2003 Ozone Precursor Study

RAQC Meeting, 17 October 2003

*** Updated 10/31/03 with final data ***

Air Pollution Control Division

Colorado Department of Public Health & Environment

Study design

- NMOCs and carbonyls

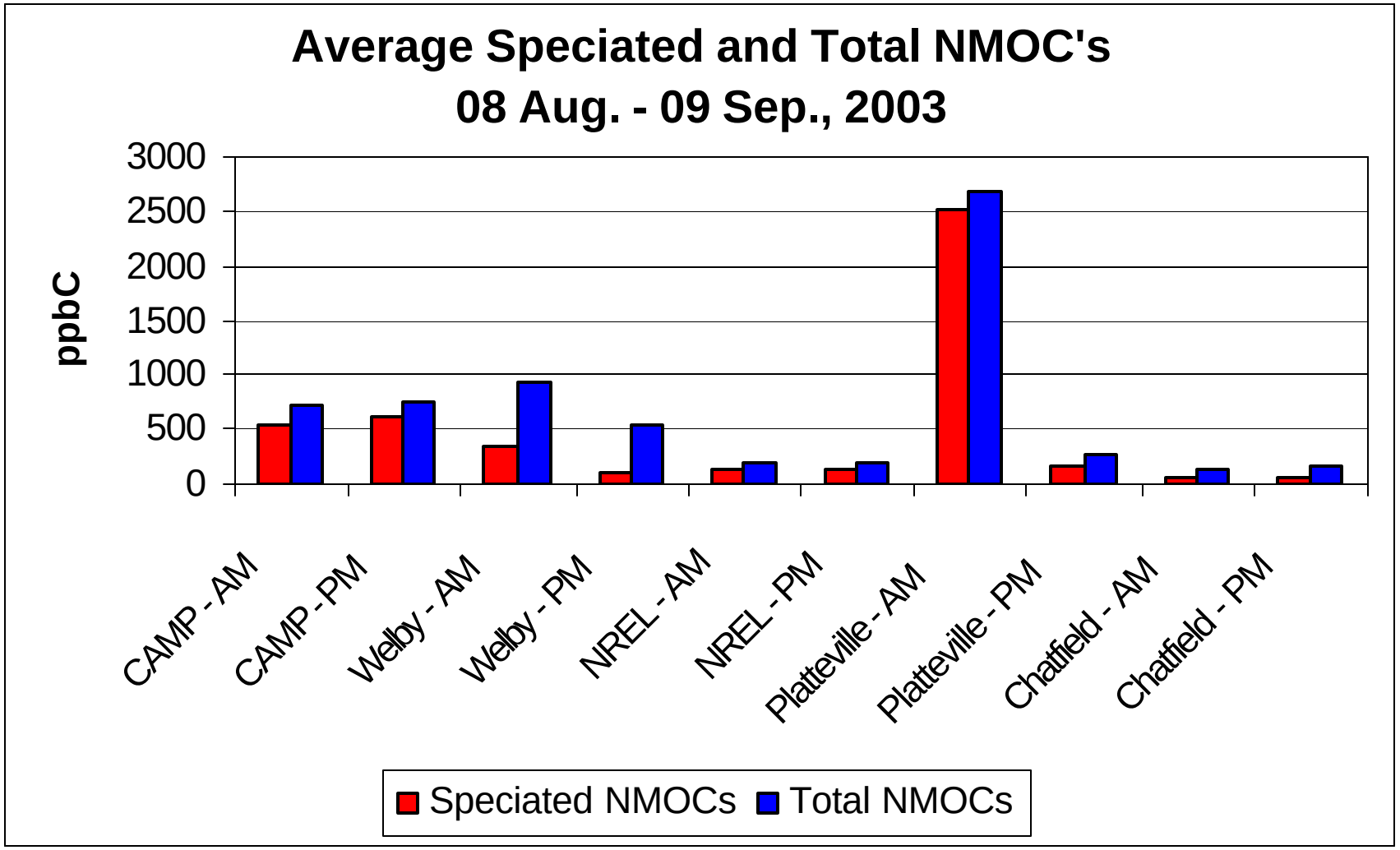
- 08 August – 09 September 2003
- AM samples (6:00 – 9:00 MDT)
- PM samples (1:00 – 4:00 MDT)

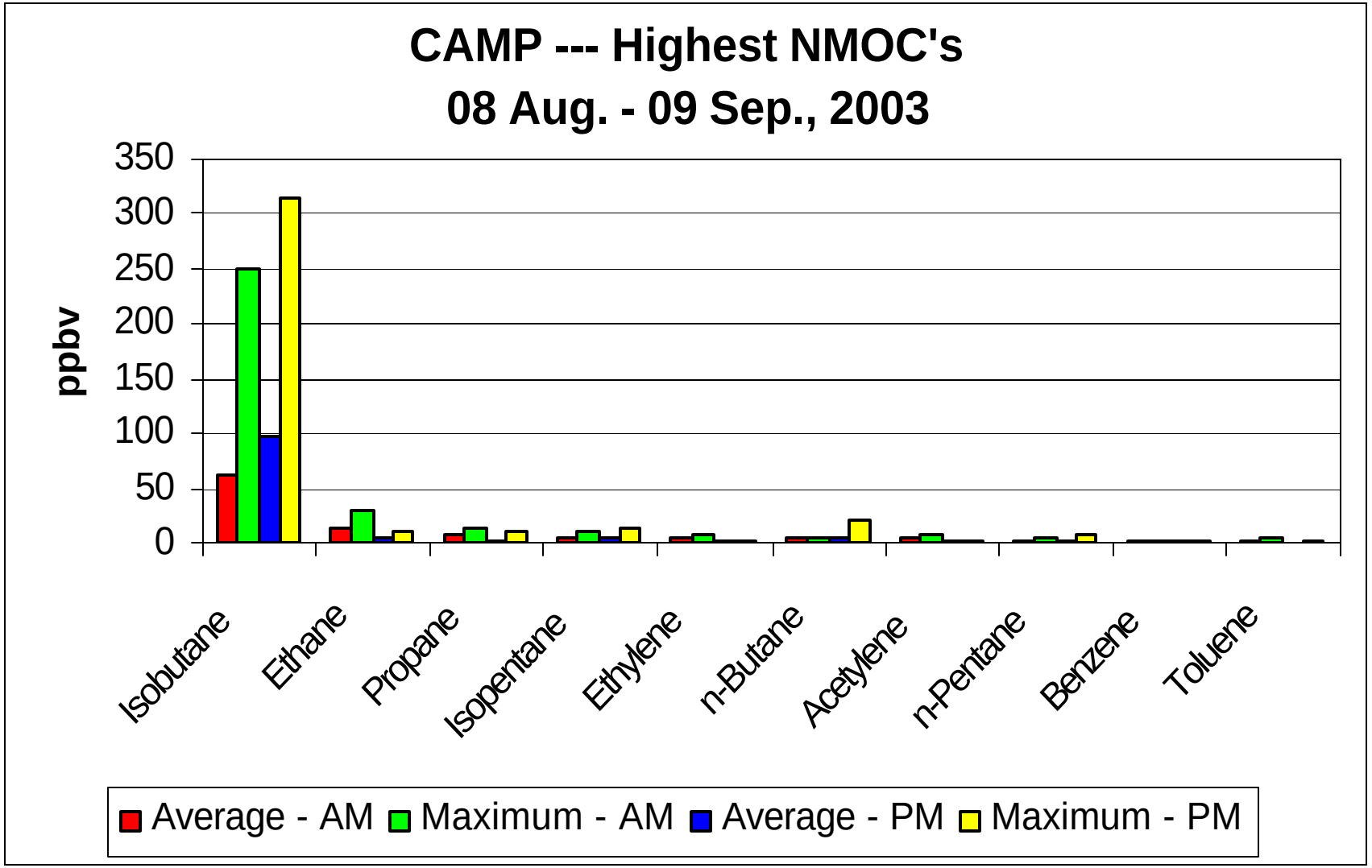
- 2 main sites (CAMP, Welby)
- 1 roving site (NREL, Platteville, Chatfield)

