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Atmospheric Measurement Techniques Discussions

Supplement of

A semi-automated system for quantifying the oxidative potential of ambient particles in aqueous extracts using the dithiothreitol (DTT) assay: results from the Southeastern Center for Air Pollution and Epidemiology (SCAPE)

T. Fang et al.

Correspondence to: R. J. Weber (rodney.weber@eas.gatech.edu)

Supporting Information (SI)

Chemical preparation and storage information:

PQN standard: 5 mM 9,10-phenanthraquinone (PQN) standard stock was made by dissolving 10.4 mg of 9,10-phenanthraquinone in 10 mL DMSO. The stock was kept in freezer when not in use. For routine analysis, final PQN standard was prepared from stock in deionized water (DI water, Nanopure Infinity^{TM} ultrapure water system; >18 MΩ cm^{-1}) before feeding to the system.

1 mM DTT: 10 mM stock DTT solution was made by dissolving 154.24 mg DTT in 100 mL DI water and stored in fridge no longer than one month. 1 mM DTT was made fresh from 10mM stock solution every time for immediate use.

0.2 mM DTNB: 0.2 mM DTNB was prepared in Methanol (MeOH), stored in fridge for no longer than 6 months.

0.08 M Tris buffer with 4 mM EDTA: Tris buffer was first prepared by dissolving 96.92 g of Tris Base and 11.69 g of EDTA in DI water. This will bring the pH to ~10. Then adjust the pH to 8.9 by adding small amount of HCl. Add DI water to make a final volume of 10 L as the stock and store in room temperature.

0.5 M Potassium Phosphate Buffer (KBuffer): 0.5 M Kbuffer was made by mixing 13.47 g of KH_2PO_4 (Monopotassium Phosphate) and 69.85 g of K_2HPO_4 (Dipotassium Phosphate) in 1 L DI water. The mixture was then chelexed using Chelex® 100 resin (BIO-RAD Laboratories, Inc., USA) to remove binding polyvalent metal ions (especially Cu and Fe).

1% w/v TCA was prepared in DI water and stored in room temperature.

Table S1. The seasonal variation on volume-normalized water-soluble DTT activity assessed by ANOVA tests

Site	Season	Average ± variance (nmol/min/m^3)		N	F	P-value	$F_{critical}$
YRK	Summer	0.28	0.01	33	0.01	0.91	7.14
	Winter	0.28	0.01	22			
RS	Fall	0.33	0.01	29	3.87	0.03	4.89
	Winter	0.36	0.02	31			
	Fall 2013	0.27	0.00	20			
GT	Summer	0.24	0.01	38	2.42	0.10	4.88
	Winter	0.25	0.02	22			
	Fall 2013	0.20	0.00	23			
JST	Summer	0.29	0.02	31	3.15	0.01	3.13
	Summer	0.29	0.00	37			
	Fall	0.34	0.01	26			
	Winter	0.43	0.03	22			
	Winter	0.33	0.04	30			
	Spring 2013	0.32	0.03	22			

Table S2. The seasonal variation on mass-normalized water-soluble DTT activity assessed by ANOVA tests

Site	Season	Mean ± variance (pmol/min/μg)		N	F	P-value	$F_{critical}$
YRK	Summer	29.76	0.16	33	15.01	3.01E-04	7.15
	Winter	42.38	0.10	21			
RS	Fall	31.15	0.02	29	1.84	0.17	3.12
	Winter	35.65	0.07	28			
	Fall 2013	32.71	0.18	20			
GT	Summer	26.16	0.05	38	19.89	1.05E-07	3.11
	Winter	30.60	0.06	20			
	Fall 2013	18.06	0.02	23			
JST	Summer	25.35	0.05	31	25.17	9.33E-19	3.13
	Summer	29.86	0.03	37			
	Fall	41.06	0.12	26			
	Winter	55.54	0.28	22			
	Winter	37.17	0.12	30			
	Winter	36.82	0.15	23			

