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Technical note: Comparison and interconversion of pH based on different standard states for aerosol acidity characterization

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Table S1. Summary of reported aerosol pH calculated by thermodynamic models

#	Location	Year	Particle size	Model	F/ R [a]	S/ MS [b]	Particulate species	Gases	pH	References
Molality based pH										
1	Beijing, China	2014	PM2.5	E-AIM-IV	F&R	S	Na^+, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-, K^+ (K^+ taken as Na^+)	NH_3, HNO_3	3.5 to 5.3 for forward mode and -2 to 10 for reverse mode.	(Song et al., 2018)
				ISORROPIA-II	F&R	S&MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-			
2	Guangzhou, China	2013	PM2.5	E-AIM-III	F	S	Na^+, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	NH_3, NO_3, HCl	2.4 ± 0.3	(Jia et al., 2018)
3	Southeastern US	2013	PM1 and PM2.5	AIOMFAC	R	MS	NH_4^+, SO_4^{2-}, organic compounds [c]	- [g]	1.4±1.2 (EQLB) 1.3±1.2 (CLLPS)	(Pye et al., 2018)
				AIOMFAC	R	MS	Na^+, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-, organic compounds [c]	- [g]	1.5±2.0 (EQLB) 1.3±2.1 (CLLPS)	
				ISORROPIA-II	R	- [g]	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	- [g]	0.7±2.5	
				ISORROPIA-II	F	- [g]	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	NH_3	1.1±0.7	

#	Location	Year	Particle size	Model	F/ R [a]	S/ MS [b]	Particulate species	Gases	pH	References
4	Beijing, China	2015& 2016	PM2.5	ISORROPIA	F	MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^- [d]	NH_3, NO_3, HCl	4.2 ± 0.5	(Liu et al., 2017)
5	Baltimore & Chicago, US	2011 to 2015	PM2.5	ISORROPIA-II	F	MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	NH_3	~1.0 to 2.7 [e]	(Battaglia et al., 2017)
6	Southeastern US	2010	PM1 & PM2.5	ISORROPIA-II	F	MS	Na^+, K^+, NH_4^+, SO_4^{2-}, NO_3^- Cl^-	NH_3, NO_3, HCl	1.9±0.5 for PM1 and 2.7±0.3 for PM2.5	(Guo et al., 2017a)
7	Beijing & Xi'an, China	2013	PM1 & PM2.5	ISORROPIA-II	F	MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^- Cl^-	NH_3	4.5 for Beijing and 5 for Xi'an	(Guo et al., 2017b)
8	Atlanta, US	2016	<18 µm [f]	ISORROPIA-II	F	- [g]	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^- Cl^-	NH_3, NO_3, HCl [h]	1 to 2 for fine particle; ~6 to ~7 for coarse particle [e]	(Fang et al., 2017)
9	Finokalia, Greece	2012	PM1 and PM10	ISORROPIA-II	F	MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^- [d]	NH_3 [i]	0.5 to 2.8	(Bougiatioti et al., 2016)
10	Northeastern US	2015	PM1	ISORROPIA-II	F	MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	NH_3 [h]	0.77 ± 0.96	(Guo et al., 2016)
11	Southeastern US	2012& 2013	PM1 and PM 2.5	ISORROPIA-II	F	MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^- [d]	NH_3	0.94 ±0.59	(Guo et al., 2015)
12	Southeastern US	2013	PM1	ISORROPIA-II	F	MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	NH_3	0-2	(Xu et al., 2015)