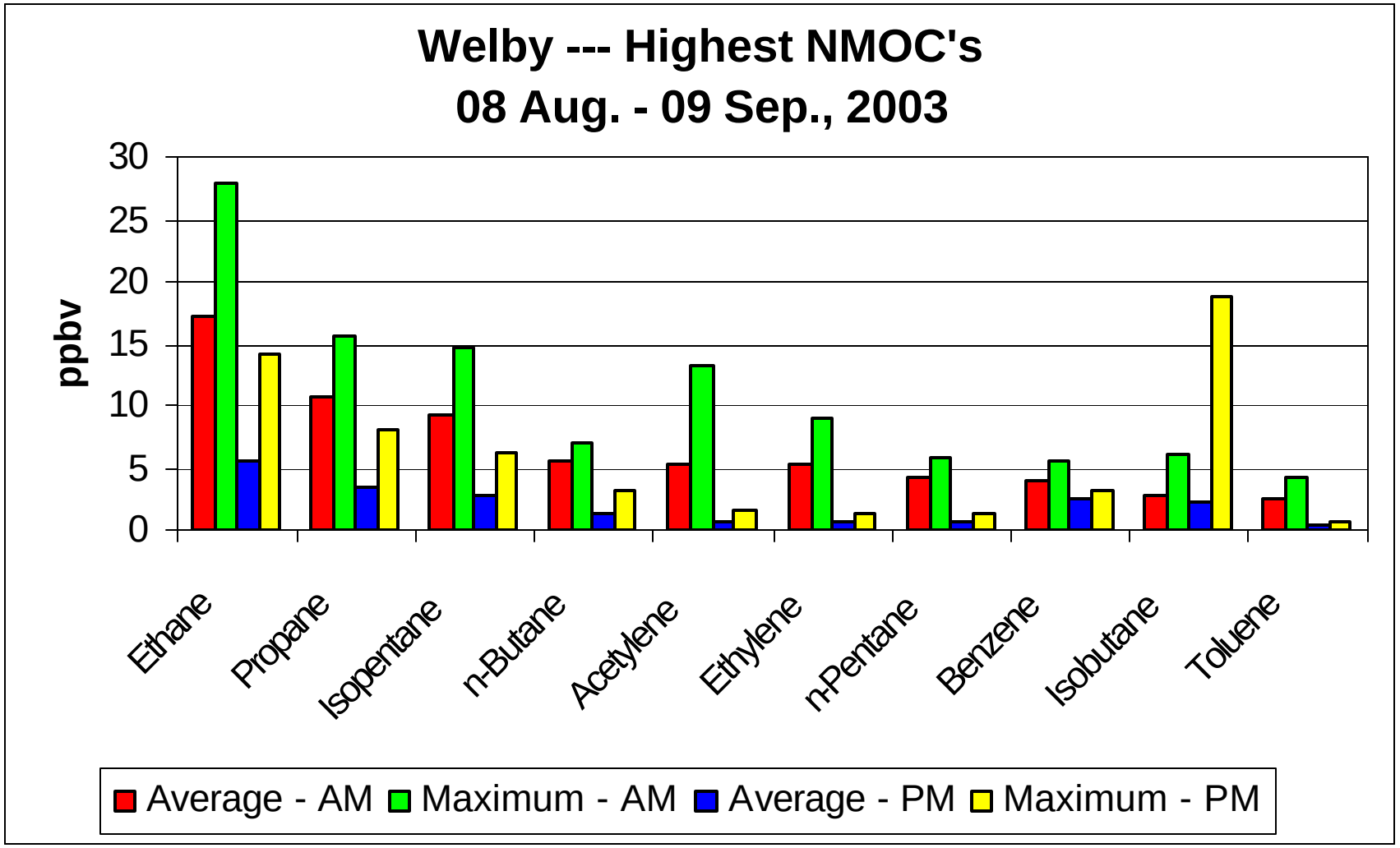
Map of sites used in 2003 study

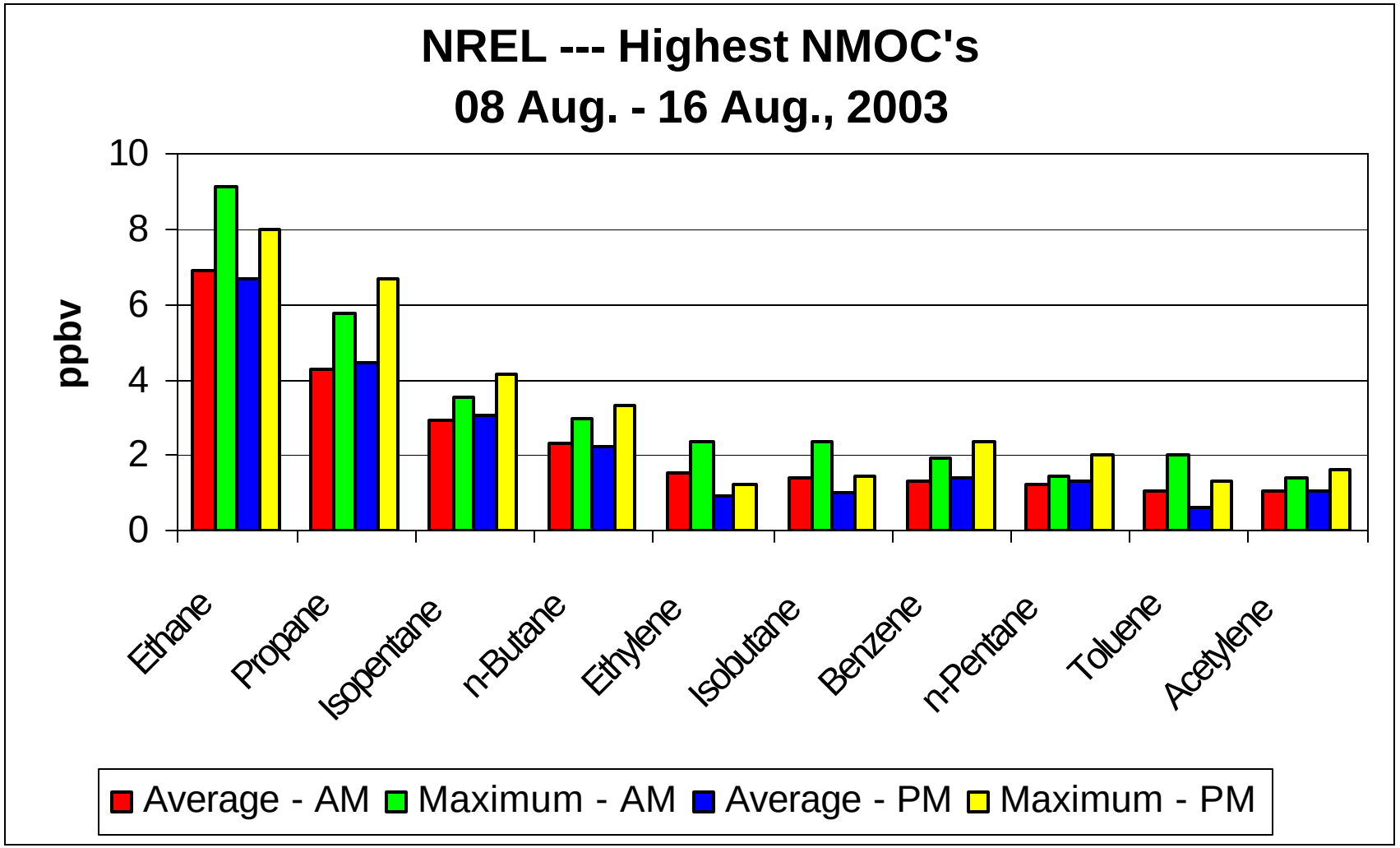
List of NMOCs (78)

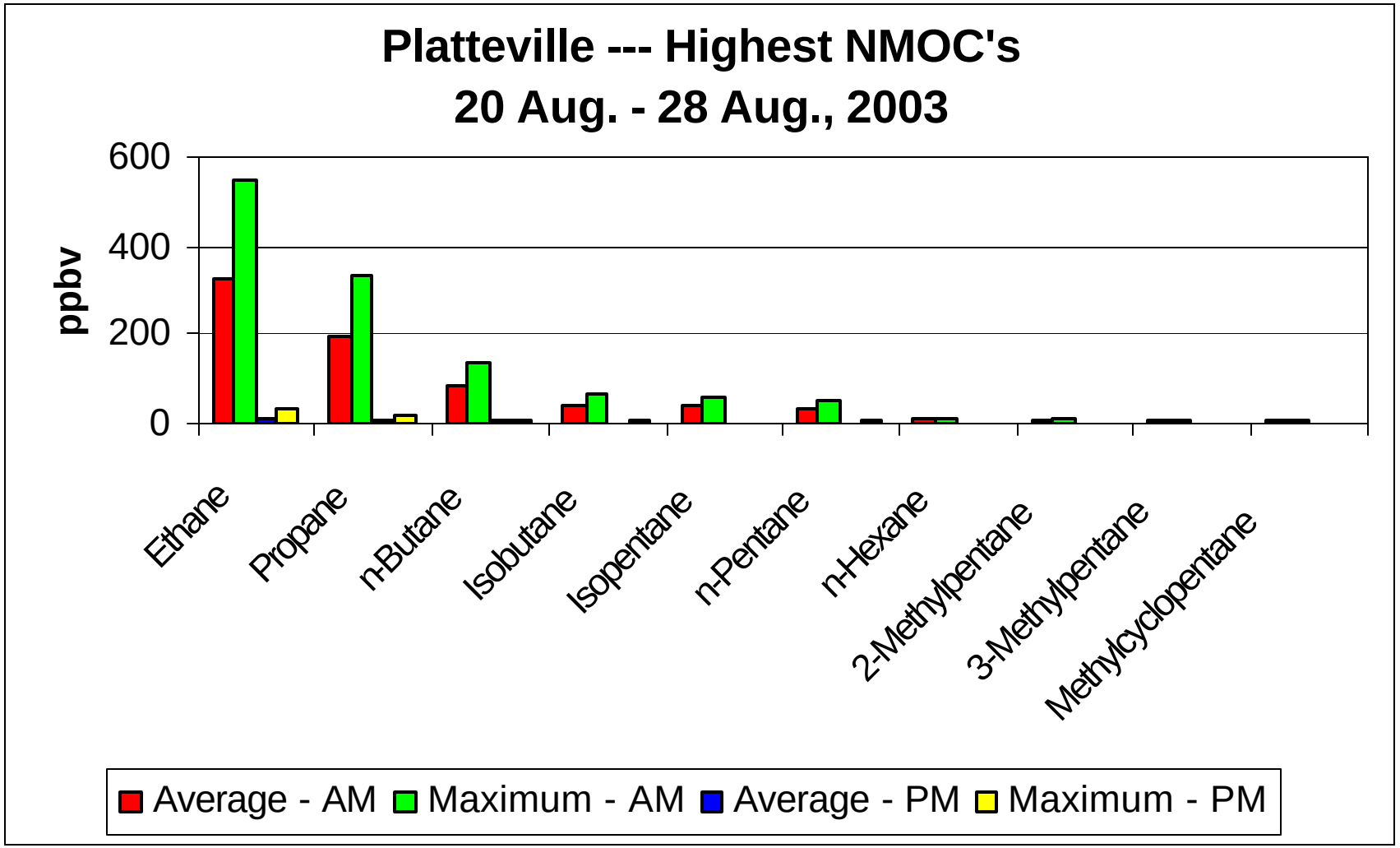
Ethylene	2-Methylpentane	Ethylbenzene
Acetylene	3-Methylpentane	m-Xylene / p-Xylene
Ethane	2-Methyl-1-pentene	Styrene
Propylene	1-Hexene	o-Xylene
Propane	2-Ethyl-1-butene	1-Nonene
Propyne	n-Hexane	n-Nonane
Isobutane	trans-2-Hexene	Isopropylbenzene
Isobutene / 1-Butene	cis-2-Hexene	a-Pinene
1,3-Butadiene	Methylcyclopentane	n-Propylbenzene
n-Butane	2,4-Dimethylpentane	m-Ethyltoluene
trans-2-Butene	Benzene	p-Ethyltoluene
cis-2-Butene	Cyclohexane	1,3,5-Trimethylbenzene
3-Methyl-1-butene	2-Methylhexane	o-Ethyltoluene
Isopentane	2,3-Dimethylpentane	b-Pinene
1-Pentene	3-Methylhexane	1,2,4-Trimethylbenzene
2-Methyl-1-butene	1-Heptene	1-Decene
n-Pentane	2,2,4-Trimethylpentane	n-Decane
Isoprene	n-Heptane	1,2,3-Trimethylbenzene
trans-2-Pentene	Methylcyclohexane	m-Diethylbenzene
cis-2-Pentene	2,2,3-Trimethylpentane	p-Diethylbenzene
2-Methyl-2-butene	2,3,4-Trimethylpentane	1-Undecene
2,2-Dimethylbutane	Toluene	n-Undecane
Cyclopentene	2-Methylheptane	1-Dodecene
4-Methyl-1-pentene	3-Methylheptane	n-Dodecane
Cyclopentane	1-Octene	1-Tridecene
2,3-Dimethylbutane	n-Octane	n-Tridecane

