Alcohol, ketone and aldehyde measurements during TRACE-P

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Instrument: GC/MS
Time resolution: 5 minutes
Sensitivity: 5-30 pptv

Compounds measured:

Alcohols	Ketones	Aldehydes
MeOH	Acetone	Acetaldehyde
EtOH	Butanone	Propanal
	Pentanone	Butanal
		Pentanal

DATA STATUS

As of latest update (Nov. 9) -

Alcohols

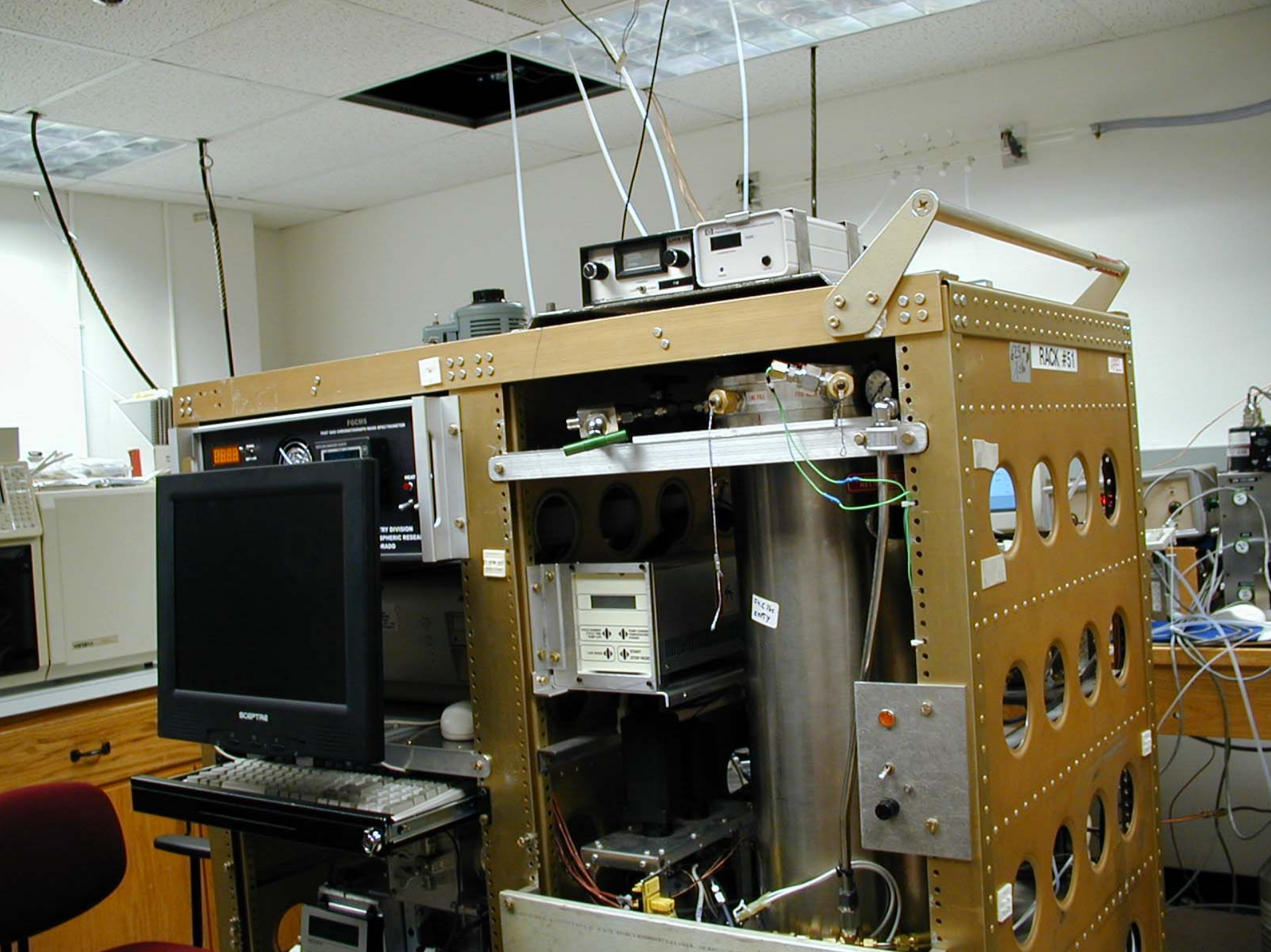
Methanol and Ethanol - OK

Ketones

Acetone and Methyl Ethyl Ketone - OK
2-pentanone - More work needed

Aldehydes

Acetaldehyde, Propanal, Butanal and Pentanal - More work needed


RACK #51
SCEPTRE

GCMS39.VI

File Edit Operate Tools Browse Window Help

Output file: c:\data\09Nov0156PM.txt

NCAR--Fast GC/MS System

Mode: In-flight run

Exit

Add text here, enter with F8

operation in laboratory

bypass A/D cards | bypass Watlow | bypass ICATS | GC 2 | close aircraft inlet | write data file

GC 1 | auto

Sample load 80

Cryofocus trap cool 30

pre cryo trap flush 30

Cryofocus 90

Injection 5

T1 5

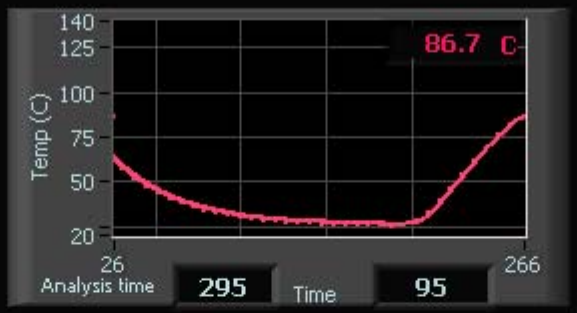
Ramp 70

T2 5

Cooldown 10

GC1

GC2



GMT time

latitude 0.00

longitude 0.00

LN2 0

static air T (C) 0.0

solar elev. relative to DC-8 0.0

aerosols (particles/ml) 0

CH4 (ppm) 0.00

GPS altitude 0

cryogenic FP (C) 0.0

load sample | cool cryo trap | pre-cryo trap flush | cryofocus | inject | T1 | T ramp | T2 | cooldown GC

