

Supplementary Information

Emerging Investigator Series: Thermodynamic and Energy Analysis of Nitrogen and Phosphorous Recovery from Wastewaters

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METHODOLOGY TO DETERMINE MOLAR MINIMUM ENERGY OF RECOVERY

To determine the molar minimum energy of nutrient recovery, \bar{E}_{\min} , mole fractions of species i in the feed, product, and retentate are required. The mole fractions of species i in the waste stream feed, $x_{i,F}$, are based on literature data.¹⁻⁷ The mole fraction and molar ratio of a species in the product, $x_{i,P}$ and $n_{i,P}$, respectively, are dependent on the targeted product, and mole fraction of species in the retentate, $x_{i,R}$, is determined by species mole balance. Mole balances are expressed as $x_{i,F}N_F + x_{i,RXN}N_{RXN} = x_{i,P}N_P + x_{i,R}N_R$ for aqueous products or $x_{i,F}N_F + n_{i,RXN}N_{RXN} = n_{i,P}N_P + x_{i,R}N_R$ for pure liquid/solid products; where the subscript i,RXN denotes the species produced or consumed in reactions. To recover products, nutrients and product co-species are consumed. Additionally, H_2O , OH^- , and H^+ may be generated or consumed for the deprotonation and protonation of NH_4^+/NH_3 and $H_3PO_4/H_2PO_4^-/HPO_4^{2-}/PO_4^{3-}$ species to capture targeted products. For the NH_4^+/NH_3 and $H_3PO_4/H_2PO_4^-/HPO_4^{2-}/PO_4^{3-}$ species, mole balances are based on TAN and TOP mole fractions, respectively. To utilize the mole balances to solve for $x_{i,R}$, scenarios with different recovery yields are modeled. Recovery yield is the amount of species, i , from the initial feed solution captured as a product, defined by $Y_{i,P} = x_{i,P}N_P/x_{i,F}N_F$ for aqueous products and $Y_{i,P} = n_{i,P}N_P/x_{i,F}N_F$ for solid/pure products.

It is important to note that pH and resultant TAN and TOP speciation influence the Gibbs free energy of a solution because of the following three factors: i) $G_{NH_3(aq)} \neq G_{NH_4^+(aq)}$, $G_{HPO_4^{2-}(aq)} \neq G_{H_2PO_4^-(aq)}$, ii) γ_i values are dependent on the species, and iii) x_i is dependent on the concentration of each species. The speciation between ammonium and ammonia, $NH_4^+ \leftrightarrow NH_3 + H^+$, is governed by eqn S(1), and the speciations between the four forms of orthophosphate, $H_3PO_4 \leftrightarrow H_2PO_4^- + H^+$, $H_2PO_4^- \leftrightarrow HPO_4^{2-} + H^+$, and $HPO_4^{2-} \leftrightarrow PO_4^{3-} + H^+$, are governed by eqns S(2), S(3), and S(4):

$$K_{a,NH_4^+} = \frac{\{NH_3\}\{H^+\}}{\{NH_4^+\}} \approx 10^{-9.24} \quad S(1)$$

$$K_{a,H_3PO_4,1} = \frac{\{H_2PO_4^-\}\{H^+\}}{\{H_3PO_4\}} \approx 10^{-2.14} \quad S(2)$$

$$K_{a,H_3PO_4,2} = \frac{\{HPO_4^{2-}\}\{H^+\}}{\{H_2PO_4^-\}} \approx 10^{-7.20} \quad S(3)$$

$$K_{a,H_3PO_4,3} = \frac{\{PO_4^{3-}\}\{H^+\}}{\{HPO_4^{2-}\}} \approx 10^{-12.37} \quad S(4)$$

where K_a is the dissociation constant for the acid and $\{i\}$ is the activity of species i . All K_a values were acquired from literature.⁸ Table S1 presents the range in pH for each waste stream and resultant speciation determined using eqns S(1)-S(4).

Table S1. Range in pH of each waste stream^{1-7,9} and resultant speciation of TAN and TOP. α_i is the fraction of TAN or TOP present as the species denoted by the subscript. The pH range is presented with “H” signifying the high-end and “L” signifying the low-end. Note that only H_2PO_4^- and HPO_4^{2-} forms of TOP are presented because H_3PO_4 and PO_4^{3-} concentrations are negligible in the waste streams.

Waste stream	pH	α_{NH_3}	$\alpha_{\text{NH}_4^+}$	$\alpha_{\text{HPO}_4^{2-}}$	$\alpha_{\text{H}_2\text{PO}_4^-}$	Predominant form of TOP
Greywater H	9	0.365	0.635	0.984	0.016	HPO_4^{2-}
Greywater L	5	5.75×10^{-5}	1.00	6.13×10^{-3}	0.994	H_2PO_4^-
2° WW effluent H	7.7	0.028	0.972	0.796	0.204	HPO_4^{2-}
2° WW effluent L	6.8	3.62×10^{-3}	0.996	0.334	0.666	H_2PO_4^-
Domestic WW H	8.5	0.154	0.846	0.984	0.016	HPO_4^{2-}
Domestic WW L	6.5	1.82×10^{-3}	9.49×10^{-7}	0.163	0.837	H_2PO_4^-
Fresh Urine H	7.5	0.018	0.982	0.661	0.339	HPO_4^{2-}
Fresh Urine L	6	5.75×10^{-4}	0.999	0.058	0.942	H_2PO_4^-
Hydrolyzed Urine H	9.2	0.477	0.523	0.990	0.010	HPO_4^{2-}
Hydrolyzed Urine L	9.0	0.365	0.635	0.984	0.016	HPO_4^{2-}

Table S2. Concentration of active species (components of products in the analysis), other forms of N, and passive species (components in the waste streams, but not in products) in waste streams examined in the analysis.^{1-7,9} Ranges are provided when available in the literature.

Species	Concentration (mM)				
	Greywater	Fresh Urine	Hydrolyzed Urine	Domestic WW	2° WW effluent
Sulfate (SO ₄ ²⁻)	0.00156-0.225	0.288-36.7	1.65-17.4	0.469	1.73
Potassium (K ⁺)	0.000510-0.0614	20.1-94.5	19.4-56.3	0.619	0.256-0.767
Magnesium (Mg ²⁺)	1.48-1.96	4.11		0.453-0.918	0.412-2.058
Nitrate (NO ₃ ⁻)					0.0714-1.42
Urea (CH ₄ N ₂ O)		125.9-264.5			
Sodium (Na ⁺)			64.9-119		1.41-17.4
Chloride (Cl ⁻)			64.9-119		1.41-17.4

MOLAR MINIMUM ENERGY EQUATIONS

The following provides the expressions for molar minimum energies to recover products from the waste streams as presented in Figures 2, 3, 5, and 6 in the main manuscript.

Figure 2. To determine \bar{E}_{\min} for recovering $\text{NH}_{3(l)}$ from all waste streams presented in Figure 2, eqn S(5) was utilized. Note that in Figure 2 all TAN was assumed to be present as NH_4^+ , while analysis presented in Figure 3 considers the speciation between NH_4^+ and NH_3 .

$$\begin{aligned} \bar{E}_{\min} = & G_{f,\text{NH}_3(l)}^0 \\ & + \frac{N_R}{N_P} \left[x_{\text{NH}_4^+,R} G_{\text{NH}_4^+} + x_{\text{H}_2\text{O},R} G_{\text{H}_2\text{O}} + x_{\text{OH}^-,R} G_{\text{OH}^-} \right. \\ & \left. + RT \left(x_{\text{NH}_4^+,R} \ln(\gamma_{\text{NH}_4^+,R} x_{\text{NH}_4^+,R}) + x_{\text{H}_2\text{O},R} \ln(\gamma_{\text{H}_2\text{O},R} x_{\text{H}_2\text{O},R}) \right) \right. \\ & \left. + x_{\text{H}^+,R} \ln(\gamma_{\text{H}^+,R} x_{\text{H}^+,R}) + x_{\text{OH}^-,R} \ln(\gamma_{\text{OH}^-,R} x_{\text{OH}^-,R}) \right] \\ & - \frac{N_F}{N_P} \left[x_{\text{NH}_4^+,F} G_{\text{NH}_4^+} + x_{\text{H}_2\text{O},F} G_{\text{H}_2\text{O}} + x_{\text{OH}^-,F} G_{\text{OH}^-} \right. \\ & \left. + RT \left(x_{\text{NH}_4^+,F} \ln(\gamma_{\text{NH}_4^+,F} x_{\text{NH}_4^+,F}) + x_{\text{H}_2\text{O},F} \ln(\gamma_{\text{H}_2\text{O},F} x_{\text{H}_2\text{O},F}) \right) \right. \\ & \left. + x_{\text{H}^+,F} \ln(\gamma_{\text{H}^+,F} x_{\text{H}^+,F}) + x_{\text{OH}^-,F} \ln(\gamma_{\text{OH}^-,F} x_{\text{OH}^-,F}) \right] \end{aligned} \quad \text{S(5)}$$

Figure 3. For the determination of \bar{E}_{\min} to recover $\text{NH}_{3(l)}$, the aqueous ammonia products (i.e., 10 M $\text{NH}_{3(\text{aq})}$, 5.0 M $\text{NH}_{3(\text{aq})}$, and 1.0 M $\text{NH}_{3(\text{aq})}$), and $(\text{NH}_4)_2\text{SO}_{4(s)}$, eqns S(6), S(7), and S(8), respectively, were utilized. The pH of all the aqueous NH_3 product streams is high (>11.7), such that $>99.7\%$ of TAN is NH_3 and NH_4^+ species are negligible. Note that in all calculations Gibbs free energy required for recovery is normalized per mole of TAN recovered.

$$\begin{aligned} \bar{E}_{\min} = & G_{f,\text{NH}_3(l)}^0 \\ & + \frac{N_R}{N_P} \left[x_{\text{NH}_4^+,R} G_{\text{NH}_4^+} + x_{\text{NH}_3,R} G_{\text{NH}_3} + x_{\text{H}_2\text{O},R} G_{\text{H}_2\text{O}} + x_{\text{OH}^-,R} G_{\text{OH}^-} \right. \\ & \left. + RT \left(x_{\text{NH}_4^+,R} \ln(\gamma_{\text{NH}_4^+,R} x_{\text{NH}_4^+,R}) + x_{\text{NH}_3,R} \ln(\gamma_{\text{NH}_3,R} x_{\text{NH}_3,R}) \right) \right. \\ & \left. + x_{\text{H}_2\text{O},R} \ln(\gamma_{\text{H}_2\text{O},R} x_{\text{H}_2\text{O},R}) + x_{\text{H}^+,R} \ln(\gamma_{\text{H}^+,R} x_{\text{H}^+,R}) + x_{\text{OH}^-,R} \ln(\gamma_{\text{OH}^-,R} x_{\text{OH}^-,R}) \right] \\ & - \frac{N_F}{N_P} \left[x_{\text{NH}_4^+,F} G_{\text{NH}_4^+} + x_{\text{NH}_3,F} G_{\text{NH}_3} + x_{\text{H}_2\text{O},F} G_{\text{H}_2\text{O}} + x_{\text{OH}^-,F} G_{\text{OH}^-} \right. \\ & \left. + RT \left(x_{\text{NH}_4^+,F} \ln(\gamma_{\text{NH}_4^+,F} x_{\text{NH}_4^+,F}) + x_{\text{NH}_3,F} \ln(\gamma_{\text{NH}_3,F} x_{\text{NH}_3,F}) \right) \right. \\ & \left. + x_{\text{H}_2\text{O},F} \ln(\gamma_{\text{H}_2\text{O},F} x_{\text{H}_2\text{O},F}) + x_{\text{H}^+,F} \ln(\gamma_{\text{H}^+,F} x_{\text{H}^+,F}) + x_{\text{OH}^-,F} \ln(\gamma_{\text{OH}^-,F} x_{\text{OH}^-,F}) \right] \end{aligned} \quad \text{S(6)}$$