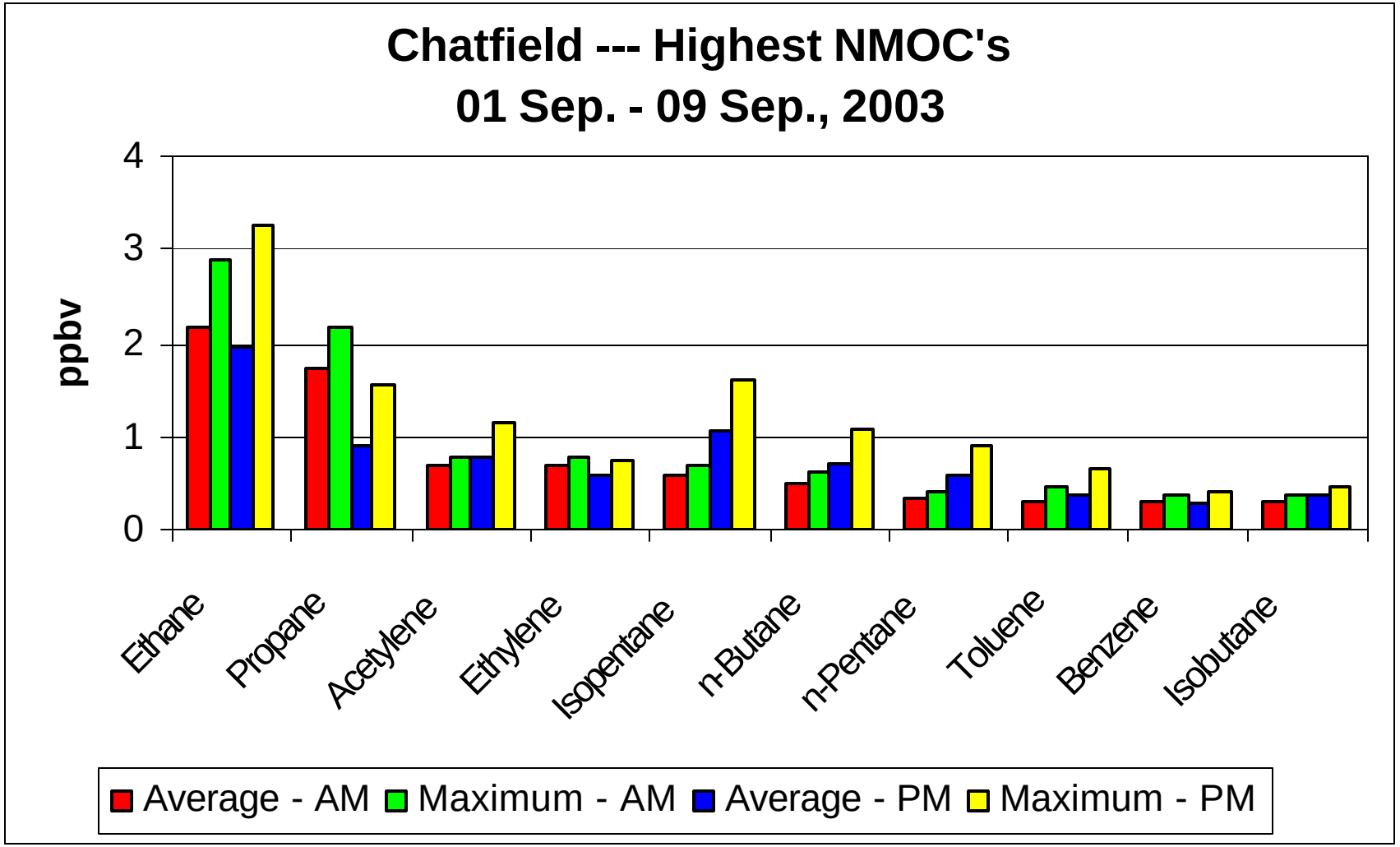

Average Speciated and Total NMOC's
08 Aug. - 09 Sep., 2003
ppbC
3000
2500
2000
1500
1000
500
0
CAMP - AM
CAMP - PM
Welby - AM
Welby - PM
NREL - AM
NREL - PM
Platteville - AM
Platteville - PM
Chatfield - AM
Chatfield - PM
Speciated NMOCs
Total NMOCs


CAMP --- Highest NMOC's
08 Aug. - 09 Sep., 2003
ppbv
350
300
250
200
150
100
50
0
Isobutane
Ethane
Propane
Isopentane
Ethylene
n-Butane
Acetylene
n-Pentane
Benzene
Toluene
Average - AM
Maximum - AM
Average - PM
Maximum - PM


Welby --- Highest NMOC's
08 Aug. - 09 Sep., 2003
ppbv
30
25
20
15
10
5
0
Ethane
Propane
Isopentane
n-Butane
Acetylene
Ethylene
n-Pentane
Benzene
Isobutane
Toluene
Average - AM
Maximum - AM
Average - PM
Maximum - PM


NREL --- Highest NMOC's
08 Aug. - 16 Aug., 2003
ppbv
10
8
6
4
2
0
Ethane
Propane
Isopentane
n-Butane
Ethylene
Isobutane
Benzene
n-Pentane
Toluene
Acetylene
Average - AM
Maximum - AM
Average - PM
Maximum - PM


Platteville --- Highest NMOC's
20 Aug. - 28 Aug., 2003
ppbv
600
400
200
0
Ethane
Propane
n-Butane
Isobutane
Isopentane
n-Pentane
n-Hexane
2-Methylpentane
3-Methylpentane
Methylcyclopentane
Average - AM
Maximum - AM
Average - PM
Maximum - PM

