Supporting Information

Predicting Organic–Inorganic Aerosol Efflorescence Using Thermodynamically Modeled Viscosity

Summary: The supporting information contains 14 pages, including 2 figures, 8 tables, and references.

Table S1. List of training datasets used for the parameterization of ERH in organic-inorganic aerosol systems. The datasets include OIR, oxygen-to-carbon ratios calculated from OIR (O:C), $T_g(\omega_{org})$, ω_{org}, viscosity, the estimated sensitivity/uncertainty of the viscosity, and ERH. All viscosity values were computed using the AIOMFAC model.

Compound	OIR	ω_{org}	O:C	$T_g(\omega_{org})$	ERH	$\log_{10}(\eta/[Pa.s])$	± $\log_{10}(\eta$ sens./[Pa.s])	Reference
Glucose ($C_6H_{12}O_6$)/AS	0.25	0.19	0.2	146.09	37	-1.56	0.02	Chang(Chang, 2020)
	0.33	0.24	0.25	149.41	34.5	-1.31	0.03	
	0.50	0.33	0.33	155.49	31.5	-0.83	0.05	
Sucrose ($C_{12}H_{22}O_{11}$)/AS	0.25	0.32	0.18	169.80	32.3	-0.74	0.03	Xu et al.(Xu et al., 2022)
	0.50	0.50	0.30	197.97	24.4	0.80	0.18	
	0.25	0.33	0.18	171.79	25.4	-0.44	0.05	Wang et al.(Wang et al., 2017a)
	0.33	0.41	0.23	182.97	21.2	0.05	0.14	
	0.50	0.51	0.30	199.51	21.1	1.28	0.28	
Glycerol ($C_3H_8O_3$)/AS	0.25	0.10	0.2	137.87	51.20	-2.12	0.01	Xu et al.(Xu et al., 2022)
	0.50	0.18	0.33	139.56	49.50	-2.00	0.01	
	1.00	0.30	0.5	142.61	45.60	-1.77	0.02	
	2.00	0.50	0.67	149.00	29.70	-1.03	0.05	
	3.00	0.61	0.75	153.53	22.80	-0.67	0.08	
	0.14	0.09	0.13	137.81	30.5	-1.78	0.02	
	0.5	0.19	0.33	139.83	41.00	-1.85	0.01	Cai et al.(Cai et al., 2017)
	0.33	0.13	0.25	138.64	42.00	-1.94	0.01	
	0.25	0.10	0.2	138.02	43.00	-1.98	0.01	
Malonic acid $C_3H_4O_4$/AS	0.25	0.18	0.67	141.65	36.70	-1.09	0.04	Xu et al.(Xu et al., 2022)
	0.50	0.25	0.44	144.32	26.50	-0.38	0.09	
	1.00	0.41	0.67	151.11	21.50	0.34	0.19	
	2.00	0.55	0.89	159.03	28.7	0.23	0.15	
	0.4286	0.23	0.4	143.45	22.6	-0.25	0.11	Braban et al.(Braban and Abbatt, 2004)
	0.1428	0.09	0.17	138.60	28	-0.99	0.05	
	0.0833	0.05	0.10	137.50	31	-1.27	0.04	
	0.6	0.17	0.5	141.41	24.3	-0.51	0.08	Parsons et al.(Parsons et al., 2004)
	0.33	0.18	0.33	141.64	30.3	-0.74	0.06	
Citric acid $C_6H_8O_7$/AS	0.25	0.21	0.29	148.97	37.30	-1.05	0.04	Xu et al[2].
	0.50	0.36	0.38	161.31	24.80	0.73	0.23	
	0.33	0.29	0.29	155.60	23	0.19	0.18	Shi at