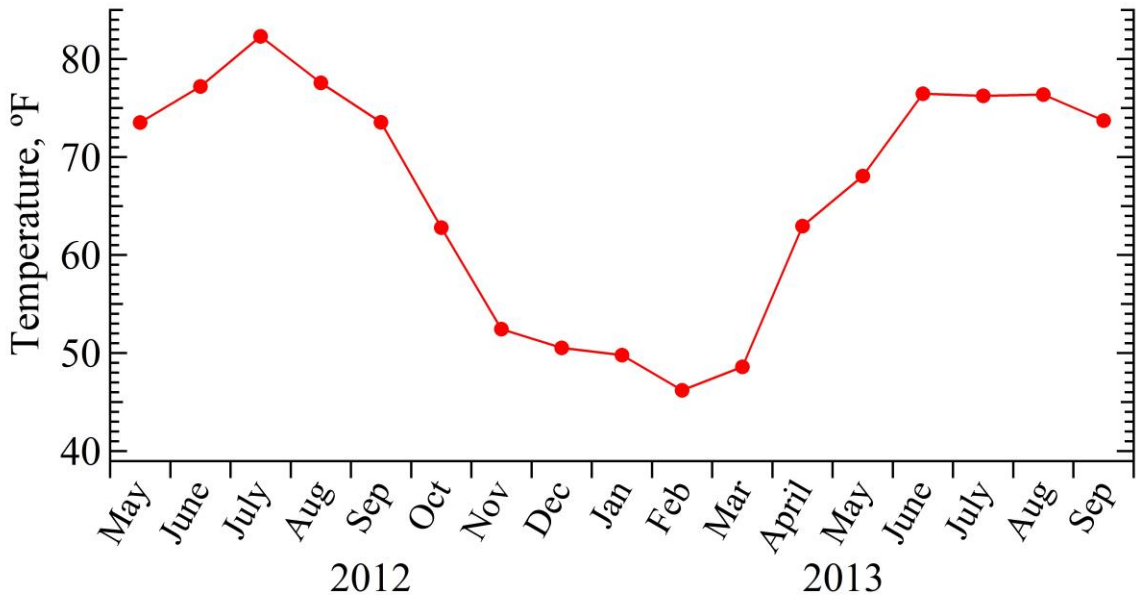

Figure S1. Temperature profile from May 2012 to September 2013 in Atlanta, GA.

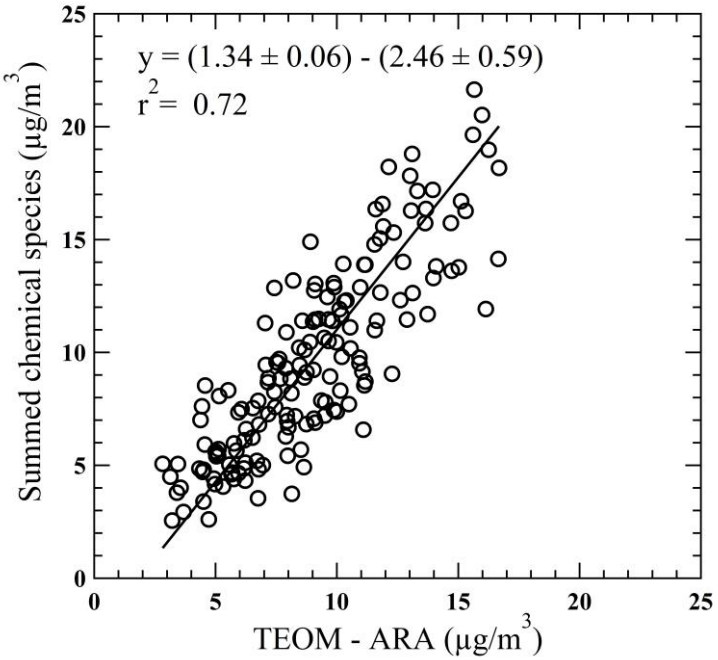

Figure S2. Comparison of estimated $PM_{2.5}$ concentration from the sum of components determined from the High Volume filters, which included: EC, organic mass (OC*1.6), ammonium sulfate and water soluble metals concentration with the $PM_{2.5}$ measured by TEOM from Atmospheric Research Analysis data archive at the SEARCH JST site. EC/OC - Sunset Laboratory TOT analyzer; water soluble metals - X-ray fluorescence instrument, XRF, Xact™ 625 Monitoring System [details would be presented in a subsequent publication (Fang et al.; in prep); $[(NH_4)_2SO_4] = \frac{MW_{(NH_4)_2SO_4}}{MW_S} \times$ [S], assuming sulfate and ammonium are all $(NH_4)_2SO_4$ and [S] (sulfur) were obtained from XRF metals analysis. (The equation was obtained by orthogonal regression.)