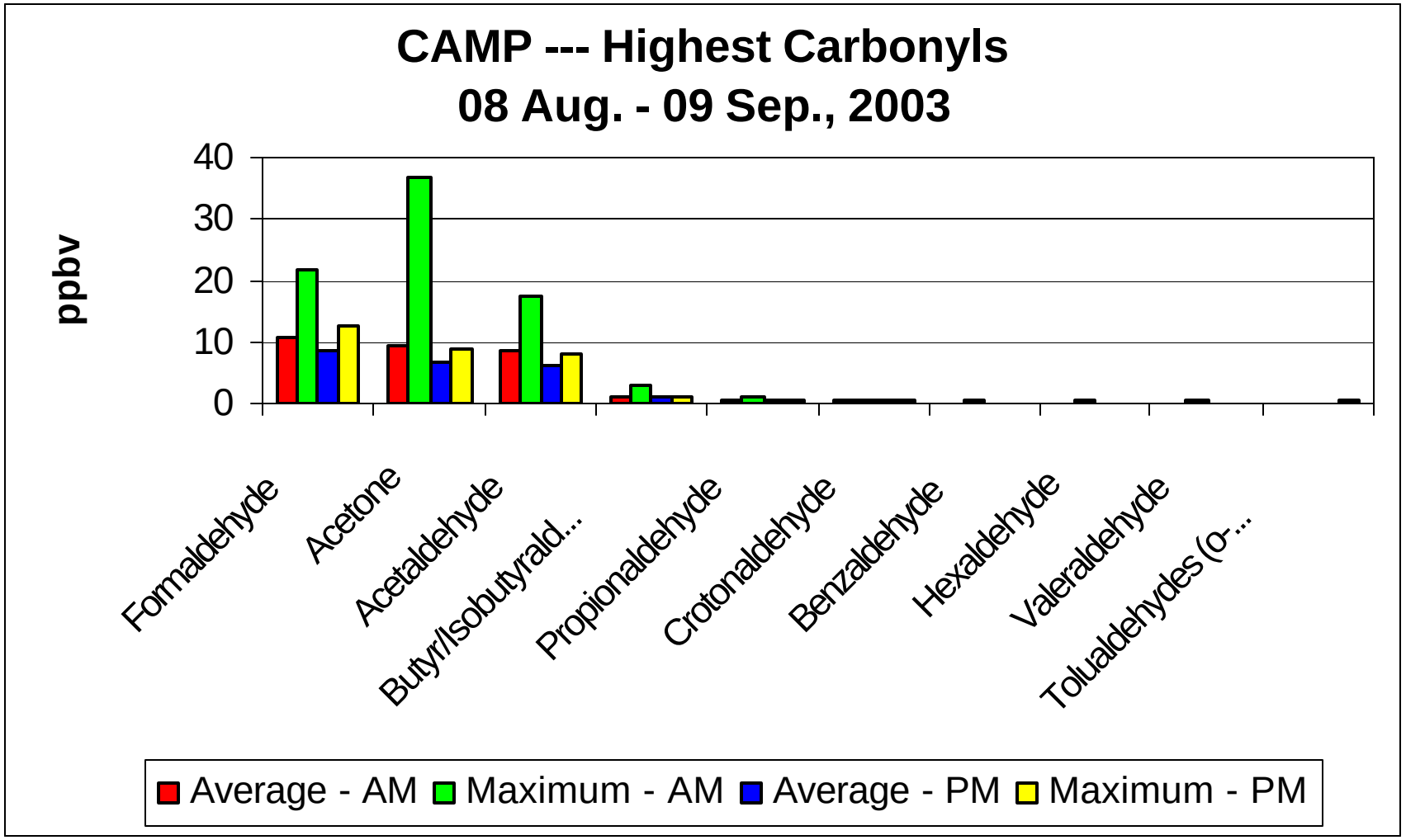

Chatfield --- Highest NMOC's
01 Sep. - 09 Sep., 2003
ppbv
4
3
2
1
0
Ethane
Propane
Acetylene
Ethylene
Isopentane
n-Butane
n-Pentane
Toluene
Benzene
Isobutane
Average - AM
Maximum - AM
Average - PM
Maximum - PM

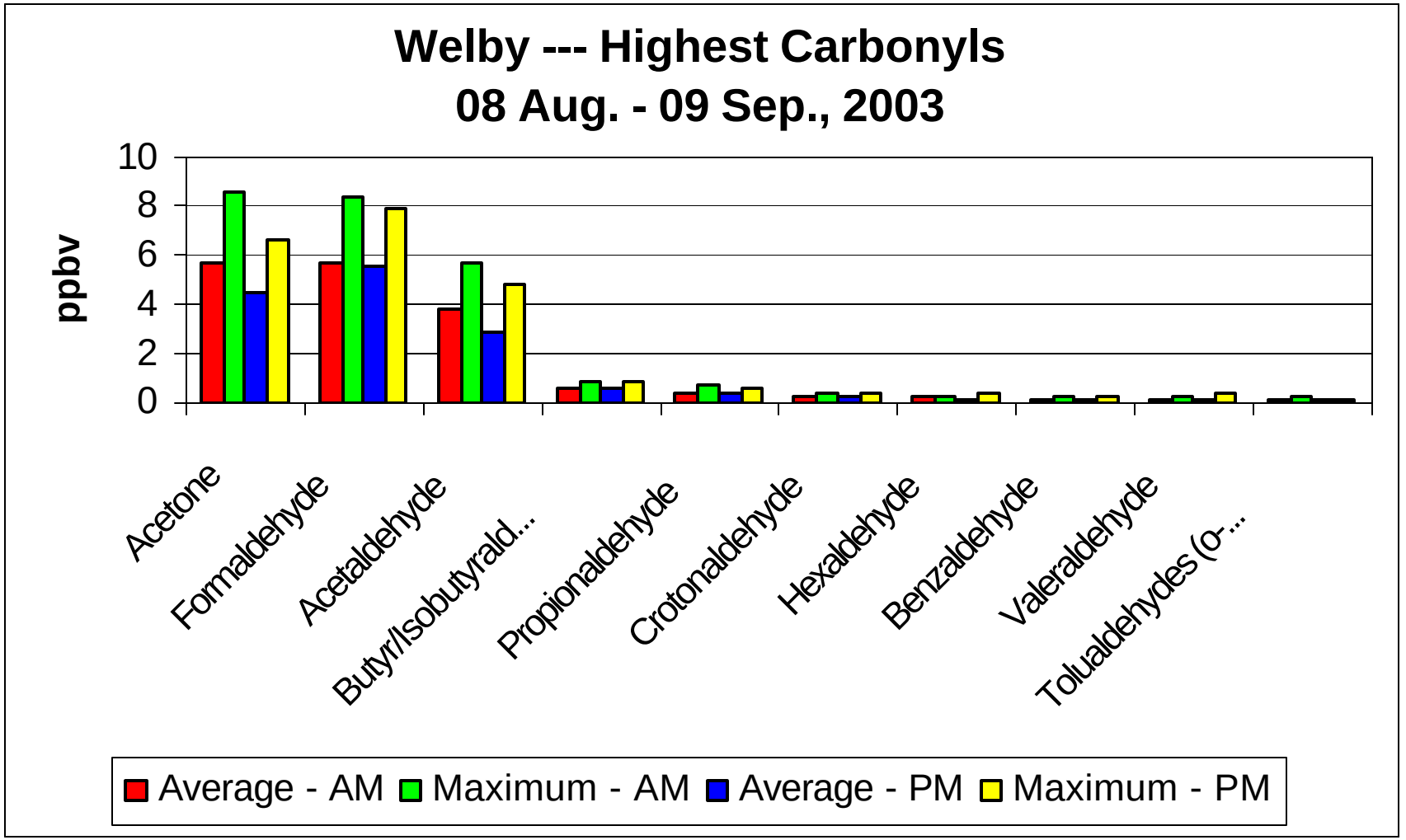
Notes on NMOCs

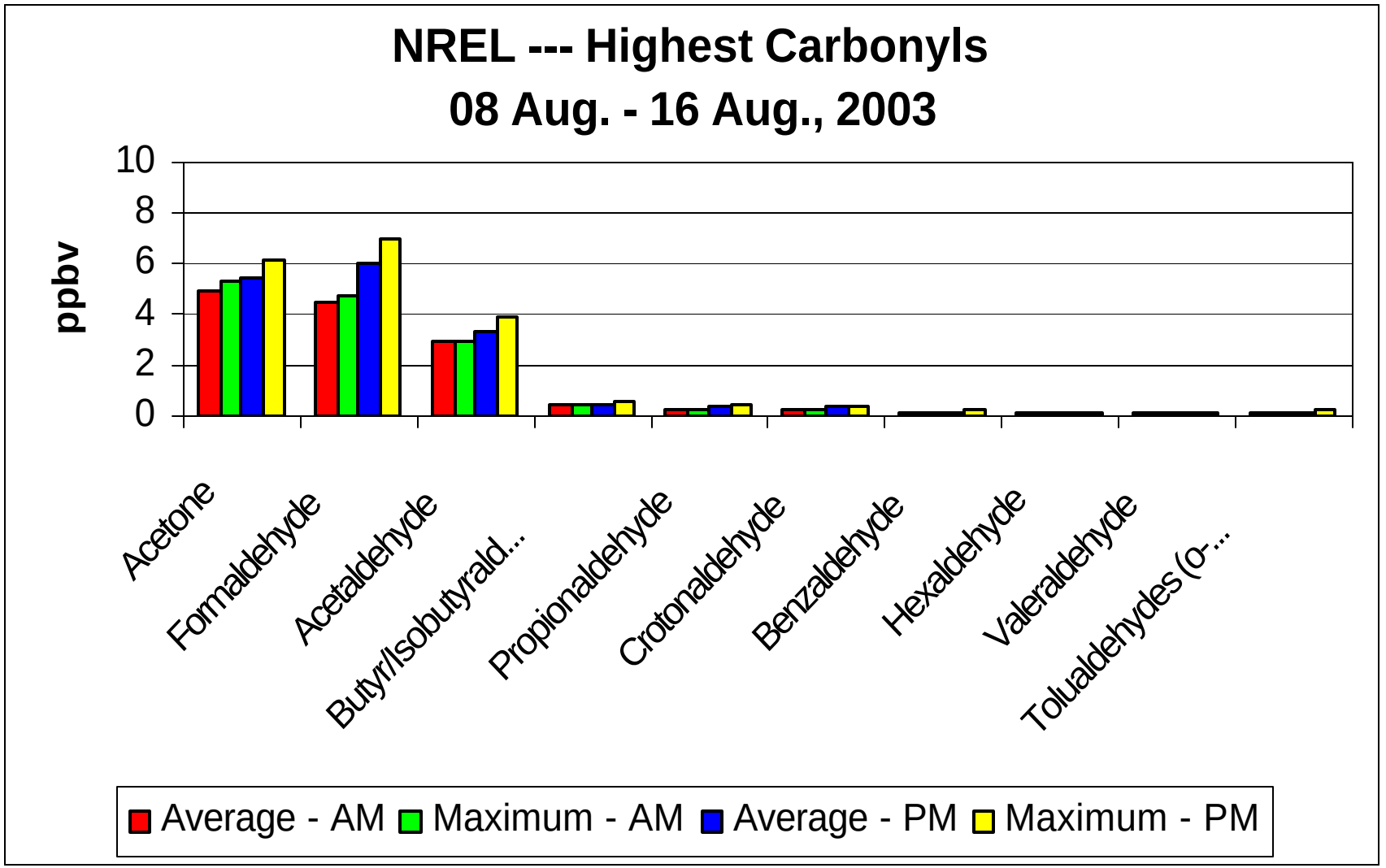
- Concentrations varied from site to site and by time of day.
- Highest compounds varied by site.
- Platteville recorded the highest overall concentrations followed by CAMP.
- In general, AM concentrations were higher than PM concentrations at Welby and Platteville. AM and PM concentrations were similar at CAMP, NREL and Chatfield.

