

# PARTICLE GENERATOR FOR ENGINE EXHAUST SIMULATION

Imad Khalek, Athanasios Mamakos, Vinay Premnath, Richard Mechler, and Daniel Preece,  
Southwest Research Institute

Robert Giannelli and Matt Spears, US Environmental Protection Agency

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# Acknowledgements

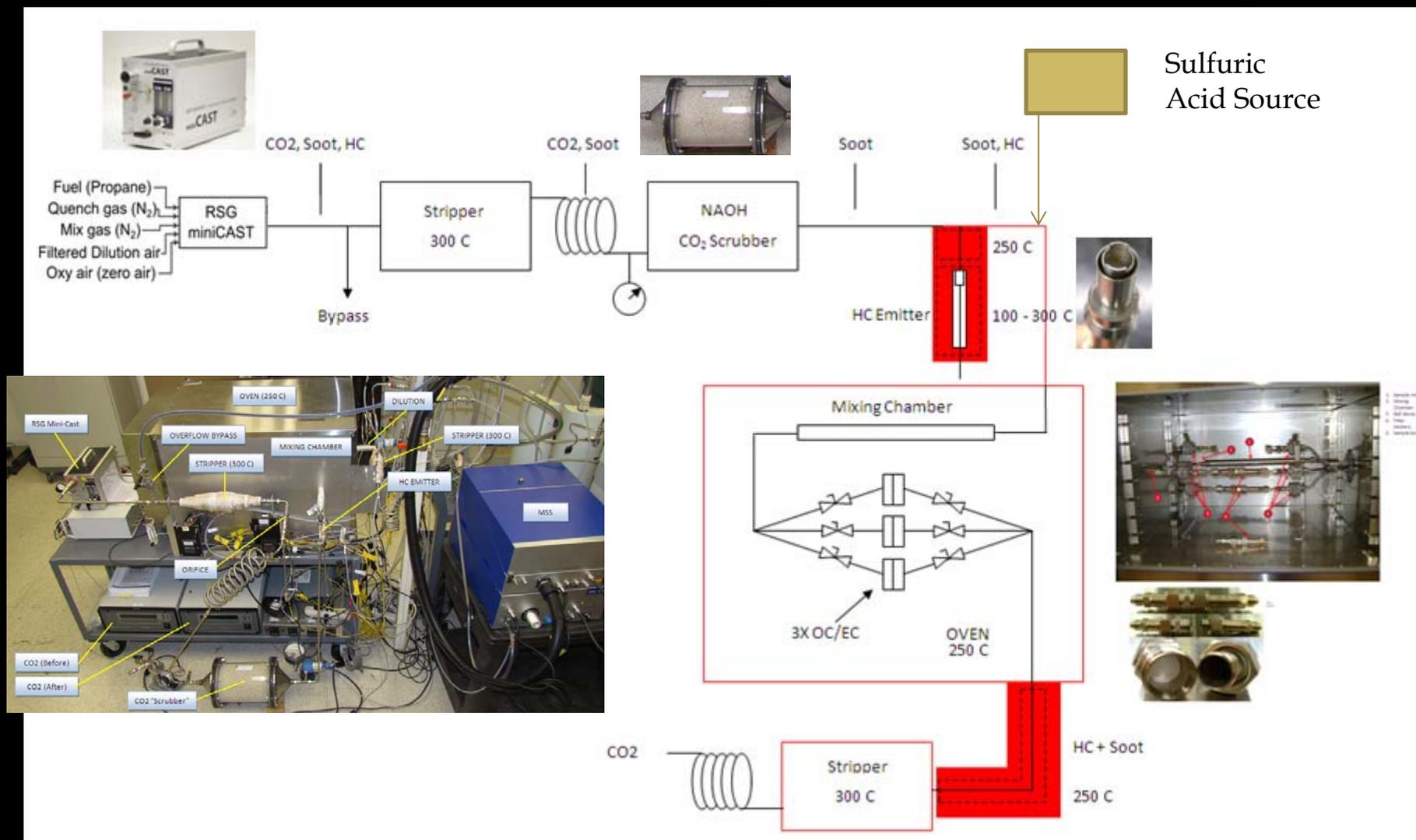
- ▣ This work is funded by the US Environmental Protection Agency



# Objectives

- ▣ This is work in progress. The objective is to develop a laboratory particle generator that can simulate engine exhaust aerosol and be used for PM research and development to assist in better understanding:
  - ▣ Gas/PM phase partitioning
  - ▣ Gas/PM phase transport & losses in sampling systems
  - ▣ Filter negative/positive artifacts
  - ▣ Particle nucleation and growth
  - ▣ Particle instrument performance and accuracy
  - ▣ Modeling using COMSOL and OpenFoam
  - ▣ Consideration of future standards related to different metrics such as particle mass and/or number
  - ▣ Other research elements

