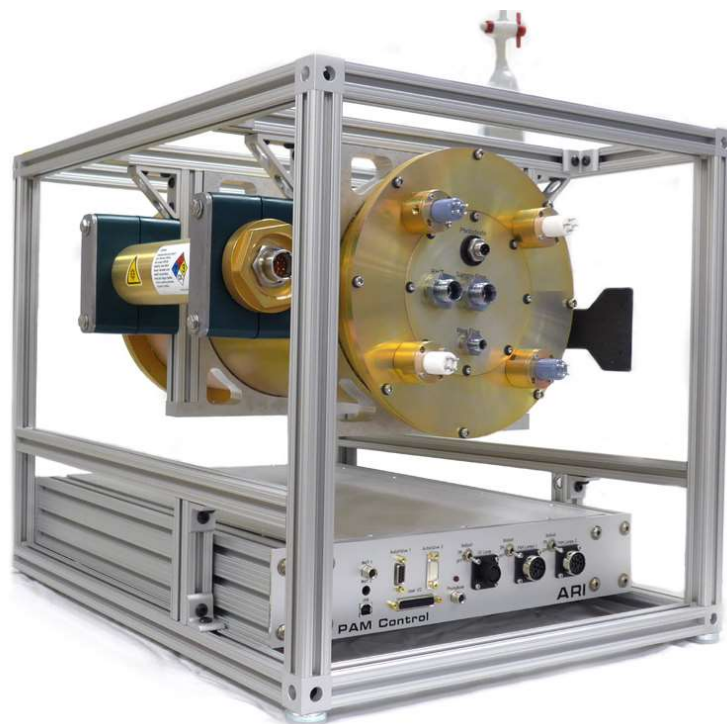


Updates on Aerodyne Potential Aerosol Mass (PAM) Oxidation Flow Reactor (OFR) **PAM**反应器的最新进展



Andy Lambe and Penglin Ye

Outline 大纲

- Overview （简介）
- Example Applications （应用实例）
- Modeling Tools （计算模拟方法）
- Summary （总结）

Introducing the concept of Potential Aerosol Mass (PAM)

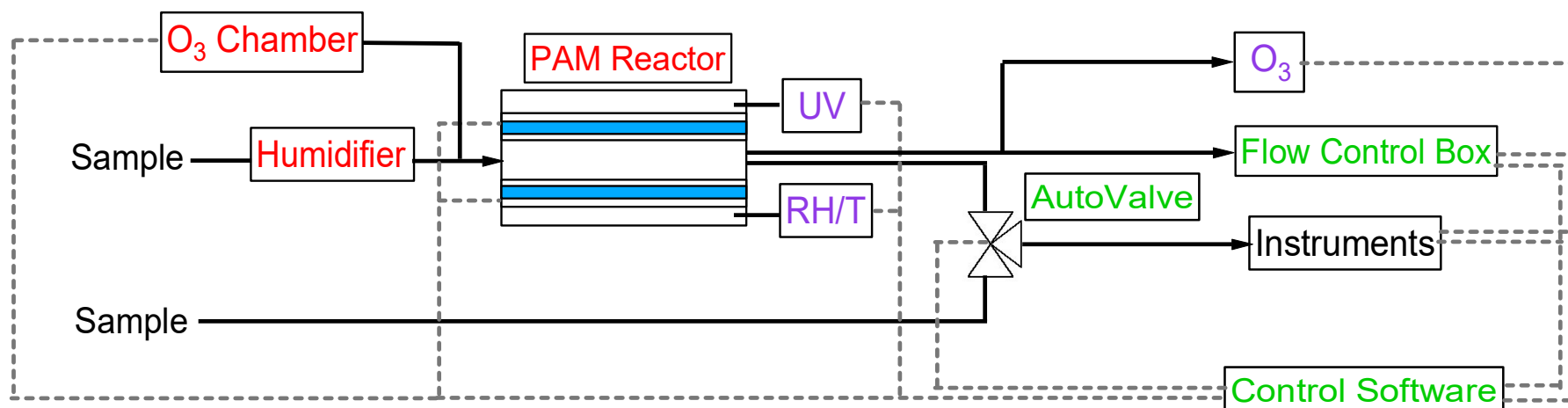
E. Kang¹, M. J. Root¹, D. W. Toohey², and W. H. Brune¹

¹Department of Meteorology, Pennsylvania State University, University Park, PA 16802, USA