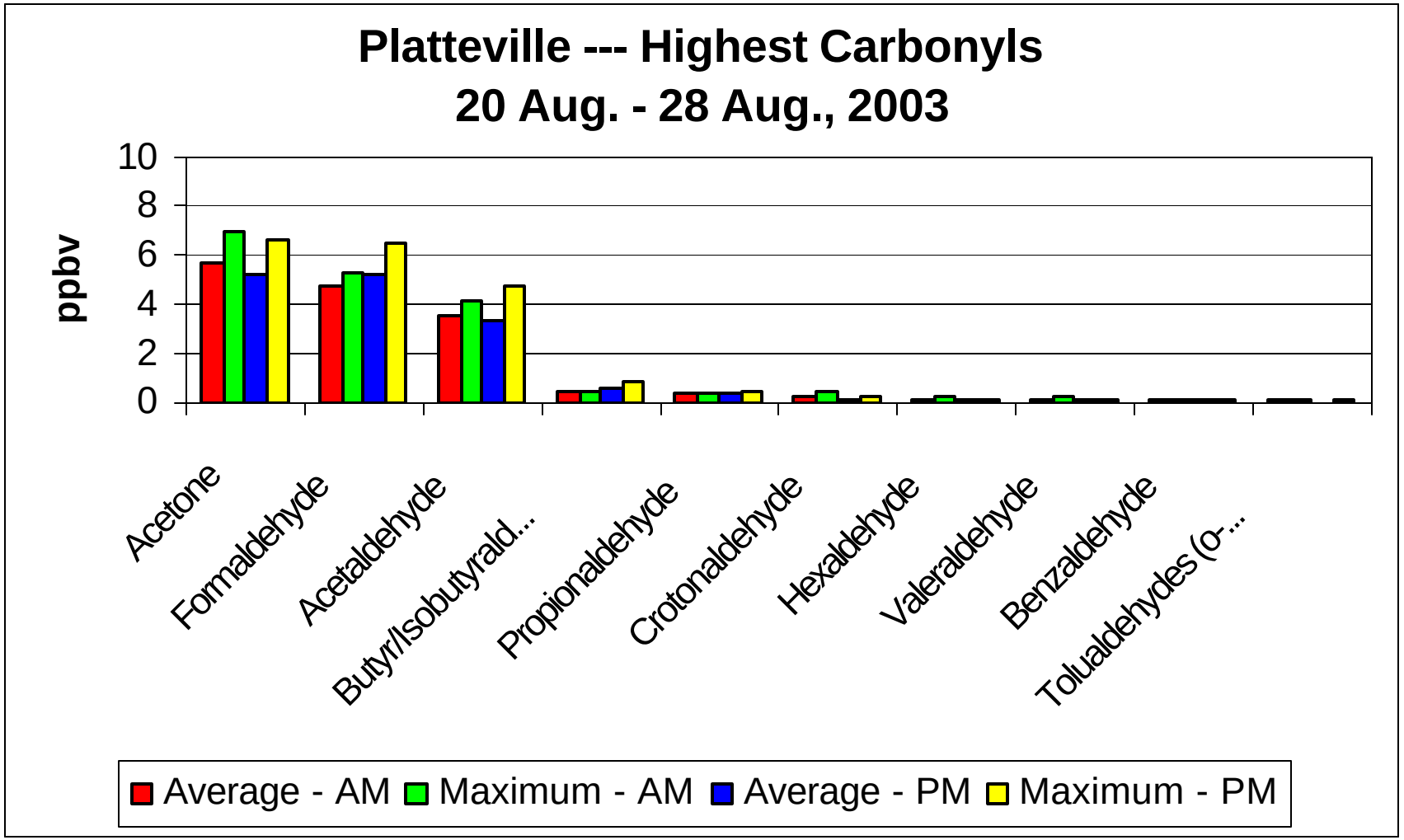
List of Carbonyls (12)

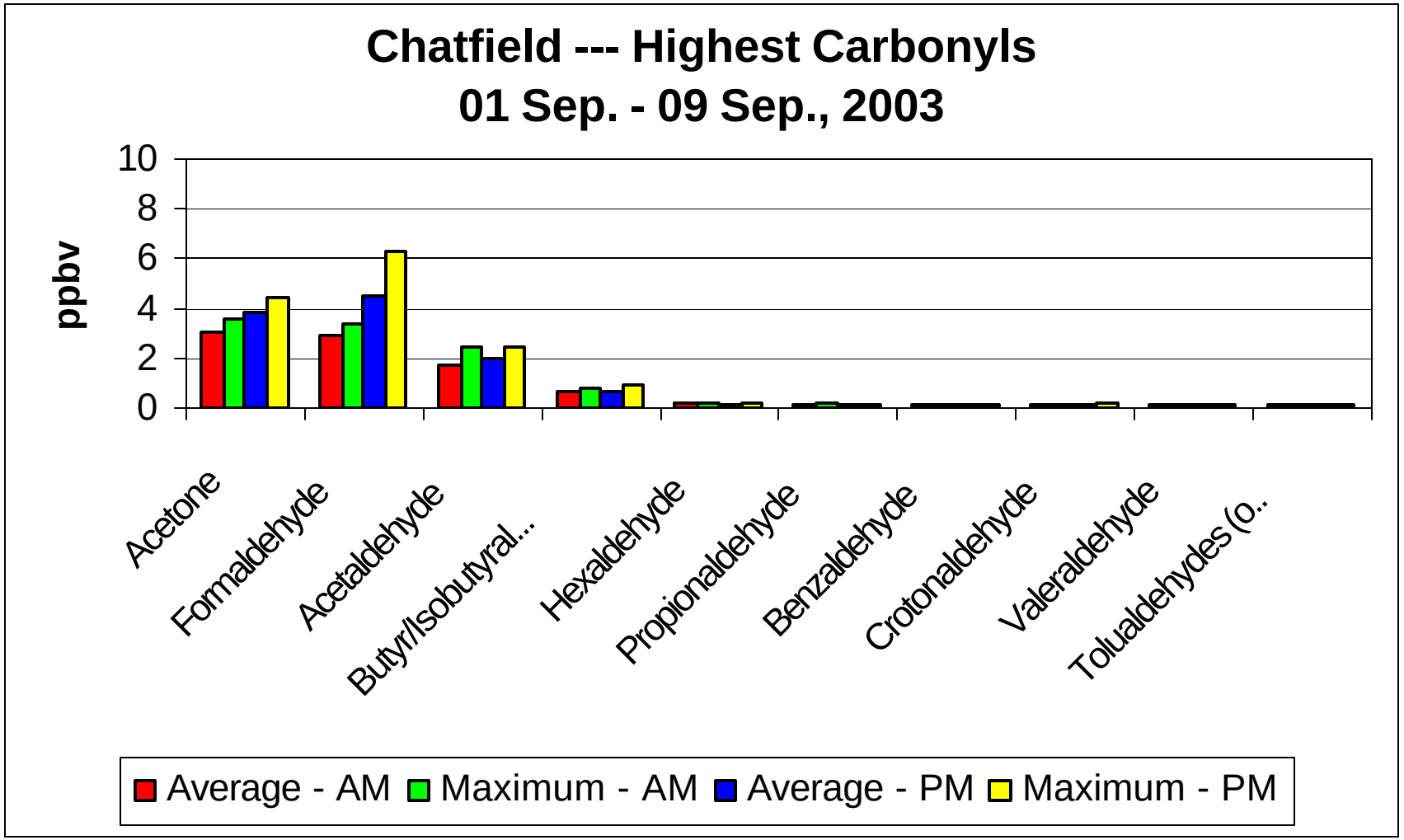
Formaldehyde
Acetaldehyde
Acetone
Propionaldehyde
Crotonaldehyde
Butyr/Isobutyraldehyde
Benzaldehyde
Isovaleraldehyde
Valeraldehyde
Tolualdehydes (o-, m-, p-)
Hexaldehyde
2,5-Dimethylbenzaldehyde


