no MeOH, no O₂)

Mineral	Temp (°C)	Naphthalene	Acenaphthylene	Biphenyl	Phenanthrene	Pyrene
Quartz	200	X	X	X	X	✓
	400	X	X	X	X	✓

Transformation Experiment

(30 min, no MeOH, no O₂)

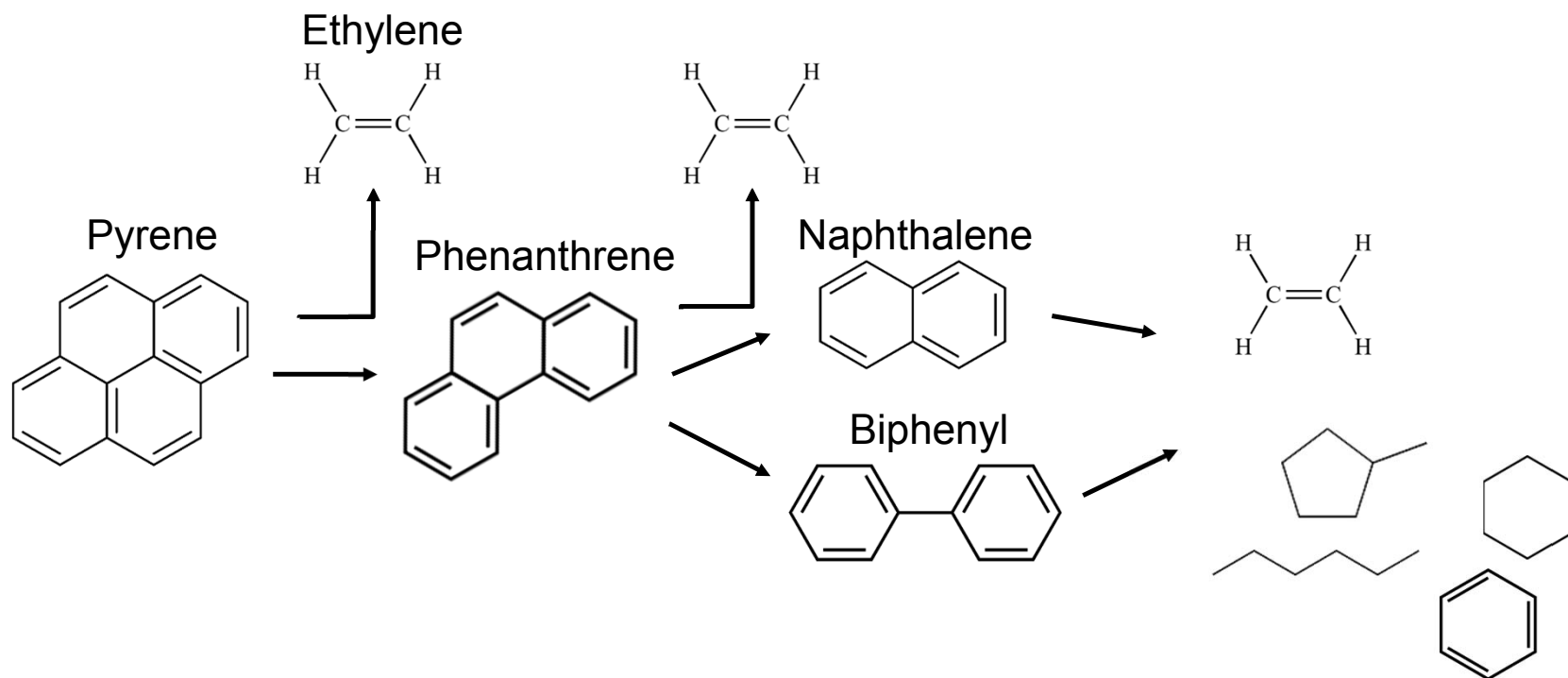


Gas Phase Results

(30 min, no MeOH, no O₂)

