Correction to "Use of Dispersive Kinetic Models for Nucleation and Denucleation to Predict Steady-State Nanoparticle Size Distributions and the Role of Ostwald Ripening"

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From eq 3 in the text, the accurate derivation of eq 4 yields

$$E_a - E_a^0 = \frac{-2\gamma v_m (r - r_0)}{r^2} \tag{A}$$

because the relationship between activation energy and particle radius is nonlinear. Given that $r_0 = 0$ for cases of nucleation-and-growth, eq A reduces to

$$g(r) = \left[\alpha\sqrt{\beta}\, e^{\left\{ -\left\{ \frac{\alpha\sqrt{\beta k_B T}\left[e^{2\gamma v_m(r-r_0)/k_B T r^2} - 1 \right]}{\sqrt{2}\sqrt{\frac{\gamma v_m(r-r_0)}{r^2}}} \right\} \right\}} \left\{ 4\gamma v_m (r - r_0) e^{\left[2\gamma v_m(r-r_0)/k_B T r^2 \right]} - k_B T r^2 \left[e^{2\gamma v_m(r-r_0)/k_B T r^2} - 1 \right] \right\} \right] \Big/ \left[4\sqrt{2 k_B T}\, r^2 \left[\frac{\gamma v_m(r-r_0)}{r^2} \right]^{3/2} \right] \tag{C}$$

noting that $E_a \leq E_a^0$ over the course of nucleation-and-growth, while $r > 0$.

On the other hand, for cases of denucleation, $E_a \geq E_a^0$ and $r \leq r_0$ over the course of the conversion. Thus

$$E_a - E_a^0 = \frac{-2\gamma v_m}{r} \tag{B}$$

which, when substituted into eq 2, gives rise to a solution that can be used to generate the plots shown in Figure 2 and Figure 3 of the paper. However, eq 5 (the solution without the assumption that $r_0 = 0$) should read

$$E_a - E_a^0 = \frac{-2\gamma v_m (r_0 - r)}{r^2} \tag{D}$$

When eq D is substituted into eq 7 in the text, the following result is obtained (in place of eq 8 in the text)
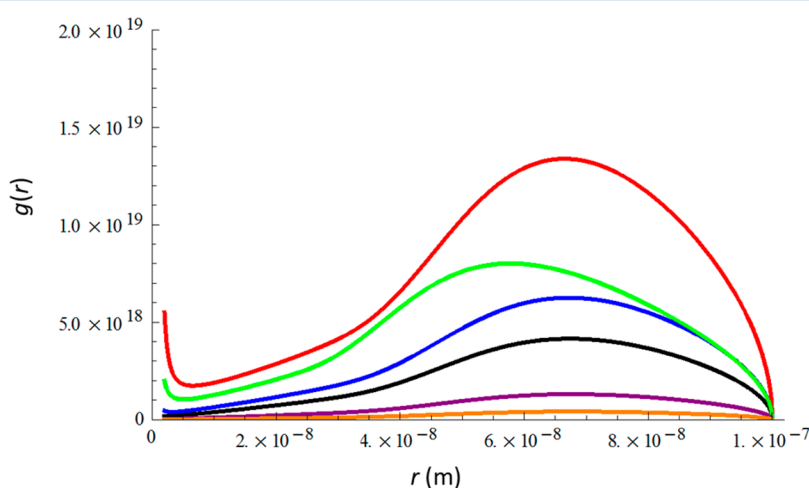

Figure 4. Theoretical molar PSDs plotted using eq E and the values for interfacial tension and monomer volume as per Figure 2. In all cases, it was assumed that $r_0 = 100$ nm. The other relevant physical parameters are: (red) $\alpha = 0.001$ s, $-\beta = 0.0002$ s^{-2}, $T = 298$ K; (black) $\alpha = 0.001$ s, $-\beta = 0.002$ s^{-2}, $T = 298$ K; (blue) $\alpha = 0.0015$ s, $-\beta = 0.002$ s^{-2}, $T = 298$ K; (green) $\alpha = 0.001$ s, $-\beta = 0.0002$ s^{-2}, $T = 498$ K; (purple) $\alpha = 0.0001$ s, $-\beta = 0.0002$ s^{-2}, $T = 298$ K; (orange) $\alpha = 0.001$ s, $-\beta = 0.2$ s^{-2}, $T = 298$ K. The abscissa is plotted from 2 to 100 nm because there is an artifact in that $g(r)$ increases rapidly as $r \to 0$ because the function is undefined at $r = 0$. The distributions are not normalized.

$$g(r) = \left[\alpha e^{-\left\{ \frac{\sqrt{2}\,\alpha\left[e^{2\gamma v_{\mathrm{m}}(r-r_0)/k_{\mathrm{B}}Tr^2}-1\right]\sqrt{\frac{\gamma v_{\mathrm{m}}(r_0-r)}{r^2}}}{\sqrt{\beta k_{\mathrm{B}}T}} \right\}} \left\{ k_{\mathrm{B}}Tr^2 - e^{[2\gamma v_{\mathrm{m}}(r-r_0)/k_{\mathrm{B}}Tr^2]}[k_{\mathrm{B}}Tr^2 + 4\gamma v_{\mathrm{m}}(r-r_0)] \right\} \right] / \left[2\sqrt{2\beta}\,(k_{\mathrm{B}}T)^{3/2}r^2\sqrt{\frac{\gamma v_{\mathrm{m}}(r_0-r)}{r^2}} \right]$$

(E)

While plots of eq E show tailing in the opposite direction to the predicted curves in Figure 2/Figure 3, they look different than the curves presented in the original Figure 4. Here, Figure 4 is reconstructed using the corrected PSD function, eq E, in place of eq 8 in the text.

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