Gas Flow

sample volume (ml) 87.5

He carrier (sccm) 3.85

grab sampling

sample (sccm) -0.9 / 0.0

He backflush (sccm) 0.06

water trap flush (sccm) -0.2 / 0.0

grab sample flow (slpm) 2.53

water trap cooling (slpm) -0.02

BPR (Torr) 801 / 800

grab sample duration (s) 36

sample trap cooling (slpm) 0.22

cryo trap cooling (slpm) 0.02

GC/MS runs 3

read | write

GC 1 fan/shutter | MS start | GC 2 fan/shutter

sample trap flush | water trap flush | column flush

Valco 1 | Valco 2 | Valco 3

Sample | Aircraft inlet | Pump isolation

Temperature (C)

Probe tip 1371.0 / 35.0

Probe inlet 1371.0 / 35.0

Inlet line 1371.0

Valco 52.1 / 50.0

GC 1 86.7 / 20.0

GC 2 25.4 / 25.0

Trap compartment 35.1 / 35.0

Water trap 35.3 / -10.0

Sample trap heat 74.1 / -110.0

Sample trap cool 76.7 / -110.0

Cryo trap heat 39.2 / 35.0

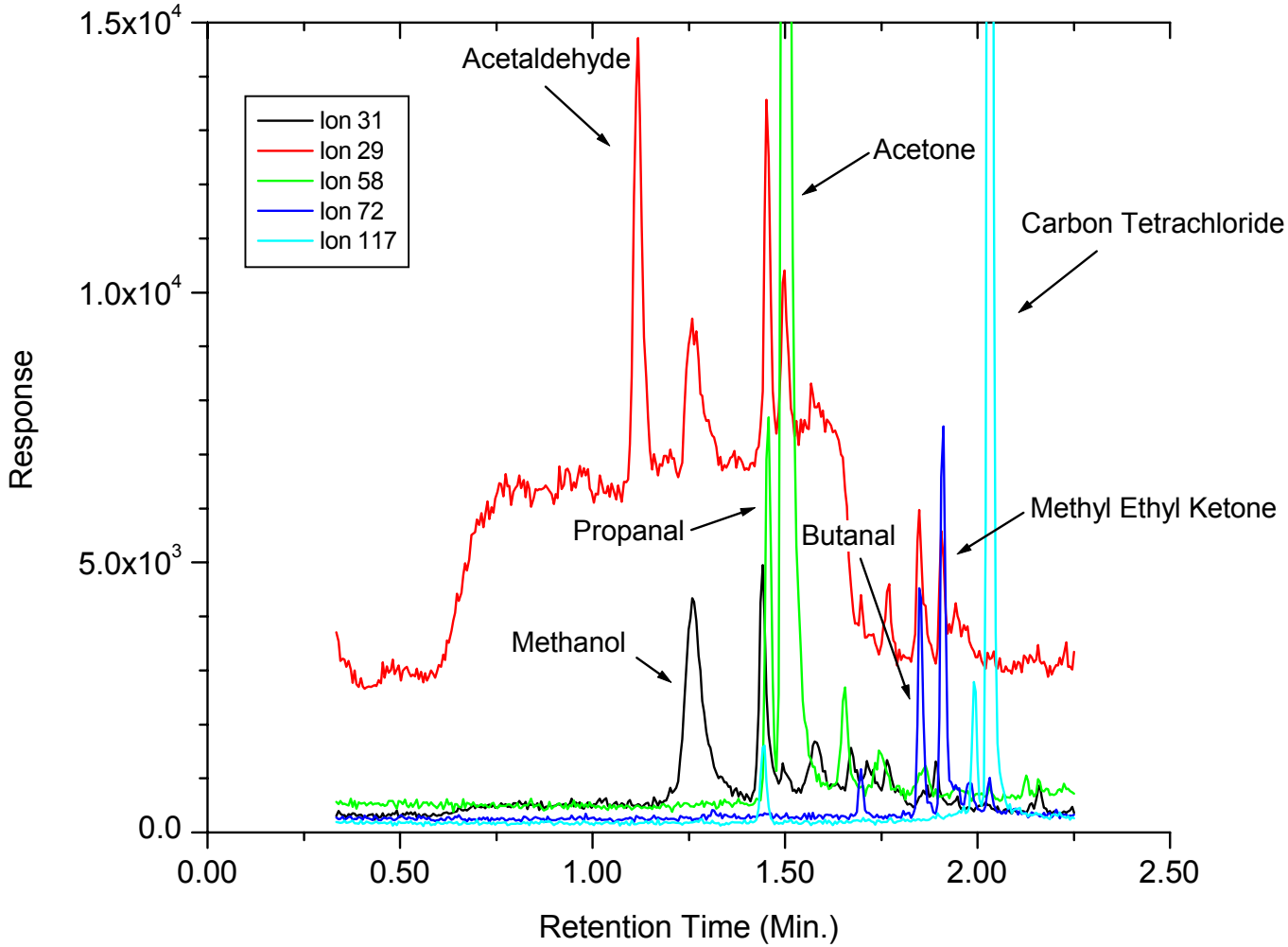
Cryo trap cool 33.9 / 35.0

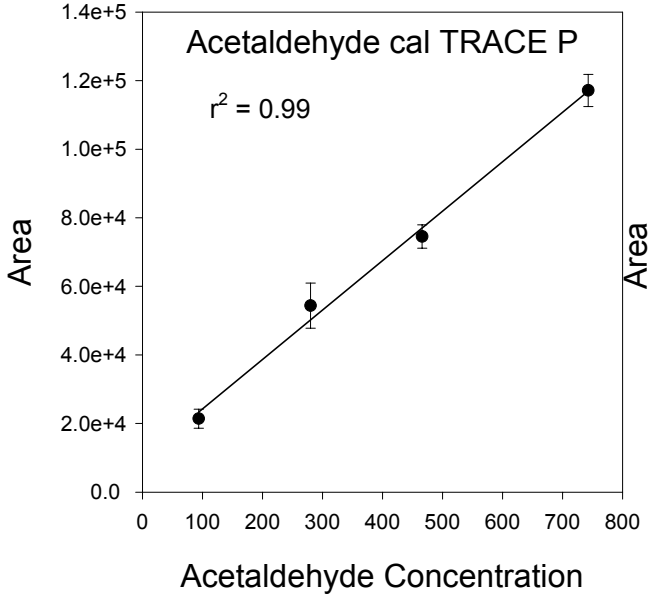
Transfer line 78.6 / 80.0

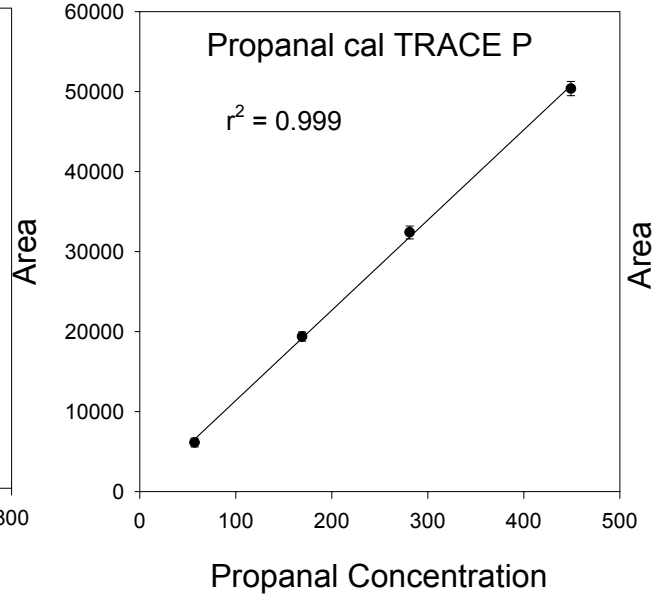
MS transfer lines 130.1 / 125.0

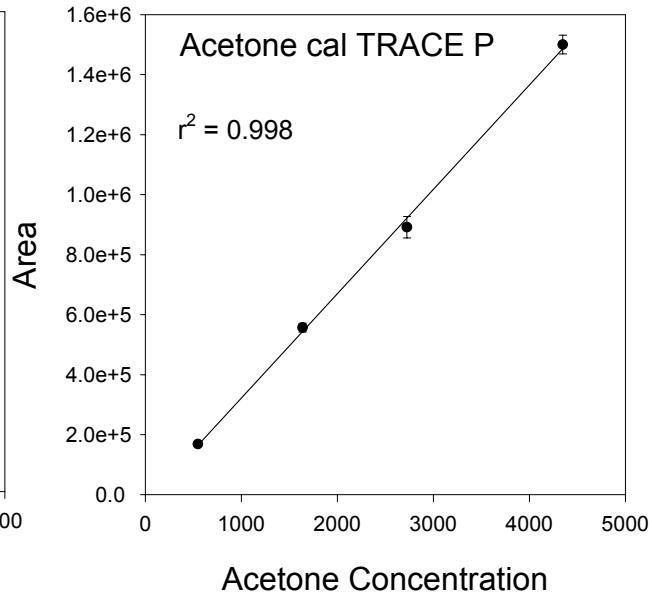
Trap compartment airspace 37.3

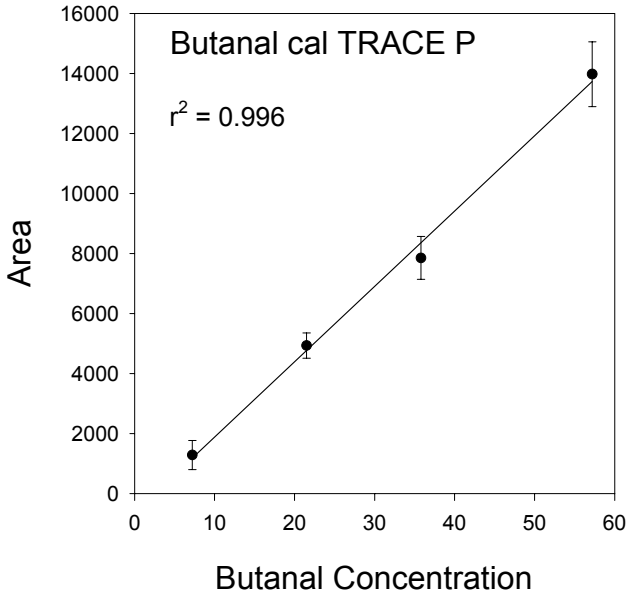
Chromatogram - Flight 10 Boundary Layer

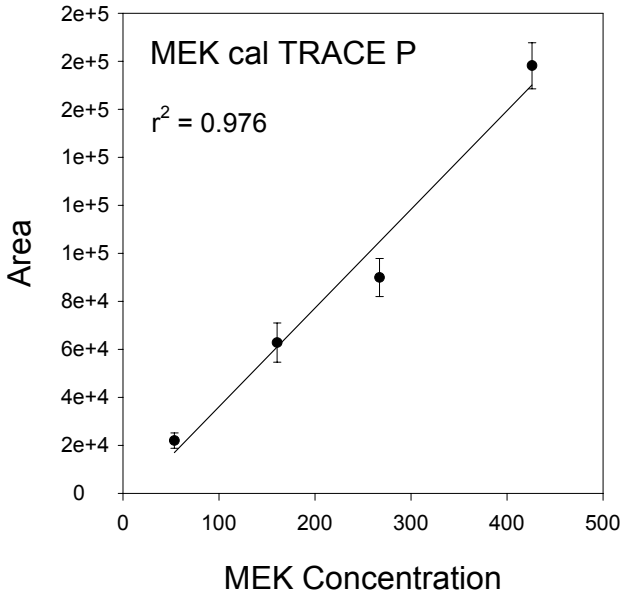



Acetaldehyde cal TRACE P
r2 = 0.99
Area
Acetaldehyde Concentration
0.0
2.0e+4
4.0e+4
6.0e+4
8.0e+4
1.0e+5
1.2e+5
1.4e+5
0
100
200
300
400
500
600
700
800