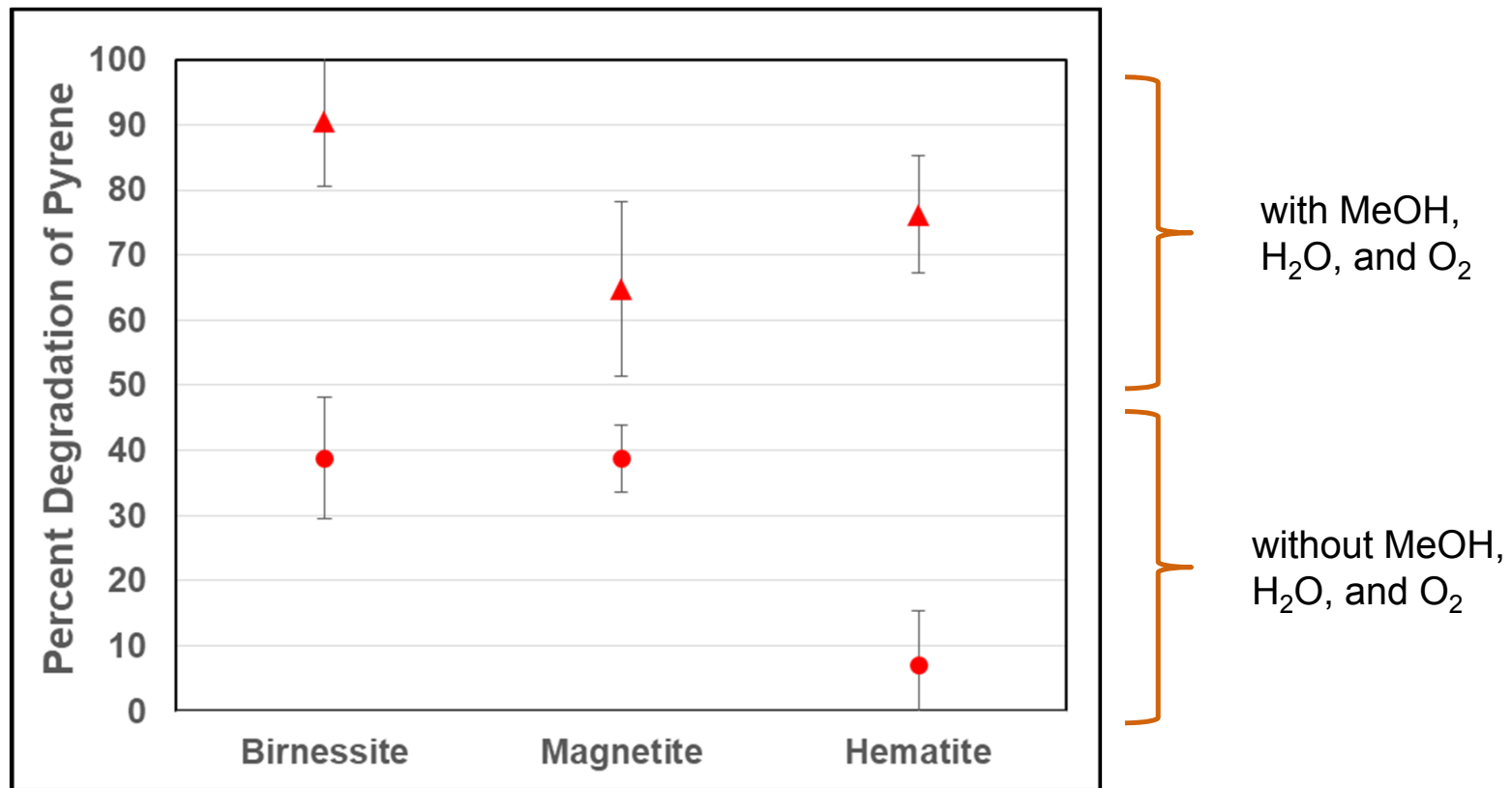
Mineral	Temp (°C)	Ethylene	6-C Cmpd's
Birnessite	150	✓	✓
	200	✓	X
	250	✓	X
Magnetite	150	✓	✓
	200	✓	X
	250	✓	X
Hematite	150	X	✓
	200	✓	✓
	250	✓	X