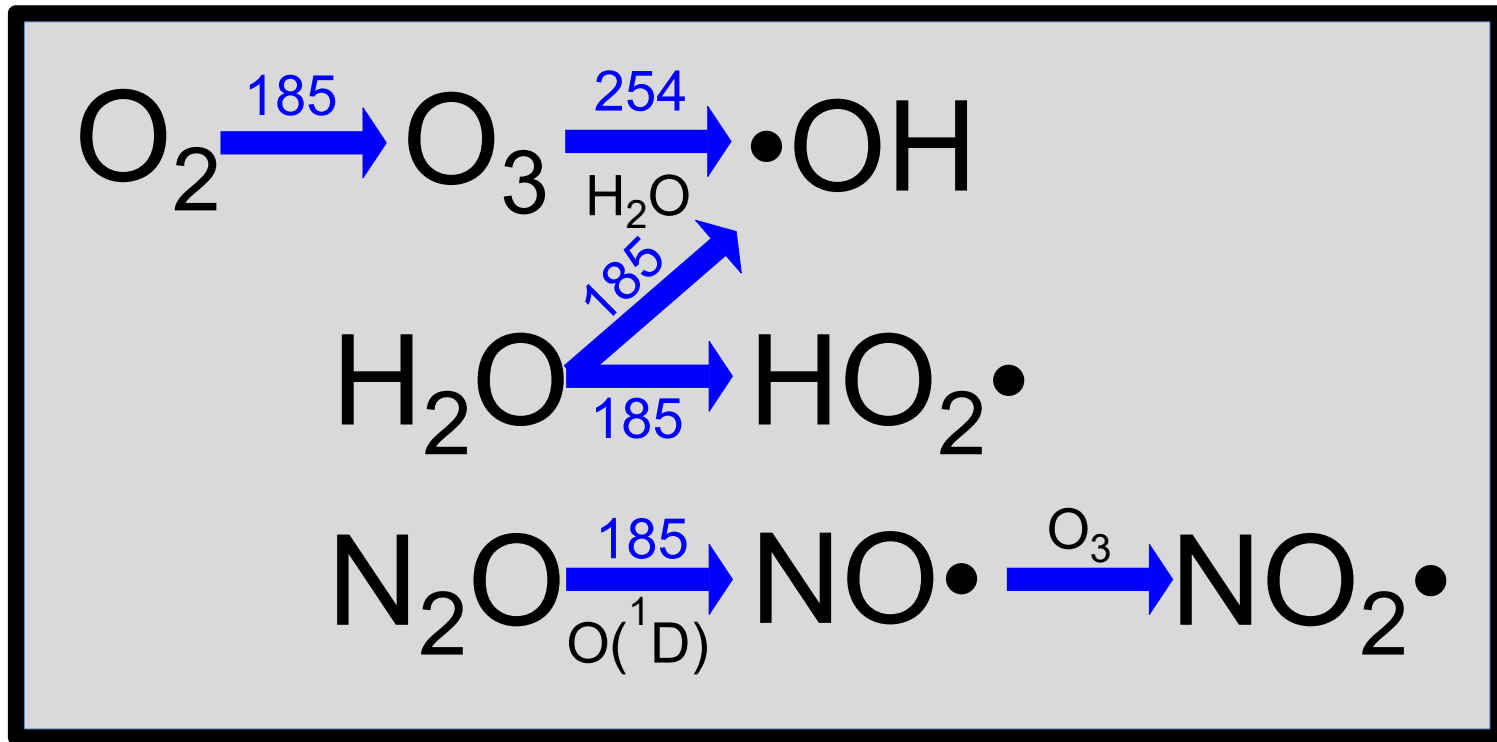
²Atmospheric and Oceanic Sciences, University of Colorado, CO 80309-0311, USA

Characterization of aerosol photooxidation flow reactors: heterogeneous oxidation, secondary organic aerosol formation and cloud condensation nuclei activity measurements