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Hardware and software details of the Kloehn Control syringe pumps (Kloehn, Inc., Las Vegas, Nevada, USA):

Pump A:

VersaPump 6, 48k resolution drive pump (P/N 55022);

12-way distribution rotary valve (P/N 24105);

10 mL syringe (P/N 17600);

Pump B:

VersaPump 3, 12k resolution drive pump (P/N 23254);

6-way distribution valve (P/N 23327);

250 µL syringe (P/N 23166);

Software: Kloehn Control version 1.04.

Kloehn Control program code for conducting the DTT method (Address 1 - pump A**;** Address 3 - pump B)**:**

Line	Line Label	Address	Command	Command Data
1		1	CONSTANT <varName> = <float>	dILarge,12
2		1	CONSTANT <varName> = <float>	AirLarge,8
3		1	CONSTANT <varName> = <float>	WasteLarge,9
4		1	CONSTANT <varName> = <float>	Kbuffer,11
5		1	CONSTANT <varName> = <float>	Tris,3
6		1	CONSTANT <varName> = <float>	TCA,4
7		1	CONSTANT <varName> = <float>	LWCC,5
8		1	CONSTANT <varName> = <float>	Sample,6
9		1	CONSTANT <varName> = <float>	DTNB,10
10		1	CONSTANT <varName> = <float>	IVLarge,1
11		1	CONSTANT <varName> = <float>	RVLarge,2
12		3	CONSTANT <varName> = <float>	dISmall,6
13		3	CONSTANT <varName> = <float>	AirSmall,4
14		3	CONSTANT <varName> = <float>	WasteSmall,1
15		3	CONSTANT <varName> = <float>	DTT,5

16		3	CONSTANT <varName> = <float>	IVSmall,2
17		3	CONSTANT <varName> = <float>	RVSmall,3
18				
19				
20	HomePosition	3	SET out2 = <bit>	1
21		3	SET out2 = <bit>	0
22		3	SET out2 = <bit>	1
23		3	SET out1 = <bit>	1
24				
25	PreloadTCA	1	VALVE_PORT = <int> [CCW]	TCA
26		1	POSITION <float> [IMM or SYNC]	1000
27		1	VALVE_PORT = <int> [CCW]	WasteLarge
28		1	POSITION <float> [IMM or SYNC]	0
29	PreloadTris	1	VALVE_PORT = <int> [CCW]	Tris
30		1	POSITION <float> [IMM or SYNC]	1000
31		1	VALVE_PORT = <int> [CCW]	WasteLarge
32		1	POSITION <float> [IMM or SYNC]	0
33	PreloadKbuffer	1	VALVE_PORT = <int> [CCW]	Kbuffer
34		1	POSITION <float> [IMM or SYNC]	1000
35		1	VALVE_PORT = <int> [CCW]	WasteLarge
36		1	POSITION <float> [IMM or SYNC]	0
37		1	VALVE_PORT = <int> [CCW]	dILarge
38		1	POSITION <float> [IMM or SYNC]	5000
39		1	VALVE_PORT = <int> [CCW]	WasteLarge
40		1	POSITION <float> [IMM or SYNC]	0
41				
42	PreloadDTNB	1	VALVE_PORT = <int> [CCW]	DTNB
43		1	POSITION <float> [IMM or SYNC]	1000
44		1	VALVE_PORT = <int> [CCW]	WasteLarge
45		1	POSITION <float> [IMM or SYNC]	0
46	PreloadDTT	3	VALVE_PORT = <int> [CCW]	DTT
47		3	SET speed = <float>	30
48		3	POSITION <float> [IMM or SYNC]	250
49		3	VALVE_PORT = <int> [CCW]	WasteSmall
50		3	POSITION <float> [IMM or SYNC]	0

