Electronic Supplementary Material (ESI) for Analyst.

Supplementary Information for "The Application of Physics-Informed Neural Networks to Hydrodynamic Voltammetry"

Haotian Chen[a], Enno Kätelhön[b], Richard G. Compton[a]*

[a] Department of Chemistry, Oxford University, South Parks Road, Oxford OX1 3QZ, Great Britain

[b] MHP Management- und IT-Beratung GmbH, Königsallee 49, 71638 Ludwigsburg, Germany

* Corresponding author.

Email address: Richard.compton@chem.ox.ac.uk (R. G. Compton)

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1 PINN Simulation of a Double Channel Electrode

The steady state transport limited currents flowing through both the generator and detector electrodes and thus the collection efficiency of double channel electrode. $C_A(X,Y)$ is predicted at steady state using a PINN. The physical constraints are:

$$\frac{\partial^2 C_A}{\partial Y^2}+\frac{\partial^2 C_A}{\partial X^2}-V_x\frac{\partial C_A}{\partial X}=0, \Omega_X\times\Omega_Y \quad 1.1$$

$$\frac{dC_A}{dY}=0, X=[0,X_1], Y=0 \quad 1.2$$

$$C_A=0, X=[X_1,X_2] \quad 1.3$$

$$\frac{dC_A}{dY}=0, X=[X_2,X_3], Y=0 \quad 1.4$$

$$C_A=1, X=[X_3,X_4] \quad 1.5$$

$$\frac{dC_A}{dY}=0, X=[X_4,X_{Channel}], Y=0 \quad 1.6$$

$$C_A=1, X=0,\Omega_Y \quad 1.7$$

$$\frac{dC_A}{dY}=0, \Omega_X, Y=Y_{channel} \quad 1.8$$

where $\Omega_X\in[0,X_{channel}]$ and $\Omega_Y\in[0,Y_{channel}]$. To enforce the constraints, the mean square error (MSE) loss functions are:

$$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{\partial^2 C_A}{\partial Y^2}+\frac{\partial^2 C_A}{\partial X^2}-V_x\frac{\partial C_A}{\partial X}\right)^2, \Omega_X \times \Omega_Y \quad 2.1$$

$$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{dC_A}{dY}\right)^2, X=[0,X_1], Y=0 \quad 2.2$$

$$\frac{1}{N}\sum_{i=1}^{N}(C_A)^2, X=[X_1,X_2] \quad 2.3$$

$$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{dC_A}{dY}\right)^2, X=[X_2,X_3], Y=0 \quad 2.4$$

$$\frac{1}{N}\sum_{i=1}^{N}(C_A-1)^2, X=[X_3,X_4] \quad 2.5$$

$$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{dC_A}{dY}\right)^2, X=[X_4, X_{Channel}], Y=0 \quad 2.6$$

$$\frac{1}{N}\sum_{i=1}^{N}(C_A-1)^2, X=0,\Omega_Y \quad 2.7$$

$$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{dC_A}{dY}\right)^2, \Omega_X, Y=Y_{channel} \quad 2.8$$

The global loss implemented in PINN is a linear combination of all the MSEs as:

$$L=\sum_{i=1}^{8} w_i MSE_i \#(3)$$

where w_i is the weight of each MSE. w is set to 1 to generate the results in this paper.

2 PINN Simulation of a Channel Electrode with CE reaction

The transport limited current of channel electrode is calculated for a CE reaction via a PINN which predicts the concentration of the two species, $C_R(X,Y)$ and $C_A(X,Y)$ in the simulation domain while satisfying the following two sets of constraints. For species R:

$$\frac{\partial^2 C_A}{\partial Y^2}+\frac{\partial^2 C_A}{\partial X^2}-V_x\frac{\partial C_A}{\partial X}+K_f C_R-K_b C_A=0 \quad 4.1$$

$$\frac{\partial C_A}{\partial Y}=0, X=[0,X_1], y=0 \quad 4.1$$

$$C_A=0, X=[X_1,X_2], y=0 \quad 4.2$$

$$\frac{\partial C_A}{\partial Y}=0, X=[X_2,X_{channel}] \quad 4.3$$

$$C_A=C_A^*, X=0, Y=[0,Y_{channel}] \quad 4.4$$

$$\frac{\partial C_A}{\partial Y}=0, X=[0,Y_{channel}], Y=Y_{channel} \quad 4.5$$

And for species A:

$$d_R\frac{\partial^2 C_R}{\partial Y^2} + d_R\frac{\partial^2 C_R}{\partial X^2} - V_x\frac{\partial C_R}{\partial X} - K_f C_R + K_b C_A = 0 \quad 5.1$$

$$\frac{\partial C_R}{\partial Y} = 0, X = [0, X_{channel}], Y = 0 \quad 5.2$$

$$C_R = C^*_R, X = 0, Y = [0, Y_{channel}] \quad 5.3$$

$$\frac{\partial C_R}{\partial Y} = 0, X = [0, X_{channel}], Y = Y_{channel} \quad 5.4$$