#	Location	Year	Particle size	Model	F/ R [a]	S/ MS [b]	Particulate species	Gases	pH	References
Molarity based pH										
13	Beijing, China	2013	$PM_{2.1}$	E-AIM-IV	R	- [g]	Na^+, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	- [g]	1.1	(Tian et al., 2018)
14	Chengdu, China	2011	0.18 to 1.8 µm	E-AIM-II	R	- [g]	SO_4^{2-}, NH_4^+, NO_3^-	- [g]	-1.11	(Cheng et al., 2015)
15	Singapore	2011	PM2.5	E-AIM-III	R	- [g]	Na^+, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	- [g]	0.48 & 0.72 (day & night)	(Behera et al., 2013)
16	Jinan, China	2006 & 2007	PM_1	E-AIM-II	R	- [g]	NH_4^+, SO_4^{2-} , NO_3^-	- [g]	−1	(Cheng et al., 2011)
17	Hong Kong	2008 &2009	PM2.5	E-AIM-III	R	- [g]	Na^+, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	- [g]	-0.45 to 0.59	(Xue et al., 2011)
18	Beijing, China	2005	PM2.5	AIM-II	R	- [g]	NH_4^+, SO_4^{2-}, NO_3^-	- [g]	−0.52±0.62	(Pathak et al., 2009)
	Shanghai, China	2005			R				−0.77±0.67	
	Lanzhou, China	2006,			R				−0.38±0.64	
	Guangzhou, China	2004			R				0.61±0.71	
19	Hong Kong	2001	PM10	AIM-II	R	- [g]	NH_4^+, SO_4^{2-}, NO_3^-	- [g]	0.25	(Pathak et al., 2004)

#	Location	Year	Particle size	Model	F/ R [a]	S/ MS [b]	Particulate species	Gases	pH	References
<u>Male fraction based pH</u>										
20	Southeastern US	1999 to 2014	PM2.5	ISORROPIA-II	F	- [g]	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	NH_3 [i]	0-2	(Weber et al., 2016)
21	Mexico City, US	2006	PM2.5	ISORROPIA-II	R	MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	- [g]	1.98	(Hennigan et al., 2015)
				E-AIM-II and IV	R	S	Na^+, NH_4^+, SO_4^{2-}, NO_3^-, and Cl^- for AIM-IV and NH_4^+, SO_4^{2-} and NO_3^- for AIM-II	- [g]	2.36	
				ISORROPIA-II,	F	MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	NH_3, HNO_3	3.31	
				E-AIM-II and IV	F	S	Na^+, NH_4^+, SO_4^{2-}, NO_3^-, Cl^- for AIM-IV and NH_4^+, SO_4^{2-}, NO_3^- for AIM-II	NH_3 and HNO_3	3.24	
22	Po Valley, Italy	2009	PM2.5	E-AIM-IV	R	- [g]	Na^+, NH_4^+, SO_4^{2-}, NO_3^-, Cl	- [g]	2.7 to 3.8	(Squizzato et al., 2013)
23	Beijing, China	2005& 2006	PM2.5	E-AIM-II	R	- [g]	NH_4^+, SO_4^{2-} and NO_3^-	- [g]	1.2 ±1.1	(He et al., 2012)
24	Pittsburgh, US	2002	PM1	E-AIM-II	R	- [g]	SO_4^{2-}, NH_4^+, NO_3^-	- [g]	~0.5 to 5 [f]	(Zhang et al., 2007)

#	Location	Year	Particle size	Model	F/ R [a]	S/ MS [b]	Particulate species	Gases	pH	References
pH not specified										
25	Beijing, China	2014& 2015	PM2.5	ISORROPIA-II	F	S	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	NH_3 [j]	7.6 ± 0.1	(He et al., 2018)
26	Beijing , China	2014	PM2.5	ISORROPIA-II	F	MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	- [g]	4.1	(Tan et al., 2018)
27	Tianjin , China	2014& 2015	PM2.5	ISORROPIA-II	F	MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	NH_3	4.9 ± 0.4	(Shi et al., 2017)
28	Beijing, China	2015	PM1	ISORROPIA-II	F	S [k]	NH_3, NH_4+, SO_4^{2-}, NO_3^-, Cl^-	NH_3	7.6 ± 0.0	(Wang et al., 2016)
	Xi'an, China	2012	PM2.5	ISORROPIA-II	F	S [k]	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-		7.0 ± 1.3	
						MS			4.4 ± 0.6	
29	Beijing, China	2013	PM2.5	ISORROPIA-II	F	MS	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^- [e]	NH_3 [j]	5.4	(Cheng et al., 2016)
					R			- [g]	6.2	
30	São Paulo, Brazil	2012	<18 µm [f]	E-AIM	R	- [g]	- [g]	- [g]	4.1 to 5.4 [e]	(Vieira-Filho et al., 2016)
31	Hong Kong	1996 to 1998	PM1	AIM-II	R	- [g]	NH_4^+, SO_4^{2-}, NO_3^-	- [g]	-2.5 to 1.5	(Yao et al., 2007)