$$\begin{aligned}
\bar{E}_{\min} = & \frac{1}{x_{\text{TAN,P}}} \left[x_{\text{NH}_3,\text{P}} G_{\text{NH}_3} + x_{\text{H}_2\text{O},\text{P}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-,\text{P}} G_{\text{OH}^-} \right. \\
& \left. + RT \left(x_{\text{NH}_3,\text{P}} \ln(\gamma_{\text{NH}_3,\text{P}} x_{\text{NH}_3,\text{P}}) + x_{\text{H}_2\text{O},\text{P}} \ln(\gamma_{\text{H}_2\text{O},\text{P}} x_{\text{H}_2\text{O},\text{P}}) \right) \right. \\
& \left. + x_{\text{H}^+,\text{P}} \ln(\gamma_{\text{H}^+,\text{P}} x_{\text{H}^+,\text{P}}) + x_{\text{OH}^-,\text{P}} \ln(\gamma_{\text{OH}^-,\text{P}} x_{\text{OH}^-,\text{P}}) \right) \left. \right] \\
+ & \frac{N_{\text{R}}}{x_{\text{TAN,P}} N_{\text{P}}} \left[x_{\text{NH}_4^+,\text{R}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{R}} G_{\text{NH}_3} + x_{\text{H}_2\text{O},\text{R}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-,\text{R}} G_{\text{OH}^-} \right. \\
& \left. + RT \left(x_{\text{NH}_4^+,\text{R}} \ln(\gamma_{\text{NH}_4^+,\text{R}} x_{\text{NH}_4^+,\text{R}}) + x_{\text{NH}_3,\text{R}} \ln(\gamma_{\text{NH}_3,\text{R}} x_{\text{NH}_3,\text{R}}) \right) \right. \\
& \left. + x_{\text{H}_2\text{O},\text{R}} \ln(\gamma_{\text{H}_2\text{O},\text{R}} x_{\text{H}_2\text{O},\text{R}}) + x_{\text{H}^+,\text{R}} \ln(\gamma_{\text{H}^+,\text{R}} x_{\text{H}^+,\text{R}}) + x_{\text{OH}^-,\text{R}} \ln(\gamma_{\text{OH}^-,\text{R}} x_{\text{OH}^-,\text{R}}) \right) \left. \right] \text{S(7)} \\
- & \frac{N_{\text{F}}}{x_{\text{TAN,P}} N_{\text{P}}} \left[x_{\text{NH}_4^+,\text{F}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{F}} G_{\text{NH}_3} + x_{\text{H}_2\text{O},\text{F}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-,\text{F}} G_{\text{OH}^-} \right. \\
& \left. + RT \left(x_{\text{NH}_4^+,\text{F}} \ln(\gamma_{\text{NH}_4^+,\text{F}} x_{\text{NH}_4^+,\text{F}}) + x_{\text{NH}_3,\text{F}} \ln(\gamma_{\text{NH}_3,\text{F}} x_{\text{NH}_3,\text{F}}) \right) \right. \\
& \left. + x_{\text{H}_2\text{O},\text{F}} \ln(\gamma_{\text{H}_2\text{O},\text{F}} x_{\text{H}_2\text{O},\text{F}}) + x_{\text{H}^+,\text{F}} \ln(\gamma_{\text{H}^+,\text{F}} x_{\text{H}^+,\text{F}}) + x_{\text{OH}^-,\text{F}} \ln(\gamma_{\text{OH}^-,\text{F}} x_{\text{OH}^-,\text{F}}) \right) \left. \right]
\end{aligned}$$

$$\begin{aligned}
\bar{E}_{\min} = & \frac{1}{2} G_{\text{f},(\text{NH}_4)_2\text{SO}_4(\text{s})}^0 \\
+ & \frac{N_{\text{R}}}{2N_{\text{P}}} \left[x_{\text{NH}_4^+,\text{R}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{R}} G_{\text{NH}_3} + x_{\text{SO}_4^{2-},\text{R}} G_{\text{SO}_4^{2-}} + x_{\text{H}_2\text{O},\text{R}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-,\text{R}} G_{\text{OH}^-} \right. \\
& \left. + RT \left(x_{\text{NH}_4^+,\text{R}} \ln(\gamma_{\text{NH}_4^+,\text{R}} x_{\text{NH}_4^+,\text{R}}) + x_{\text{NH}_3,\text{R}} \ln(\gamma_{\text{NH}_3,\text{R}} x_{\text{NH}_3,\text{R}}) + \right. \right. \\
& \left. \left. x_{\text{SO}_4^{2-},\text{R}} \ln(\gamma_{\text{SO}_4^{2-},\text{R}} x_{\text{SO}_4^{2-},\text{R}}) + x_{\text{H}_2\text{O},\text{R}} \ln(\gamma_{\text{H}_2\text{O},\text{R}} x_{\text{H}_2\text{O},\text{R}}) + \right. \right. \\
& \left. \left. x_{\text{H}^+,\text{R}} \ln(\gamma_{\text{H}^+,\text{R}} x_{\text{H}^+,\text{R}}) + x_{\text{OH}^-,\text{R}} \ln(\gamma_{\text{OH}^-,\text{R}} x_{\text{OH}^-,\text{R}}) \right) \right. \\
- & \frac{N_{\text{F}}}{2N_{\text{P}}} \left[x_{\text{NH}_4^+,\text{F}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{F}} G_{\text{NH}_3} + x_{\text{SO}_4^{2-},\text{F}} G_{\text{SO}_4^{2-}} + x_{\text{H}_2\text{O},\text{F}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-,\text{F}} G_{\text{OH}^-} \right. \\
& \left. + RT \left(x_{\text{NH}_4^+,\text{F}} \ln(\gamma_{\text{NH}_4^+,\text{F}} x_{\text{NH}_4^+,\text{F}}) + x_{\text{NH}_3,\text{F}} \ln(\gamma_{\text{NH}_3,\text{F}} x_{\text{NH}_3,\text{F}}) + \right. \right. \\
& \left. \left. x_{\text{SO}_4^{2-},\text{F}} \ln(\gamma_{\text{SO}_4^{2-},\text{F}} x_{\text{SO}_4^{2-},\text{F}}) + x_{\text{H}_2\text{O},\text{F}} \ln(\gamma_{\text{H}_2\text{O},\text{F}} x_{\text{H}_2\text{O},\text{F}}) + \right. \right. \\
& \left. \left. x_{\text{H}^+,\text{F}} \ln(\gamma_{\text{H}^+,\text{F}} x_{\text{H}^+,\text{F}}) + x_{\text{OH}^-,\text{F}} \ln(\gamma_{\text{OH}^-,\text{F}} x_{\text{OH}^-,\text{F}}) \right) \right. \left. \right] \text{S(8)}
\end{aligned}$$

For the determination of \bar{E}_{\min} to recover different phosphate products, $\text{KMgPO}_4 \cdot 6 \text{H}_2\text{O}_{(\text{s})}$ (potassium magnesium phosphate), $\text{NH}_4\text{MgPO}_4 \cdot 6\text{H}_2\text{O}_{(\text{s})}$ (struvite), $\text{KH}_2\text{PO}_4_{(\text{s})}$ (potassium phosphate), and $\text{NH}_4\text{H}_2\text{PO}_4_{(\text{s})}$ (monoammonium phosphate), eqns S(9), S(10), S(11), and S(12) were respectively employed.

$$\begin{aligned}
\bar{E}_{\min} &= G_{f,\text{KMgPO}_4 \cdot 6\text{H}_2\text{O(s)}}^0 \\
&+ \frac{N_{\text{R}}}{N_{\text{P}}} \left[x_{\text{K}^+,\text{R}} G_{\text{K}^+} + x_{\text{Mg}^{2+},\text{R}} G_{\text{Mg}^{2+}} + x_{\text{H}_2\text{PO}_4^-, \text{R}} G_{\text{H}_2\text{PO}_4^-} + x_{\text{HPO}_4^{2-}, \text{R}} G_{\text{HPO}_4^{2-}} + x_{\text{H}_2\text{O},\text{R}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-, \text{R}} G_{\text{OH}^-} \right. \\
&\quad \left. + RT \left(x_{\text{K}^+,\text{R}} \ln(\gamma_{\text{K}^+,\text{R}} x_{\text{K}^+,\text{R}}) + x_{\text{Mg}^{2+},\text{R}} \ln(\gamma_{\text{Mg}^{2+},\text{R}} x_{\text{Mg}^{2+},\text{R}}) \right. \right. \\
&\quad \left. \left. + x_{\text{H}_2\text{PO}_4^-, \text{R}} \ln(\gamma_{\text{H}_2\text{PO}_4^-, \text{R}} x_{\text{H}_2\text{PO}_4^-, \text{R}}) + x_{\text{HPO}_4^{2-}, \text{R}} \ln(\gamma_{\text{HPO}_4^{2-}, \text{R}} x_{\text{HPO}_4^{2-}, \text{R}}) \right. \right. \\
&\quad \left. \left. + x_{\text{H}_2\text{O},\text{R}} \ln(\gamma_{\text{H}_2\text{O},\text{R}} x_{\text{H}_2\text{O},\text{R}}) + x_{\text{H}^+,\text{R}} \ln(\gamma_{\text{H}^+,\text{R}} x_{\text{H}^+,\text{R}}) + x_{\text{OH}^-, \text{R}} \ln(\gamma_{\text{OH}^-, \text{R}} x_{\text{OH}^-, \text{R}}) \right) \right] \\
&- \frac{N_{\text{F}}}{N_{\text{P}}} \left[x_{\text{K}^+,\text{F}} G_{\text{K}^+} + x_{\text{Mg}^{2+},\text{F}} G_{\text{Mg}^{2+}} + x_{\text{H}_2\text{PO}_4^-, \text{F}} G_{\text{H}_2\text{PO}_4^-} + x_{\text{HPO}_4^{2-}, \text{F}} G_{\text{HPO}_4^{2-}} + x_{\text{H}_2\text{O},\text{F}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-, \text{F}} G_{\text{OH}^-} \right. \\
&\quad \left. + RT \left(x_{\text{K}^+,\text{F}} \ln(\gamma_{\text{K}^+,\text{F}} x_{\text{K}^+,\text{F}}) + x_{\text{Mg}^{2+},\text{F}} \ln(\gamma_{\text{Mg}^{2+},\text{F}} x_{\text{Mg}^{2+},\text{F}}) \right. \right. \\
&\quad \left. \left. + x_{\text{H}_2\text{PO}_4^-, \text{F}} \ln(\gamma_{\text{H}_2\text{PO}_4^-, \text{F}} x_{\text{H}_2\text{PO}_4^-, \text{F}}) + x_{\text{HPO}_4^{2-}, \text{F}} \ln(\gamma_{\text{HPO}_4^{2-}, \text{F}} x_{\text{HPO}_4^{2-}, \text{F}}) \right. \right. \\
&\quad \left. \left. + x_{\text{H}_2\text{O},\text{F}} \ln(\gamma_{\text{H}_2\text{O},\text{F}} x_{\text{H}_2\text{O},\text{F}}) + x_{\text{H}^+,\text{F}} \ln(\gamma_{\text{H}^+,\text{F}} x_{\text{H}^+,\text{F}}) + x_{\text{OH}^-, \text{F}} \ln(\gamma_{\text{OH}^-, \text{F}} x_{\text{OH}^-, \text{F}}) \right) \right] \quad \text{S(9)}
\end{aligned}$$