								al.(Shi et al., 2017)
1,2,6-Hexanetriol $C_6H_{14}O_3$/AS	1.00	0.37	0.25	146.84	47.45	-1.70	0.02	Ma et al.(Ma et al., 2021)
	0.25	0.13	0.1	139.31	46.4	-2.07	0.01	
	2.00	0.56	0.34	154.76	43.2	-1.07	0.05	
Oxalic acid $C_2H_2O_4$/AS	1.00	0.34	1	148.31	44.3	0.06	0.07	Wang et al.(Wang et al., 2017b)
	3.00	0.45	1.50	154.08	64.4	-2.79	0.02	
	0.33	0.17	0.5	141.42	34.4	0.27	0.13	
Glutaric acid $C_5H_8O_4$/AS	1.5	0.24	0.48	144.07	22	0.34	0.24	Pant et al.(Pant et al., 2004)
	0.1111	0.02	0.08	136.65	32	-1.50	0.02	
	1.00	0.07	0.4	137.96	36.5	-0.81	0.07	Wu(Wu, 2017)
DEMA/AS Diethyl malonic acid	2.00	0.63	0.38	167.99	43.06	-0.20	0.13	Huang et al.(Huang et al., 2024)
DMSA/AS 2,2-Dimethyl succinic acid	2.00	0.60	0.45	164.55	42.04	-0.39	0.11	
DMGA/AS 3,3-Dimethyl glutaric acid	2.00	0.63	0.38	167.99	43.49	-0.20	0.13	
HMMA/AS DL-4-Hydroxy-3-methoxymandelic acid	2.00	0.65	0.38	180.87	38.74	-0.13	0.11	
Oxalic acid/KCl $C_2H_2O_4$	0.33	0.12	0.5	139.90	73	-2.59	0.00	Wang(Wang, 2018)
	1	0.27	1	145.59	72	-2.23	0.01	
	3	0.40	1.5	151.47	75	-1.97	0.00	
Malonic acid/KCl $C_3H_4O_4$	0.33	0.19	0.33	141.20	53	-2.27	0.01	
	1	0.03	0.67	153.00	42	-1.48	0.03	
Maleic acid/KCl $C_4H_4O_4$	0.33	0.22	0.25	143.36	44	-2.13	0.01	
	1	0.51	0.5	156.45	33	-1.13	0.06	
	3	0.72	0.75	172.18	33	-1.90	0.12	
Glutaric acid/NaCl $C_5H_8O_4$	0.33	0.18	0.2	141.95	66	-2.34	0.00	Ghorai et al.(Ghorai et al., 2014)
	1	0.01	0.4	152.97	59	-1.89	0.01	
	0.25	0.20	0.16	142.41	45	-2.07	0.01	Pant et al.(Pant et al., 2004)
	1.5	0.64	0.48	165.94	39	-0.85	0.07	
	2.33	0.75	0.56	175.63	31	0.02	0.16	
Malonic acid /NaCl $C_3H_4O_4$	0.33	0.56	0.33	141.20	62	-2.22	0.00	Ghorai et al.(Ghorai et al., 2014)
	0.50	0.63	0.44	146.81	36.2	-1.48	0.02	Laskina et

								al.(Laskina et al., 2015)
Glycerol /$NaNO_3$ ($C_3H_8O_3$)	1.00	0.43	0.5	146.49	32	-0.66	0.08	Yu et al.(Yu et al., 2012)
	0.50	0.27	0.33	141.84	35.7	-1.07	0.05	
	0.125	0.07	0.11	137.37	57	-2.03	0.01	Ren et al.(Ren et al., 2016)
	0.25	0.14	0.2	138.77	51	-1.76	0.02	
	0.5	0.52	0.33	141.15	47	-1.57	0.03	
	1	0.42	0.5	146.19	35	-0.86	0.06	
	2	0.64	0.67	154.92	15	0.35	0.26	
Sucrose/$NaNO_3$ ($C_{12}H_{22}O_{11}$)	0.25	0.45	0.18	189.01	20.7	1.95	0.07	Ji et al.(Ji et al., 2017)
	0.125	0.28	0.10	164.79	25.4	0.27	0.05	

Table S2. The validation dataset for predicting ERH in mixed aerosol systems consists of 12 organic compounds and 4 inorganic salts.

