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LETTER TO THE EDITOR

Concentration profile curvature for diffusion processes with simultaneous irreversible reaction

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In a recent paper, Thiagarajan et al. [1] explored the utility of a perturbation method for solving the following differential equation [Equation (11) in their paper]:

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} = \frac{ku}{1+\alpha u} \quad (k \text{ and } \alpha \text{ are constants}) \tag{1}$$

subject to two different sets of boundary conditions:

$$\text{Case 1: } u(0) = 1, u(1) = 0; \quad \text{Case 2: } u(0) = 1, \frac{\mathrm{d}u}{\mathrm{d}x}(1) = 0.$$

Figures 1 and 3 in their paper depict $u(x)$ profiles for Case 1 and 2, respectively, for the parameter ranges $0.01 \leq k \leq 10$ and $0.01 \leq \alpha \leq 10$. The authors' figures show excellent agreement between the results of calculations based on their perturbation solution to (1), which they provided in detail, and their numerical solution to (1), for which they provided a Matlab program listing.

We are puzzled by the $u(x)$ profiles in Figures 1c and 3c, which were calculated with $\alpha = 10$ and k assigned the aforementioned range of values. Portions of these profiles, and in some cases their entireties, are concave downward, i.e., $\frac{\mathrm{d}^2u}{\mathrm{d}x^2} < 0$. Notwithstanding the overlap of results based on two different analyses, the downward concavity is inconsistent with (1), the right-hand side of which cannot be negative. Such behavior is notably absent from the $u(x)$ profiles in Figures 1a, 1b, 3a and 3b, which were calculated with α fixed at considerably lower values.

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It is also worth noting that:

- Using the authors' Matlab code for the *numerical* solution to (1), we were able to replicate the numerical results depicted in Figures 1a, 1b, 3a and 3b; but were unable to replicate those in Figures 1c and 3c.
- Using the authors' *perturbation* solution for Case 1 [Equations (14) and (16) in their paper], we replicated their analytical results, including not only the curves in Figures 1a and 1b with the expected upward concavity, but also those in Figure 1c with the anomalous downward concavity.

References

1. S. Thiagarajan, A. Meena, S. Anitha, L. Rajendran, Analytical expression of the steady-state catalytic current of mediated bioelectrocatalysis and the application of He's Homotopy perturbation method. J. Math. Chem. **49**, 1727–1740 (2011)