$$\begin{aligned}
\bar{E}_{\min} &= G_{f,\text{NH}_4\text{MgPO}_4 \cdot 6\text{H}_2\text{O(s)}}^0 \\
&+ \frac{N_{\text{R}}}{N_{\text{P}}} \left[\left(x_{\text{NH}_4^+,\text{R}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{R}} G_{\text{NH}_3} + x_{\text{Mg}^{2+},\text{R}} G_{\text{Mg}^{2+}} + x_{\text{H}_2\text{PO}_4^-, \text{R}} G_{\text{H}_2\text{PO}_4^-} + \right. \right. \\
&\quad \left. \left. x_{\text{HPO}_4^{2-}, \text{R}} G_{\text{HPO}_4^{2-}} + x_{\text{H}_2\text{O},\text{R}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-, \text{R}} G_{\text{OH}^-} \right) \right. \\
&\quad \left. + RT \left(x_{\text{NH}_4^+,\text{R}} \ln(\gamma_{\text{NH}_4^+,\text{R}} x_{\text{NH}_4^+,\text{R}}) + x_{\text{NH}_3,\text{R}} \ln(\gamma_{\text{NH}_3,\text{R}} x_{\text{NH}_3,\text{R}}) + \right. \right. \\
&\quad \left. \left. x_{\text{Mg}^{2+},\text{R}} \ln(\gamma_{\text{Mg}^{2+},\text{R}} x_{\text{Mg}^{2+},\text{R}}) + x_{\text{H}_2\text{PO}_4^-, \text{R}} \ln(\gamma_{\text{H}_2\text{PO}_4^-, \text{R}} x_{\text{H}_2\text{PO}_4^-, \text{R}}) + \right. \right. \\
&\quad \left. \left. x_{\text{HPO}_4^{2-}, \text{R}} \ln(\gamma_{\text{HPO}_4^{2-}, \text{R}} x_{\text{HPO}_4^{2-}, \text{R}}) + x_{\text{H}_2\text{O},\text{R}} \ln(\gamma_{\text{H}_2\text{O},\text{R}} x_{\text{H}_2\text{O},\text{R}}) + \right. \right. \\
&\quad \left. \left. x_{\text{H}^+,\text{R}} \ln(\gamma_{\text{H}^+,\text{R}} x_{\text{H}^+,\text{R}}) + x_{\text{OH}^-, \text{R}} \ln(\gamma_{\text{OH}^-, \text{R}} x_{\text{OH}^-, \text{R}}) \right) \right] \\
&- \frac{N_{\text{F}}}{N_{\text{P}}} \left[\left(x_{\text{NH}_4^+,\text{F}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{F}} G_{\text{NH}_3} + x_{\text{Mg}^{2+},\text{F}} G_{\text{Mg}^{2+}} + x_{\text{H}_2\text{PO}_4^-, \text{F}} G_{\text{H}_2\text{PO}_4^-} + \right. \right. \\
&\quad \left. \left. x_{\text{HPO}_4^{2-}, \text{F}} G_{\text{HPO}_4^{2-}} + x_{\text{H}_2\text{O},\text{F}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-, \text{F}} G_{\text{OH}^-} \right) \right. \\
&\quad \left. + RT \left(x_{\text{NH}_4^+,\text{F}} \ln(\gamma_{\text{NH}_4^+,\text{F}} x_{\text{NH}_4^+,\text{F}}) + x_{\text{NH}_3,\text{F}} \ln(\gamma_{\text{NH}_3,\text{F}} x_{\text{NH}_3,\text{F}}) + \right. \right. \\
&\quad \left. \left. x_{\text{Mg}^{2+},\text{F}} \ln(\gamma_{\text{Mg}^{2+},\text{F}} x_{\text{Mg}^{2+},\text{F}}) + x_{\text{H}_2\text{PO}_4^-, \text{F}} \ln(\gamma_{\text{H}_2\text{PO}_4^-, \text{F}} x_{\text{H}_2\text{PO}_4^-, \text{F}}) + \right. \right. \\
&\quad \left. \left. x_{\text{HPO}_4^{2-}, \text{F}} \ln(\gamma_{\text{HPO}_4^{2-}, \text{F}} x_{\text{HPO}_4^{2-}, \text{F}}) + x_{\text{H}_2\text{O},\text{F}} \ln(\gamma_{\text{H}_2\text{O},\text{F}} x_{\text{H}_2\text{O},\text{F}}) + \right. \right. \\
&\quad \left. \left. x_{\text{H}^+,\text{F}} \ln(\gamma_{\text{H}^+,\text{F}} x_{\text{H}^+,\text{F}}) + x_{\text{OH}^-, \text{F}} \ln(\gamma_{\text{OH}^-, \text{F}} x_{\text{OH}^-, \text{F}}) \right) \right] \quad \text{S(10)}
\end{aligned}$$

$$\begin{aligned}
\bar{E}_{\min} &= G_{f,\text{KH}_2\text{PO}_4(\text{s})}^0 \\
&+ \frac{N_{\text{R}}}{N_{\text{P}}} \left[\begin{aligned} &x_{\text{K}^+,\text{R}} G_{\text{K}^+} + x_{\text{H}_2\text{PO}_4^-\text{,R}} G_{\text{H}_2\text{PO}_4^-} + x_{\text{HPO}_4^{2-}\text{,R}} G_{\text{HPO}_4^{2-}} + x_{\text{H}_2\text{O,R}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-\text{,R}} G_{\text{OH}^-} \\ &+ RT \left(\begin{aligned} &x_{\text{K}^+,\text{R}} \ln(\gamma_{\text{K}^+,\text{R}} x_{\text{K}^+,\text{R}}) + x_{\text{H}_2\text{PO}_4^-\text{,R}} \ln(\gamma_{\text{H}_2\text{PO}_4^-\text{,R}} x_{\text{H}_2\text{PO}_4^-\text{,R}}) + \\ &x_{\text{HPO}_4^{2-}\text{,R}} \ln(\gamma_{\text{HPO}_4^{2-}\text{,R}} x_{\text{HPO}_4^{2-}\text{,R}}) + x_{\text{H}_2\text{O,R}} \ln(\gamma_{\text{H}_2\text{O,R}} x_{\text{H}_2\text{O,R}}) + \\ &x_{\text{H}^+\text{,R}} \ln(\gamma_{\text{H}^+\text{,R}} x_{\text{H}^+\text{,R}}) + x_{\text{OH}^-\text{,R}} \ln(\gamma_{\text{OH}^-\text{,R}} x_{\text{OH}^-\text{,R}}) \end{aligned} \right) \end{aligned} \right] \\
&- \frac{N_{\text{F}}}{N_{\text{P}}} \left[\begin{aligned} &x_{\text{K}^+,\text{F}} G_{\text{K}^+} + x_{\text{H}_2\text{PO}_4^-\text{,F}} G_{\text{H}_2\text{PO}_4^-} + x_{\text{HPO}_4^{2-}\text{,F}} G_{\text{HPO}_4^{2-}} + x_{\text{H}_2\text{O,F}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-\text{,F}} G_{\text{OH}^-} \\ &+ RT \left(\begin{aligned} &x_{\text{K}^+,\text{F}} \ln(\gamma_{\text{K}^+,\text{F}} x_{\text{K}^+,\text{F}}) + x_{\text{H}_2\text{PO}_4^-\text{,F}} \ln(\gamma_{\text{H}_2\text{PO}_4^-\text{,F}} x_{\text{H}_2\text{PO}_4^-\text{,F}}) + \\ &x_{\text{HPO}_4^{2-}\text{,F}} \ln(\gamma_{\text{HPO}_4^{2-}\text{,F}} x_{\text{HPO}_4^{2-}\text{,F}}) + x_{\text{H}_2\text{O,F}} \ln(\gamma_{\text{H}_2\text{O,F}} x_{\text{H}_2\text{O,F}}) + \\ &x_{\text{H}^+\text{,F}} \ln(\gamma_{\text{H}^+\text{,F}} x_{\text{H}^+\text{,F}}) + x_{\text{OH}^-\text{,F}} \ln(\gamma_{\text{OH}^-\text{,F}} x_{\text{OH}^-\text{,F}}) \end{aligned} \right) \end{aligned} \right] \quad \text{S(11)}
\end{aligned}$$

$$\begin{aligned}
\bar{E}_{\min} &= G_{f,\text{NH}_4\text{H}_2\text{PO}_4(\text{s})}^0 \\
&+ \frac{N_{\text{R}}}{N_{\text{P}}} \left[\begin{aligned} &\left(\begin{aligned} &x_{\text{NH}_4^+\text{,R}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{R}} G_{\text{NH}_3} + x_{\text{H}_2\text{PO}_4^-\text{,R}} G_{\text{H}_2\text{PO}_4^-} + \\ &x_{\text{HPO}_4^{2-}\text{,R}} G_{\text{HPO}_4^{2-}} + x_{\text{H}_2\text{O,R}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-\text{,R}} G_{\text{OH}^-} \end{aligned} \right) \\ &+ RT \left(\begin{aligned} &x_{\text{NH}_4^+\text{,R}} \ln(\gamma_{\text{NH}_4^+\text{,R}} x_{\text{NH}_4^+\text{,R}}) + x_{\text{NH}_3,\text{R}} \ln(\gamma_{\text{NH}_3,\text{R}} x_{\text{NH}_3,\text{R}}) \\ &+ x_{\text{H}_2\text{PO}_4^-\text{,R}} \ln(\gamma_{\text{H}_2\text{PO}_4^-\text{,R}} x_{\text{H}_2\text{PO}_4^-\text{,R}}) + x_{\text{HPO}_4^{2-}\text{,R}} \ln(\gamma_{\text{HPO}_4^{2-}\text{,R}} x_{\text{HPO}_4^{2-}\text{,R}}) \\ &+ x_{\text{H}_2\text{O,R}} \ln(\gamma_{\text{H}_2\text{O,R}} x_{\text{H}_2\text{O,R}}) + x_{\text{H}^+\text{,R}} \ln(\gamma_{\text{H}^+\text{,R}} x_{\text{H}^+\text{,R}}) + x_{\text{OH}^-\text{,R}} \ln(\gamma_{\text{OH}^-\text{,R}} x_{\text{OH}^-\text{,R}}) \end{aligned} \right) \end{aligned} \right] \\
&- \frac{N_{\text{F}}}{N_{\text{P}}} \left[\begin{aligned} &\left(\begin{aligned} &x_{\text{NH}_4^+\text{,F}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{F}} G_{\text{NH}_3} + x_{\text{H}_2\text{PO}_4^-\text{,F}} G_{\text{H}_2\text{PO}_4^-} + \\ &x_{\text{HPO}_4^{2-}\text{,F}} G_{\text{HPO}_4^{2-}} + x_{\text{H}_2\text{O,F}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-\text{,F}} G_{\text{OH}^-} \end{aligned} \right) \\ &+ RT \left(\begin{aligned} &x_{\text{NH}_4^+\text{,F}} \ln(\gamma_{\text{NH}_4^+\text{,F}} x_{\text{NH}_4^+\text{,F}}) + x_{\text{NH}_3,\text{F}} \ln(\gamma_{\text{NH}_3,\text{F}} x_{\text{NH}_3,\text{F}}) \\ &+ x_{\text{H}_2\text{PO}_4^-\text{,F}} \ln(\gamma_{\text{H}_2\text{PO}_4^-\text{,F}} x_{\text{H}_2\text{PO}_4^-\text{,F}}) + x_{\text{HPO}_4^{2-}\text{,F}} \ln(\gamma_{\text{HPO}_4^{2-}\text{,F}} x_{\text{HPO}_4^{2-}\text{,F}}) \\ &+ x_{\text{H}_2\text{O,F}} \ln(\gamma_{\text{H}_2\text{O,F}} x_{\text{H}_2\text{O,F}}) + x_{\text{H}^+\text{,F}} \ln(\gamma_{\text{H}^+\text{,F}} x_{\text{H}^+\text{,F}}) + x_{\text{OH}^-\text{,F}} \ln(\gamma_{\text{OH}^-\text{,F}} x_{\text{OH}^-\text{,F}}) \end{aligned} \right) \end{aligned} \right] \quad \text{S(12)}
\end{aligned}$$