[a] calculated using the AIOMFAC model

[b] experimentally measured

Compound	OIR	ERH	$\log_{10}(\eta/[Pa.s])$	Reference
HXT/AS/SUS	1:1:0	46	-1.70 [a]	Hu et al.(Hu et al., 2025)
	1:1:0.1	46.8	-1.53 [a]	
	1:1:0.25	41	-0.98 [a]	
	1:1:0.5	25	0.78 [a]	
	1:1:0.75	25	1.43 [a]	
HXT/AS/GLY	1:1:0	45	-1.68 [a]	
	1:1:0.1	46	-1.66 [a]	
	1:1:0.25	48	-1.67 [a]	
	1:1:0.5	48	-1.58 [a]	
	1:1:0.75	46	-1.46 [a]	
	1:1:1	42	-1.27 [a]	
HXT/AS/CA	1:1:0	45	-1.68 [a]	
	1:1:0.1	40	-1.25 [a]	
	1:1:0.25	37.5	-0.73 [a]	
	1:1:0.5	35	-0.019 [a]	
	1:1:0.75	35	0.45 [a]	
HMMA/AS	0.34	40.3	-1.57 [a]	Bertram et al.(Bertram et al., 2011)
	0.92	39.8	-0.99 [a]	
	2.06	37.8	-0.057 [a]	
DHBA/AS	0.21	33.6	-0.76 [a]	
	0.39	36.7	-0.82 [a]	
	0.63	34.2	-0.84 [a]	
	0.95	32.9	-0.83 [a]	
DMSA/AS	0.35	32.9	-1.35 [a]	
	0.61	33.9	-1.07 [a]	
	1.12	40.3	-0.82 [a]	
	1.38	32.1	-0.12 [a]	
Maleic acid/ $NaNO_3$	1：3	0	3.75 [a]	Chang(Chang, 2020)
	1：1	0	3.73 [a]	
	3：1	0	3.72 [a]	
Glutaric acid/NaCl	3：1	0	3.38 [a]	Pant et al.(Pant et al., 2004)
Malonic acid /KCl	3：1	0	3.51 [a]	Wang(Wang, 2018)
Raffinose/AS	1：1	0	6.00 [b]	Ushijima et al.(Ushijima et al., 2021)

Citric acid /AS	1：1	0	7.54 [b]	Sheldon et al.(S. Sheldon et al., 2023)
	2：1	0	7.54 [b]	
	3：1	0	7.70 [b]	

Table S3. Functional group decomposition of organic compounds in AIOMFAC.

Compound	Subgroup	Quantity
Sucrose ($C_{12}H_{22}O_{11}$)	CH_2_hydroxy	3
	CH_hydroxy	5
	OH	8
	CHO(ether)	3
	C	1
Glucose ($C_6H_{12}O_6$)	CH_2_hydroxy	1
	CH_hydroxy	4
	OH	5
	CHO(ether)	1
1,2,6-Hexanetriol ($C_6H_{14}O_3$)	CH_2[alc]	3
	CH	1
	CH_2	2
	OH	3
DMSA 2,2-Dimethyl succinic	C	1
	CH_3	2
	CH_2	1
	COOH	2
DMGA 3,3-Dimethyl glutaric acid	CH_3	2
	CH_2	2
	C	1
	COOH	2
DEMA Diethyl malonic acid	C	1
	CH_3	2
	CH_2	2
	COOH	2
DHBA 2,5-Dihydroxybenzoic acid	ACH	3
	AC	1
	ACOH	2
	COOH	1
HMMA DL-4-Hydroxy-3-methoxymandelic acid	ACH	3
	ACH	2
	ACOH	1
	CH_3O	1
	CH-[OH]	1
	OH	1
	COOH	1

Table S4. Comparison of the experimentally measured T_g of organic compounds with values predicted using the method of Li et al. and the method of Armeli et al.

T_g/K	Glucose	Sucrose	Glycerol	Citric acid	1,2,6-Hexanetriol
$T_{g\ literature}$(Armeli Iapichino et al., 2023)	303	334	186	284.35	204.15
$T_{g\ Li}$(Li et al., 2020)	253.32	350.97	181.38	274.53	192.25
$T_{g\ Armeli}$(Armeli et al., 2023)	188.4	230.5	156.6	186.3	167.7

Model	Mean Error	Mean Absolute Error	Relative Mean Absolute Error	Standard Deviation
$T_{g\ Li}$	-11.81 K	18.60 K	24.02 K	24.07 K
$T_{g\ Armeli}$	-76.40 K	76.40 K	87.18 K	40.21 K

Table S5. The equation obtained after linearly regressing various physicochemical parameters with ERH and the R^2.

Parameter	**R^2**	**Fitting equation**
O:C	0.08	y=32.96+13.46x
ω_{org}	0.06	y=44.00-17.042x
$T_g(\omega_{org})$	0.14	y=89.79-0.34x
Viscosity	0.65	y=27.40-10.23x

Table S6. Prediction model for ERH using multivariate function fitting with O:C, ω_{org}, and T_g as input variables.