# PM Generator (Housed in SwRI Nanoparticle Laboratory)



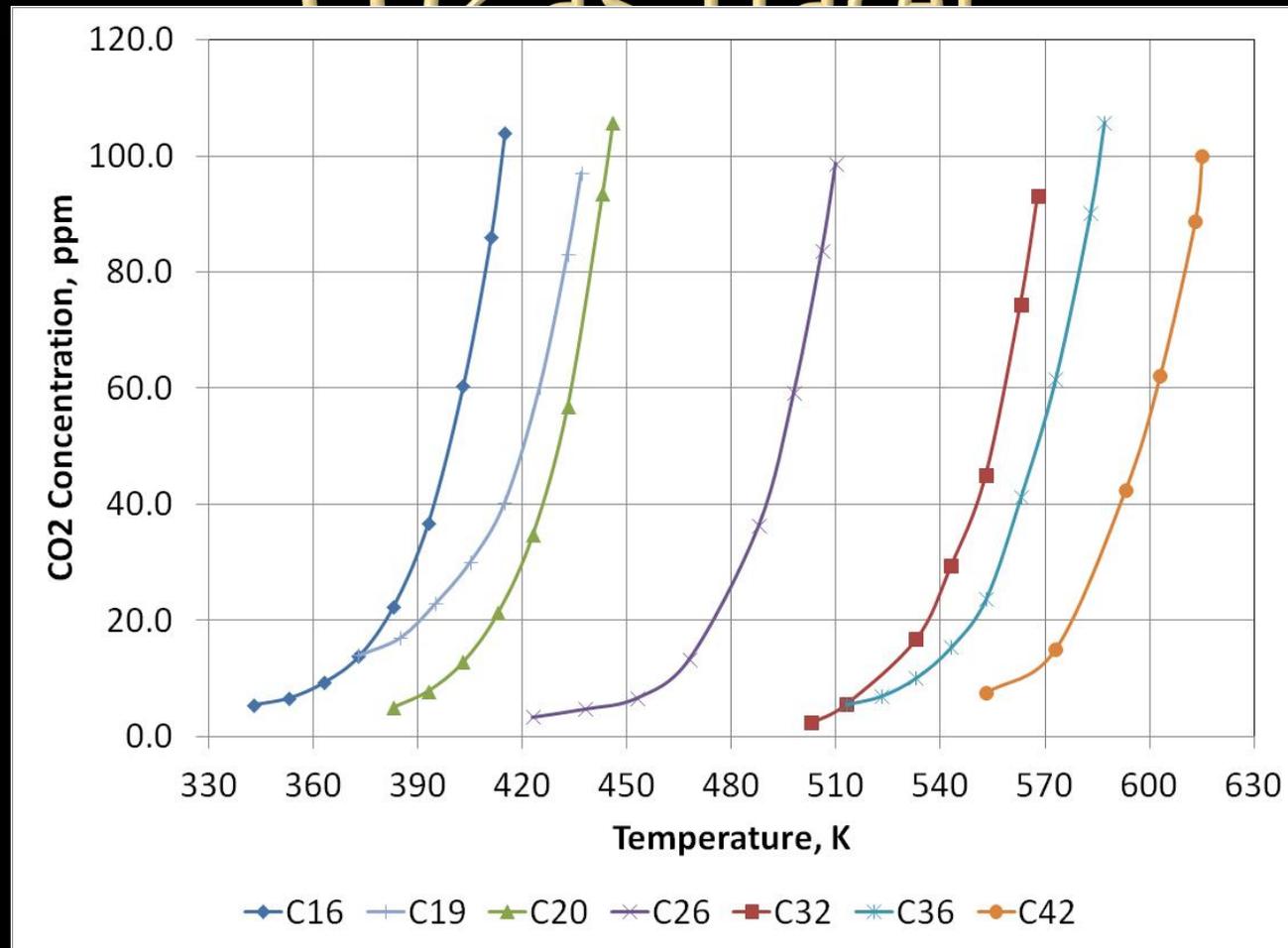
Elemental Carbon + Hydrocarbons (C<sub>1</sub>-C<sub>42</sub>) + H<sub>2</sub>SO<sub>4</sub>

# Features

- ▣ Elemental Carbon or Soot
  - Min-CAST + Catalytic Stripper
- ▣ HC Source
  - Developed a HC generator
  - Controlled C16 to C42 (alkanes for now but flexible to add any other compounds)
  - Concentration range: 0 to 100 ppmC
  - CO<sub>2</sub> for hydrocarbon detection
- ▣ Sulfuric Acid Source
  - SO<sub>2</sub> + catalytic stripper + H<sub>2</sub>O
  - Concentration range: 0 to 100 ppm
  - SO<sub>2</sub> for H<sub>2</sub>SO<sub>4</sub> detection
- ▣ Other Sources like ammonia and can be easily added



# Generating Different Hydrocarbon Profiles & Using CO<sub>2</sub> as Tracer



HC Mass Concentration Range from 0 to ~ 60 mg/m<sup>3</sup>



# HC Recovery Using CO<sub>2</sub>

	Measured	CO <sub>2</sub> -Based	% Difference	
	mg/m <sup>3</sup>	mg/m <sup>3</sup>		
C16	16.74	17.20	2.7%	
C20	28.82	29.85	3.6%	
C26	29.45	29.50	0.2%	
C32	34.95	34.66	-0.8%	
C36	31.48	29.82	-5.3%	
C42	26.45	21.62	-18.3%	
Measured: Weight Difference before and after				
CO <sub>2</sub> -Based: Based on CO <sub>2</sub> Measurement Downstream of Catalytic Stripper				

HC was transported at 250°C

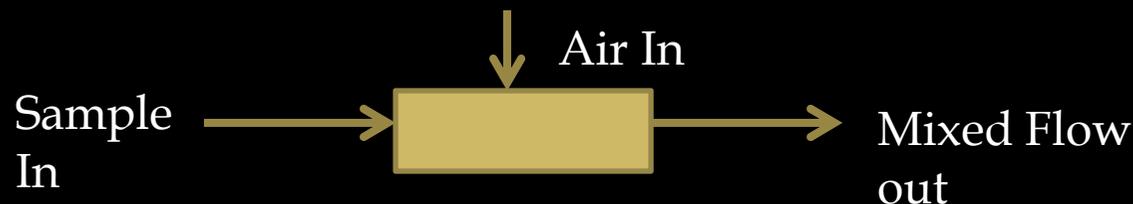
Catalytic Stripper was operated at 300°C