Propanal cal TRACE P
r2 = 0.999
Area
Propanal Concentration
0
10000
20000
30000
40000
50000
60000
0
100
200
300
400
500


Acetone cal TRACE P
r2 = 0.998
Area
Acetone Concentration
0.0
2.0e+5
4.0e+5
6.0e+5
8.0e+5
1.0e+6
1.2e+6
1.4e+6
1.6e+6
0
1000
2000
3000
4000
5000


Butanal cal TRACE P
r2 = 0.996
Area
Butanal Concentration
0
2000
4000
6000
8000
10000
12000
14000
16000
0
10
20
30
40
50
60


MEK cal TRACE P
r2 = 0.976
Area
MEK Concentration
0
2e+4
4e+4
6e+4
8e+4
1e+5
1e+5
1e+5
1e+5
2e+5
2e+5
2e+5
0
100
200
300
400
500

Problems

- Ozone interference from valve rotor

Compounds affected -
Acetaldehyde
Propanal
Butanal
Pentanal
Acetone

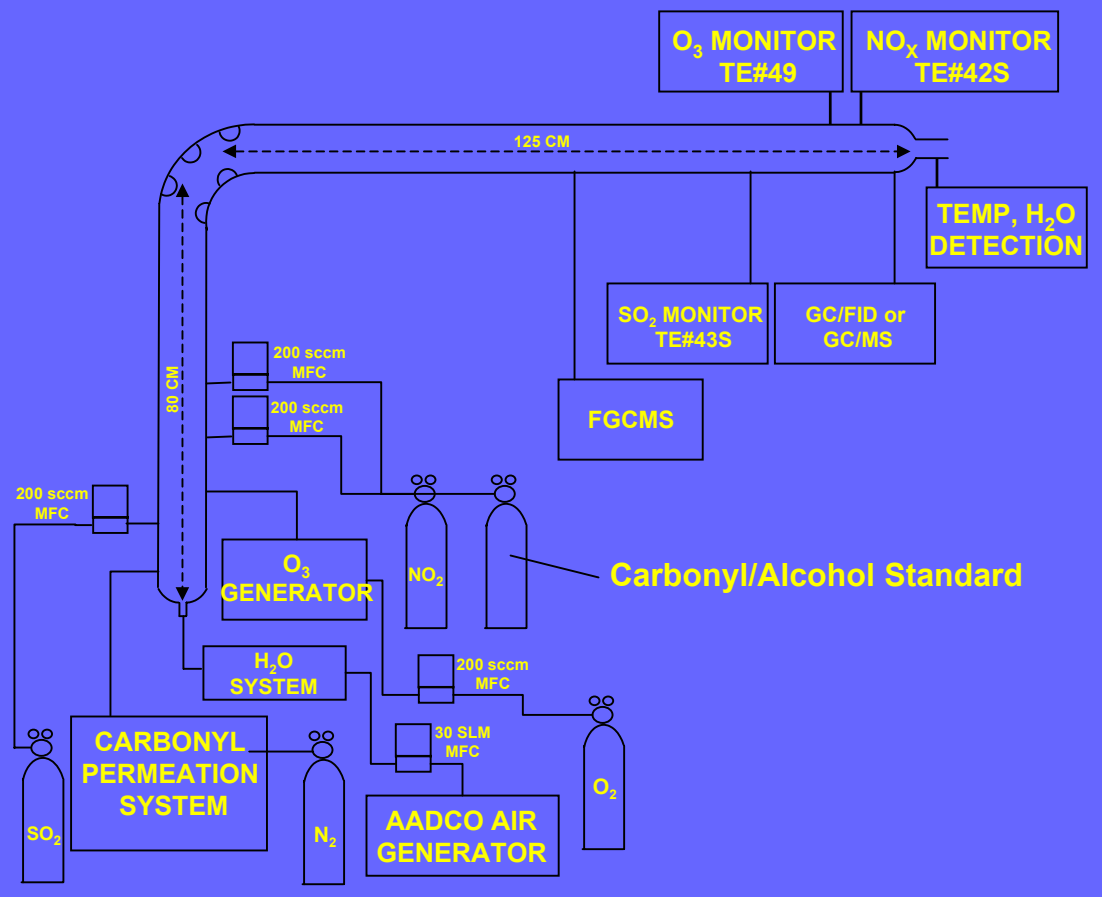
Compounds **NOT** affected -
Methanol
Ethanol
Methyl Ethyl Ketone
2-Pentanone

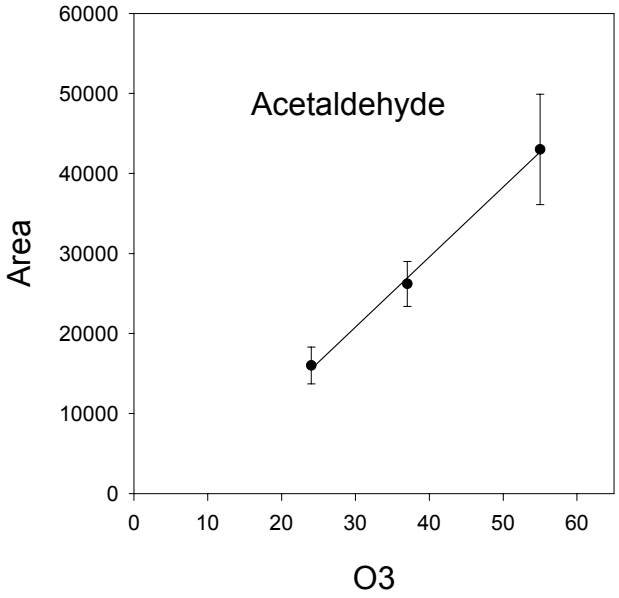
- Pressure effects from undersized sampling pump (at >10 km)