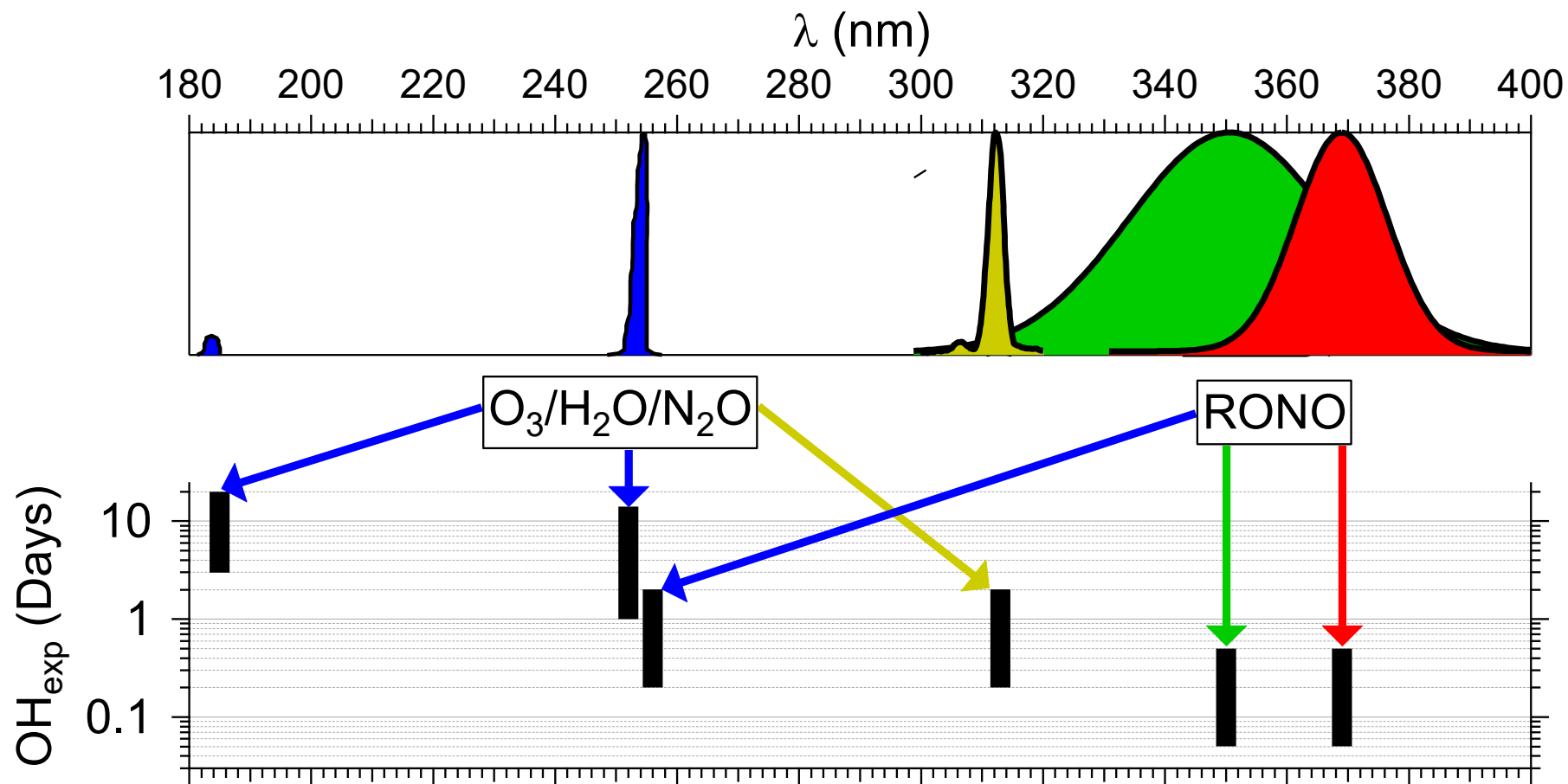
A. T. Lambe^{1,2}, A. T. Ahern^{1,2}, L. R. Williams², J. G. Slowik³, J. P. S. Wong³, J. P. D. Abbatt³, W. H. Brune⁴,
 N. L. Ng², J. P. Wright¹, D. R. Croasdale¹, D. R. Worsnop², P. Davidovits¹, and T. B. Onasch^{1,2}



- Oxidant generation (氧化剂制备)
- Measurement of photochemical conditions (测量光化学参数)
- Hardware control, data acquisition (硬件控制, 数据采集)



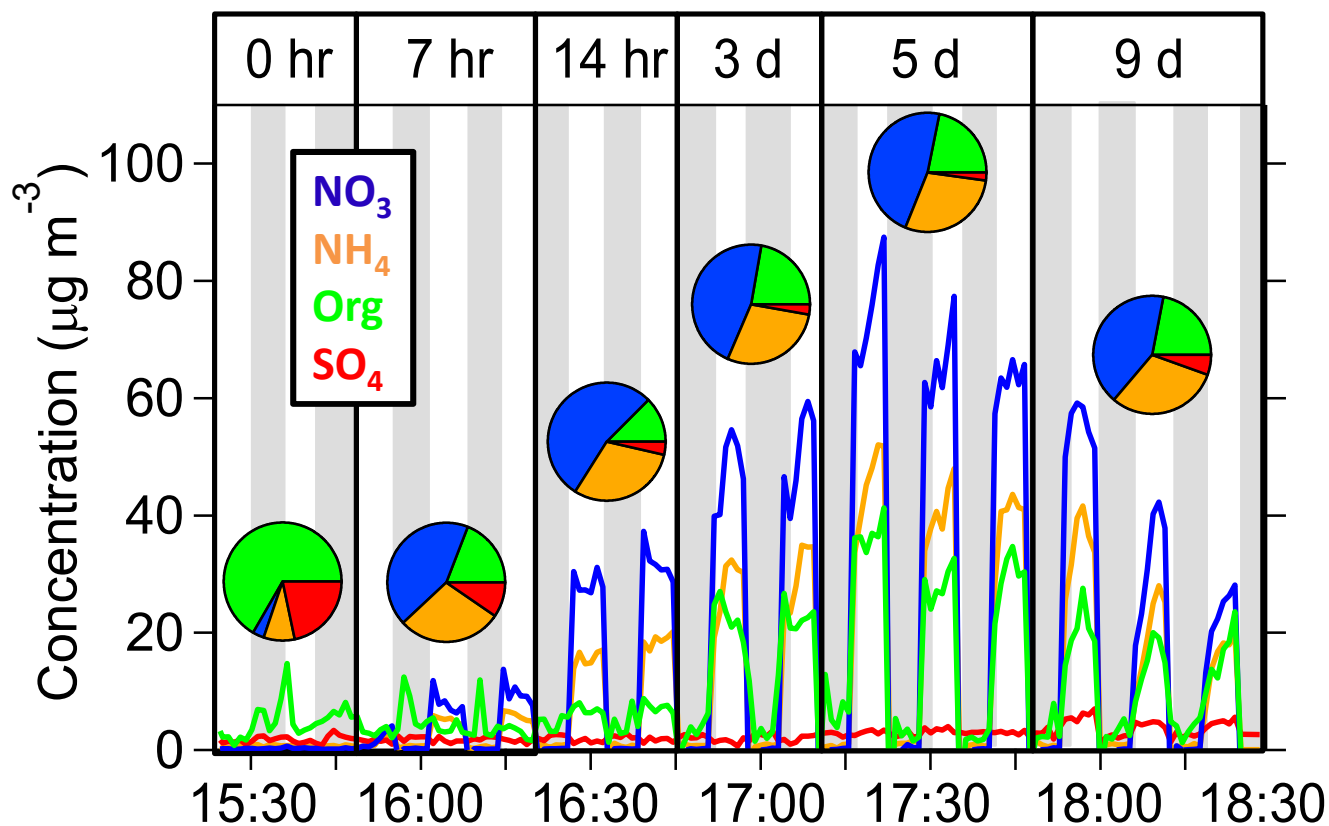
- “OFR₁₈₅”: Easiest and most efficient method
(最简洁高效的方法)
- “OFR₂₅₄”: More flexible method
(比较灵活的方法)