51				
52			DO	
53	ChangeSample	3	SET out1 = <bit>	0
54		3	SET out1 = <bit>	1
55				
56				
57	PreloadSample	1	VALVE_PORT = <int> [CCW]	Sample
58		1	SET speed = <float>	400
59		1	POSITION <float> [IMM or SYNC]	1000
60		1	VALVE_PORT = <int> [CCW]	WasteLarge
61		1	POSITION <float> [IMM or SYNC]	0
62		1	DELAY <float>	1
63				
64	CleanLarge+Small		DO	
65		1	VALVE_PORT = <int> [CCW]	dILarge
66		1	POSITION <float> [IMM or SYNC]	5000
67		1	VALVE_PORT = <int> [CCW]	WasteLarge
68		1	POSITION <float> [IMM or SYNC]	0
69		3	VALVE_PORT = <int> [CCW]	dISmall
70		3	POSITION <float> [IMM or SYNC]	250
71		3	VALVE_PORT = <int> [CCW]	WasteSmall
72		3	POSITION <float> [IMM or SYNC]	0
73			LOOP <int>	3
74				
75	LoadReactionVial	1	VALVE_PORT = <int> [CCW]	Kbuffer
76		1	POSITION <float> [IMM or SYNC]	1000
77		1	VALVE_PORT = <int> [CCW]	RVLarge
78		1	POSITION <float> [IMM or SYNC]	0
79		1	VALVE_PORT = <int> [CCW]	Sample
80		1	POSITION <float> [IMM or SYNC]	3500
81		1	DELAY <float>	1
82		1	VALVE_PORT = <int> [CCW]	RVLarge
83		1	POSITION <float> [IMM or SYNC]	0
84		1	VALVE_PORT = <int> [CCW]	AirLarge
85		1	POSITION <float> [IMM or SYNC]	2000
86		1	VALVE_PORT = <int> [CCW]	RVLarge

87		1	POSITION <float> [IMM or SYNC]	0
88		1	VALVE_PORT = <int> [CCW]	dILarge
89		1	POSITION <float> [IMM or SYNC]	5000
90		1	VALVE_PORT = <int> [CCW]	WasteLarge
91		1	POSITION <float> [IMM or SYNC]	0
92		3	VALVE_PORT = <int> [CCW]	DTT
93		3	POSITION <float> [IMM or SYNC]	250
94		3	VALVE_PORT = <int> [CCW]	RVSmall
95		3	SET speed = <float>	40
96		3	POSITION <float> [IMM or SYNC]	0
97		3	VALVE_PORT = <int> [CCW]	DTT
98		3	SET speed = <float>	30
99		3	POSITION <float> [IMM or SYNC]	250
100		3	VALVE_PORT = <int> [CCW]	RVSmall
101		3	SET speed = <float>	40
102		3	POSITION <float> [IMM or SYNC]	0
103		3	VALVE_PORT = <int> [CCW]	AirSmall
104		3	POSITION <float> [IMM or SYNC]	250
105		3	VALVE_PORT = <int> [CCW]	RVSmall
106		3	POSITION <float> [IMM or SYNC]	0
107		1	VALVE_PORT = <int> [CCW]	AirLarge
108		1	POSITION <float> [IMM or SYNC]	5000
109		1	VALVE_PORT = <int> [CCW]	RVLarge
110		1	SET speed = <float>	1000
111		1	POSITION <float> [IMM or SYNC]	0
112			DO	
113		3	VALVE_PORT = <int> [CCW]	dISmall
114		3	SET speed = <float>	30
115		3	POSITION <float> [IMM or SYNC]	250
116		3	VALVE_PORT = <int> [CCW]	WasteSmall
117		3	POSITION <float> [IMM or SYNC]	0
118			LOOP <int>	3
119				
120			DO	
121	LoadTCA	1	VALVE_PORT = <int> [CCW]	TCA