The system seems to suggest losses of C<sub>42</sub> at temperature of 250°C



# Normal Alkanes Nucleation in Simple Tee Diluter

- ▣ Problem Statement:
  - In our earlier work, we had several publications on the effect of dilution conditions on particle formation and growth:
  - We indentified :
    - ▣ Dilution ratio, dilution air temperature, residence time, relative humidity, transfer tube temperature as playing a major in effecting total particle number and size
  - We did not investigate the effect of diluter design on particle formation and growth in a systematic way
- ▣ The goal of these activities is to look at various diluter designs to study particle nucleation and growth starting with simple Tee diluter (aided with modeling)



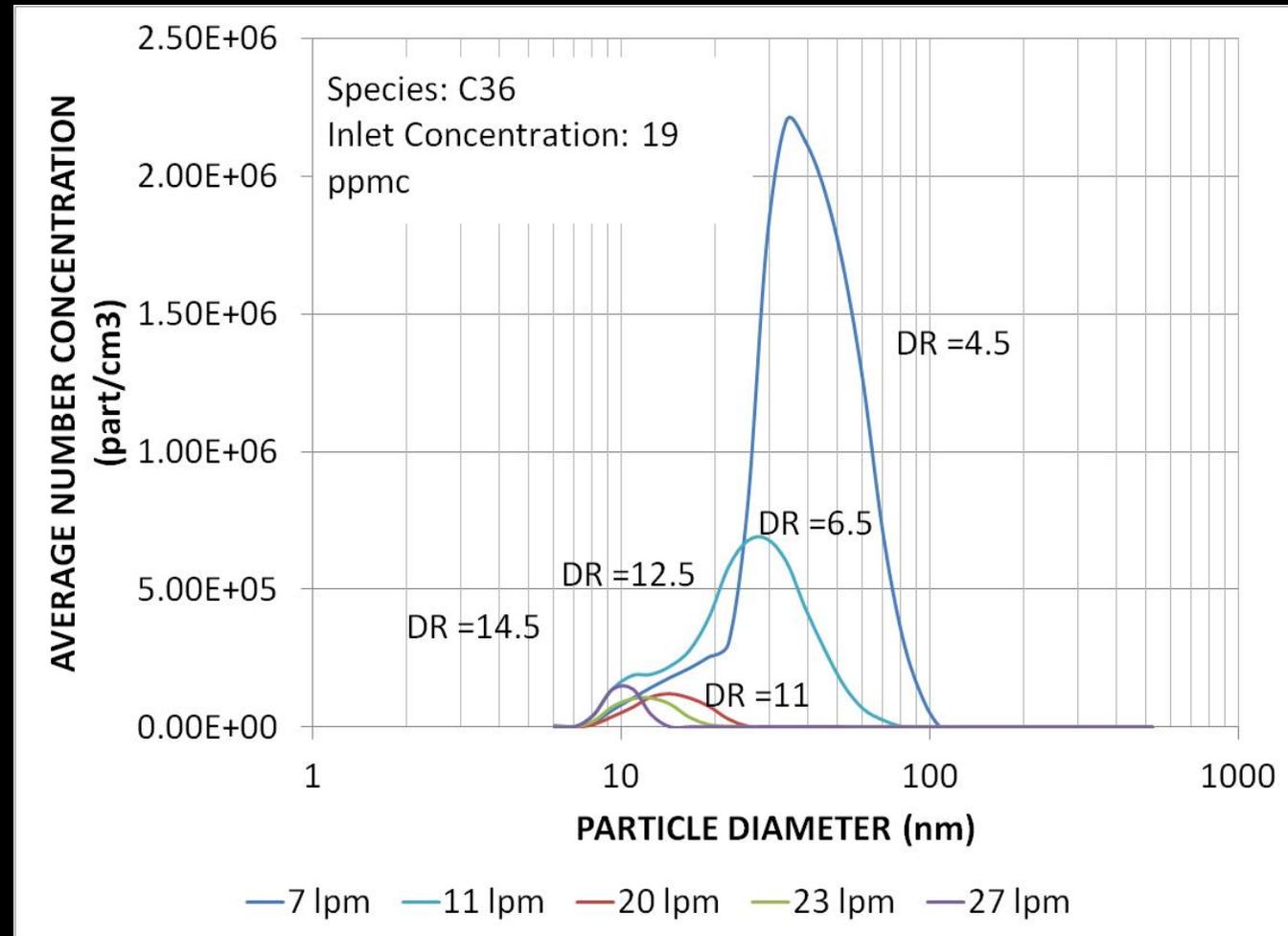
# Normal Alkanes Nucleation

- ▣ Ei-, Do-, Hexa-cosane (C20, C22, and C26) did not nucleate and grow using the following parameters:
  - Saturation pressure ratio of ~2000
  - Sample Temperature 250C
  - Dilution air temperature 25C
  - Dilution Ratio 4.5 to 14.5
- ▣ Only Dotria- and Hexatria-contane (C32 and C36) nucleated and grew, but required **extremely high saturation pressure ratio**