Figure 5. For the determination of \bar{E}_{\min} to recover $\text{NH}_3(\text{l})$ and 1.0 M $\text{NH}_3(\text{aq})$ at various recovery yields from hydrolyzed urine and 2° treated WW effluent eqns S(6) and S(7) were respectively applied. Inputs of $x_{\text{NH}_3,\text{F}}$ and $x_{\text{NH}_4^+,\text{F}}$ are dependent on the speciation of TAN in the feed (i.e., fraction of TAN as NH_3 , α_{NH_3} , and as NH_4^+ , $\alpha_{\text{NH}_4^+}$; where $x_{\text{NH}_3} = \alpha_{\text{NH}_3} x_{\text{TAN}}$ and

$x_{\text{NH}_4^+} = \alpha_{\text{NH}_4^+} x_{\text{TAN}}$). Inputs of $x_{\text{NH}_3,\text{R}}$ and $x_{\text{NH}_4^+,\text{R}}$ are dependent on the speciation of TAN in the retentate as well as the TAN material balance, $x_{\text{TAN},\text{F}} N_{\text{F}} + x_{\text{TAN},\text{RXN}} N_{\text{RXN}} = x_{\text{TAN},\text{P}} N_{\text{P}} + x_{\text{TAN},\text{R}} N_{\text{R}}$. For 2° treated WW effluent systems, NH_4^+ was assumed to be predominant in the feed and retentate due to both streams having $\text{pH} \ll \text{pK}_a$. For hydrolyzed urine systems, speciation of TAN in the feed was evaluated using a model urine solution (Table S7) with Visual Minteq.¹⁰ To calculate $x_{\text{TAN},\text{R}}$, the TAN material balance was applied. Then, $x_{\text{NH}_3,\text{R}}$ and $x_{\text{NH}_4^+,\text{R}}$ were calculated using Visual Minteq to determine pH , $\alpha_{\text{NH}_3,\text{R}}$, and $\alpha_{\text{NH}_4^+,\text{R}}$ (Tables S8 and S9).

Figure 6. For the determination of \bar{E}_{min} to recover 1.0 M $\text{KNO}_3(\text{aq})$, 1.0 M $\text{NH}_4\text{NO}_3(\text{aq})$, $\text{KNO}_3(\text{s})$, and $\text{NH}_4\text{NO}_3(\text{s})$ from 2° treated WW effluent, eqns S(13), S(14), S(15), and S(16), respectively, were used. For 1.0 M $\text{urea}(\text{aq})$ and $\text{urea}(\text{s})$ recovery from hydrolyzed urine, eqns S(17) and S(18) were used, respectively. In this analysis, all recovery energies were normalized per mole of nitrogen recovered.

$$\begin{aligned}
 \bar{E}_{\text{min}} = & \frac{1}{x_{\text{NO}_3^-, \text{P}}} \left[\begin{array}{l} x_{\text{K}^+, \text{P}} G_{\text{K}^+} + x_{\text{NO}_3^-, \text{P}} G_{\text{NO}_3^-} + x_{\text{H}_2\text{O}, \text{P}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-, \text{P}} G_{\text{OH}^-} \\ + RT \left(\begin{array}{l} x_{\text{K}^+, \text{P}} \ln(\gamma_{\text{K}^+, \text{P}} x_{\text{K}^+, \text{P}}) \\ + x_{\text{NO}_3^-, \text{P}} \ln(\gamma_{\text{NO}_3^-, \text{P}} x_{\text{NO}_3^-, \text{P}}) + x_{\text{H}_2\text{O}, \text{P}} \ln(\gamma_{\text{H}_2\text{O}, \text{P}} x_{\text{H}_2\text{O}, \text{P}}) \\ + x_{\text{H}^+, \text{P}} \ln(\gamma_{\text{H}^+, \text{P}} x_{\text{H}^+, \text{P}}) + x_{\text{OH}^-, \text{P}} \ln(\gamma_{\text{OH}^-, \text{P}} x_{\text{OH}^-, \text{P}}) \end{array} \right) \end{array} \right] \\
 + & \frac{N_{\text{R}}}{x_{\text{NO}_3^-, \text{P}} N_{\text{P}}} \left[\begin{array}{l} x_{\text{K}^+, \text{R}} G_{\text{K}^+} + x_{\text{NO}_3^-, \text{R}} G_{\text{NO}_3^-} + x_{\text{H}_2\text{O}, \text{R}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-, \text{R}} G_{\text{OH}^-} \\ + RT \left(\begin{array}{l} x_{\text{K}^+, \text{R}} \ln(\gamma_{\text{K}^+, \text{R}} x_{\text{K}^+, \text{R}}) \\ + x_{\text{NO}_3^-, \text{R}} \ln(\gamma_{\text{NO}_3^-, \text{R}} x_{\text{NO}_3^-, \text{R}}) + x_{\text{H}_2\text{O}, \text{R}} \ln(\gamma_{\text{H}_2\text{O}, \text{R}} x_{\text{H}_2\text{O}, \text{R}}) \\ + x_{\text{H}^+, \text{R}} \ln(\gamma_{\text{H}^+, \text{R}} x_{\text{H}^+, \text{R}}) + x_{\text{OH}^-, \text{R}} \ln(\gamma_{\text{OH}^-, \text{R}} x_{\text{OH}^-, \text{R}}) \end{array} \right) \end{array} \right] \\
 - & \frac{N_{\text{F}}}{x_{\text{NO}_3^-, \text{P}} N_{\text{P}}} \left[\begin{array}{l} x_{\text{K}^+, \text{F}} G_{\text{K}^+} + x_{\text{NO}_3^-, \text{F}} G_{\text{NO}_3^-} + x_{\text{H}_2\text{O}, \text{F}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-, \text{F}} G_{\text{OH}^-} \\ + RT \left(\begin{array}{l} x_{\text{K}^+, \text{F}} \ln(\gamma_{\text{K}^+, \text{F}} x_{\text{K}^+, \text{F}}) \\ + x_{\text{NO}_3^-, \text{F}} \ln(\gamma_{\text{NO}_3^-, \text{F}} x_{\text{NO}_3^-, \text{F}}) + x_{\text{H}_2\text{O}, \text{F}} \ln(\gamma_{\text{H}_2\text{O}, \text{F}} x_{\text{H}_2\text{O}, \text{F}}) \\ + x_{\text{H}^+, \text{F}} \ln(\gamma_{\text{H}^+, \text{F}} x_{\text{H}^+, \text{F}}) + x_{\text{OH}^-, \text{F}} \ln(\gamma_{\text{OH}^-, \text{F}} x_{\text{OH}^-, \text{F}}) \end{array} \right) \end{array} \right] \quad \text{S(13)}
 \end{aligned}$$

$$\begin{aligned}
\bar{E}_{\min} = & \frac{1}{2x_{\text{TAN,P}}} \left[x_{\text{NH}_4^+,\text{P}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{P}} G_{\text{NH}_3} + x_{\text{NO}_3^-\text{,P}} G_{\text{NO}_3^-} + x_{\text{H}_2\text{O,P}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-\text{,P}} G_{\text{OH}^-} \right. \\
& + RT \left(\begin{aligned} & x_{\text{NH}_4^+,\text{P}} \ln(\gamma_{\text{NH}_4^+,\text{P}} x_{\text{NH}_4^+,\text{P}}) + x_{\text{NH}_3,\text{P}} \ln(\gamma_{\text{NH}_3,\text{P}} x_{\text{NH}_3,\text{P}}) \\ & + x_{\text{NO}_3^-\text{,P}} \ln(\gamma_{\text{NO}_3^-\text{,P}} x_{\text{NO}_3^-\text{,P}}) + x_{\text{H}_2\text{O,P}} \ln(\gamma_{\text{H}_2\text{O,P}} x_{\text{H}_2\text{O,P}}) \\ & + x_{\text{H}^+,\text{P}} \ln(\gamma_{\text{H}^+,\text{P}} x_{\text{H}^+,\text{P}}) + x_{\text{OH}^-\text{,P}} \ln(\gamma_{\text{OH}^-\text{,P}} x_{\text{OH}^-\text{,P}}) \end{aligned} \right) \\
& + \frac{N_{\text{R}}}{2x_{\text{TAN,P}} N_{\text{P}}} \left[x_{\text{NH}_4^+,\text{R}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{R}} G_{\text{NH}_3} + x_{\text{NO}_3^-\text{,R}} G_{\text{NO}_3^-} + x_{\text{H}_2\text{O,R}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-\text{,R}} G_{\text{OH}^-} \right. \\
& + RT \left(\begin{aligned} & x_{\text{NH}_4^+,\text{R}} \ln(\gamma_{\text{NH}_4^+,\text{R}} x_{\text{NH}_4^+,\text{R}}) + x_{\text{NH}_3,\text{R}} \ln(\gamma_{\text{NH}_3,\text{R}} x_{\text{NH}_3,\text{R}}) \\ & + x_{\text{NO}_3^-\text{,R}} \ln(\gamma_{\text{NO}_3^-\text{,R}} x_{\text{NO}_3^-\text{,R}}) + x_{\text{H}_2\text{O,R}} \ln(\gamma_{\text{H}_2\text{O,R}} x_{\text{H}_2\text{O,R}}) \\ & + x_{\text{H}^+,\text{R}} \ln(\gamma_{\text{H}^+,\text{R}} x_{\text{H}^+,\text{R}}) + x_{\text{OH}^-\text{,R}} \ln(\gamma_{\text{OH}^-\text{,R}} x_{\text{OH}^-\text{,R}}) \end{aligned} \right) \\
& - \frac{N_{\text{F}}}{2x_{\text{TAN,P}} N_{\text{P}}} \left[x_{\text{NH}_4^+,\text{F}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{F}} G_{\text{NH}_3} + x_{\text{NO}_3^-\text{,F}} G_{\text{NO}_3^-} + x_{\text{H}_2\text{O,F}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-\text{,F}} G_{\text{OH}^-} \right. \\
& + RT \left(\begin{aligned} & x_{\text{NH}_4^+,\text{F}} \ln(\gamma_{\text{NH}_4^+,\text{F}} x_{\text{NH}_4^+,\text{F}}) + x_{\text{NH}_3,\text{F}} \ln(\gamma_{\text{NH}_3,\text{F}} x_{\text{NH}_3,\text{F}}) \\ & + x_{\text{NO}_3^-\text{,F}} \ln(\gamma_{\text{NO}_3^-\text{,F}} x_{\text{NO}_3^-\text{,F}}) + x_{\text{H}_2\text{O,F}} \ln(\gamma_{\text{H}_2\text{O,F}} x_{\text{H}_2\text{O,F}}) \\ & + x_{\text{H}^+,\text{F}} \ln(\gamma_{\text{H}^+,\text{F}} x_{\text{H}^+,\text{F}}) + x_{\text{OH}^-\text{,F}} \ln(\gamma_{\text{OH}^-\text{,F}} x_{\text{OH}^-\text{,F}}) \end{aligned} \right) \left. \right] \quad \text{S(14)}
\end{aligned}$$