#	Location	Year	Particle size	Model	F/ R [a]	S/ MS [b]	Particulate species	Gases	pH	References
32	Hong Kong	2000	PM2.5	AIM-II	R	- [g]	NH_4^+, SO_4^{2-}, NO_3^-	- [g]	-0.4	(Yao et al., 2006)
				SCAPE2	F	- [g]	Na^+, K^+, Ca^{2+}, Mg^{2+}, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	NH_3, NO_3, HCl	2.3	
				ISORROPIA-I	F	- [g]	Na^+, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	NH_3, NO_3, HCl	3.9	
				SCAPE2	F	- [g]	Na^+, NH_4^+, SO_4^{2-}, NO_3^-, Cl^-	NH_3, NO_3, HCl	1.9	

Note: [a] *F* means forward and *R* means reverse. [b] *S* means stable and *MS* means metastable. [c] Organic compounds were considered either in complete liquid–liquid phase separation (CLLPS) or equilibrium (EQLB) mode; Ca^{2+}, K^+ and Mg^{2+} were taken as Na^+. [d] Aerosol water content associated with organic compounds considered; [e] Data extracted from figure; [f] Size segregated samples; [g] - means not specified; [h] Assuming NH_4^+ (total) = NH_3 (gas phase) +NH_4^+ (particle phase); [i] Estimated based on iteration; [j] NH_3 estimated based on empirical equation; [k] Obtained from Song et al. (2018).

Table S2. A summary of estimation methods of parameters for pH calculation based on different standard states.

Parameter	E-AIM-IV	ISORROPIA-II	AIOMFAC
Molar fraction			
x_H	output	Eq. (7)	output
f_H	output	1 [a]	Eq. (4)
Molality			
m_H	output	output	output
γ_H	Eq. (4)	1 [a]	output
Molarity			
c_H	Eq. (8) [b]	Eq. (8) [b]	Eq. (8) [b]
y_H	Eq. (6)	1 [a]	Eq. (6)

Note: [a] Activity coefficient is assumed to be 1; [b] the density of aerosol solution is based on the result from E-AIM-IV.

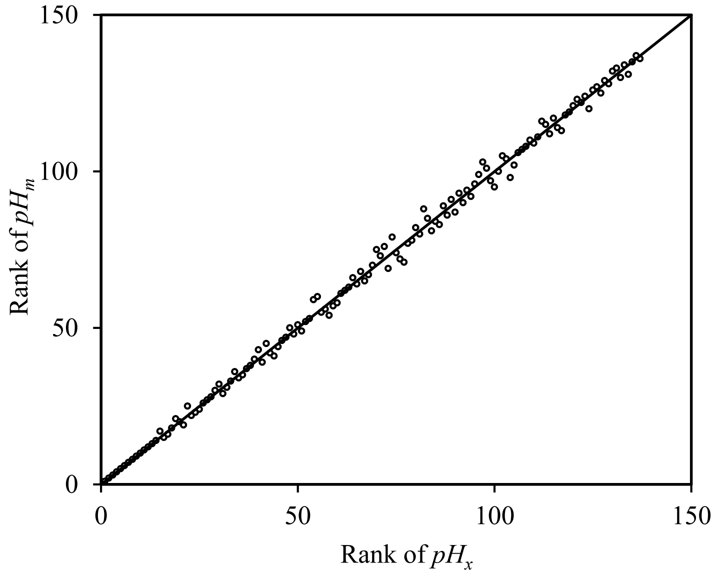

Figure S1. Comparison of the rank of pH_x and pH_m

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