The MSE loss functions consider both eqn(4) and eqn(5) are:

$$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{\partial^2 C_A}{\partial Y^2} + \frac{\partial^2 C_A}{\partial X^2} - V_x\frac{\partial C_A}{\partial X} + K_f C_R - K_b C_A\right)^2, \Omega_X \times \Omega_Y \quad 6.1$$

$$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{\partial C_A}{\partial Y}\right)^2, X = [0, X_1], y = 0 \quad 6.2$$

$$\frac{1}{N}\sum_{i=1}^{N}(C_A)^2, X = [X_1, X_2], y = 0 \quad 6.3$$

$$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{\partial C_A}{\partial Y}\right)^2, X = [X_2, X_{channel}] \quad 6.4$$

$$\frac{1}{N}\sum_{i=1}^{N}(C_A - C^*_A)^2, X = 0, Y = [0, Y_{channel}] \quad 6.5$$

$$\frac{\partial C_A}{\partial Y} = 0, X = [0, Y_{channel}], Y = Y_{channel} \quad 6.6$$

$$\frac{1}{N}\sum_{i=1}^{N}\left(d_R\frac{\partial^2 C_R}{\partial Y^2} + d_R\frac{\partial^2 C_R}{\partial X^2} - V_x\frac{\partial C_R}{\partial X} - K_f C_R + K_b C_A\right)^2, \Omega_X \times \Omega_Y \quad 6.7$$

$$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{\partial C_R}{\partial Y}\right)^2, X = [0, X_{channel}], Y = 0 \quad 6.8$$

$$\frac{1}{N}\sum_{i=1}^{N}(C_R - C^*_R)^2, X = 0, Y = [0, Y_{channel}] \quad 6.9$$

$$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{\partial C_R}{\partial Y}\right)^2, X = [0, X_{channel}], Y = Y_{channel} \quad 6.10$$

The global loss is thus a linear combination of eqn(6) as:

$$L = \sum_{i=1}^{10} w_i MSE_i \#(7)$$

To predict mass transport of two species, two independent neural networks are first constructed, specializing in predicting C_R and C_A respectively. Then the two networks are connected via the physical constraints implemented according to eqn(6) and a schematic illustration is shown in Figure S 1. Implementation using TensorFlow can be found at https://github.com/nmerovingian/PINN-Hydrodynamic-Voltammetry.

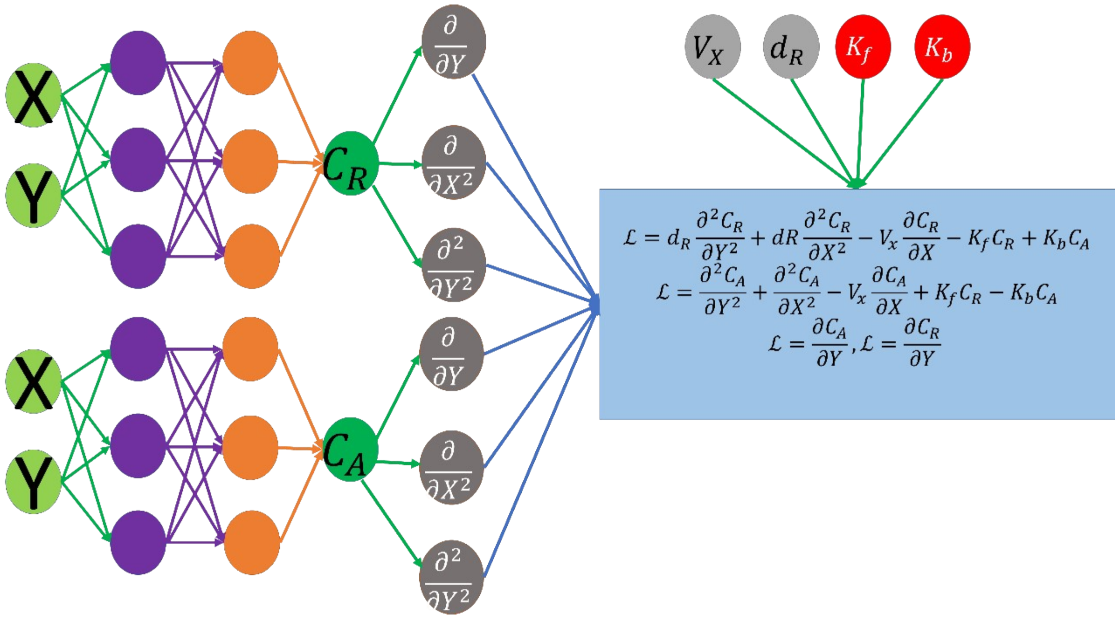

Figure S 1. Schematic illustration of the structure of the PINN when predicting channel electrode transport limited current for a CE reaction. It shows two fully-connected neural network, each specializing in predicting the concentration of one species, which are then connected together by the physical constraints.

3 Computational time

The simulations were run using a Nvidia V100 GPU and 12 allocated CPU cores using the Advanced Research Computing (ARC) facility at the University of Oxford. We also performed the simulations on a desktop without a GPU and equipped with E5-2640 v4 CPU* 2 (20 CPU cores in total) and 16 GB of RAM. The computational time of the three models mentioned in the paper is compared in Table 1.

Table 1, Computational time at a cluster and a desktop

	Cluster	Desktop
Single microband channel electrode	1-2 hours	4-6 hours
Double microband channel electrode	0.5-1 hours	2-3 hours
Single microband channel electrode with CE reaction	~ 3 hours	~ 7 hours