OVERVIEW – OXIDANT GENERATION

Secondary Organic Aerosol Formation from in-Use Motor Vehicle Emissions Using a Potential Aerosol Mass Reactor

Daniel S. Tkacik,^{†,§} Andrew T. Lambe,[‡] Shantanu Jathar,[§] Xiang Li,^{¶,||} Albert A. Presto,^{¶,||} Yunliang Zhao,^{¶,||} Donald Blake,[‡] Simone Meinardi,[‡] John T. Jayne,[‡] Philip L. Croteau,[‡] and Allen L. Robinson^{*,¶,||}

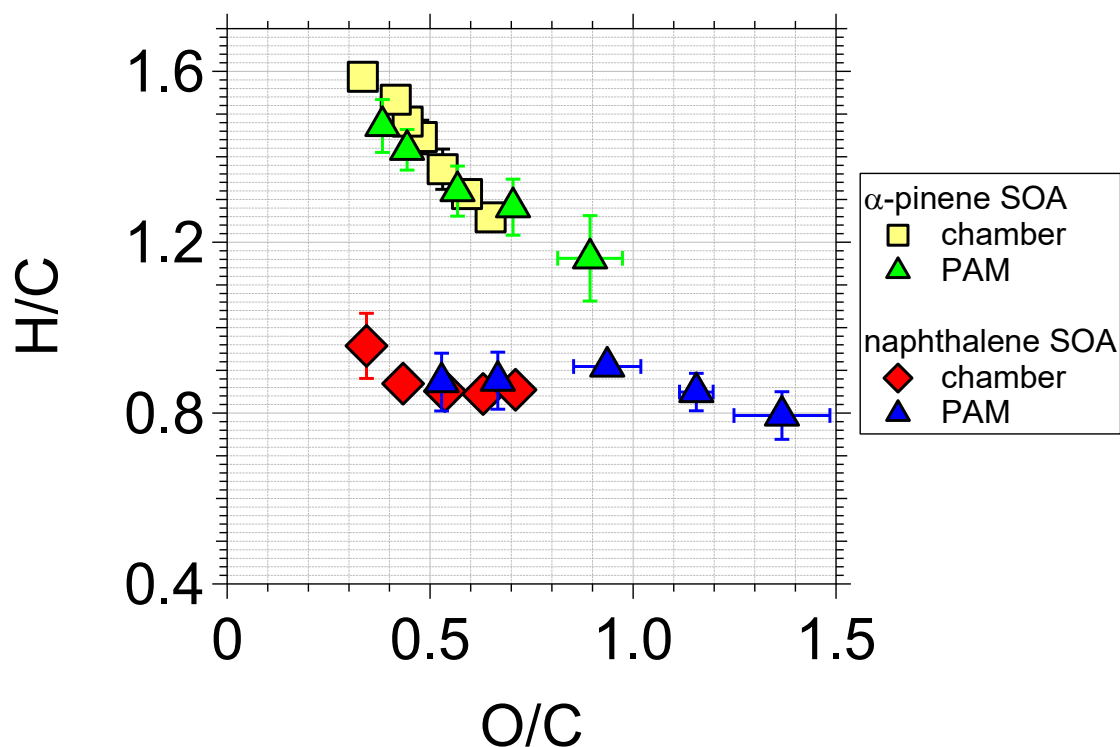


- “Potential Aerosol Mass” of emission sources (来自排放源的潜在气溶胶)
- Transition from “functionalization” to “fragmentation” (形成官能团到碳链断开的渐变)