CAMP --- Highest Carbonyls
08 Aug. - 09 Sep., 2003
ppbv
40
30
20
10
0
Formaldehyde
Acetone
Acetaldehyde
Butyr/Isobutyrald...
Propionaldehyde
Crotonaldehyde
Benzaldehyde
Hexaldehyde
Valeraldehyde
Tolualdehydes (o-...
Average - AM
Maximum - AM
Average - PM
Maximum - PM


Welby --- Highest Carbonyls
08 Aug. - 09 Sep., 2003
ppbv
10
8
6
4
2
0
Acetone
Formaldehyde
Acetaldehyde
Butyr/Isobutyrald...
Propionaldehyde
Crotonaldehyde
Hexaldehyde
Benzaldehyde
Valeraldehyde
Tolualdehydes (o-...
Average - AM
Maximum - AM
Average - PM
Maximum - PM


NREL --- Highest Carbonyls
08 Aug. - 16 Aug., 2003
ppbv
10
8
6
4
2
0
Acetone
Formaldehyde
Acetaldehyde
Butyr/Isobutyrald...
Propionaldehyde
Crotonaldehyde
Benzaldehyde
Hexaldehyde
Valeraldehyde
Tolualdehydes (o-...
Average - AM
Maximum - AM
Average - PM
Maximum - PM


Platteville --- Highest Carbonyls
20 Aug. - 28 Aug., 2003
ppbv
10
8
6
4
2
0
Acetone
Formaldehyde
Acetaldehyde
Butyr/Isobutyrald...
Propionaldehyde
Crotonaldehyde
Hexaldehyde
Valeraldehyde
Benzaldehyde
Tolualdehydes (o-...
Average - AM
Maximum - AM
Average - PM
Maximum - PM

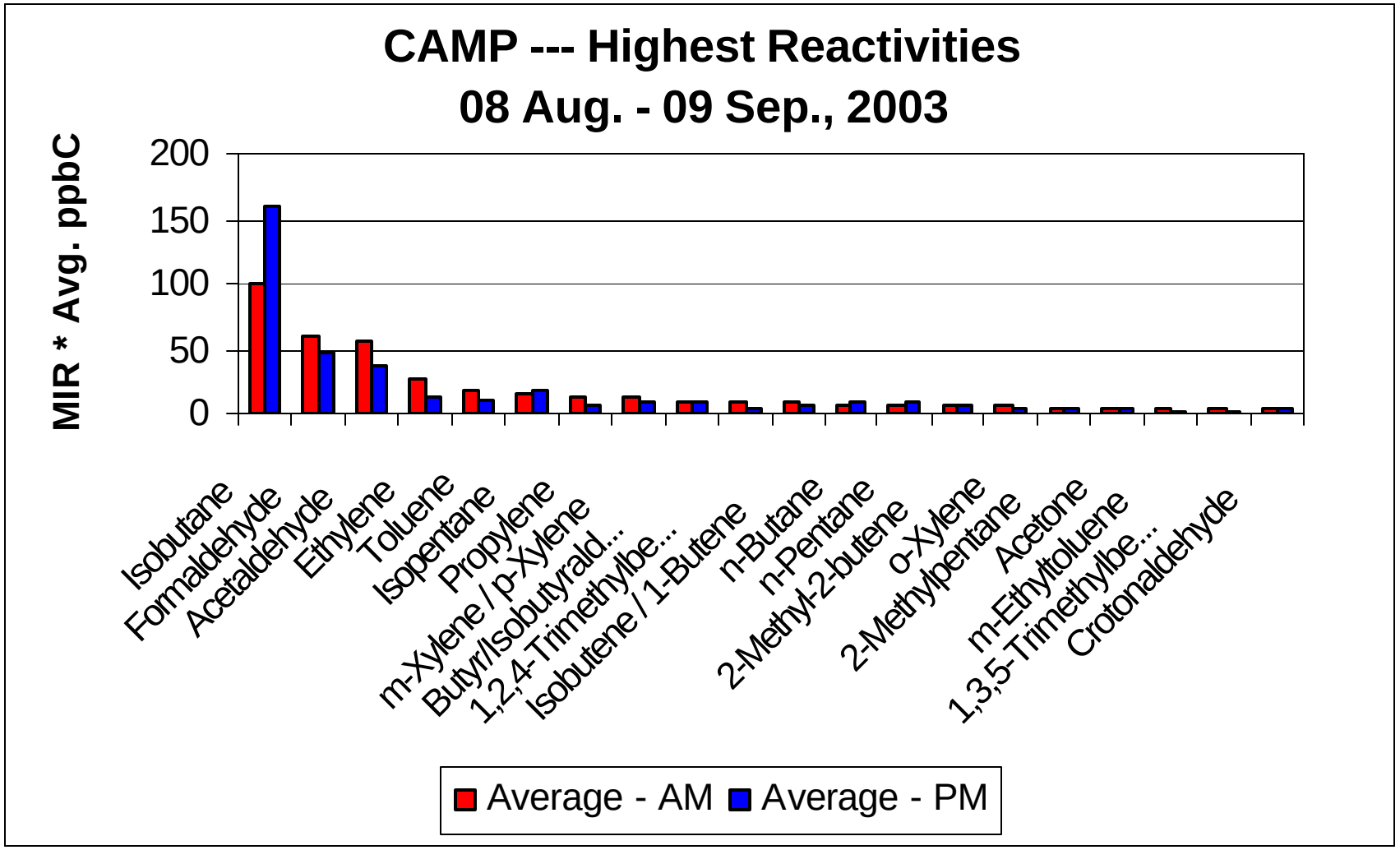

Chatfield --- Highest Carbonyls
01 Sep. - 09 Sep., 2003
ppbv
10
8
6
4
2
0
Acetone
Formaldehyde
Acetaldehyde
Butyr/Isobutyral...
Hexaldehyde
Propionaldehyde
Benzaldehyde
Crotonaldehyde
Valeraldehyde
Tolualdehydes (o..
Average - AM
Maximum - AM
Average - PM
Maximum - PM

