Physics-Informed Neural Networks for Accelerating Prodrug Delivery System Design

Quinn Stein, Humphrey Yiu, Ali Ozel

School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, United Kingdom

1 Aim & Objectives

Develop a data-driven physics-informed neural network (PINN) framework for characterising mass transport in drug delivery systems. This framework will:

- Determine the diffusion coefficient of Rhodamine B as a model prodrug.
- Validate the framework across varied experimental conditions to confirm physical consistency.
- Provide a framework for characterising transport in porous implants.
- Accelerate rational design and screening of hydrogel formulations for localised drug delivery.

2 Methodology

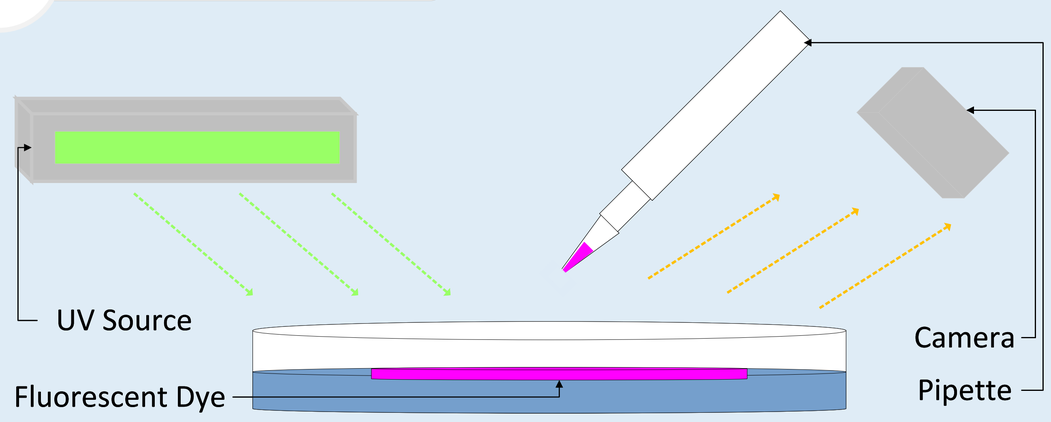

Figure 1. Stage 1: Experimental study

Stage 1: An experimental study to track rhodamine diffusion via imaging of fluorescent emissions excited by UV source (Fig. 1).

Stage 2: Mathematical and computational modelling (Fig. 2)[1]. PINN loss function is informed by stage 1 data and diffusion Equation PDE.

