Corrigendum

Thermodynamic yield predictions for biodegradation through oxygenase activation reactions

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There is a discrepancy between Tables 2 and 3 and Equations (18) and (20) in this paper. Equations (18) and (20) show the mineralization of NTA and EDTA as deprotonated anions (NTA^{3-} and $EDTA^{4-}$) and provide computed ΔG^{01}_{eD} for this case. Tables 2 and 3 provide calculations based on the stoichiometry of the *protonated* forms, H_3NTA and H_4EDTA. Since the ΔG^{01}_{f} values for NTA and EDTA given in Appendix A are estimated following Mavrovouniotis (1991), a method that assumes carboxylic groups are *deprotonated*, the stochiometry and associated yield calculations in Tables 2 and 3 are incorrect. This discrepancy in selecting the form for the stoichiometry introduces an error into the calculated values that is carried through the tables. The corrected tables appear here. Values that have been corrected are shown in bold.

The correction indicated here improves the predictions from the original stoichiometric yield prediction method of McCarty and the new oxygenase-catalyzed stoichiometric yield prediction method. However, the correction does not change the overall conclusion of this paper that the new method significantly improves yield prediction for electron donor pathways that are catalyzed by oxygenase enzymes. The original method errors are reduced from 80% and 120% to 63% and 88%, respectively for NTA and EDTA. The new oxygenase method errors are reduced from 44% and 22% to 30% and 8%, respectively for NTA and EDTA.

One other point should also be corrected. As my group has continued to work on EDTA biodegradation modeling, we sought to confirm the yield values published by Henneken et al. (1995, 1998). Henneken et al. (1998) report a yield of 0.271 g CDW/g EDTA and a maintenance coefficient of 15.5 mg EDTA/g CDW-hour. In VanBriesen (2001), I assumed 0.271 g CDW/g EDTA was the *observed* yield and used the maintenance costs and observed maximum cell growth rate to estimate the theoretical yield as 0.245 C-mole cells/C-mole EDTA. However, recent communications with Henneken confirm that 0.271 g CDW/g EDTA is actually a *theoretical* yield value computed from their observation and the maintenance coefficient and growth rate. Thus, the correction of this value shown after Equation (21) in VanBriesen (2001) is unnecessary and only a unit conversion is needed. The yield that should be shown after Equation (21) and in Table 3 is 0.266 C-mole cells/C-mole EDTA.

References

Henneken LB, Nortemann B & Hempel DC (1995) Influence of physiological conditions on EDTA degradation. Appl. Microbiol. Biotechnol. 44: 190–197

Henneken L, Nortemann B & Hempel DC (1998) Biological degradation of EDTA: reaction kinetics and technical approach. J. Chem. Technol. Biotechnol. 73: 144–152

Mavrovouniotis ML (1991) Estimation of standard Gibbs energy changes of biotransformations. J. Biol. Chem. 266: 14440–14445

Table 2. Key parameters and calculated values for NTA mineralization reactions

Parameter	Original McCarty method	New oxygenase method
ΔG_D^{01} (kJ/mole)	**580.32**	**891.72**
γ_S (degree of reductance of substrate)	3	3
γ_C (degree of reductance of cells)	4.2	4.2
EQs (electrons in 1 mole substrate)	18	18
N_O (electrons invested in oxygenase reaction)	0	4
N_T (electrons transferred)	18	14
$\Delta G_{e\text{-}ox}^{01}$ (kJ/eeq) = ΔG_{eA}^{01}	−78.14	−78.14
ΔG_{eD}^{01} (kJ/eeq)	**32.24**	–
$(\Delta G_{eD}^{01})^{ox}$ (kJ/eeq)	–	**41.37**
ΔG_{eR}^{01} (kJ/eeq)	**−110.38**	**−119.51**
ΔG_{eCS}^{01} (kJ/eeq)	**32.24**	**32.24**
$\Delta G_{e\text{-}cells}^{01}$ (kJ/eeq)	34.75	34.75
$\Delta G_{e\text{-}syn}^{01}$ (kJ/eeq) following Equation (9)	**40.6**	**40.6**
κ	0.6	0.6
f_{ox}	0	0.22
$T = N_T/EQs = f_s^0 + f_e^0$	1	0.78
f_s^0	**0.62**	**0.50**
f_e^0	**0.38**	**0.28**
Predicted yield (Cmole/Cmole); following Equation (3)	**0.44**	**0.35**
Experimental yield (Cmole/Cmole)	0.271	0.271
Error $\left(\frac{\lvert \text{ExpYield} - \text{PredYield} \rvert}{\text{ExpYield}} * 100\%\right)$	**+63%**	**+30%**

Table 3. Key parameter and calculated values for EDTA mineralization reactions

Parameter	Original McCarty method	New oxygenase method
ΔG_D^{01} (kJ/mole)	**1088.08**	**2343.36**
γ_S (degree of reductance of substrate)	3.4	3.4
γ_C (degree of reductance of cells)	4.2	4.2
EQs (electrons in 1 mole substrate)	34	34
N_O (electrons invested in oxygenase reaction)	0	16
N_T (electrons transferred)	34	18
$\Delta G_{e\text{-}ox}^{01}$ (kJ/eeq) = ΔG_{eA}^{01}	−78.14	−78.14
ΔG_{eD}^{01} (kJ/eeq)	**32.02**	–
$(\Delta G_{eD}^{01})^{ox}$ (kJ/eeq)	–	**60.73**
ΔG_{eR}^{01} (kJ/eeq)	**−110.16**	**−138.87**
ΔG_{eCS}^{01} (kJ/eeq)	**32.02**	**32.02**
$\Delta G_{e\text{-}cells}^{01}$ (kJ/eeq)	34.75	34.75
$\Delta G_{e\text{-}syn}^{01}$ (kJ/eeq) following Equation (9)	**41.0**	**41.0**
κ	0.6	0.6
f_{ox}	0	0.47
$T = N_T/EQs = f_s^0 + f_e^0$	1	0.53
f_s^0	**0.62**	**0.36**
f_e^0	**0.38**	**0.17**
Predicted yield (Cmole/Cmole); following Equation (3)	**0.50**	**0.29**
Experimental yield (Cmole/Cmole)	**0.266**	**0.266**
Error $\left(\frac{\lvert \text{ExpYield} - \text{PredYield} \rvert}{\text{ExpYield}} * 100\%\right)$	**+88%**	**+8%**