$$\begin{aligned}
\bar{E}_{\min} = & G_{\text{f,KNO}_3(\text{s})}^0 \\
& + \frac{N_{\text{R}}}{N_{\text{P}}} \left[\begin{aligned} & x_{\text{K}^+,\text{R}} G_{\text{K}^+} + x_{\text{NO}_3^-\text{,R}} G_{\text{NO}_3^-} + x_{\text{H}_2\text{O,R}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-\text{,R}} G_{\text{OH}^-} \\ & + RT \left(\begin{aligned} & x_{\text{K}^+,\text{R}} \ln(\gamma_{\text{K}^+,\text{R}} x_{\text{K}^+,\text{R}}) + x_{\text{NO}_3^-\text{,R}} \ln(\gamma_{\text{NO}_3^-\text{,R}} x_{\text{NO}_3^-\text{,R}}) \\ & + x_{\text{H}_2\text{O,R}} \ln(\gamma_{\text{H}_2\text{O,R}} x_{\text{H}_2\text{O,R}}) + x_{\text{H}^+,\text{R}} \ln(\gamma_{\text{H}^+,\text{R}} x_{\text{H}^+,\text{R}}) + x_{\text{OH}^-\text{,R}} \ln(\gamma_{\text{OH}^-\text{,R}} x_{\text{OH}^-\text{,R}}) \end{aligned} \right) \end{aligned} \right] \quad \text{S(15)} \\
& - \frac{N_{\text{F}}}{N_{\text{P}}} \left[\begin{aligned} & x_{\text{K}^+,\text{F}} G_{\text{K}^+} + x_{\text{NO}_3^-\text{,F}} G_{\text{NO}_3^-} + x_{\text{H}_2\text{O,F}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-\text{,F}} G_{\text{OH}^-} \\ & + RT \left(\begin{aligned} & x_{\text{K}^+,\text{F}} \ln(\gamma_{\text{K}^+,\text{F}} x_{\text{K}^+,\text{F}}) + x_{\text{NO}_3^-\text{,F}} \ln(\gamma_{\text{NO}_3^-\text{,F}} x_{\text{NO}_3^-\text{,F}}) \\ & + x_{\text{H}_2\text{O,F}} \ln(\gamma_{\text{H}_2\text{O,F}} x_{\text{H}_2\text{O,F}}) + x_{\text{H}^+,\text{F}} \ln(\gamma_{\text{H}^+,\text{F}} x_{\text{H}^+,\text{F}}) + x_{\text{OH}^-\text{,F}} \ln(\gamma_{\text{OH}^-\text{,F}} x_{\text{OH}^-\text{,F}}) \end{aligned} \right) \end{aligned} \right]
\end{aligned}$$

$$\begin{aligned}
\bar{E}_{\min} &= \frac{1}{2} G_{\text{f,NH}_4\text{NO}_3(\text{s})}^0 \\
&+ \frac{N_{\text{R}}}{2N_{\text{P}}} \left[+RT \left(x_{\text{NH}_4^+,\text{R}} \ln(\gamma_{\text{NH}_4^+,\text{R}} x_{\text{NH}_4^+,\text{R}}) + x_{\text{NH}_3,\text{R}} \ln(\gamma_{\text{NH}_3,\text{R}} x_{\text{NH}_3,\text{R}}) + x_{\text{NO}_3^-\text{,R}} \ln(\gamma_{\text{NO}_3^-\text{,R}} x_{\text{NO}_3^-\text{,R}}) \right) \right. \\
&\quad \left. + x_{\text{H}_2\text{O},\text{R}} \ln(\gamma_{\text{H}_2\text{O},\text{R}} x_{\text{H}_2\text{O},\text{R}}) + x_{\text{H}^+,\text{R}} \ln(\gamma_{\text{H}^+,\text{R}} x_{\text{H}^+,\text{R}}) + x_{\text{OH}^-\text{,R}} \ln(\gamma_{\text{OH}^-\text{,R}} x_{\text{OH}^-\text{,R}}) \right) \Big] \\
&- \frac{N_{\text{F}}}{2N_{\text{P}}} \left[+RT \left(x_{\text{NH}_4^+,\text{F}} \ln(\gamma_{\text{NH}_4^+,\text{F}} x_{\text{NH}_4^+,\text{F}}) + x_{\text{NH}_3,\text{F}} \ln(\gamma_{\text{NH}_3,\text{F}} x_{\text{NH}_3,\text{F}}) + x_{\text{NO}_3^-\text{,F}} \ln(\gamma_{\text{NO}_3^-\text{,F}} x_{\text{NO}_3^-\text{,F}}) \right) \right. \\
&\quad \left. + x_{\text{H}_2\text{O},\text{F}} \ln(\gamma_{\text{H}_2\text{O},\text{F}} x_{\text{H}_2\text{O},\text{F}}) + x_{\text{H}^+,\text{F}} \ln(\gamma_{\text{H}^+,\text{F}} x_{\text{H}^+,\text{F}}) + x_{\text{OH}^-\text{,F}} \ln(\gamma_{\text{OH}^-\text{,F}} x_{\text{OH}^-\text{,F}}) \right) \Big]
\end{aligned} \tag{S16}$$

$$\begin{aligned}
\bar{E}_{\min} &= \frac{1}{2x_{\text{CO}(\text{NH}_2)_2,\text{P}} N_{\text{P}}} \left[+RT \left(x_{\text{CO}(\text{NH}_2)_2,\text{P}} \ln(\gamma_{\text{CO}(\text{NH}_2)_2,\text{P}} x_{\text{CO}(\text{NH}_2)_2,\text{P}}) + x_{\text{H}_2\text{O},\text{P}} \ln(\gamma_{\text{H}_2\text{O},\text{P}} x_{\text{H}_2\text{O},\text{P}}) \right) \right. \\
&\quad \left. + x_{\text{H}^+,\text{P}} \ln(\gamma_{\text{H}^+,\text{P}} x_{\text{H}^+,\text{P}}) + x_{\text{OH}^-\text{,P}} \ln(\gamma_{\text{OH}^-\text{,P}} x_{\text{OH}^-\text{,P}}) \right) \Big] \\
&+ \frac{N_{\text{R}}}{2x_{\text{CO}(\text{NH}_2)_2,\text{P}} N_{\text{P}}} \left[+RT \left(x_{\text{CO}(\text{NH}_2)_2,\text{R}} \ln(\gamma_{\text{CO}(\text{NH}_2)_2,\text{R}} x_{\text{CO}(\text{NH}_2)_2,\text{R}}) + x_{\text{H}_2\text{O},\text{R}} \ln(\gamma_{\text{H}_2\text{O},\text{R}} x_{\text{H}_2\text{O},\text{R}}) \right) \right. \\
&\quad \left. + x_{\text{H}^+,\text{R}} \ln(\gamma_{\text{H}^+,\text{R}} x_{\text{H}^+,\text{R}}) + x_{\text{OH}^-\text{,R}} \ln(\gamma_{\text{OH}^-\text{,R}} x_{\text{OH}^-\text{,R}}) \right) \Big] \\
&- \frac{N_{\text{F}}}{2x_{\text{CO}(\text{NH}_2)_2,\text{P}} N_{\text{P}}} \left[+RT \left(x_{\text{CO}(\text{NH}_2)_2,\text{F}} \ln(\gamma_{\text{CO}(\text{NH}_2)_2,\text{F}} x_{\text{CO}(\text{NH}_2)_2,\text{F}}) + x_{\text{H}_2\text{O},\text{F}} \ln(\gamma_{\text{H}_2\text{O},\text{F}} x_{\text{H}_2\text{O},\text{F}}) \right) \right. \\
&\quad \left. + x_{\text{H}^+,\text{F}} \ln(\gamma_{\text{H}^+,\text{F}} x_{\text{H}^+,\text{F}}) + x_{\text{OH}^-\text{,F}} \ln(\gamma_{\text{OH}^-\text{,F}} x_{\text{OH}^-\text{,F}}) \right) \Big]
\end{aligned} \tag{S17}$$

$$\begin{aligned}
\bar{E}_{\min} &= G_{\text{f,CO}(\text{NH}_2)_2(\text{s})}^0 \\
&+ \frac{N_{\text{R}}}{2N_{\text{P}}} \left[+RT \left(x_{\text{CO}(\text{NH}_2)_2,\text{R}} \ln(\gamma_{\text{CO}(\text{NH}_2)_2,\text{R}} x_{\text{CO}(\text{NH}_2)_2,\text{R}}) + x_{\text{H}_2\text{O},\text{R}} \ln(\gamma_{\text{H}_2\text{O},\text{R}} x_{\text{H}_2\text{O},\text{R}}) \right) \right. \\
&\quad \left. + x_{\text{H}^+,\text{R}} \ln(\gamma_{\text{H}^+,\text{R}} x_{\text{H}^+,\text{R}}) + x_{\text{OH}^-\text{,R}} \ln(\gamma_{\text{OH}^-\text{,R}} x_{\text{OH}^-\text{,R}}) \right) \Big] \\
&- \frac{N_{\text{F}}}{2N_{\text{P}}} \left[+RT \left(x_{\text{CO}(\text{NH}_2)_2,\text{F}} \ln(\gamma_{\text{CO}(\text{NH}_2)_2,\text{F}} x_{\text{CO}(\text{NH}_2)_2,\text{F}}) + x_{\text{H}_2\text{O},\text{F}} \ln(\gamma_{\text{H}_2\text{O},\text{F}} x_{\text{H}_2\text{O},\text{F}}) \right) \right. \\
&\quad \left. + x_{\text{H}^+,\text{F}} \ln(\gamma_{\text{H}^+,\text{F}} x_{\text{H}^+,\text{F}}) + x_{\text{OH}^-\text{,F}} \ln(\gamma_{\text{OH}^-\text{,F}} x_{\text{OH}^-\text{,F}}) \right) \Big]
\end{aligned} \tag{S18}$$

For the determination of \bar{E}_{\min} to recover $\text{NH}_{3(l)}$ and 1.0 M $\text{NH}_{3(aq)}$ from waste streams excluding Na^+ and Cl^- species in the analysis, eqns S(6) and S(7) were respectively applied. For the determination of \bar{E}_{\min} to recover $\text{NH}_{3(l)}$ and 1.0 M $\text{NH}_{3(aq)}$ from waste streams including Na^+ and Cl^- species in the analysis, eqns S(19) and S(20) were respectively applied. The \bar{E}_{\min} values are presented in Table S6 and discussed in the main manuscript.