Effect of oxidant concentration, exposure time, and seed particles on secondary organic aerosol chemical composition and yield

A. T. Lambe^{1,2}, P. S. Chhabra^{2,*}, T. B. Onasch^{1,2}, W. H. Brune³, J. F. Hunter⁴, J. H. Kroll⁴, M. J. Cummings¹, J. F. Brogan¹, Y. Parmar¹, D. R. Worsnop², C. E. Kolb², and P. Davidovits¹

¹Chemistry Department, Boston College, Chestnut Hill, MA, USA

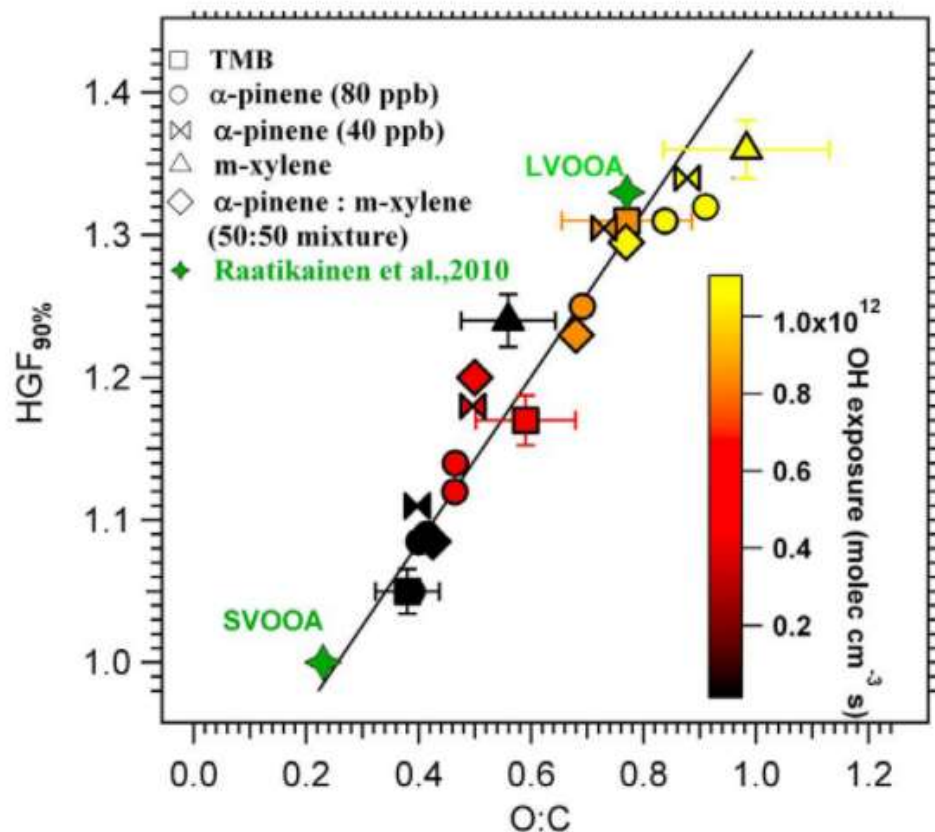


- SOA composition over multigeneration oxidation
(经过多次氧化后的二次气溶胶组成)

EXAMPLE APPLICATIONS - AMS

Relationship between aerosol oxidation level and hygroscopic properties of laboratory generated secondary organic aerosol (SOA) particles

P. Massoli,¹ A. T. Lambe,^{1,2} A. T. Ahern,^{1,2} L. R. Williams,¹ M. Ehn,³ J. Mikkilä,³
M. R. Canagaratna,¹ W. H. Brune,⁴ T. B. Onasch,¹ J. T. Jayne,¹ T. Petäjä,³ M. Kulmala,³
A. Laaksonen,⁵ C. E. Kolb,¹ P. Davidovits,² and D. R. Worsnop^{1,3,5}