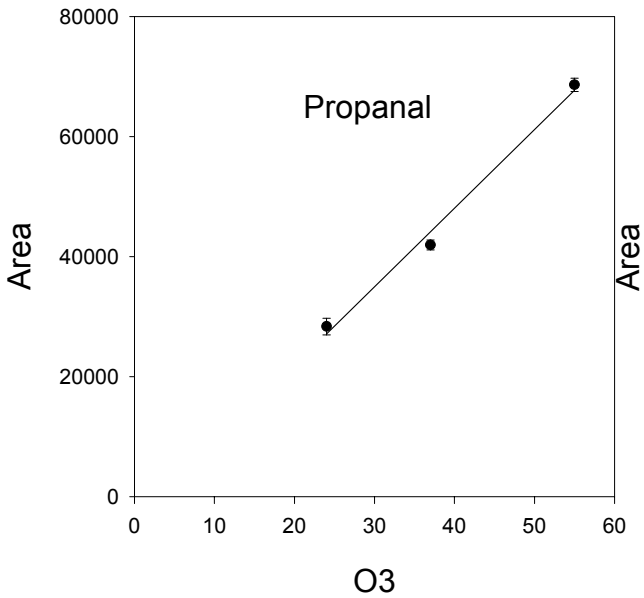
Compounds affected -
Acetaldehyde
Propanal
Butanal
Pentanal

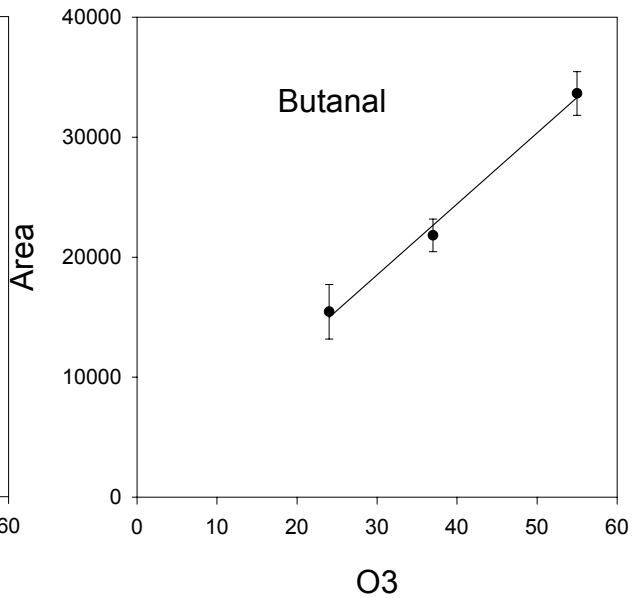
Compounds **NOT** affected -
Methanol
Ethanol
Acetone
Methyl Ethyl Ketone
2-Pentanone