# Example of C36 Nucleation at Various Dilution Ratios

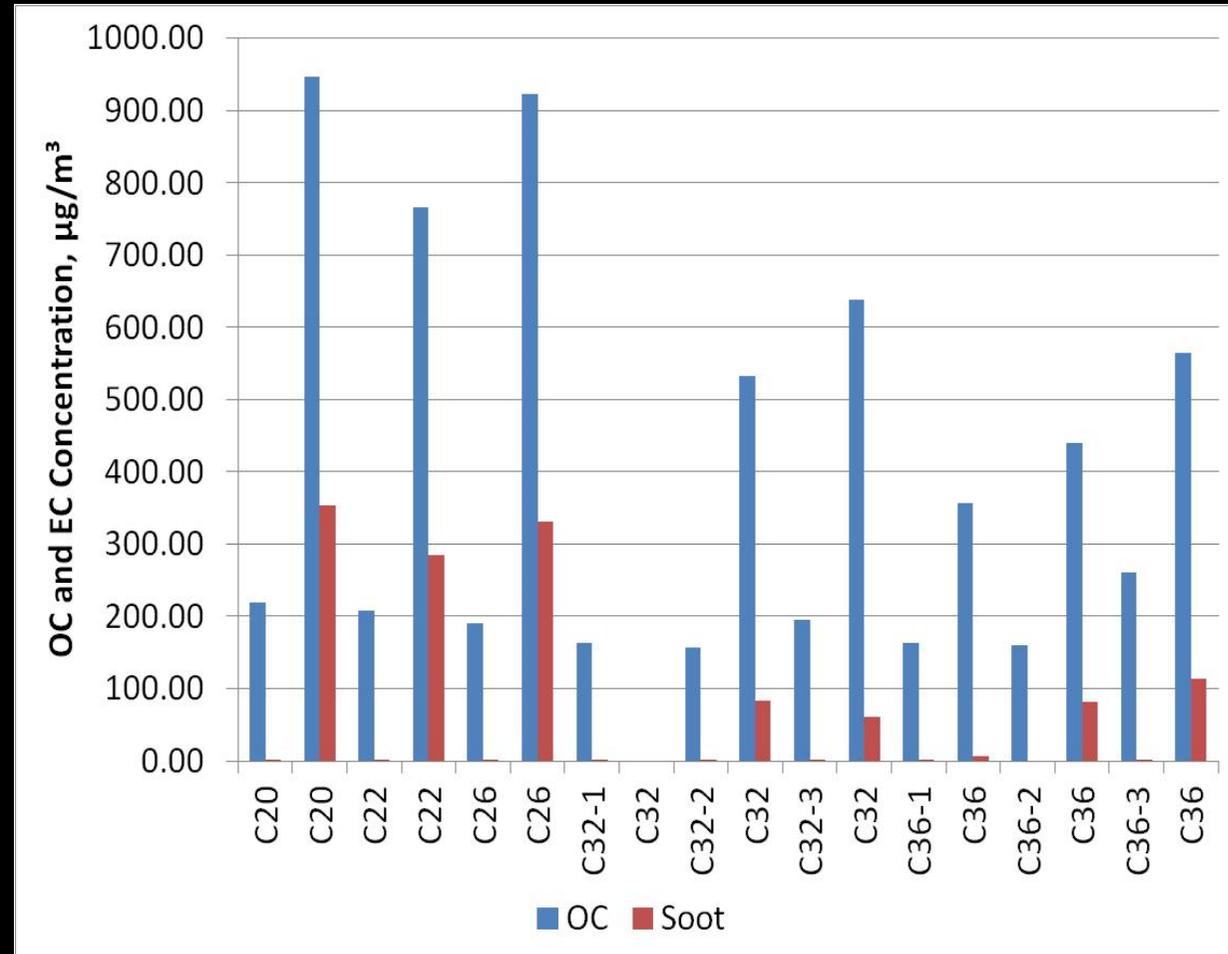
- It takes an extremely high saturation pressure ratio to nucleate and grow normal alkanes
- Significant part of the material is lost to the walls of the sampling system.
- The OC recovery after the lowest dilution was about ~8%