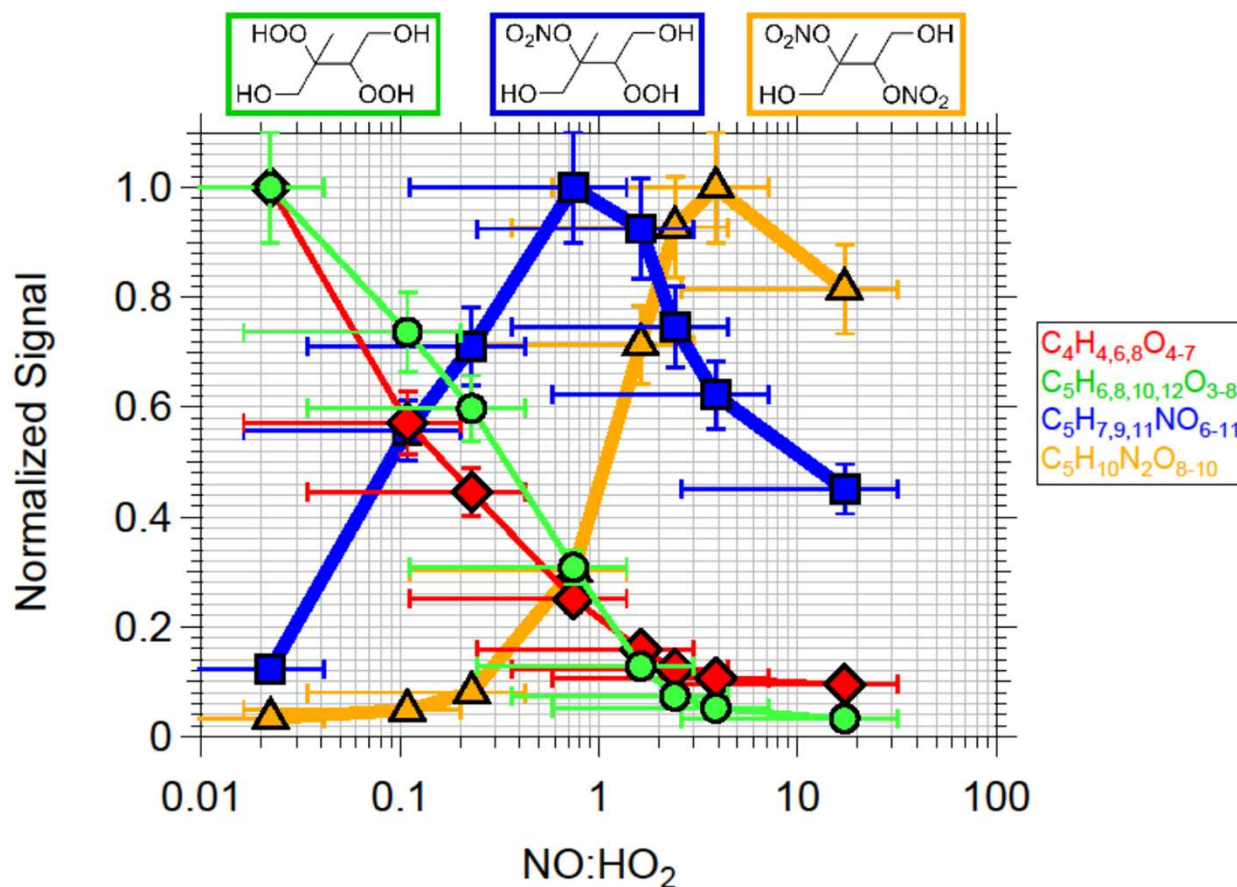


- Correlation of SOA composition and hygroscopicity
(二次气溶胶组成和吸湿性的相关性)

EXAMPLE APPLICATIONS - AMS

Controlled nitric oxide production via $O(^1D)+N_2O$ reactions for use in oxidation flow reactor studies

Andrew Lambe^{1,2}, Paola Massoli¹, Xuan Zhang¹, Manjula Canagaratna¹, John Nowak^{1,*}, Chao Yan³, Wei Nie^{4,3}, Timothy Onasch^{1,2}, John Jayne¹, Charles Kolb¹, Paul Davidovits², Douglas Worsnop^{1,3}, and William Brune⁵



- Molecular tracers for “low-NO” and “high-NO” conditions
 (高、低一氧化氮浓度条件下的分子标识物)

EXAMPLE APPLICATIONS - CIMS

**Modeling the Radical Chemistry in an Oxidation Flow Reactor:
Radical Formation and Recycling, Sensitivities, and the OH Exposure
Estimation Equation**

Rui Li,^{*,†,§} Brett B. Palm,^{‡,||} Amber M. Ortega,^{‡,§} James Hlywiak,[⊥] Weiwei Hu,^{‡,||} Zhe Peng,^{‡,||}
Douglas A. Day,^{‡,||} Christoph Knote,^{¶,V} William H. Brune,[⊥] Joost A. de Gouw,^{‡,||}
and Jose L. Jimenez^{*,‡,||}