$$\begin{aligned}
\bar{E}_{\min} = & G_{f,\text{NH}_{3(l)}}^0 \\
& + \frac{N_{\text{R}}}{N_{\text{P}}} \left[\begin{aligned} & x_{\text{NH}_4^+,\text{R}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{R}} G_{\text{NH}_3} + x_{\text{H}_2\text{O},\text{R}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-,\text{R}} G_{\text{OH}^-} + x_{\text{Na}^+,\text{R}} G_{\text{Na}^+} + x_{\text{Cl}^-,\text{R}} G_{\text{Cl}^-} \\ & + RT \left(\begin{aligned} & x_{\text{NH}_4^+,\text{R}} \ln(\gamma_{\text{NH}_4^+,\text{R}} x_{\text{NH}_4^+,\text{R}}) + x_{\text{NH}_3,\text{R}} \ln(\gamma_{\text{NH}_3,\text{R}} x_{\text{NH}_3,\text{R}}) \\ & + x_{\text{H}_2\text{O},\text{R}} \ln(\gamma_{\text{H}_2\text{O},\text{R}} x_{\text{H}_2\text{O},\text{R}}) + x_{\text{H}^+,\text{R}} \ln(\gamma_{\text{H}^+,\text{R}} x_{\text{H}^+,\text{R}}) + x_{\text{OH}^-,\text{R}} \ln(\gamma_{\text{OH}^-,\text{R}} x_{\text{OH}^-,\text{R}}) \\ & + x_{\text{Na}^+,\text{R}} \ln(\gamma_{\text{Na}^+,\text{R}} x_{\text{Na}^+,\text{R}}) + x_{\text{Cl}^-,\text{R}} \ln(\gamma_{\text{Cl}^-,\text{R}} x_{\text{Cl}^-,\text{R}}) \end{aligned} \right) \end{aligned} \right] \\
& - \frac{N_{\text{F}}}{N_{\text{P}}} \left[\begin{aligned} & x_{\text{NH}_4^+,\text{F}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{F}} G_{\text{NH}_3} + x_{\text{H}_2\text{O},\text{F}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-,\text{F}} G_{\text{OH}^-} + x_{\text{Na}^+,\text{F}} G_{\text{Na}^+} + x_{\text{Cl}^-,\text{F}} G_{\text{Cl}^-} \\ & + RT \left(\begin{aligned} & x_{\text{NH}_4^+,\text{F}} \ln(\gamma_{\text{NH}_4^+,\text{F}} x_{\text{NH}_4^+,\text{F}}) + x_{\text{NH}_3,\text{F}} \ln(\gamma_{\text{NH}_3,\text{F}} x_{\text{NH}_3,\text{F}}) \\ & + x_{\text{H}_2\text{O},\text{F}} \ln(\gamma_{\text{H}_2\text{O},\text{F}} x_{\text{H}_2\text{O},\text{F}}) + x_{\text{H}^+,\text{F}} \ln(\gamma_{\text{H}^+,\text{F}} x_{\text{H}^+,\text{F}}) + x_{\text{OH}^-,\text{F}} \ln(\gamma_{\text{OH}^-,\text{F}} x_{\text{OH}^-,\text{F}}) \\ & + x_{\text{Na}^+,\text{F}} \ln(\gamma_{\text{Na}^+,\text{F}} x_{\text{Na}^+,\text{F}}) + x_{\text{Cl}^-,\text{F}} \ln(\gamma_{\text{Cl}^-,\text{F}} x_{\text{Cl}^-,\text{F}}) \end{aligned} \right) \end{aligned} \right] \quad \text{S(19)}
\end{aligned}$$

$$\begin{aligned}
\bar{E}_{\min} = & \frac{1}{x_{\text{TAN,P}}} \left[\begin{aligned} & x_{\text{NH}_3,\text{P}} G_{\text{NH}_3} + x_{\text{H}_2\text{O,P}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-, \text{P}} G_{\text{OH}^-} + x_{\text{Na}^+, \text{P}} G_{\text{Na}^+} + x_{\text{Cl}^-, \text{P}} G_{\text{Cl}^-} \\ & + RT \left(\begin{aligned} & x_{\text{NH}_3,\text{P}} \ln(\gamma_{\text{NH}_3,\text{P}} x_{\text{NH}_3,\text{P}}) + x_{\text{H}_2\text{O,P}} \ln(\gamma_{\text{H}_2\text{O,P}} x_{\text{H}_2\text{O,P}}) \\ & + x_{\text{H}^+, \text{P}} \ln(\gamma_{\text{H}^+, \text{P}} x_{\text{H}^+, \text{P}}) + x_{\text{OH}^-, \text{P}} \ln(\gamma_{\text{OH}^-, \text{P}} x_{\text{OH}^-, \text{P}}) \\ & + x_{\text{Na}^+, \text{P}} \ln(\gamma_{\text{Na}^+, \text{P}} x_{\text{Na}^+, \text{P}}) + x_{\text{Cl}^-, \text{P}} \ln(\gamma_{\text{Cl}^-, \text{P}} x_{\text{Cl}^-, \text{P}}) \end{aligned} \right) \end{aligned} \right] \\
+ \frac{N_{\text{R}}}{x_{\text{TAN,P}} N_{\text{P}}} & \left[\begin{aligned} & x_{\text{NH}_4^+, \text{R}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{R}} G_{\text{NH}_3} + x_{\text{H}_2\text{O,R}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-, \text{R}} G_{\text{OH}^-} + x_{\text{Na}^+, \text{R}} G_{\text{Na}^+} + x_{\text{Cl}^-, \text{R}} G_{\text{Cl}^-} \\ & + RT \left(\begin{aligned} & x_{\text{NH}_4^+, \text{R}} \ln(\gamma_{\text{NH}_4^+, \text{R}} x_{\text{NH}_4^+, \text{R}}) + x_{\text{NH}_3,\text{R}} \ln(\gamma_{\text{NH}_3,\text{R}} x_{\text{NH}_3,\text{R}}) \\ & + x_{\text{H}_2\text{O,R}} \ln(\gamma_{\text{H}_2\text{O,R}} x_{\text{H}_2\text{O,R}}) + x_{\text{H}^+, \text{R}} \ln(\gamma_{\text{H}^+, \text{R}} x_{\text{H}^+, \text{R}}) + x_{\text{OH}^-, \text{R}} \ln(\gamma_{\text{OH}^-, \text{R}} x_{\text{OH}^-, \text{R}}) \\ & + x_{\text{Na}^+, \text{R}} \ln(\gamma_{\text{Na}^+, \text{R}} x_{\text{Na}^+, \text{R}}) + x_{\text{Cl}^-, \text{R}} \ln(\gamma_{\text{Cl}^-, \text{R}} x_{\text{Cl}^-, \text{R}}) \end{aligned} \right) \end{aligned} \right] \\
- \frac{N_{\text{F}}}{x_{\text{TAN,P}} N_{\text{P}}} & \left[\begin{aligned} & x_{\text{NH}_4^+, \text{F}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{F}} G_{\text{NH}_3} + x_{\text{H}_2\text{O,F}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-, \text{F}} G_{\text{OH}^-} + x_{\text{Na}^+, \text{F}} G_{\text{Na}^+} + x_{\text{Cl}^-, \text{F}} G_{\text{Cl}^-} \\ & + RT \left(\begin{aligned} & x_{\text{NH}_4^+, \text{F}} \ln(\gamma_{\text{NH}_4^+, \text{F}} x_{\text{NH}_4^+, \text{F}}) + x_{\text{NH}_3,\text{F}} \ln(\gamma_{\text{NH}_3,\text{F}} x_{\text{NH}_3,\text{F}}) \\ & + x_{\text{H}_2\text{O,F}} \ln(\gamma_{\text{H}_2\text{O,F}} x_{\text{H}_2\text{O,F}}) + x_{\text{H}^+, \text{F}} \ln(\gamma_{\text{H}^+, \text{F}} x_{\text{H}^+, \text{F}}) + x_{\text{OH}^-, \text{F}} \ln(\gamma_{\text{OH}^-, \text{F}} x_{\text{OH}^-, \text{F}}) \\ & + x_{\text{Na}^+, \text{F}} \ln(\gamma_{\text{Na}^+, \text{F}} x_{\text{Na}^+, \text{F}}) + x_{\text{Cl}^-, \text{F}} \ln(\gamma_{\text{Cl}^-, \text{F}} x_{\text{Cl}^-, \text{F}}) \end{aligned} \right) \end{aligned} \right] \tag{S(20)}
\end{aligned}$$

ACTIVITY COEFFICIENT MODELS

Davies Approximation for Ion Activity Coefficients in Dilute Systems. The Davies approximation, eqn S(21), is an empirical extension of the Debye-Huckel theory that can be used to estimate activity coefficients in solutions with ionic strengths, I , <0.5 M. For solutions with ionic strengths comparable to or lower than hydrolyzed urine, the Davies approximation for activity coefficients resulted in the best agreement with experimental results compared to other methods, including the B-dot and Millero-Screiber methods.¹¹

$$\log \gamma = -Az^2 \left(\frac{\sqrt{I}}{1+\sqrt{I}} - 0.3I \right) \quad \text{S(21)}$$

Here, $A = 1.82 \times 10^6 (\epsilon T)^{-3/2} \approx 0.509$, z is the valency of the ion, ϵ is the dielectric constant, T is absolute temperature. $I = 0.5 \sum C_i z_i^2$ and C is the concentration of ion.

The Davies approximation was applied to calculate the activity coefficient for ions, including NH_4^+ , SO_4^{2-} , H_2PO_4^- , HPO_4^{2-} , Mg^{2+} , K^+ , Na^+ , Cl^- , and NO_3^- , for all streams that fit the criteria, $I \leq 0.5$, which includes the simplified versions of hydrolyzed urine that only include nutrients and co-species components, fresh urine, domestic WW effluent, 2° WW effluent, and greywater. Not that this method is not applicable for determining activity coefficients of neutral components, such as, urea, $\text{CO}(\text{NH}_2)_2$.

Non-Random Two Liquid Model for NH_3 and H_2O Activity Coefficients in Concentrated Product Streams of 1.0 M, 5.0 M and 10 M $\text{NH}_3(\text{aq})$. The Non-Random Two Liquid (NRTL) model for a binary mixture, eqns S(22)-S(24), is widely applied in phase-equilibria calculations for the quantification of activity coefficients. The NRTL method has been used to determine $\gamma_{\text{H}_2\text{O}}$ and γ_{NH_3} in binary $\text{NH}_3/\text{H}_2\text{O}$ systems.^{12, 13}

$$\ln \gamma_1 = x_2 \left[\tau_{21} \left(\frac{G_{21}}{x_1 + x_2 G_{21}} \right)^2 + \frac{\tau_{12} G_{12}}{(x_2 + x_1 G_{12})^2} \right] \quad \text{S(22)}$$

$$\ln \gamma_2 = x_1 \left[\tau_{12} \left(\frac{G_{12}}{x_2 + x_1 G_{12}} \right)^2 + \frac{\tau_{21} G_{21}}{(x_1 + x_2 G_{21})^2} \right] \quad \text{S(23)}$$

$$\left\{ \begin{array}{l} \ln G_{12} = -\alpha_{12}\tau_{12} \\ \ln G_{21} = -\alpha_{21}\tau_{21} \\ \tau_{12} = \tau_{12}^{(0)} + \frac{\tau_{12}^{(1)}}{T} \\ \tau_{21} = \tau_{21}^{(0)} + \frac{\tau_{21}^{(1)}}{T} \end{array} \right. \quad S(24)$$

Here, G_{12} and G_{21} are interaction energy parameters, τ_{12} and τ_{21} are dimensionless interaction parameters, at reference point 0 and state point 1, and α_{12} and α_{21} are non-randomness parameters. Parameters values from literature were used for the calculations.^{12, 13} The NRTL method was applied to determine $\gamma_{\text{H}_2\text{O}}$ and γ_{NH_3} in binary TAN/H₂O streams, where nearly all TAN is present as NH₃; product streams 1.0 M NH_{3(aq)}, 5.0 M NH_{3(aq)}, and 10 NH_{3(aq)} met these criteria.