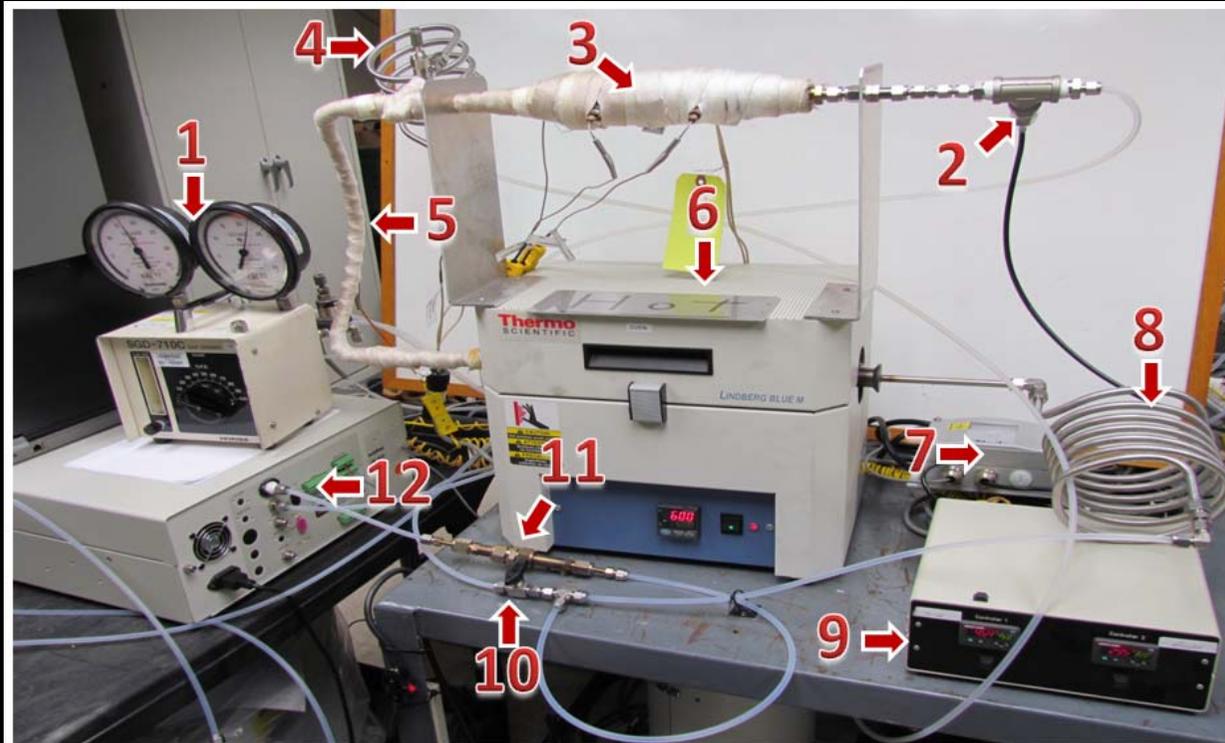


# Hydrocarbon Transport in the Presence and Absence of Soot

- Significant HC loss was observed in the absence of soot. Soot acts as a transport mechanism of species
- This poses a challenge to the measurement of toxic compounds emitted from modern engines with DPF in the absence of soot.



# Sulfuric Acid Generation System

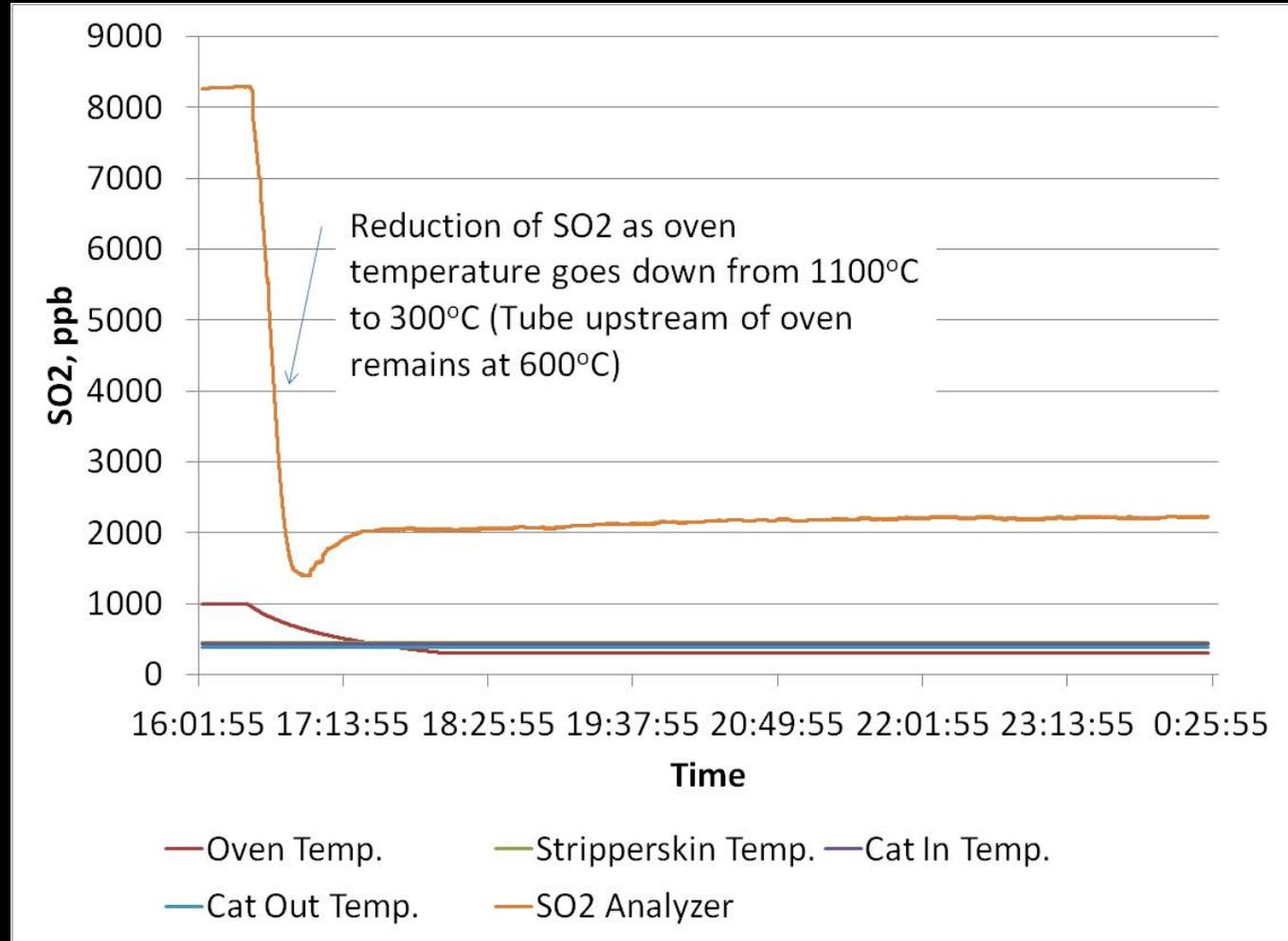


- |                                      |                            |                  |
|--------------------------------------|----------------------------|------------------|
| 1. Gas Divider                       | 6. Oven                    | 11. TX Filter    |
| 2. RH Sensor                         | 7. RH Analyzer             | 12. SO2 Analyzer |
| 3. Catalyst                          | 8. Cooling Coil Oven Out   |                  |
| 4. Bypass After Catalyst             | 9. Temperature Control Box |                  |
| 5. Heated Tube from Catalyst to Oven | 10. Bypass After Oven      |                  |