122		1	SET speed = <float>	400
123		1	POSITION <float> [IMM or SYNC]	1000
124		1	VALVE_PORT = <int> [CCW]	IVLarge
125		1	POSITION <float> [IMM or SYNC]	0
126		1	VALVE_PORT = <int> [CCW]	AirLarge
127		1	POSITION <float> [IMM or SYNC]	1000
128		1	VALVE_PORT = <int> [CCW]	IVLarge
129		1	POSITION <float> [IMM or SYNC]	0
130		1	VALVE_PORT = <int> [CCW]	dILarge
131		1	POSITION <float> [IMM or SYNC]	1500
132		1	VALVE_PORT = <int> [CCW]	WasteLarge
133		1	POSITION <float> [IMM or SYNC]	0
134				
135	CleanLWCC	1	VALVE_PORT = <int> [CCW]	dILarge
136		1	POSITION <float> [IMM or SYNC]	5000
137		1	VALVE_PORT = <int> [CCW]	LWCC
138		1	POSITION <float> [IMM or SYNC]	0
139				
140	Draw	3	VALVE_PORT = <int> [CCW]	RVSmall
141		3	POSITION <float> [IMM or SYNC]	250
142		3	VALVE_PORT = <int> [CCW]	WasteSmall
143		3	POSITION <float> [IMM or SYNC]	0
144		3	VALVE_PORT = <int> [CCW]	RVSmall
145		3	POSITION <float> [IMM or SYNC]	250
146		3	VALVE_PORT = <int> [CCW]	WasteSmall
147		3	POSITION <float> [IMM or SYNC]	0
148		3	VALVE_PORT = <int> [CCW]	RVSmall
149		3	POSITION <float> [IMM or SYNC]	250
150		3	VALVE_PORT = <int> [CCW]	WasteSmall
151		3	POSITION <float> [IMM or SYNC]	180
152		3	VALVE_PORT = <int> [CCW]	IVSmall
153		3	POSITION <float> [IMM or SYNC]	80
154		3	VALVE_PORT = <int> [CCW]	RVSmall
155		3	POSITION <float> [IMM or	0

			SYNC]	
156		3	VALVE_PORT = <int> [CCW]	AirSmall
157		3	POSITION <float> [IMM or SYNC]	250
158		3	VALVE_PORT = <int> [CCW]	RVSmall
159		3	POSITION <float> [IMM or SYNC]	0
160		3	VALVE_PORT = <int> [CCW]	AirSmall
161		3	POSITION <float> [IMM or SYNC]	250
162		3	VALVE_PORT = <int> [CCW]	IVSmall
163		3	POSITION <float> [IMM or SYNC]	0
164				
165	LoadTris	1	VALVE_PORT = <int> [CCW]	Tris
166		1	POSITION <float> [IMM or SYNC]	2000
167		1	VALVE_PORT = <int> [CCW]	IVLarge
168		1	POSITION <float> [IMM or SYNC]	0
169		1	VALVE_PORT = <int> [CCW]	AirLarge
170		1	POSITION <float> [IMM or SYNC]	1000
171		1	VALVE_PORT = <int> [CCW]	IVLarge
172		1	POSITION <float> [IMM or SYNC]	0
173		1	VALVE_PORT = <int> [CCW]	dILarge
174		1	POSITION <float> [IMM or SYNC]	5000
175		1	VALVE_PORT = <int> [CCW]	WasteLarge
176		1	POSITION <float> [IMM or SYNC]	0
177				
178	LoadDTNB	1	VALVE_PORT = <int> [CCW]	DTNB
179		1	POSITION <float> [IMM or SYNC]	500
180		1	VALVE_PORT = <int> [CCW]	IVLarge
181		1	POSITION <float> [IMM or SYNC]	0
182		1	VALVE_PORT = <int> [CCW]	dILarge
183		1	POSITION <float> [IMM or SYNC]	1800
184		1	VALVE_PORT = <int> [CCW]	IVLarge
185		1	POSITION <float> [IMM or SYNC]	0
186		1	VALVE_PORT = <int> [CCW]	IVLarge
187		1	POSITION <float> [IMM or SYNC]	5000
188		1	VALVE_PORT = <int> [CCW]	IVLarge