Degradation Pathway

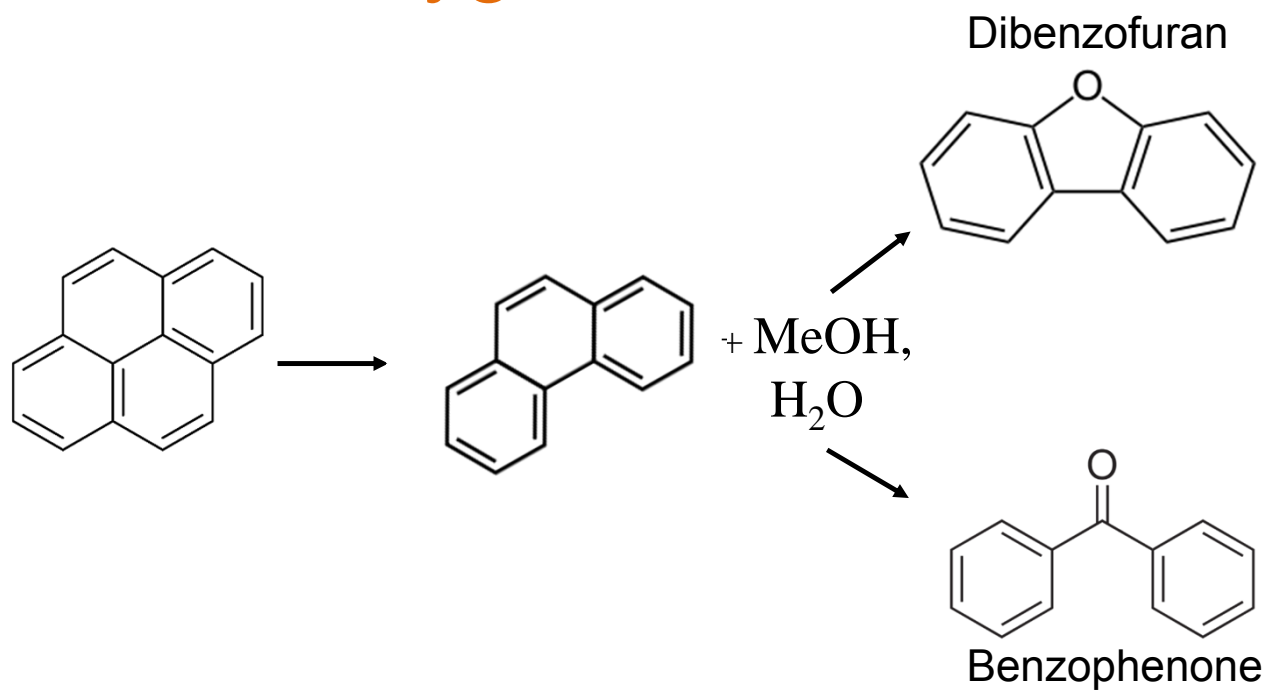


Transformation Experiment

(150 °C, 30 min, MeOH, H₂O, and O₂)



Degradation Pathway with Oxygen Source



Conclusions

Increased temperature (up to 400 °C) leads to increased degradation of pyrene

Mineral composition affects extent of degradation and by-product formation

Degradation occurs through sequential loss of ethylene fragments

Oxygen source (CH_3OH , H_2O) changes by-products formed

Future Work

Conduct flow-through experiments

Perform experiments in a real soil with known mineralogy

Determine surface oxidation state before and after treatment

Acknowledgements

Lynn Katz, PhD

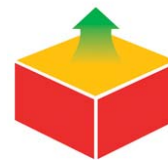
Charles Werth, PhD

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