“PAM_chem”模型

#	reactions	reaction rate constant
1	$O_2 + h\nu (185 \text{ nm}) \rightarrow 2O(^1P)$	$1.1 \times 10^{-20} \times \text{flux}_{185}^a$
2	$O_3 + h\nu (254 \text{ nm}) \rightarrow O_2 + O(^1D)$	$1.03 \times 10^{-17} \times \text{flux}_{254}^b$
3	$H_2O_2 + h\nu (185 \text{ nm}) \rightarrow HO_2 + H$	$1 \times 10^{-19} \times \text{flux}_{185}$
4	$H_2O_2 + h\nu (254 \text{ nm}) \rightarrow 2OH$	$6.7 \times 10^{-20} \times \text{flux}_{254}$
5	$HO_2 + h\nu (254 \text{ nm}) \rightarrow OH + O(^1D)$	$2.63 \times 10^{-19} \times \text{flux}_{254} + 3.68 \times 10^{-18} \times \text{flux}_{185}$
6	$HO_2 + h\nu (185 \text{ nm}) \rightarrow OH + O(^1D)$	
7	$H_2O + h\nu (185 \text{ nm}) \rightarrow OH + H$	$6.78 \times 10^{-38} \times \text{flux}_{185}$
8	$O(^1D) + H_2O \rightarrow 2OH$	$1.63 \times 10^{-16} e^{60/T}$
9	$O(^1D) + N_2 \rightarrow O(^1P)$	$2.15 \times 10^{-11} e^{110/T}$
10	$O(^1D) + O_2 \rightarrow O(^1P)$	$3.3 \times 10^{-11} e^{55/T}$
11	$O(^1D) + CO_2 \rightarrow O(^1P) + CO_2$	$7.5 \times 10^{-11} e^{115/T}$
12	$O(^1D) + O_3 \rightarrow 2O_2$	1.20×10^{-10}
13	$O(^1D) + O_3 \rightarrow O_2 + O + O$	1.20×10^{-10}
14	$O(^1D) + H_2 \rightarrow OH + H$	1.20×10^{-10}
15	$O(^1D) + N_2 + M \rightarrow N_2O$	$2.8 \times 10^{-36} M(300/T)^{0.9}$
16	$O(^1D) + N_2O \rightarrow N_2 + O_2 \text{ or } 2NO$	$1.19 \times 10^{-16} e^{20/T}$
17	$O + OH \rightarrow O_2 + H$	$2.2 \times 10^{-11} e^{180/T}$
18	$O + HO_2 \rightarrow OH + O_2$	$3.0 \times 10^{-11} e^{200/T}$
19	$O + H_2O_2 \rightarrow OH + HO_2$	$1.4 \times 10^{-12} e^{-2000/T}$
20	$O + O_3 \rightarrow 2O_2$	$8.0 \times 10^{-12} e^{-2060/T}$
21	$H + O_3 \rightarrow OH + O_2$	$1.4 \times 10^{-10} e^{-470/T}$
22	$OH + O_3 \rightarrow HO_2 + O_2$	$1.7 \times 10^{-12} e^{-940/T}$
23	$HO_2 + NO \rightarrow OH + NO_2$	$3.5 \times 10^{-12} e^{270/T}$
24	$HO_2 + O_3 \rightarrow OH + 2O_2$	$1.0 \times 10^{-14} e^{-490/T}$
25	$OH + HO_2 \rightarrow H_2O + O_2$	$4.8 \times 10^{-11} e^{250/T}$
26	$H + HO_2 \rightarrow 2OH$	7.20×10^{-11}
27	$H + HO_2 \rightarrow O + H_2O$	1.60×10^{-12}
28	$H + HO_2 \rightarrow O_2 + H_2$	6.90×10^{-12}
29	$OH + H_2 \rightarrow H_2O + H$	$2.8 \times 10^{-12} e^{-1800/T}$
30	$OH + OH \rightarrow H_2O + O$	1.80×10^{-12}
31	$O + NO_2 \rightarrow NO + O_2$	$5.1 \times 10^{-12} e^{210/T}$
32	$O + NO_2 \rightarrow O_2 + NO_2$	1.0×10^{-11}
33	$O + HO_2NO_2 \rightarrow \text{products}$	$7.80 \times 10^{-11} e^{-3400/T}$
34	$H + NO_2 \rightarrow OH + NO$	$4.0 \times 10^{-10} e^{-340/T}$
35	$OH + NO_2 \rightarrow HO_2 + NO_2$	2.2×10^{-11}
36	$OH + HONO \rightarrow H_2O + NO_2$	$1.80 \times 10^{-11} e^{-390/T}$
37	$HO_2 + NO_3 \rightarrow OH + NO_2 + O_2$	3.5×10^{-12}
38	$NO + NO_3 \rightarrow 2NO_2$	$1.50 \times 10^{-11} e^{170/T}$
39	$NO_3 + NO_3 \rightarrow 2NO_2 + O_2$	$8.5 \times 10^{-13} e^{-2450/T}$
41	$\tilde{NO} + O_3 \rightarrow NO_2 + O_2$	$3.0 \times 10^{-12} e^{-1500/T}$
42	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.2 \times 10^{-13} e^{-2450/T}$
43	$HO_2 + NO_2 + M \rightarrow HONO_2 + M$	$\text{Eq}(1)^b$
	$HO_2 + NO_2 + M \rightarrow HOONO + M$	
44	$OH + HNO_3 \rightarrow \text{products}$	$1.3 \times 10^{-12} e^{380/T}$
45	$OH + H_2O_2 \rightarrow H_2O + HO_2$	1.80×10^{-12}
46	$OH + NO_2 + M \rightarrow HNO_3 + M$	$\text{Eq}(1)$
47	$O + O_2 + M \rightarrow O_3 + M$	$6.0 \times 10^{-33} M(300/T)^{2.4}$
48	$H + O_2 + M \rightarrow HO_2 + M$	$\text{Eq}(1)$
49	$OH + OH + M \rightarrow H_2O_2 + M$	$\text{Eq}(1)$
50	$OH + SO_2 + M \rightarrow HOSO_2 + M$	$\text{Eq}(1)$
51	$HOSO_2 + O_2 \rightarrow HO_2 + SO_3$	$1.3^{-12} e^{-330/T}$
52	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	$(3.0 \times 10^{-13} e^{460/T} + 2.1 \times 10^{-13} \text{Me}^{920/T}) \times (1 + 1.4e^{-23} H_2O \times 10^{2200/T})$
53	$O + NO + M \rightarrow NO_2 + M$	$\text{Eq}(1)$
54	$O + NO_2 + M \rightarrow NO_3 + M$	$\text{Eq}(1)$
55	$NO_2 + NO_3 + M \rightarrow N_2O_5 + M$	$\text{Eq}(1)$
56	$OH + CO + M \rightarrow H + CO_2 + M$	$\text{Eq}(2)^c$
57	$OH + CO + M \rightarrow HOCO + M$	$\text{Eq}(1)$
58	$HOCO + O_2 \rightarrow HO_2 + CO_2$	1.5×10^{-12}