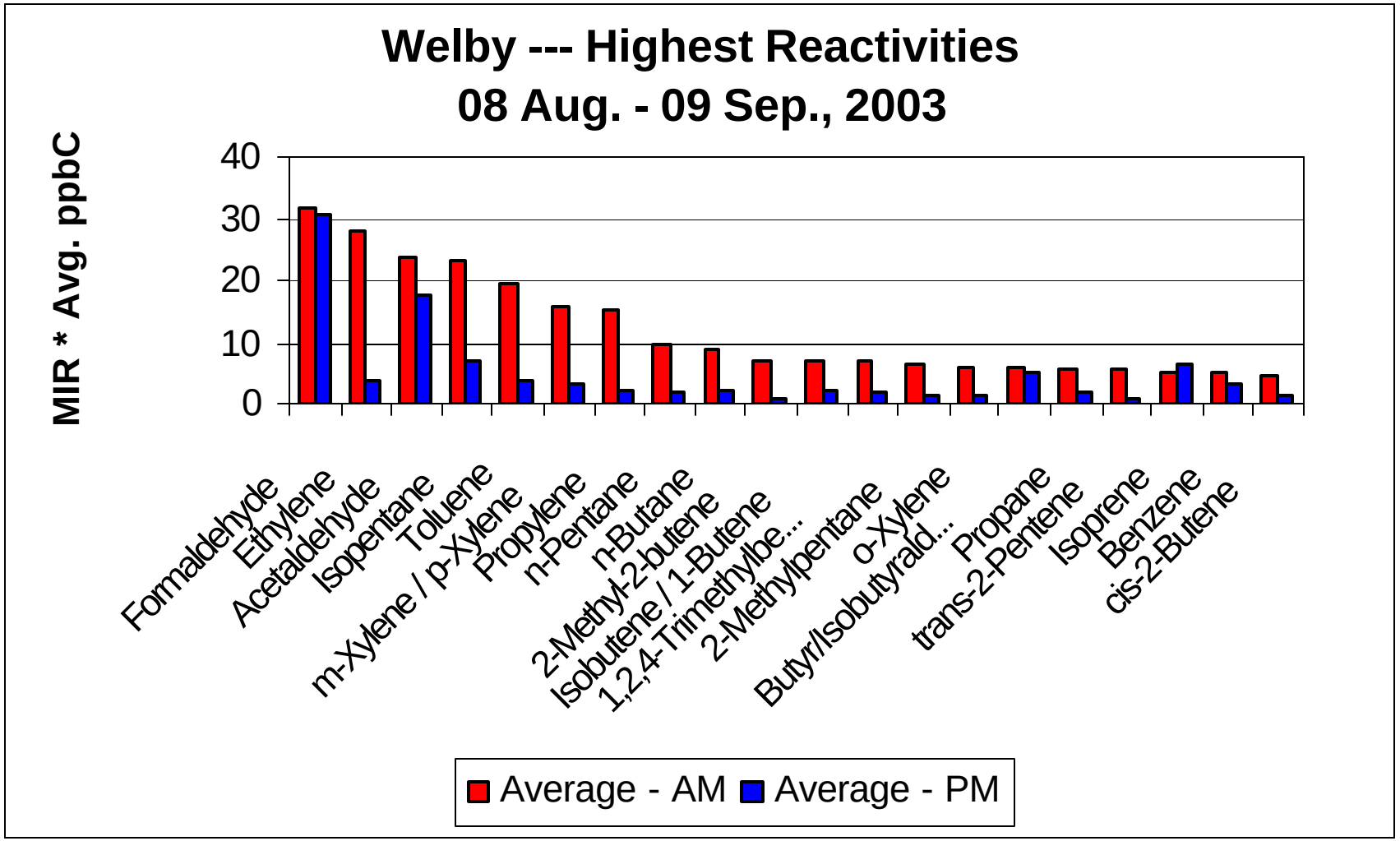
Notes on Carbonyls

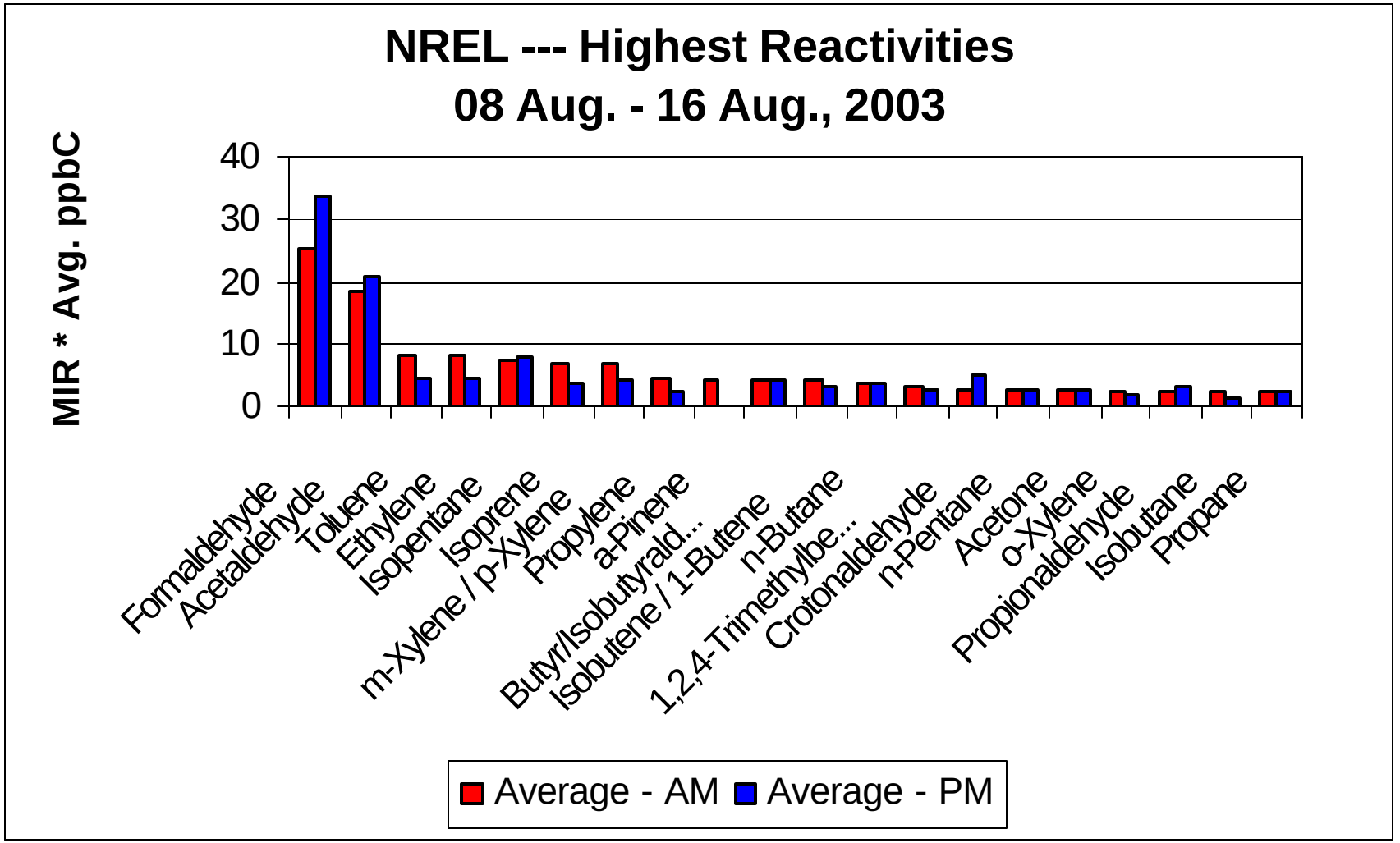
- Concentrations varied from site to site.
- Highest compounds varied by site.
- CAMP recorded the highest overall concentrations followed by Welby.
- In general, no significant differences in concentrations based on time of day.

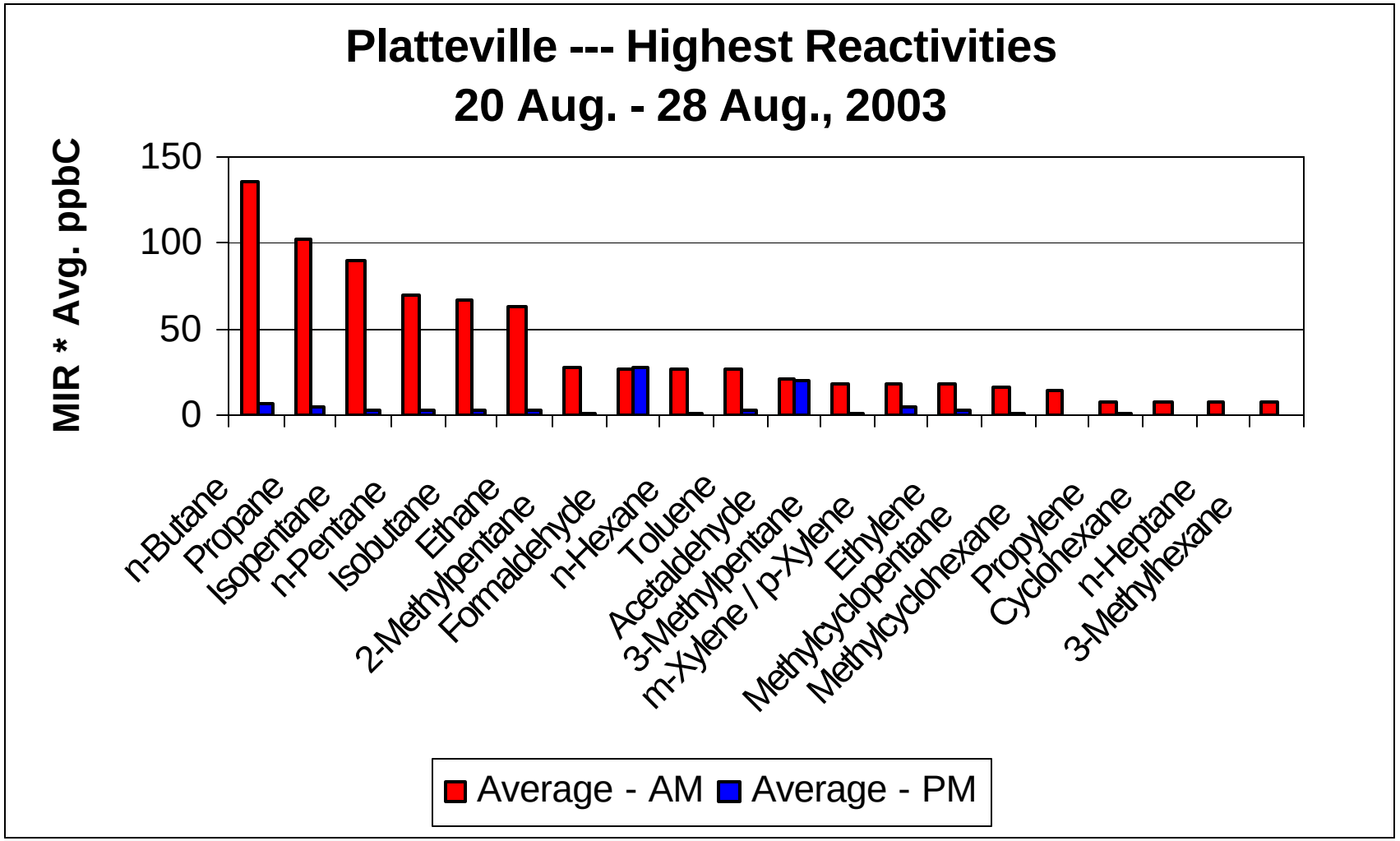
Maximum Incremental Reactivity (mole O_3 / mole C)

