

Erratum list for “*Digital Simulation in Electrochemistry*”

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A number of errors in the book have been pointed out to me by sharp-eyed readers. Please let me know if you see any others.

- Page 13: the statement just after (2.29) should read
“so that one p -unit corresponds to $25.69/n$ mV.”
Thanks to Dr. Fekner (Lublin, Poland) who pointed this out.

- Page 23: equation (2.79) should read

$$G = \sqrt{K} \operatorname{erf} \sqrt{KT} + \frac{\exp(-KT)}{\sqrt{\pi T}}. \quad (2.79)$$

- Page 27: equation (2.99) should read

$$i(t) = n\mathcal{F}Ac_b \sqrt{\frac{n\mathcal{F}Dv}{\mathcal{R}T}}. \quad (2.99)$$

- Page 105, top: Feldberg [231] is cited as the originator of exponentially expanding space intervals. However, earlier in the same year (1981), Seeber and Stefani [501] described the same grid expansion scheme. This earlier work was inadvertently overlooked in the book, and the paper is only cited in the context of unequal time intervals. Apologies to Seeber and Stefani for this lapse.
- Page 110, last line of the first paragraph: the calculation of H_1 is in error, the correct value being 0.0195691. Thanks to Dr. Fekner (Lublin, Poland) for pointing this out. I had neglected to multiply by $X_{lim} = 6$.
Also, although this is not an error as such, the citation in line 3 of that paragraph to Martínez-Ortiz is now out of date, and [385] should now read F. Martínez-Ortiz, N. Zoroa, A. Molina C. Serna and E. Laborda, *Electrochim. Acta* **54** (2009) 1042-1055. (24.2.2011)
- Page 160, line 7 after equation (9.30). There is a reference to the book by Lapidus and Pinder, page 19-; this should be page 39 instead.

- Page 194, equation (11.2): there is a plain F instead of the gothic, and the equation should read

$$\rho = R_u \frac{n\mathcal{F}}{\mathcal{RT}} n\mathcal{F} D^{\frac{1}{2}} c^* \sqrt{\frac{n\mathcal{F}v}{\mathcal{RT}}} . \quad (1)$$

- Page 196, equation (11.12): the symbol γ_c was left out on both sides of the equation, which should read

$$G'_c + \frac{\gamma_c \rho}{\delta T} (G'_c + G'_A) = \gamma_c + \frac{\gamma_c \rho}{\delta T} (G_c + G_A) . \quad (11.12)$$

This affects also the fifth row of the Jacobian matrix (11.20), where again both of these terms need correcting in the same manner, and that equation becomes

$$\vec{J} \equiv \begin{bmatrix} 1 & -\exp(p) & 0 & 0 & 0 & -\exp(p)C_{B,0} \\ V_A & 0 & 1 & 0 & 0 & 0 \\ 0 & V_B & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & \frac{\gamma_c \rho}{\delta T} & 0 & 1 + \frac{\gamma_c \rho}{\delta T} & 0 \\ 0 & 0 & -\rho & 0 & -\rho & 1 \end{bmatrix} . \quad (11.20)$$

Finally, in Fig. 11.1, the correction makes the capacitive curve (dotted, lowest curve) much smaller in its swings. I have corrected the example program LSV4IRC as presented in my own web page under Examples, but this was not possible at the Springer site.

- Page 203, equation (12.4): the equation should read

$$i(t) = n\mathcal{F}D \int_{r=0}^a 2\pi r \left. \frac{\partial c}{\partial z} \right|_{z=0} dr . \quad (12.4)$$

- Page 206: equation (12.19) should read

$$I(T) = \int_{R=0}^1 \frac{\pi R}{2} \left. \frac{\partial C}{\partial Z} \right|_{Z=0} dR . \quad (12.19)$$

This comes about as a result of normalising the current value to the Saito steady state value, $4n\mathcal{F}Dac_b$, as given in (12.5) on page 204.

- Page 207; not actually an error, but an improvement: I have received new values for the last two coefficients in (12.24), extended to more decimals, and they are, respectively, -0.120031163 and 0.0132727696. The new values were kindly communicated to me by Dr. Peter Mahon, Swinbourne, Australia. (6.12.2007).

- Page 208: the section from equation (12.26) to equation (12.28) should read as:

$$\frac{\partial C}{\partial T} = \frac{1}{P^2} \left(\frac{\partial^2 C}{\partial R^2} + \frac{1}{R} \frac{\partial C}{\partial R} + \frac{\partial^2 C}{\partial Z^2} \right) \quad (12.26)$$

with $T = t/\tau$ and

$$\tau = \frac{\mathcal{RT}}{n\mathcal{F}v} \quad (12.27)$$

making P , the ratio of disk radius to the Nernst diffusion layer thickness for the duration τ equal to

$$P = \frac{a}{\sqrt{D\tau}} = (a^2 n\mathcal{F}v / R\mathcal{T}D)^{\frac{1}{2}}. \quad (12.28)$$

- Page 208: equation (12.29) should read

$$\frac{i(T)}{n\mathcal{F}Dc^*l} = \frac{1}{\sqrt{\pi T}} + 1. \quad (12.29)$$

Also, this equation is incorrectly attributed to Szabo et al, but in fact originated with K. Aoki, K. Tokuda and H. Matsuda, *Denki Kagaku* **54** (1986) 1010.

- Page 228, Table 12.2; the entries for **OAS** are incorrect. The correct Table should be

Table 12.2: Parameter values for the diffusion equations in the AF and OAS spaces. For better readability, the symbols $\theta' \equiv \frac{\pi}{2}\theta$ and $\Gamma' \equiv \frac{\pi}{2}\Gamma$ are used.

| Parameter | AF | OAS |
|------------|----------------------------------|---|
| F | $\theta^2 + \tan^2 \Gamma'$ | $\frac{1}{\cos^2 \Gamma'} (\cos^2 \theta' + \sin^2 \theta' \sin^2 \Gamma')$ |
| a_θ | $1 - \theta^2$ | $\frac{4}{\pi^2}$ |
| b_θ | -2θ | $\frac{2}{\pi} \cot \Gamma'$ |
| a_Γ | $\frac{4}{\pi^2} \cos^2 \Gamma'$ | $\frac{4}{\pi^2} \cos^2 \Gamma'$ |
| b_Γ | 0 | 0 |

- Page 303: not actually an error but an advance. The subroutine `U_DERIV` has now been superseded by the new routine `FORNBERG.f90`, downloadable from this page. It is based on the algorithm by Fornberg, *Math. Comp.* 51 (1988) 699. It does not compute the coefficients via Taylor expansions and a linear system, but in a recursive process. It can return derivatives of any given degree, at any given point in (or indeed outside) a given set of coordinates, including the zero-degree “derivative”, which is an interpolation. Whereas `U_DERIV` begins to fail badly after about 11 points, the new routine can handle up to 15 points accurately, and even up to (as tested) 21 points, it still delivers good values. (Feb 21, 2008)
- Page 313, ref. 1: the URL is incomplete. The proper URL is <http://hsl.rl.ac.uk/archive/hslarchive.html>