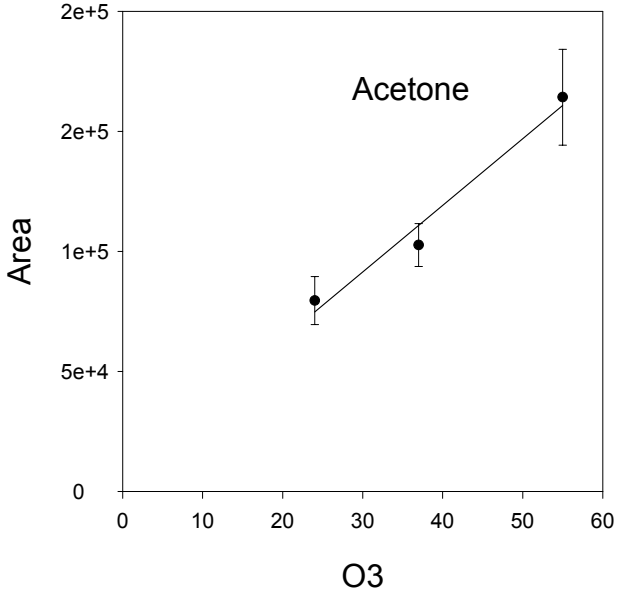
NCAR Calibration Facility

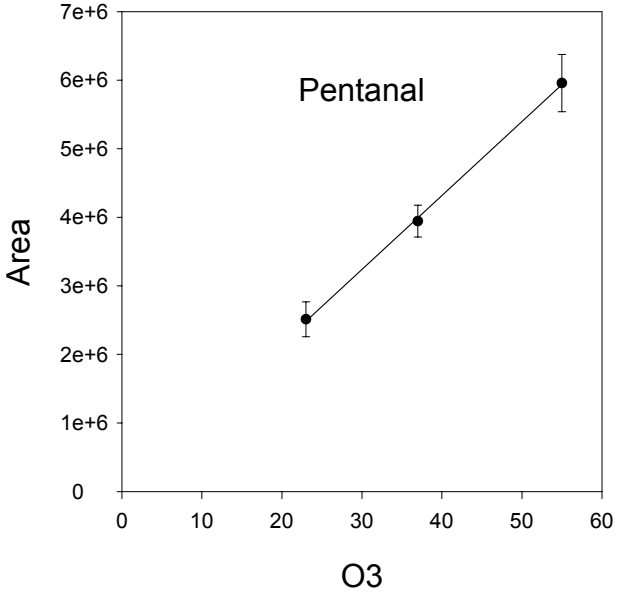



Acetaldehyde
Area
O3
0
10000
20000
30000
40000
50000
60000
0
10
20
30
40
50
60


Propanal
Area
O3
0
20000
40000
60000
80000
0
10
20
30
40
50
60


Butanal
Area
O3
0
10000
20000
30000
40000
0
10
20
30
40
50
60


Acetone
Area
O3
0
5e+4
1e+5
2e+5
2e+5
0
10
20
30
40
50
60


Pentanal
Area
O3
0
1e+6
2e+6
3e+6
4e+6
5e+6
6e+6
7e+6
0
10
20
30
40
50
60

Calibration Gas Intercomparison

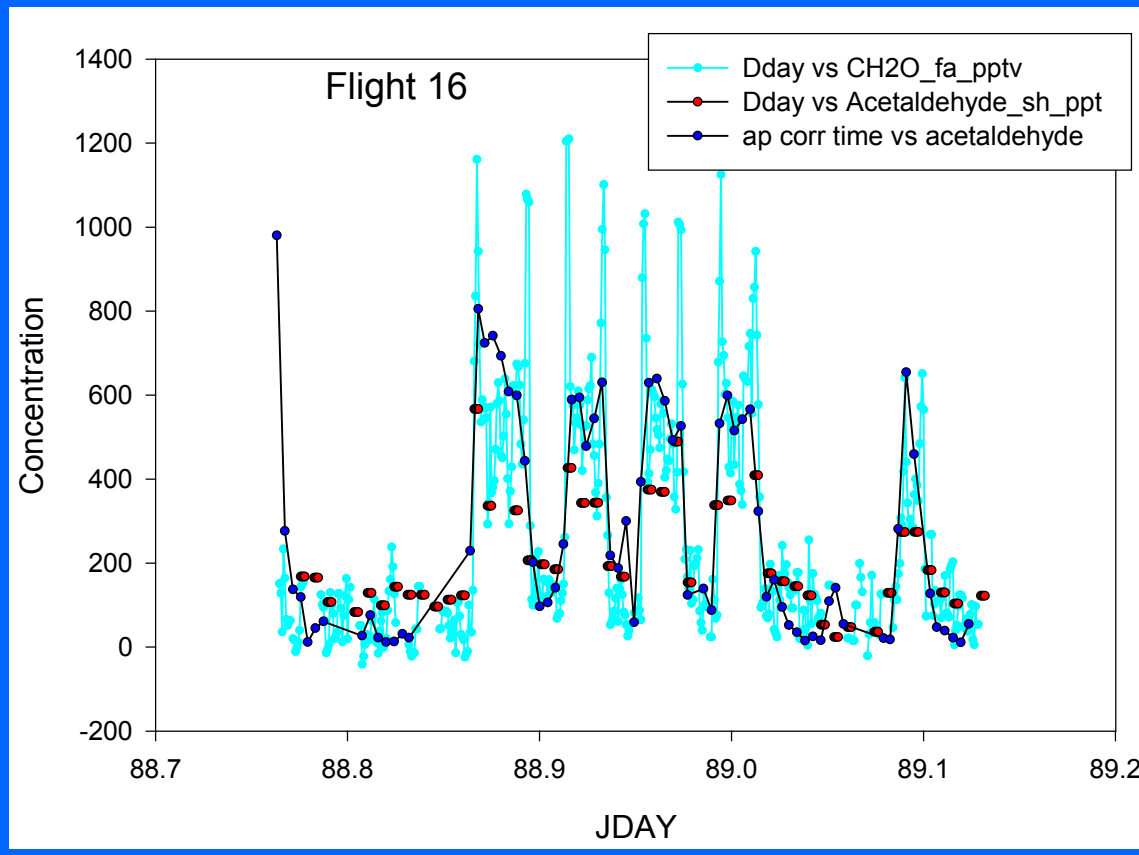
HS Calibration Cylinder - ~ 1 ppm Acetone, Methanol, Ethanol, Acetaldehyde

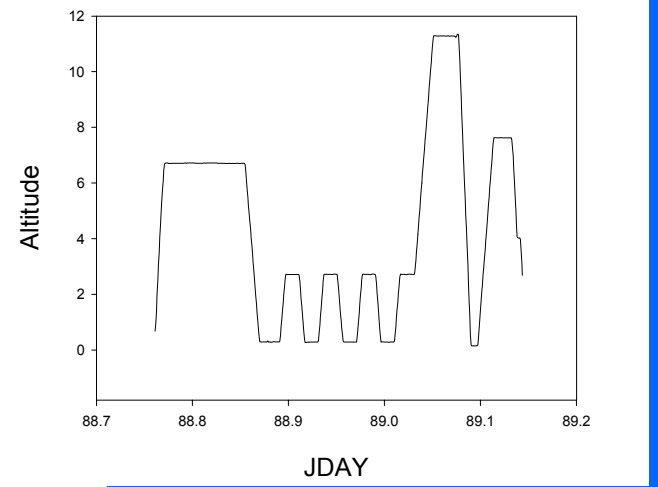
FGCMS Calibration Cylinder - 556 ppb Acetone, 52 ppb MEK, 412 ppb Methanol, 54 ppb Ethanol, 102 ppb Acetaldehyde, 43 ppb Propanal, 11 ppb Butanal, 39 ppb Carbon Tetrachloride

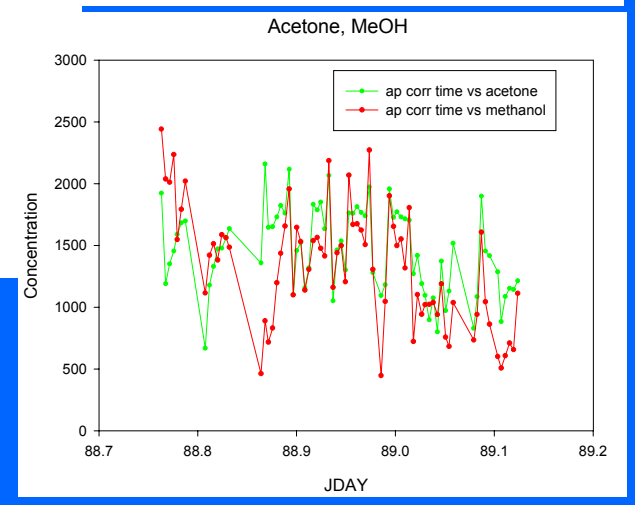
Diluted into ultraclean zero air at ambient humidity

Compound	FGCMS standard (RF) (ppt/count)	HS standard (RF) (ppt/count)	% difference
Acetone	2.25×10^{-3}	2.0×10^{-3}	11.8
Methyl Ethyl Ketone	1.85×10^{-3}	n/a	
Methanol	2.35×10^{-2}	1.77×10^{-2}	28.1
Ethanol	1.97×10^{-2}	1.18×10^{-2}	50.3
Acetaldehyde	1.30×10^{-2}	1.07×10^{-2}	19.4
Propanal	3.40×10^{-3}	n/a	
Butanal	2.39×10^{-3}	n/a	