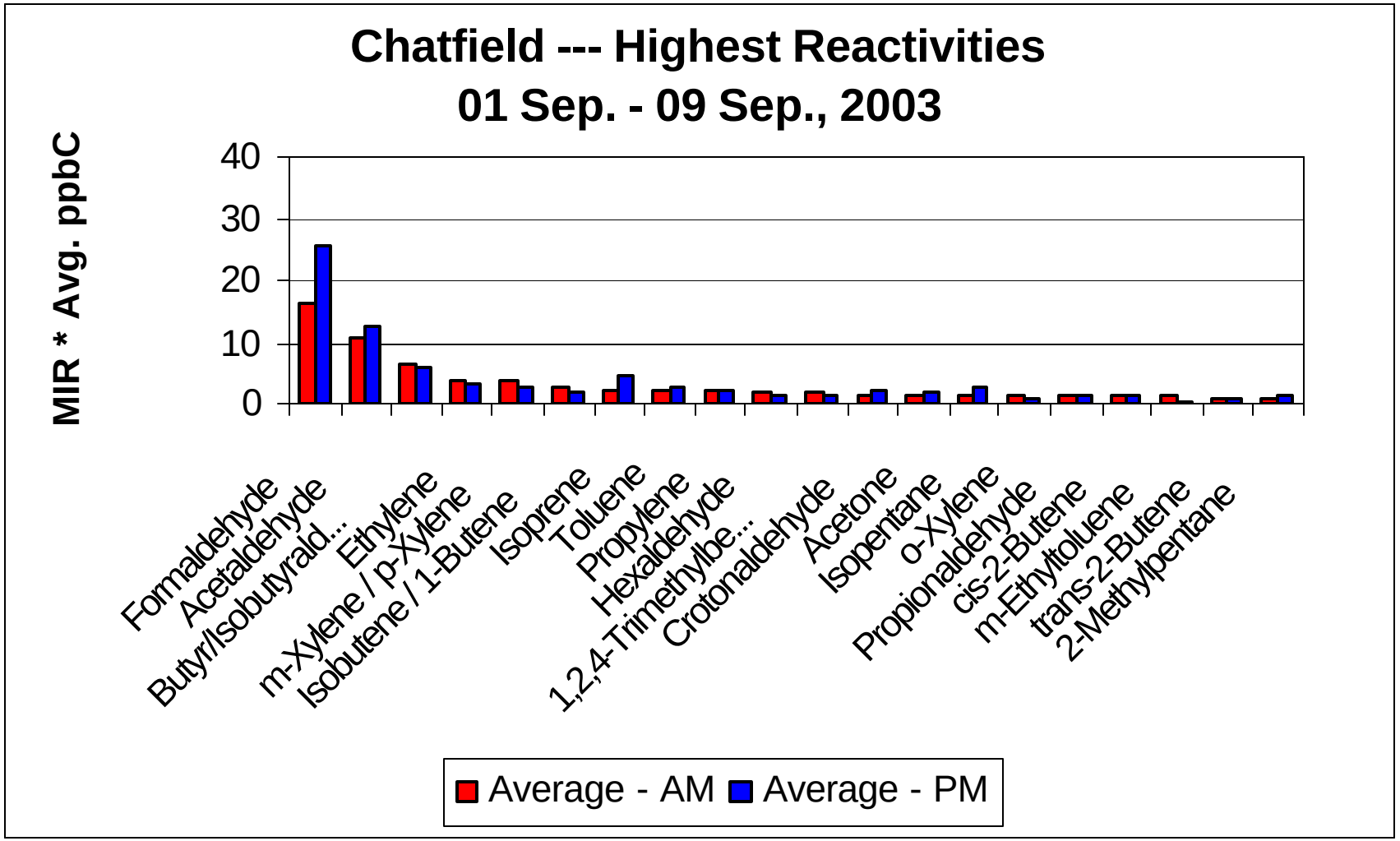
Ethylene	2.65	2-Methylpentane	0.53	Ethylbenzene	0.77
Acetylene	0.34	3-Methylpentane	0.62	m-Xylene / p-Xylene	2.05
Ethane	0.10	2-Methyl-1-pentene	1.51	Styrene	0.53
Propylene	3.38	1-Hexene	1.79	o-Xylene	2.07
Propane	0.17	2-Ethyl-1-butene	1.46	1-Nonene	0.80
Propyne	1.79	n-Hexane	0.43	n-Nonane	0.28
Isobutane	0.41	trans-2-Hexene	2.44	Isopropylbenzene	0.65
Isobutene / 1-Butene	2.42	cis-2-Hexene	2.44	a-Pinene	1.22
1,3-Butadiene	3.79	Methylcyclopentane	0.70	n-Propylbenzene	0.61
n-Butane	0.40	2,4-Dimethylpentane	0.49	m-Ethyltoluene	2.61
trans-2-Butene	4.06	Benzene	0.22	p-Ethyltoluene	1.04
cis-2-Butene	3.86	Cyclohexane	0.42	1,3,5-Trimethylbenzene	3.12
3-Methyl-1-butene	2.03	2-Methylhexane	0.41	o-Ethyltoluene	1.84
Isopentane	0.50	2,3-Dimethylpentane	0.46	b-Pinene	0.93
1-Pentene	2.26	3-Methylhexane	0.55	1,2,4-Trimethylbenzene	2.00
2-Methyl-1-butene	1.89	1-Heptene	1.23	1-Decene	0.66
n-Pentane	0.46	2,2,4-Trimethylpentane	0.43	n-Decane	0.24
Isoprene	3.03	n-Heptane	0.38	1,2,3-Trimethylbenzene	3.13
trans-2-Pentene	2.99	Methylcyclohexane	0.58	m-Diethylbenzene	2.35
cis-2-Pentene	2.99	2,2,3-Trimethylpentane	---	p-Diethylbenzene	0.94
2-Methyl-2-butene	4.22	2,3,4-Trimethylpentane	0.36	1-Undecene	0.56
2,2-Dimethylbutane	0.40	Toluene	1.09	n-Undecane	0.21
Cyclopentene	2.08	2-Methylheptane	0.35	1-Dodecene	0.51
4-Methyl-1-pentene	1.81	3-Methylheptane	0.40	n-Dodecane	0.19
Cyclopentane	0.78	1-Octene	1.00	1-Tridecene	0.44
2,3-Dimethylbutane	0.34	n-Octane	0.32	n-Tridecane	0.18
Formaldehyde	5.61	Crotonaldehyde	3.64	Valeraldehyde	2.05
Acetaldehyde	3.13	Butyr/Isobutyraldehyde	2.35	Tolualdehydes (o-, m-, p-)	-0.17
Acetone	0.17	Benzaldehyde	-0.19	Hexaldehyde	1.71
Propionaldehyde	3.18	Isovaleraldehyde	1.96	2,5-Dimethylbenzaldehyde	---


CAMP --- Highest Reactivities
08 Aug. - 09 Sep., 2003
MIR * Avg. ppbC
200
150
100
50
0
Isobutane
Formaldehyde
Acetaldehyde
Ethylene
Toluene
Isopentane
Propylene
m-Xylene / p-Xylene
Butyr/Isobutyrald...
1,2,4-Trimethylbe...
Isobutene / 1-Butene
n-Butane
n-Pentane
2-Methyl-2-butene
o-Xylene
2-Methylpentane
Acetone
m-Ethyltoluene
1,3,5-Trimethylbe...
Crotonaldehyde
Average - AM
Average - PM


Welby --- Highest Reactivities
08 Aug. - 09 Sep., 2003
MIR * Avg. ppbC
40
30
20
10
0
Formaldehyde
Ethylene
Acetaldehyde
Isopentane
Toluene
m-Xylene / p-Xylene
Propylene
n-Pentane
n-Butane
2-Methyl-2-butene
Isobutene / 1-Butene
1,2,4-Trimethylbe...
2-Methylpentane
o-Xylene
Butyr/Isobutyrald...
Propane
trans-2-Pentene
Isoprene
Benzene
cis-2-Butene
Average - AM
Average - PM


NREL --- Highest Reactivities
08 Aug. - 16 Aug., 2003
MIR * Avg. ppbC
40
30
20
10
0
Formaldehyde
Acetaldehyde
Toluene
Ethylene
Isopentane
Isoprene
m-Xylene / p-Xylene
Propylene
a-Pinene
Butyr/Isobutyrald...
Isobutene / 1-Butene
n-Butane
1,2,4-Trimethylbe...
Crotonaldehyde
n-Pentane
Acetone
o-Xylene
Propionaldehyde
Isobutane
Propane
Average - AM
Average - PM


Platteville --- Highest Reactivities
20 Aug. - 28 Aug., 2003
MIR * Avg. ppbC
150
100
50
0
n-Butane
Propane
Isopentane
n-Pentane
Isobutane
Ethane
2-Methylpentane
Formaldehyde
n-Hexane
Toluene
Acetaldehyde
3-Methylpentane
m-Xylene / p-Xylene
Ethylene
Methylcyclopentane
Methylcyclohexane
Propylene
Cyclohexane
n-Heptane
3-Methylhexane
Average - AM
Average - PM


Chatfield --- Highest Reactivities
01 Sep. - 09 Sep., 2003
MIR * Avg. ppbC
40
30
20
10
0
Formaldehyde
Acetaldehyde
Butyr/Isobutyrald...
Ethylene
m-Xylene / p-Xylene
Isobutene / 1-Butene
Isoprene
Toluene
Propylene
Hexaldehyde
1,2,4-Trimethylbe...
Crotonaldehyde
Acetone
Isopentane
o-Xylene
Propionaldehyde
cis-2-Butene
m-Ethyltoluene
trans-2-Butene
2-Methylpentane
Average - AM
Average - PM

Notes on Reactivities

- MIRs from Carter, SAPRC99 model, updated 2/5/2003.
- Reactivities varied from site to site and by time of day.
- Highest reactivities/compounds varied by site.
- CAMP recorded the highest overall reactivities followed by Platteville.
- In general, AM reactivities were higher than PM reactivities at Welby and Platteville. AM and PM reactivities were more similar at CAMP, NREL and Chatfield.

To be done…..

- Obtain ozone data and meteorological data for the sample days.
- NMOC/NOx ratios.
- Put final data files on RAQC website.