Experimentally Measured Osmotic and Activity Coefficients for Urea-Water Solutions. To account for nonideal behavior of urea, CO(NH₂)₂, and H₂O, reported literature values for $\gamma_{\text{CO(NH}_2)_2}$ and $\gamma_{\text{H}_2\text{O}}$ determined using vapor pressure osmometry data were utilized. For CO(NH₂)₂ concentrations ranging from 0.0103 to 1.6927 M, $\gamma_{\text{CO(NH}_2)_2} = -0.0663C_{\text{CO(NH}_2)_2} + 0.9976$ and $\gamma_{\text{H}_2\text{O}} = -0.0328C_{\text{CO(NH}_2)_2} + 0.9987$.¹⁴ Urea and water activity coefficients at CO(NH₂)₂ concentrations relevant to the analysis in this study were calculated with the linear relationships.

Activity Coefficients for 1.0 M KNO_{3(aq)} and 1.0 M NH₄NO_{3(aq)} recovery. To account for nonideal behavior in systems with $I > 0.5$ M, specifically, 1.0 M KNO_{3(aq)} and 1.0 M NH₄NO_{3(aq)}, activity coefficients based on isopiestic data¹⁵ at compositions relevant to the analysis were utilized.

Table S3. Standard state Gibbs free energy of formation for species in an aqueous solution.^{16, 17}

Species in Aqueous Solution	G_i^0 (kJ/mol)
NH ₄ ⁺	-79.3
NH ₃	-26.6
SO ₄ ²⁻	-744.5
H ₂ PO ₄ ⁻	-1130.2
HPO ₄ ²⁻	-1089.2
PO ₄ ³⁻	-1081.7
K ⁺	-283.3
Mg ²⁺	-454.8
NO ₃ ⁻	-111.3
H ₂ O	-237.1
OH ⁻	-157.2
H ⁺	0.0

Table S4. Standard state Gibbs free energy of formation for liquid and solid products.¹⁶⁻¹⁸ For urea, CO(NH₂)₂, the Gibbs free energy of dissolution, or the change in Gibbs free energy from CO(NH₂)_{2(aq)} to CO(NH₂)_{2(s)}, $G_{f,CO(NH_2)_2(s)}^0 - G_{f,CO(NH_2)_2(aq)}^0$ is presented.^{19, 20}

Product	$G_{f,P}^0$ (kJ/mol)
NH _{3(l)}	-16.410
(NH ₄) ₂ SO _{4(s)}	-901.7
(NH ₄)H ₂ PO _{4(s)}	-1210.38
KMgPO ₄ ·6H ₂ O _(s)	-3241
NH ₄ MgPO ₄ ·6H ₂ O _(s)	-3051.1
KH ₂ PO _{4(s)}	-1415.85
KNO _{3(s)}	-394.93
NH ₄ NO _{3(s)}	-183.9
CO(NH ₂) _{2(s)}	-5.77

Table S5. Molar minimum energies of recovery, \bar{E}_{\min} , for TAN products from each waste stream presented in Figure 3A of the main manuscript. \bar{E}_{\min} values are calculated at low and high TAN concentrations in the waste stream and low and high waste stream pH, *i.e.*, four \bar{E}_{\min} values calculated for each recovery scenario. The high and low wastewater pH ranges are respectively indicated by H and L, which correspond to the H and L \bar{E}_{\min} values. Also shown is the percent decrease in \bar{E}_{\min} of solution L relative to solution H (*i.e.*, from low to high pH range).

Product	Type of WW	High pH (H)	Low pH (L)	\bar{E}_{\min} (kJ/mol-TAN)					
				Low [TAN]			High [TAN]		
				H	L	Decrease from L to H (%)	H	L	Decrease from L to H (%)
(NH₄)₂SO₄(s)	Greywater	9	5	59.73	62.24	4.03	43.12	45.66	5.58
	2° WW effluent	7.7	6.8	53.37	53.56	0.36	39.94	39.75	0.47
	Domestic WW	8.5	6.5	43.15	44.28	2.54	38.28	39.44	2.94
	Fresh Urine	7.5	6	36.45	36.59	0.38	29.22	29.35	0.46
	Hydrolyzed Urine	9.2	9	25.45	26.24	2.99	21.02	21.73	3.28
NH₃(l)	Greywater	9	5	83.64	100.38	16.67	72.97	89.72	18.67
	2° WW effluent	7.7	6.8	98.66	99.63	0.97	85.08	86.06	1.13
	Domestic WW	8.5	6.5	82.48	89.11	7.44	77.51	84.16	7.90
	Fresh Urine	7.5	6	79.87	80.54	0.83	77.53	78.20	0.86
	Hydrolyzed Urine	9.2	9	51.63	57.26	9.83	49.81	55.44	10.15
10 M NH₃(aq)	Greywater	9	5	67.64	85.28	20.68	56.97	74.63	23.67
	2° WW effluent	7.7	6.8	83.49	84.52	1.22	69.92	70.95	1.46
	Domestic WW	8.5	6.5	67.00	74.01	9.47	62.03	69.06	10.18
	Fresh Urine	7.5	6	64.73	65.44	1.09	62.39	63.10	1.13
	Hydrolyzed Urine	9.2	9	35.37	41.27	14.30	33.57	39.46	14.93
5.0 M NH₃(aq)	Greywater	9	5	54.14	82.45	34.34	54.14	71.80	24.60
	2° WW effluent	7.7	6.8	80.67	81.70	1.26	67.09	68.12	1.52
	Domestic WW	8.5	6.5	64.17	71.18	9.84	59.20	66.23	10.61
	Fresh Urine	7.5	6	61.90	62.61	1.13	59.56	60.27	1.18
	Hydrolyzed Urine	9.2	9	32.57	38.46	15.32	30.81	36.69	16.01
1.0 M NH₃(aq)	Greywater	9	5	48.10	76.41	37.05	48.10	65.76	26.86
	2° WW effluent	7.7	6.8	74.63	75.65	1.36	61.05	62.09	1.67
	Domestic WW	8.5	6.5	58.13	65.14	10.76	53.17	60.20	11.69
	Fresh Urine	7.5	6	55.86	56.62	1.34	53.52	54.36	1.54
	Hydrolyzed Urine	9.2	9	26.80	33.07	18.96	25.35	32.03	20.86

Table S6. Molar minimum energies of recovery, \bar{E}_{\min} , for TOP products from each waste stream presented in Figure 3B of the main manuscript. \bar{E}_{\min} values are calculated at low and high TOP and co-species concentrations in the waste stream and low and high waste stream pH, *i.e.*, four \bar{E}_{\min} values calculated for each recovery scenario. The high and low wastewater pH ranges are respectively indicated by H and L, which correspond to the H and L \bar{E}_{\min} values. Also shown is the percent decrease in \bar{E}_{\min} of solution L relative to solution H (*i.e.*, from low to high pH range).

Product	Type of WW	High pH (H)	Low pH (L)	\bar{E}_{\min} (kJ/mol-TOP)					
				Low [TOP] and [Co-species]			High [TOP] and [Co-species]		
				H	L	Decrease from L to H (%)	H	L	Decrease from L to H (%)
KMgPO₄·6(H₂O)_(s)	Greywater	9	5	126.25	165.50	23.72	99.08	138.28	28.35
	2° WW effluent	7.7	6.8	106.56	125.56	15.13	96.30	114.97	16.24
	Domestic WW	8.5	6.5	90.99	124.47	26.89	87.92	120.80	27.22
	Fresh Urine	7.5	6	88.31	110.12	19.81	83.84	105.53	20.55
	Hydrolyzed Urine	9.2	9						
NH₄MgPO₄·6H₂O_(s)	Greywater	9	5	108.07	147.60	26.78	79.79	119.16	33.04
	2° WW effluent	7.7	6.8	102.84	120.90	14.93	81.54	99.27	17.86
	Domestic WW	8.5	6.5	78.25	110.91	29.45	70.12	102.31	31.46
	Fresh Urine	7.5	6	75.07	95.65	21.52	71.53	91.83	22.11
	Hydrolyzed Urine	9.2	9						
KH₂PO_{4(s)}	Greywater	9	5	91.09	90.47	-0.69	64.68	63.72	-1.51
	2° WW effluent	7.7	6.8	55.81	57.50	2.93	48.54	50.02	2.95
	Domestic WW	8.5	6.5	50.94	51.25	0.61	48.94	48.85	-0.20
	Fresh Urine	7.5	6	37.18	37.69	1.35	32.84	32.15	-2.14
	Hydrolyzed Urine	9.2	9	42.28	41.26	-2.47	38.97	38.00	-2.56
NH₄H₂PO_{4(s)}	Greywater	9	5	84.26	86.05	2.08	58.97	60.51	2.54
	2° WW effluent	7.7	6.8	65.87	67.74	2.76	49.04	50.43	2.74
	Domestic WW	8.5	6.5	51.90	53.39	2.79	46.14	46.63	1.06
	Fresh Urine	7.5	6	41.77	39.71	-5.18	39.26	35.48	-10.63
	Hydrolyzed Urine	9.2	9	36.48	36.59	0.28	34.45	34.53	0.24

METHODOLOGY TO DETERMINE THE MOLAR MINIMUM ENERGY TO RECOVER N FROM HYDROLYZED URINE AT $Y > 0$

For $\text{NH}_3(\text{l})$ and 1.0 M $\text{NH}_3(\text{aq})$ recovery from hydrolyzed urine, the speciation of TAN in the feed and retentate are not equal. Using Visual Minteq, pH and TAN speciation in the feed and retentate systems at various recovery yields were determined. To capture the buffering capacity of typical hydrolyzed urine, a model solution, consisting of typical concentrations of TAN, HCO_3^- , SO_4^{2-} , and TOP found in hydrolyzed urine (Table S7) was applied as the initial feed stream. TAN material balances were used to determine TAN mole fractions in the retentate. Then, Visual Minteq was used to determine the pH, α_{NH_3} , and $\alpha_{\text{NH}_4^+}$ for the feed and retentate streams in each recovery scenario (Tables S8 for $\text{NH}_3(\text{l})$ recovery and S8 for 1.0 M $\text{NH}_3(\text{aq})$ recovery). TAN speciation and material balance were used to determine NH_4^+ and NH_3 mole fractions in each stream, which were inputted into eqns S(10) and S(11) to calculate \bar{E}_{min} for $\text{NH}_3(\text{l})$ and 1.0 M $\text{NH}_3(\text{aq})$, respectively.

Table S7. Model hydrolyzed urine solution composition consisting of typical TAN, HCO_3^- , SO_4^{2-} , and TOP concentrations found in hydrolyzed urine. The target pH, 9.1, is the mid-range pH of hydrolyzed urine.

Salt	Concentration (M)
NH_4^+	0.424
Na^+	0.068
H^+	0.066
CO_3^{2-}	0.212
SO_4^{2-}	0.01
PO_4^{3-}	0.024
Cl^-	0.042

Table S8. Visual Minteq outputs for hydrolyzed urine feed and retentate streams in $\text{NH}_3(\text{l})$ product recovery scenarios at various recovery yields.

Stream	pH	$\alpha_{\text{NH}_3,\text{R}}$	$\alpha_{\text{NH}_4^+,\text{R}}$
Feed	9.106	0.420	0.580
Retentate at $Y = 0$	9.106	0.420	0.580
Retentate at $Y = 0.005$	9.096	0.418	0.582
Retentate at $Y = 0.2$	8.812	0.272	0.728
Retentate at $Y = 0.5$	6.911	4.666×10^{-3}	0.995
Retentate at $Y = 0.8$	5.843	4.007×10^{-4}	0.999
Retentate at $Y = 1$	2.278	1.091×10^{-7}	1.000

Table S9. Visual Minteq outputs for hydrolyzed urine feed and retentate streams in 1.0 M $\text{NH}_3(\text{aq})$ product recovery scenarios at various recovery yields.

