

Droplet-Size Distribution Effects on Urea–Water Spray Evaporation and Decomposition: Knowledge of Sauter Mean Diameter (SMD) is not Sufficient

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Thirteen key chemical reactions and fifteen species involved in urea decomposition

Table S1. Evaporation and Chemical Reactions involving Urea and Its Derivatives [38].

R1	urea (l) + HNCO (l) $\rightleftharpoons$ biu (s)
R2	urea (l) + HNCO (l) $\rightleftharpoons$ biu (l)
R3	biu (l) + HNCO (l) $\rightleftharpoons$ triu (s)
R4	triu (s) $\rightarrow$ cya (s) + NH ₃
R5	triu (s) $\rightarrow$ amd (s) + H ₂ O(g)
R6	2 urea (l) $\rightarrow$ biu (l) + NH ₃
R7	biu (l) + urea (l) $\rightarrow$ triu (s) + NH ₃
R8	cya (s) $\rightarrow$ cya (g)
R9	urea (g) $\rightleftharpoons$ urea (l)
R10	HNCO (g) $\rightleftharpoons$ HNCO (l)
R11	urea (l) $\rightleftharpoons$ urea (s)
R12	biu (l) $\rightleftharpoons$ biu (s)
R13	amd (s) $\rightleftharpoons$ amd (g)

Progress variable normalization

$$\varphi = \frac{\varphi - \varphi[0]}{\varphi[\text{end}] - \varphi[0]} \quad (\text{Eq. S1})$$

$$\varphi = \varphi + (1 - \varphi[0])$$

The variable φ is normalized to lie in the interval [0, 1].

Ambient temperatures and droplet radii

Table S2. Ambient temperatures and droplet radii used for tabulation.

r_0 (μm)	15	25	35	45	55	65	75	85	95	105
	115	125	135	145	155	165	175	185	195	205
T_g (K)	350	360	370	380	390	400	410	420	430	440
	450	460	470	480	490	500	510	520	530	540
	550	560	570	580	590	600	610	620	630	640
	650	660	670	680	690	700				

Rosin–Rammler, double-hump and the SMD particle size distributions

The Rosin-Rammler particle size distribution:

$$f_{RR}(x; \lambda, n, A, B) = \frac{\frac{n}{\lambda} \left(\frac{x}{\lambda}\right)^{(n-1)} e^{-\left(\frac{x}{\lambda}\right)^n}}{e^{-\left(\frac{A}{\lambda}\right)^n} - e^{-\left(\frac{B}{\lambda}\right)^n}}, \quad (\text{Eq. S2})$$

$f_{RR}(x; \lambda, n, A, B)$ is the probability density function, λ is the scale parameter, n is the shape parameter, A and B are bounds for the radius of the droplet. The double-hump particle size distribution:

$$f_{DH}(x; \lambda_1, \lambda_2, n, A, B) = (1 - \alpha)f_{RR}(x; \lambda_1, n, A, B) + \alpha f_{RR}(x; \lambda_2, n, A, B), \quad (\text{Eq. S3})$$

$f_{RR}(x; \lambda, n, A, B)$ is the Rosin-Rammler probability density function, α the humps ratio.

The SMD (The SMD discrete):

$$SMD = \frac{\sum_i n_i d_i^3}{\sum_i n_i d_i^2}, \quad (\text{Eq. S4})$$

d_i diameter of droplet i , n_i number of droplets of diameter d_i

All the properties given in the table produced by the tabulation process

Table S3. Concise summary of table numbers, descriptions, and units.

Table	Description	Units
0	Progress variable φ	– (dimensionless, 0-1)
1	$d\varphi/dt$	1/s
2	droplet radius ² / initial radius ²	– (dimensionless ratio, 0-1)
3	Mass of droplet	g
4	Temperature at droplet center	K
5	Density of droplet	kg/m ³
6	H ₂ O mass fraction	– (dimensionless, 0-1)
7	Urea(s) mass fraction	– (dimensionless, 0-1)
8	Urea(l) mass fraction	– (dimensionless, 0-1)
9	HNCO(l) mass fraction	– (dimensionless, 0-1)
10	BIU(l) mass fraction	– (dimensionless, 0-1)
11	BIU(s) mass fraction	– (dimensionless, 0-1)
12	TRIU mass fraction	– (dimensionless, 0-1)
13	CYA(s) mass fraction	– (dimensionless, 0-1)
14	AMMD(s) mass fraction	– (dimensionless, 0-1)
15	H ₂ O evaporation rate	kg/s
16	Ammonia evaporation rate	kg/s
17	CYA(g) evaporation rate	kg/s
18	AMMD(g) evaporation rate	kg/s
19	UREA(g) evaporation rate	kg/s
20	HNCO(g) evaporation rate	kg/s
21	Heat flux through gas phase	J/s
22	Time	s
23	Evaporation rate of droplet	kg/s

Table S4. Data Representation with Indexes.

Index	Symbol	Substance
0	h2o_l	H ₂ O(l)
1	ur_s	Urea (s)
2	ur_l	Urea (l)
3	hnco_l	HNCO (l)
4	biu_l	biuret (l)
5	biu_s	biuret (s)
6	triu_s	triuret (s)
7	cya_s	cyanuric acid (s)
8	amd_s	ammelide (s)
9	h2o_g	H ₂ O (g)
10	nh3_g	NH ₃ (g)
11	cya_g	cyanuric acid (g)
12	amd_g	ammelide (g)
13	ur_g	Urea (g)
14	hnco_g	HNCO (g)

Table S5. Composition abbreviations.

Abbreviation	Composition
urea	ur_s+ur_l+ur_g
res_l	hnco_l+biu_l
res_s	biu_s+triu_s+cya_s+amd_s
Res_g	cya_g+amd_g+hnco_g
nh3	nh3_g

Chemical compounds involved in urea water solution (UWS) decomposition

Table S6. Species in liquid chemistry mechanism, phase abbreviation.

Abbreviation	Species name	Chemical formula	Molecular mass (g/mol)
h2o	water	H ₂ O	18.02
ur	urea	CO(NH ₂) ₂	60.06
nh3	ammonia	NH ₃	17.03
hnco	isocyanic acid	HNCO	43.03
cya	cyanuric acid	C ₃ H ₃ N ₃ O ₃	129.08
biu	biuret	C ₂ H ₅ N ₃ O ₂	103.08
triu	triuret	C ₃ H ₆ N ₄ O ₃	146.11
amd	ammelide	C ₃ H ₄ N ₄ O ₂	129.10

Phase	Abbreviation
gas	g
liquid	l
solid	s