189		1	POSITION <float> [IMM or SYNC]	0
190		1	VALVE_PORT = <int> [CCW]	AirLarge
191		1	POSITION <float> [IMM or SYNC]	5000
192		1	VALVE_PORT = <int> [CCW]	IVLarge
193		1	POSITION <float> [IMM or SYNC]	0
194				
195	IVtoLWCC	1	VALVE_PORT = <int> [CCW]	IVLarge
196		1	POSITION <float> [IMM or SYNC]	4700
197		1	VALVE_PORT = <int> [CCW]	WasteLarge
198		1	POSITION <float> [IMM or SYNC]	4000
199		1	VALVE_PORT = <int> [CCW]	LWCC
200		1	SET speed = <float>	400
201		1	POSITION <float> [IMM or SYNC]	0
202				
203	RinseIV	1	VALVE_PORT = <int> [CCW]	IVLarge
204		1	SET speed = <float>	400
205		1	POSITION <float> [IMM or SYNC]	2000
206		1	VALVE_PORT = <int> [CCW]	WasteLarge
207		1	POSITION <float> [IMM or SYNC]	0
208			DO	
209		1	VALVE_PORT = <int> [CCW]	dILarge
210		1	POSITION <float> [IMM or SYNC]	5000
211		1	VALVE_PORT = <int> [CCW]	IVLarge
212		1	POSITION <float> [IMM or SYNC]	0
213		1	VALVE_PORT = <int> [CCW]	dILarge
214		1	POSITION <float> [IMM or SYNC]	3000
215		1	VALVE_PORT = <int> [CCW]	IVLarge
216		1	POSITION <float> [IMM or SYNC]	0
217		1	VALVE_PORT = <int> [CCW]	IVLarge
218		1	POSITION <float> [IMM or SYNC]	5000
219		1	VALVE_PORT = <int> [CCW]	WasteLarge
220		1	POSITION <float> [IMM or SYNC]	0
221		1	VALVE_PORT = <int> [CCW]	IVLarge
222		1	POSITION <float> [IMM or SYNC]	5000

223		1	VALVE_PORT = <int> [CCW]	WasteLarge
224		1	POSITION <float> [IMM or SYNC]	0
225			LOOP <int>	2
226			LOOP <int>	5
227				
228	RinseRV	1	VALVE_PORT = <int> [CCW]	RVLarge
229		1	POSITION <float> [IMM or SYNC]	5000
230		1	VALVE_PORT = <int> [CCW]	WasteLarge
231		1	POSITION <float> [IMM or SYNC]	0
232			DO	
233		1	VALVE_PORT = <int> [CCW]	dILarge
234		1	POSITION <float> [IMM or SYNC]	5000
235		1	VALVE_PORT = <int> [CCW]	RVLarge
236		1	POSITION <float> [IMM or SYNC]	0
237		1	VALVE_PORT = <int> [CCW]	dILarge
238		1	POSITION <float> [IMM or SYNC]	3000
239		1	VALVE_PORT = <int> [CCW]	RVLarge
240		1	POSITION <float> [IMM or SYNC]	0
241		1	VALVE_PORT = <int> [CCW]	RVLarge
242		1	POSITION <float> [IMM or SYNC]	5000
243		1	VALVE_PORT = <int> [CCW]	WasteLarge
244		1	POSITION <float> [IMM or SYNC]	0
245		1	VALVE_PORT = <int> [CCW]	RVLarge
246		1	POSITION <float> [IMM or SYNC]	5000
247		1	VALVE_PORT = <int> [CCW]	WasteLarge
248		1	POSITION <float> [IMM or SYNC]	0
249			LOOP <int>	2
250				
251	RecleanLWCC	1	VALVE_PORT = <int> [CCW]	dILarge
252		1	POSITION <float> [IMM or SYNC]	5000
253		1	VALVE_PORT = <int> [CCW]	LWCC
254		1	POSITION <float> [IMM or SYNC]	0
255				
256			LOOP <int>	14