# Using SO<sub>2</sub> Measurement as Surrogate for SO<sub>3</sub>

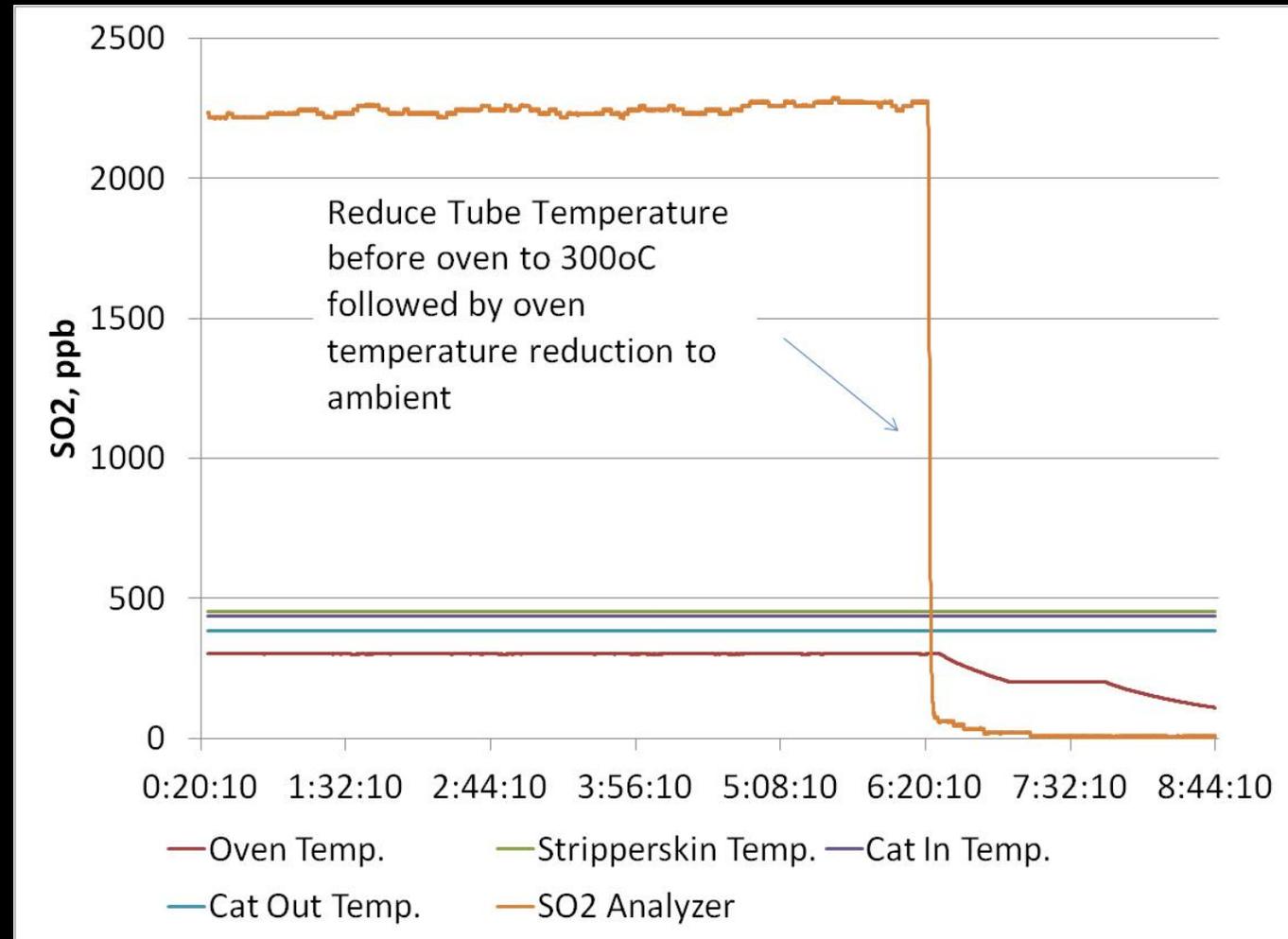
As the oven temperature is reduced, SO<sub>2</sub> concentration decreases