Parameter	R^2	Fitting equation
O:C, $T_g(\omega_{org})$, ω_{org}	0.25	ERH=68.93+18.15(O:C)-0.22($T_g(\omega_{org})$) -15.83(ω_{org})

	Value	Std. Error	t-value	Prob>t
Constant	68.933	19.708	3.498	0.001
"O:C"	18.148	5.924	3.064	0.003
" $T_g(\omega_{org})$"	-0.217	0.140	-1..544	0.128
"ω_{org}"	-15.827	11.709	-1.352	0.181

Table S7. Comparison of multivariate ERH prediction models incorporating viscosity, O:C, ω_{org}, and T_g with the viscosity-ERH model.

Parameter	**R^2**	**Fitting equation**	**Sig F change**
Viscosity	0.65	y=-10.23(viscosity)+27.40	0.000
Viscosity, O:C, $T_g(\omega_{org})$, ω_{org}	0.69	y=3.57(O:C)+0.25 ($T_g(\omega_{org})$) - 2.62(ω_{org})-12.157(viscosity)-13.43	0.031

Parameter	Value	Std. Error	t-value	Prob>|t|
Constant	27.390	1.439	19.029	0.000
"Viscosity"	-10.230	0.946	-10.833	0.000
Constant	13.428	15.434	-0.870	0.388
"O:C"	3.569	4.121	0.866	0.390
"Viscosity"	-12.157	1.294	-9.394	0.000
"$T_g(\omega_{org})$"	0.250	0.103	2.425	0.018
"ω_{org}"	-2.621	7.676	-0.341	0.734

Table S8. Comparison and parameter analysis of the multivariate ERH prediction model (using viscosity, O:C, ω_{org}, and T_g as input variables) versus the bivariate viscosity-T_g model.

Parameter	R^2	Fitting equation	Sig F change
Viscosity, $T_g(\omega_{org})$	0.691	$y=0.251(T_g(\omega_{org}))-12.579(\text{Viscosity})-13.284$	<0.001
Viscosity, O:C, $T_g(\omega_{org})$, ω_{org}	0.695	$y=3.569(\text{O:C})+0.25\ (T_g(\omega_{org}))-2.621(\omega_{org})-12.157(\text{Viscosity})-13.428$	0.685

Parameter	Value	Std. Error	t-value	Prob>|t|
Constant	-13.284	13.700	0.970	0.336
"Viscosity"	-12.579	1.187	10.598	0.000
"$T_g(\omega_{org})$"	0.251	0.084	2.984	0.004
Intercept	-13.428	15.434	-0.870	0.388
"O:C"	3.569	4.121	0.866	0.390
"Viscosity"	-12.157	1.294	-9.394	0.000
"$T_g(\omega_{org})$"	0.250	0.103	2.425	0.018
"ω_{org}"	-2.621	7.676	-0.341	0.734