- Developed by Bill Brune（由Brune教授开发）
- Included with delivered PAM systems, compile in Matlab（用Matlab写的程序预装在已售的PAM中）

OFR_Exposure_Estimator

Oxidation Flow Reactor Exposure Estimator v2.3

Zhe Peng and Jose-Luis Jimenez

Common inputs

Water vapor mixing ratio: 0.01

External OH reactivity (s^{-1}): 20

Residence time (s): 100

Select an input option

☒ OFR185 Option 1
☐ OFR185 Option 2
☐ OFR254 Option 1
☐ OFR254 Option 2

OFR185

Enter

Photon flux at 185 nm ($photons\ cm^{-2}\ s^{-1}$): $1e+13$

or

Output O_3 concentration ($molecules\ cm^{-3}$): $4e+12$

OFR254

Initial O_3 concentration (ppm): 20

Enter

Photon flux at 254 nm ($photons\ cm^{-2}\ s^{-1}$): $2e+14$

or

Ratio between input and output O_3 : 0.95

Also make the plots of relative importance of

☐ 185 nm photon flux ☐ 254 nm photon flux
☐ $O(^1D)$ ☐ $O(^3P)$ ☐ O_3
 to OH (Figs. 1-5 of Peng et al. ACP 2016)

Calculate Exposures

Readme

University of Colorado Boulder

Atmos. Meas. Tech., 8, 4863–4890, 2015
 www.atmos-meas-tech.net/8/4863/2015/
 doi:10.5194/amt-8-4863-2015
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Atmospheric
Measurement
Techniques

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HO_x radical chemistry in oxidation flow reactors with low-pressure mercury lamps systematically examined by modeling

Z. Peng^{1,2}, D. A. Day^{1,2}, H. Stark^{1,2,3}, R. Li^{1,4,5}, J. Lee-Taylor^{1,2}, B. B. Palm^{1,2}, W. H. Brune⁶, and J. L. Jimenez^{1,2}

Atmos. Chem. Phys., 16, 4283–4305, 2016
 www.atmos-chem-phys.net/16/4283/2016/
 doi:10.5194/acp-16-4283-2016
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Atmospheric
Chemistry
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Non-OH chemistry in oxidation flow reactors for the study of atmospheric chemistry systematically examined by modeling

Zhe Peng^{1,2}, Douglas A. Day^{1,2}, Amber M. Ortega^{1,3,a}, Brett B. Palm^{1,2}, Weiwei Hu^{1,2}, Harald Stark^{1,2,5}, Rui Li^{1,3,4,b}, Kostas Tsigaridis⁶, William H. Brune⁷, and Jose L. Jimenez^{1,2}

- Developed by Zhe Peng and Jose Jimenez (由Peng Zhe博士和Jimenez教授开发)
- Download from PAM wiki, compile in Igor (用IGOR写的程序可以从PAM wiki下载)

Additional Resources 更多资源

- PAMwiki: <https://sites.google.com/site/pamwiki/home>
- Email lists: pamusers@googlegroups.com,
aerodyne-pam-users@aerodyne.com, cacc-support@aerodyne.com
- Asian PAM users:

Serial #	Institution
005	Institute of Earth Environment, Chinese Academy of Sciences (中国科学院地球环境研究所)
007	Hankuk University of Foreign Studies
009	Peking University (北京大学)
012	National University of Singapore
014	Anhui Institute for Optics and Fine Mechanics, Hefei Institutes of Physical Science, Chinese Academy of Sciences (中国科学院安徽光学精密机械研究所, 合肥物质科学研究院)
018	Tsinghua University (清华大学)

- Please ask me questions during the meeting. (欢迎随时与我讨论) Thank you!