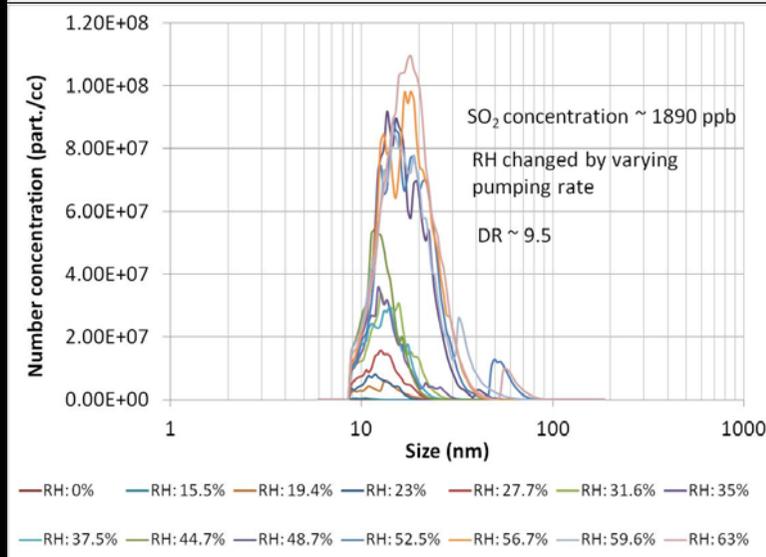
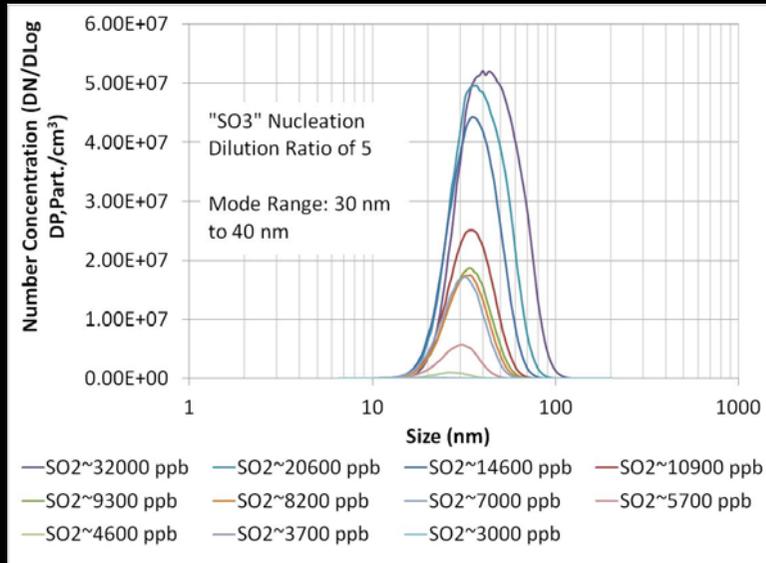
# Complete Loss of SO<sub>3</sub> with Oven Temperature Down to Ambient

- At 1100°C, we were able to decompose 95% of the SO<sub>3</sub> formed
- The literature suggests a temperature of 1250°C is needed for complete decomposition (Noglik et al., *J. of Solar Energy Engineering*, 2009)