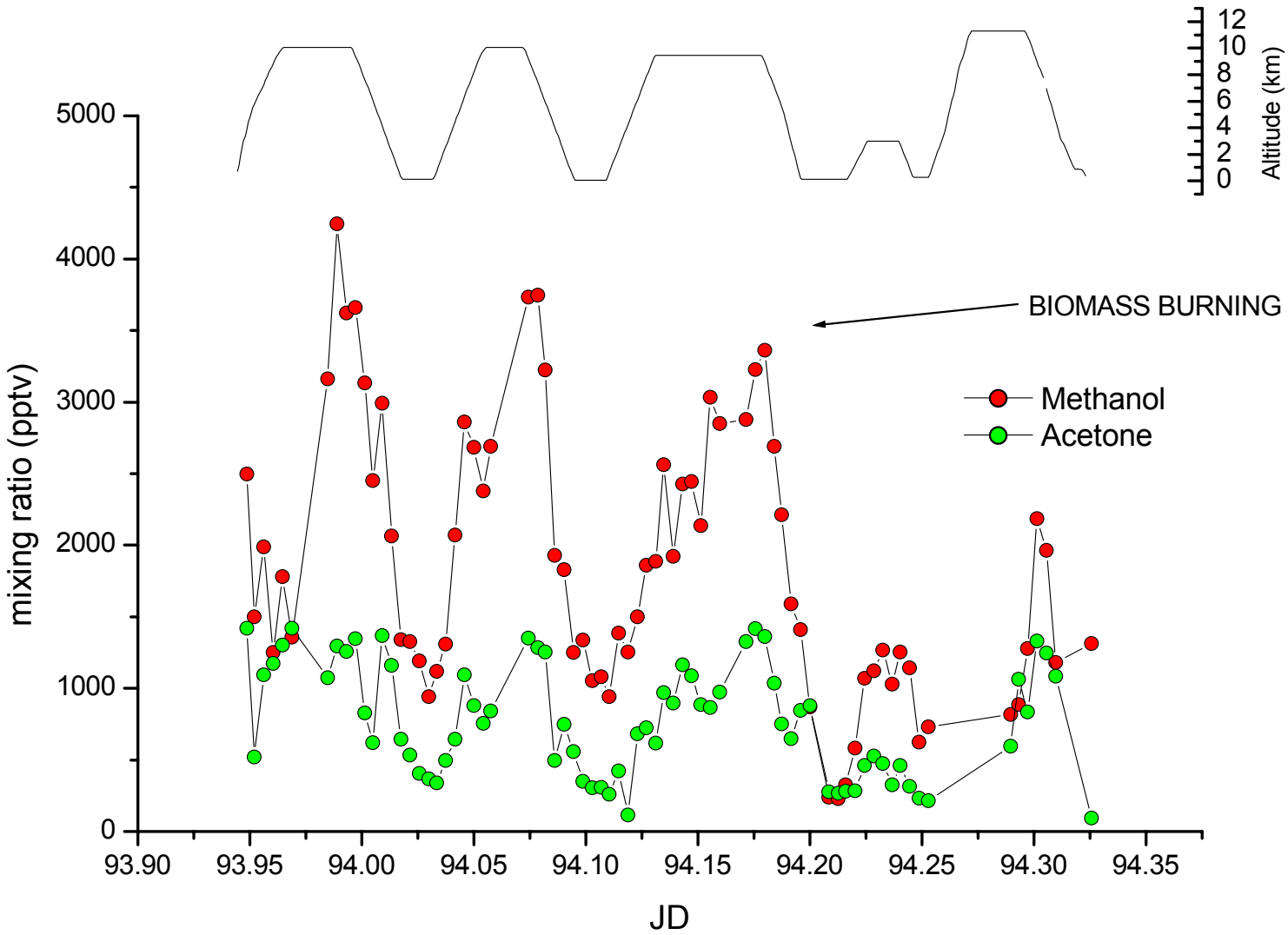
Sunrise Experiment

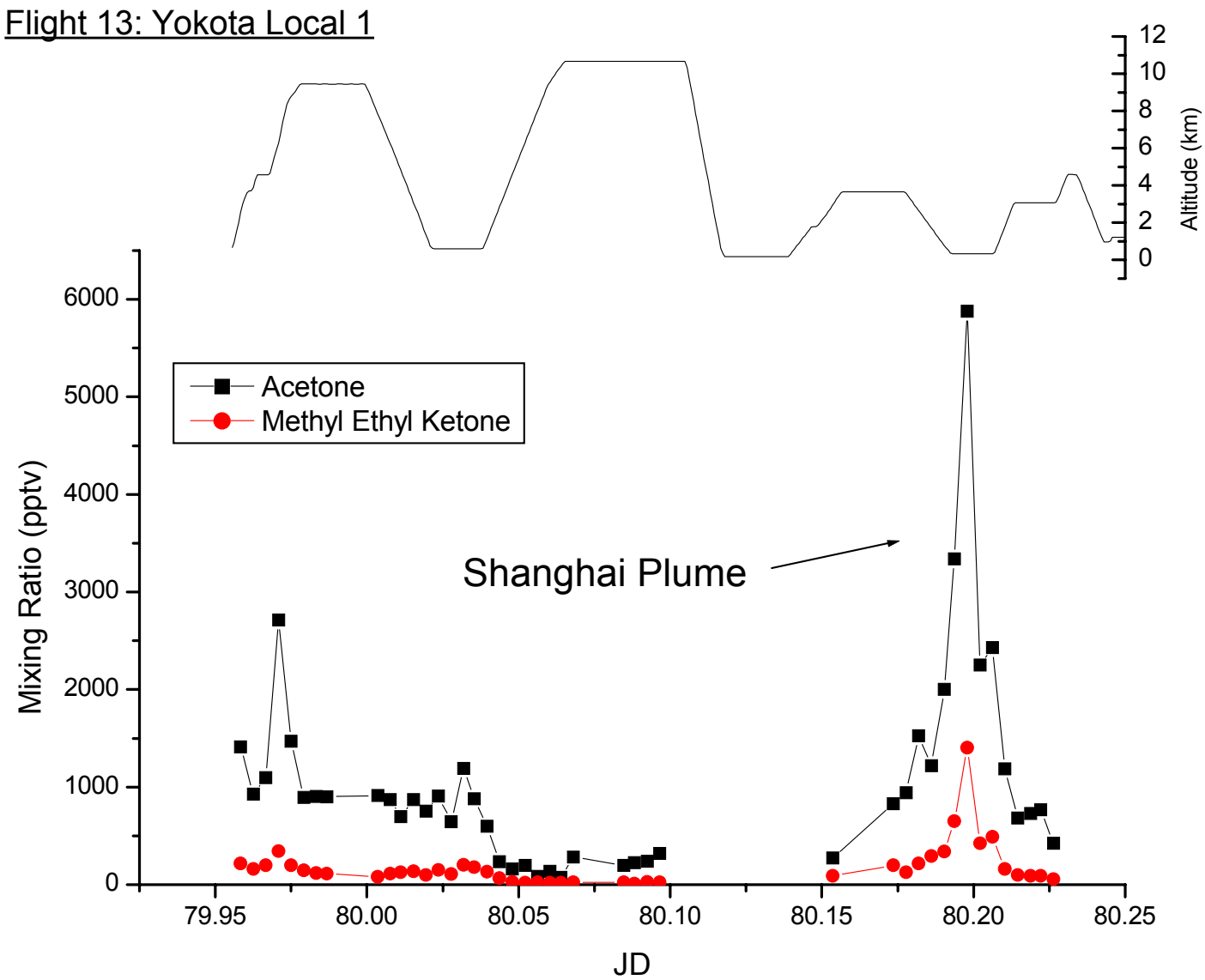






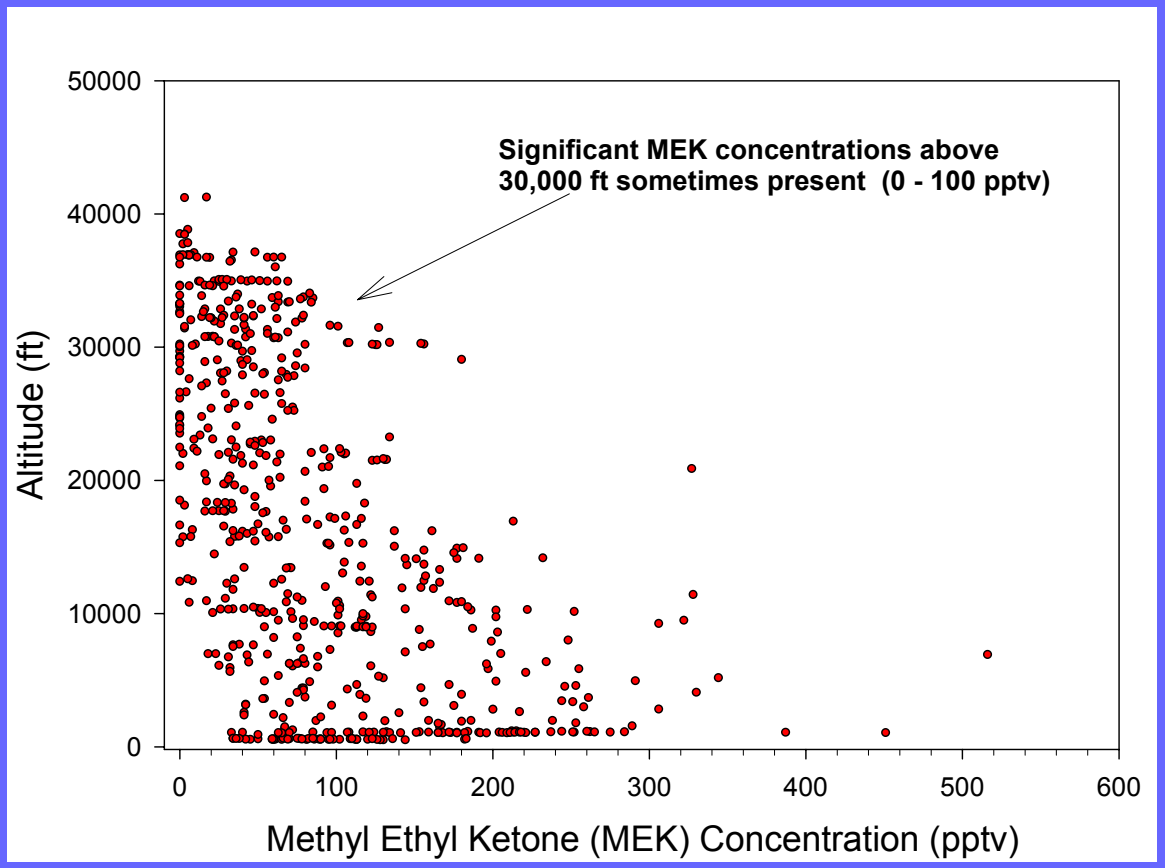
Flight 18 (Yakota - Kona Transit)




Flight 13: Yokota Local 1
Altitude (km)
12
10
8
6
4
2
0
Mixing Ratio (pptv)
6000
5000
4000
3000
2000
1000
0
Acetone
Methyl Ethyl Ketone
Shanghai Plume
79.95
80.00
80.05
80.10
80.15
80.20
80.25
JD

Detection of Methyl Ethyl Ketone in the upper troposphere

NASA TRACE -P Experiment, Spring 2001, Missions 10 -20, Preliminary Data



Eric Apel, NCAR
Dan Riemer, UM

Potentially contributes to HOx budget through photolysis
Lifetime approximately 1/4 that of acetone
Previously not included in budgets

Conclusions and Outlook:

Alcohols and carbonyls measured
- -some problems w/aldehydes discovered post-flight
- -in process of correcting data
- -instrument being modified and improved

Unanswered questions: Ocean as a source of aldehydes?
comparison w/Singh after data correction

Potential Papers:

Instrument paper. The instrument used has never been described – it will be described in this paper

Distributions of methanol and ethanol during TRACE-P. A paper examining the distributions, sources, and sinks for these compounds.

Distributions of ketones during TRACE-P. A paper examining the distributions, sources, and sinks for these compounds.