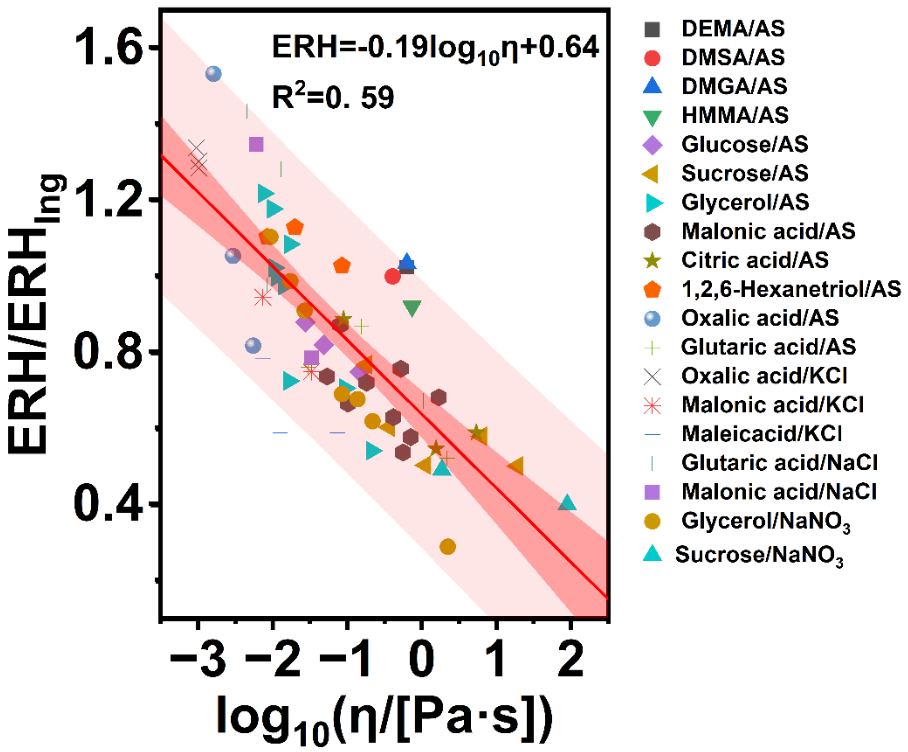

Figure S1. Linear fitting of aerosol normalized ERH for different organic-inorganic aerosols by using viscosity ($\log_{10}\eta$) as the predictor. The ERH of the organic-inorganic mixture systems was normalized according to the ERH of the inorganic salt in the mixture, i.e., ERH/ERH_{Ing}. Data points are color- and shape-coded to distinguish between different organic and inorganic aerosol species. The red solid line represents the linear regression fit between viscosity and ERH. The dark pink band indicates the 95% confidence interval, while the light pink band shows the prediction interval. DEMA represents Diethyl malonic acid, DMSA represents 2,2-Dimethyl succinic acid, DMGA represents 3,3-Dimethyl glutaric acid, HMMA represents DL-4-Hydroxy-3-methoxymandelic acid and DHBA represents 2,5-Dihydroxybenzoic acid.

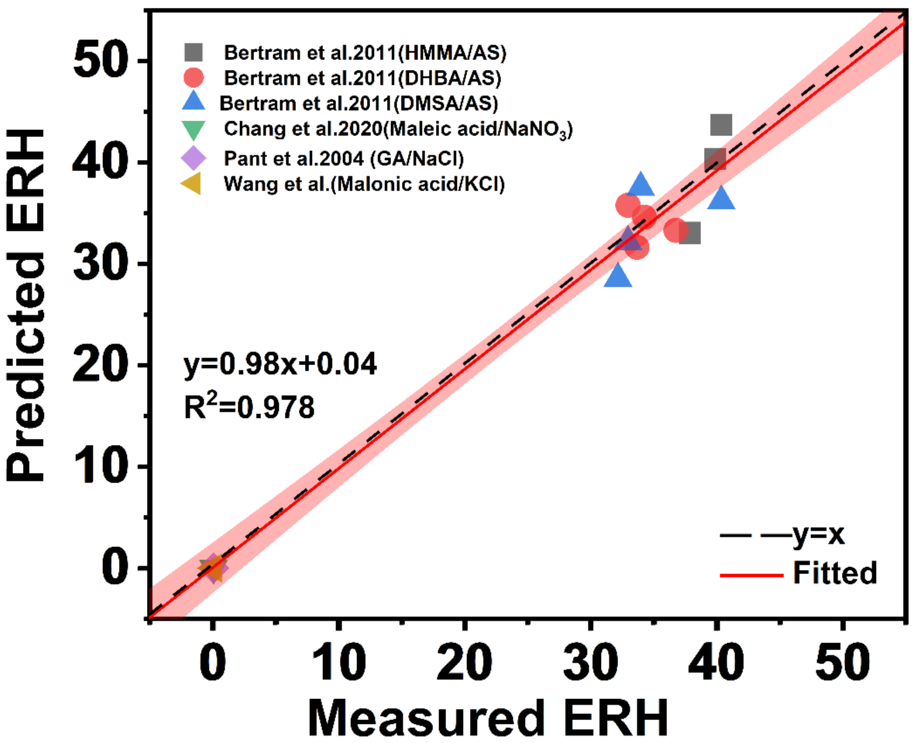

Fig S2. Comparison of measured ERH values versus model predicted ERH values based on the viscosity-T_g-ERH model. The black dashed line denotes the y=x, and the red line representing the linear regression fit to the data, along with the corresponding coefficient of determination (R^2), R^2=0.978. The pale pink shading represents the 95% confidence interval.

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