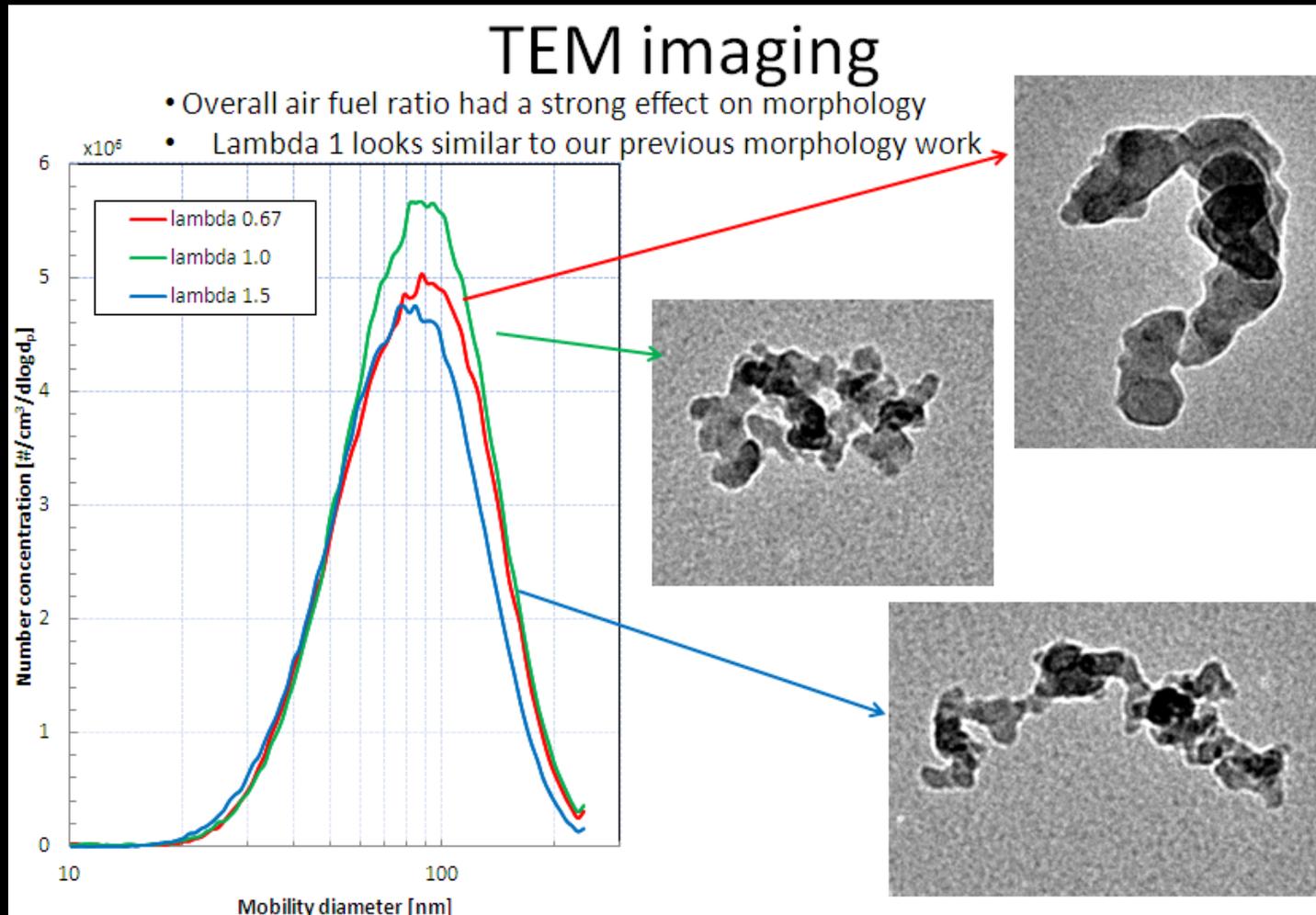


# SO<sub>3</sub> or SO<sub>4</sub> and Sulfuric Acid Nucleation



- ❑ SO<sub>3</sub> or SO<sub>4</sub> nucleation produced larger size distributions than that of sulfuric acid
- ❑ The increase in water significantly enhanced sulfuric acid nucleation and growth. Even at high concentration, the mode of the distribution on a number basis did not exceed 20 nm. This is what we typically see in engine exhaust nucleation and growth, but the growth is typically via hydrocarbons
- ❑ At very high water content (> 16% in exhaust, ~Natural Gas), large mode started to appear, especially on a mass basis.

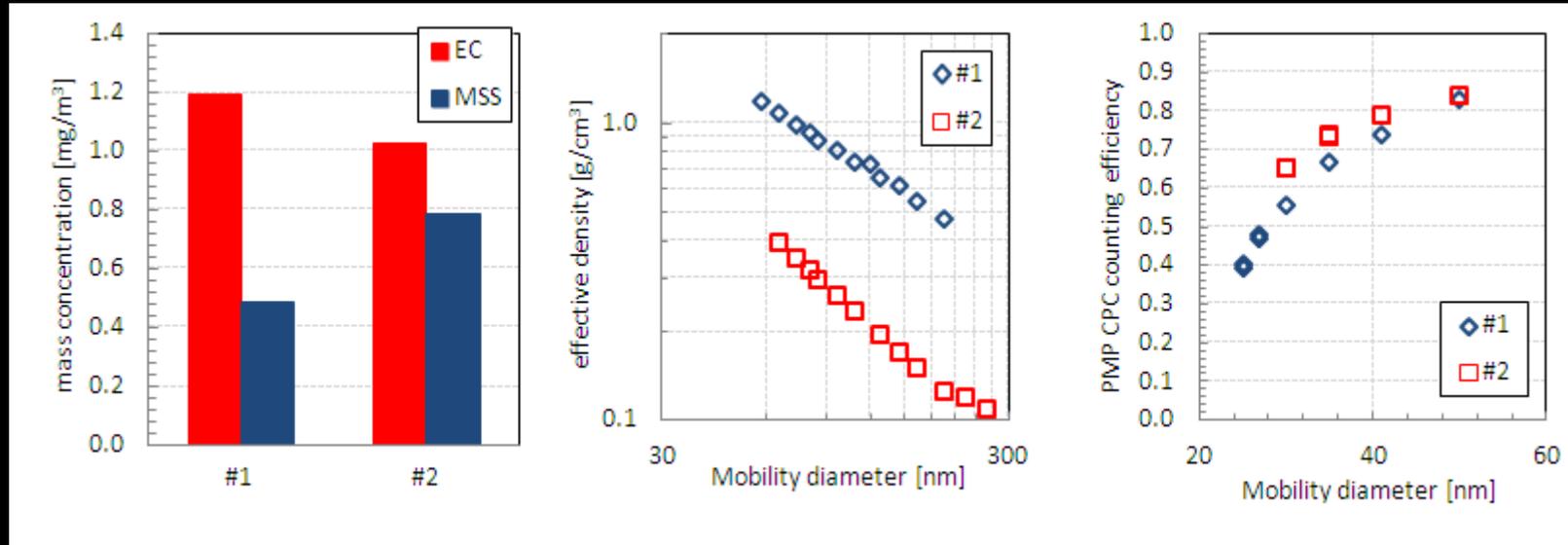
# Different Soot Morphology



In-kind support of TEM images and analyses were provided by Argonne National Laboratory



# MINICAST AEROSOL CHARACTERIZATION



#1	#2
60 mlpm $\text{C}_3\text{H}_8$	60 mlpm $\text{C}_3\text{H}_8$
0 mlpm $\text{N}_2$	275 mlpm $\text{N}_2$
1 lpm air	1.85 lpm air
$d_g$ at $\sim 70$ nm	$d_g$ at $\sim 80$ nm

miniCAST operating conditions had a strong effect on the light absorption, effective density and particle affinity for butanol.

*Characterization of Combustion Aerosol Produced by a Mini-CAST and Treated in a Catalytic Stripper*  
Mamakos, Khalek, Giannelli & Spears, AS&T, vol 47, issue 8, May 2013



# Summary

- ▣ A “quiet” Particle Generator has been developed to investigate various fundamental processes of aerosol formation and growth
- ▣ We have recently added modeling efforts to gain more fundamental insights to the experimental findings
- ▣ A final report for 2013 activities will be issued by September 31, 2013
- ▣ We expect to continue working with the system in FY2014 , starting October 1, 2013.