Stream	pH	$\alpha_{\text{NH}_3,\text{R}}$	$\alpha_{\text{NH}_4^+,\text{R}}$
Feed	9.106	0.420	0.580
Retentate at $Y = 0$	9.106	0.420	0.580
Retentate at $Y = 0.005$	9.095	0.417	0.587
Retentate at $Y = 0.2$	8.813	0.272	0.728
Retentate at $Y = 0.5$	6.900	4.550×10^{-3}	0.995
Retentate at $Y = 0.8$	5.823	5.754×10^{-10}	1.000
Retentate at $Y = 1$	2.097	5.754×10^{-10}	1.000

IMPACT OF RECOVERY YIELD ON MOLAR MINIMUM ENERGY OF RECOVERY

The \bar{E}_{\min} trends of $\text{NH}_3(\text{l})$ and 1.0 M $\text{NH}_3(\text{aq})$ recovery from hydrolyzed urine as a function of recovery yield are not monotonic, but instead exhibit L-shaped rebounds with initial sharp decreases and followed by gradual increases. To further investigate the underlying reasons for these trends, \bar{E}_{\min} for $\text{NH}_3(\text{l})$ recovery from hydrolyzed urine, eqn S(10), was separated into its contributing terms, A and B , and term B is then further separated into terms C and D (eqns S(25), S(26), S(27), and S(28), respectively). The term that contributes most to the L-shape rebound is B ($= C + D$), i.e., the terms C and D dictate the change in \bar{E}_{\min} with different recovery yields. C represents the difference in Gibbs free energy of formation of $\text{NH}_4^+(\text{aq})$ moles in the retentate and feed normalized by moles of product captured; similarly, D is the difference in Gibbs free energy of formation of $\text{NH}_4^+(\text{aq})$ moles in the retentate and feed normalized by moles of product captured. Note that $G_{\text{NH}_4^+}$ and G_{NH_3} are constant values of -79.3 kJ/mol and -26.6 kJ/mol, respectively.

$$\begin{aligned}
 A = G_{f,\text{NH}_3(\text{l})}^0 + \frac{N_{\text{R}}}{N_{\text{P}}} \left[RT \left(\begin{aligned} &x_{\text{NH}_4^+,\text{R}} \ln(\gamma_{\text{NH}_4^+,\text{R}} x_{\text{NH}_4^+,\text{R}}) + x_{\text{NH}_3,\text{R}} \ln(\gamma_{\text{NH}_3,\text{R}} x_{\text{NH}_3,\text{R}}) \\ &+ x_{\text{H}_2\text{O},\text{R}} \ln(\gamma_{\text{H}_2\text{O},\text{R}} x_{\text{H}_2\text{O},\text{R}}) + x_{\text{H}^+,\text{R}} \ln(\gamma_{\text{H}^+,\text{R}} x_{\text{H}^+,\text{R}}) \\ &+ x_{\text{OH}^-,\text{R}} \ln(\gamma_{\text{OH}^-,\text{R}} x_{\text{OH}^-,\text{R}}) \end{aligned} \right) \right] \\
 - \frac{N_{\text{F}}}{N_{\text{P}}} \left[RT \left(\begin{aligned} &x_{\text{NH}_4^+,\text{F}} \ln(\gamma_{\text{NH}_4^+,\text{F}} x_{\text{NH}_4^+,\text{F}}) + x_{\text{NH}_4^+,\text{F}} \ln(\gamma_{\text{NH}_4^+,\text{F}} x_{\text{NH}_4^+,\text{F}}) \\ &+ x_{\text{H}_2\text{O},\text{F}} \ln(\gamma_{\text{H}_2\text{O},\text{F}} x_{\text{H}_2\text{O},\text{F}}) + x_{\text{H}^+,\text{F}} \ln(\gamma_{\text{H}^+,\text{F}} x_{\text{H}^+,\text{F}}) \\ &+ x_{\text{OH}^-,\text{F}} \ln(\gamma_{\text{OH}^-,\text{F}} x_{\text{OH}^-,\text{F}}) \end{aligned} \right) \right] \quad \text{S(25)} \\
 - \frac{N_{\text{F}}}{N_{\text{P}}} \left[x_{\text{NH}_4^+,\text{F}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{F}} G_{\text{NH}_3} + x_{\text{H}_2\text{O},\text{F}} G_{\text{H}_2\text{O}} + x_{\text{OH}^-,\text{F}} G_{\text{OH}^-} \right]
 \end{aligned}$$

$$B = \frac{N_{\text{R}}}{N_{\text{P}}} \left[x_{\text{NH}_4^+,\text{R}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{R}} G_{\text{NH}_3} \right] - \frac{N_{\text{F}}}{N_{\text{P}}} \left[x_{\text{NH}_4^+,\text{F}} G_{\text{NH}_4^+} + x_{\text{NH}_3,\text{F}} G_{\text{NH}_3} \right] \quad \text{S(26)}$$

$$C = \frac{N_{\text{R}}}{N_{\text{P}}} \left[x_{\text{NH}_4^+,\text{R}} G_{\text{NH}_4^+} \right] - \frac{N_{\text{F}}}{N_{\text{P}}} \left[x_{\text{NH}_4^+,\text{F}} G_{\text{NH}_4^+} \right] \quad \text{S(27)}$$

$$D = \frac{N_R}{N_P} \left[x_{\text{NH}_3, \text{R}} G_{\text{NH}_3} \right] - \frac{N_F}{N_P} \left[x_{\text{NH}_3, \text{F}} G_{\text{NH}_3} \right] \quad \text{S(28)}$$

Figure S1 displays the contributions of each term toward \bar{E}_{min} and shows that C follows an L-shaped rebound (i.e., a sharp decrease with increasing Y followed by a more gradual increase with increasing Y), which is similar to the \bar{E}_{min} trend. Initially, C decreases as Y increases, indicating that the difference between moles of NH_4^+ in the feed and retentate decreases with the initial increase in Y . This is due to the decline in retentate pH with higher recovery yields, which corresponds to increased $\alpha_{\text{NH}_4^+, \text{R}}$ and decreased $\alpha_{\text{NH}_3, \text{R}}$ (see Tables S8 and S9 for pH and speciation in the feed and retentate at different recovery yields). Although increased recovery yield results in lower TAN in the retentate, a higher fraction of TAN remaining in the retentate speciates to NH_4^+ , thus C initially decreases with higher recovery yield. However, once the pH of the retentate is sufficiently lower than the $\text{p}K_{\text{a}}$, such that NH_4^+ is predominant compared to NH_3 , additional increase in Y results in reduced NH_4^+ in the retentate. At this point, C begins to increase with higher recovery yield. D follows the opposite trend as C with an initial sharp increase with higher recovery yields followed by a gradual decrease with higher recovery yields. Initially, $\text{NH}_{3(\text{aq})}$ in the retentate are lost to both the product and protonation to NH_4^+ . Then, once essentially all TAN is present as NH_3 , increases in Y no longer result in significant changes to speciation, thus D increases.

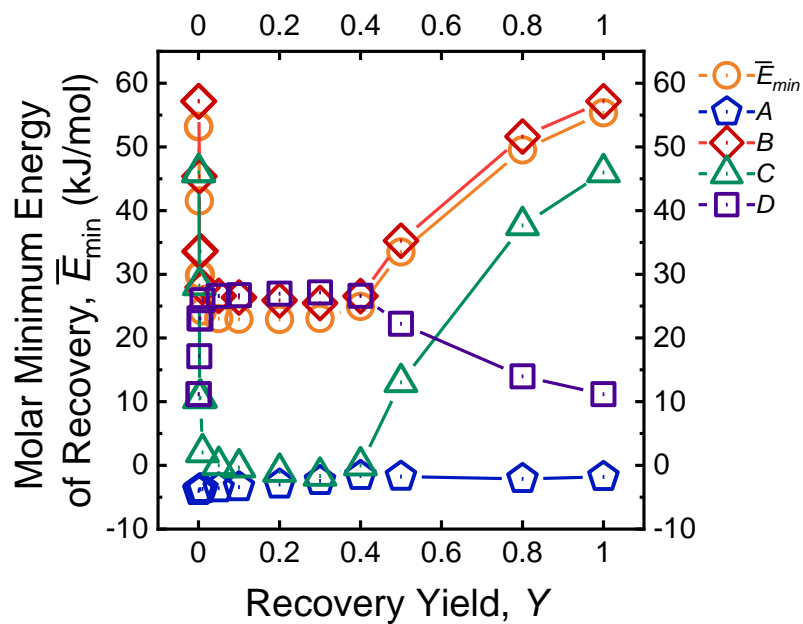


Figure S1. Molar minimum energy, \bar{E}_{min} , as a function of recovery yield to recover $\text{NH}_{3(l)}$ from hydrolyzed urine and the contributing terms A , B , C , and D .

Table S10. The change in the sum of the standard state Gibbs free energy of individual ions, $\sum x_i G_i$, between the final state (product and retentate) and initial state (waste stream feed); denoted by $\Delta \sum x_i G_i$. Note that a range is provided for $\text{NH}_4\text{NO}_3(\text{aq})$ and $\text{NH}_4\text{NO}_3(\text{s})$ recoveries because this value is dependent on pH of the waste stream.

Waste Stream	Product	$\Delta \sum x_i G_i$
Secondary wastewater effluent	$\text{KNO}_3(\text{s})$	-0.330
	$\text{NH}_4\text{NO}_3(\text{s})$	5.797-7.569
	$\text{KNO}_3(\text{aq})$	0.000
	$\text{NH}_4\text{NO}_3(\text{aq})$	-0.002
Fresh urine	$\text{Urea}(\text{aq})$	0.000
	$\text{Urea}(\text{s})$	-5.774

Table S11. Molar minimum energy for recovery of select products, $\text{NH}_3(\text{l})$ and $1.0 \text{ M NH}_3(\text{aq})$, from waste streams of secondary wastewater effluent and hydrolyzed urine calculated with the exclusion and inclusion of passive species, Na^+ and Cl^- . All calculations considered nutrients and co-species of TAN, H_2O , H^+ , and OH^- . Eqns S(6) and S(7) were applied for the determination of \bar{E}_{min} to recover $\text{NH}_3(\text{l})$ and $1.0 \text{ M NH}_3(\text{aq})$, from waste streams excluding Na^+ and Cl^- species. Eqns S(19) and S(20) were applied for the determination of \bar{E}_{min} . Note that the mid-range pH and TAN concentration in each waste stream were utilized in the analysis, thus the mid-range molar minimum energy of recovery is reported. The percent increase in molar minimum energy for recovery observed when including Na^+ and Cl^- species in the analysis is also presented for each recovery scenario.

Waste Stream	Product	Specific Minimum Energy for Recovery, \bar{E}_{min} (kJ/mol)		
		Excluding Na^+ and Cl^- Species	Including Na^+ and Cl^- Species	Percent Increase (%)
Secondary WW Effluent	$\text{NH}_3(\text{l})$	87.45	87.48	0.22
Secondary WW Effluent	$1.0 \text{ M NH}_3(\text{aq})$	63.46	63.70	0.38
Hydrolyzed Urine	$\text{NH}_3(\text{l})$	50.47	50.52	0.10
Hydrolyzed Urine	$1.0 \text{ M NH}_3(\text{aq})$	26.39	26.89	1.89

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