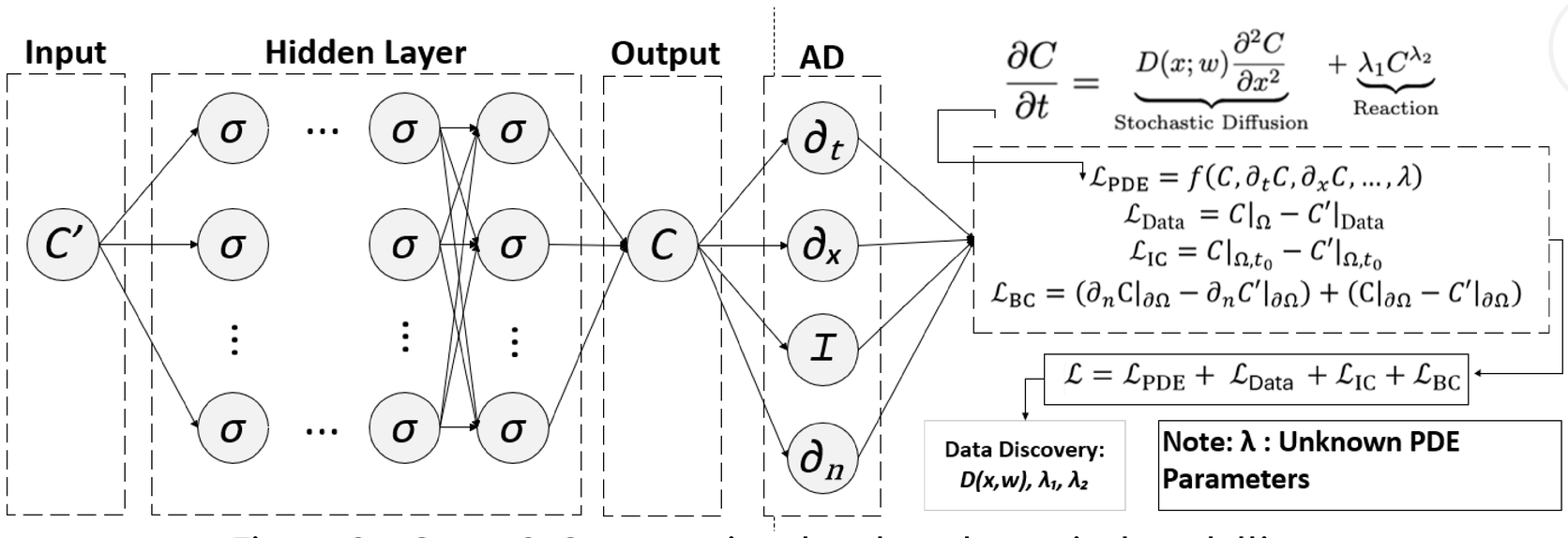

Figure 2 – Stage 2: Computational and mathematical modelling

3 Porous Media: Hydrogels

Hydrogels are water-swollen polymer networks with high biocompatibility. Tunable structural properties allow for variance in porosity (Fig. 4) for targeted release of therapeutics. Two gels are trailed in our work:

- CMC–ODex: carboxymethylated chitosan with periodate-oxidised dextran
- Gelatin–ODex: gelatin with periodate-oxidised dextran

Both gels loaded with prodrug mimic Rhodamine B as a prodye.

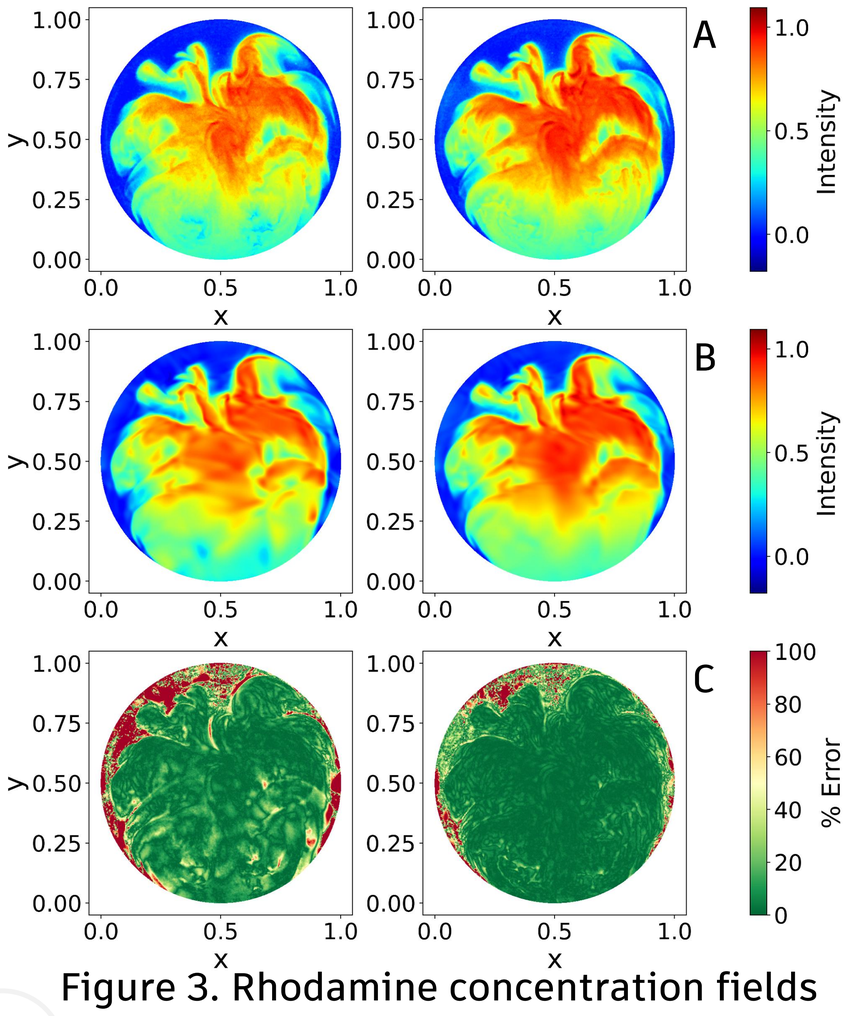

Figure 3. Rhodamine concentration fields

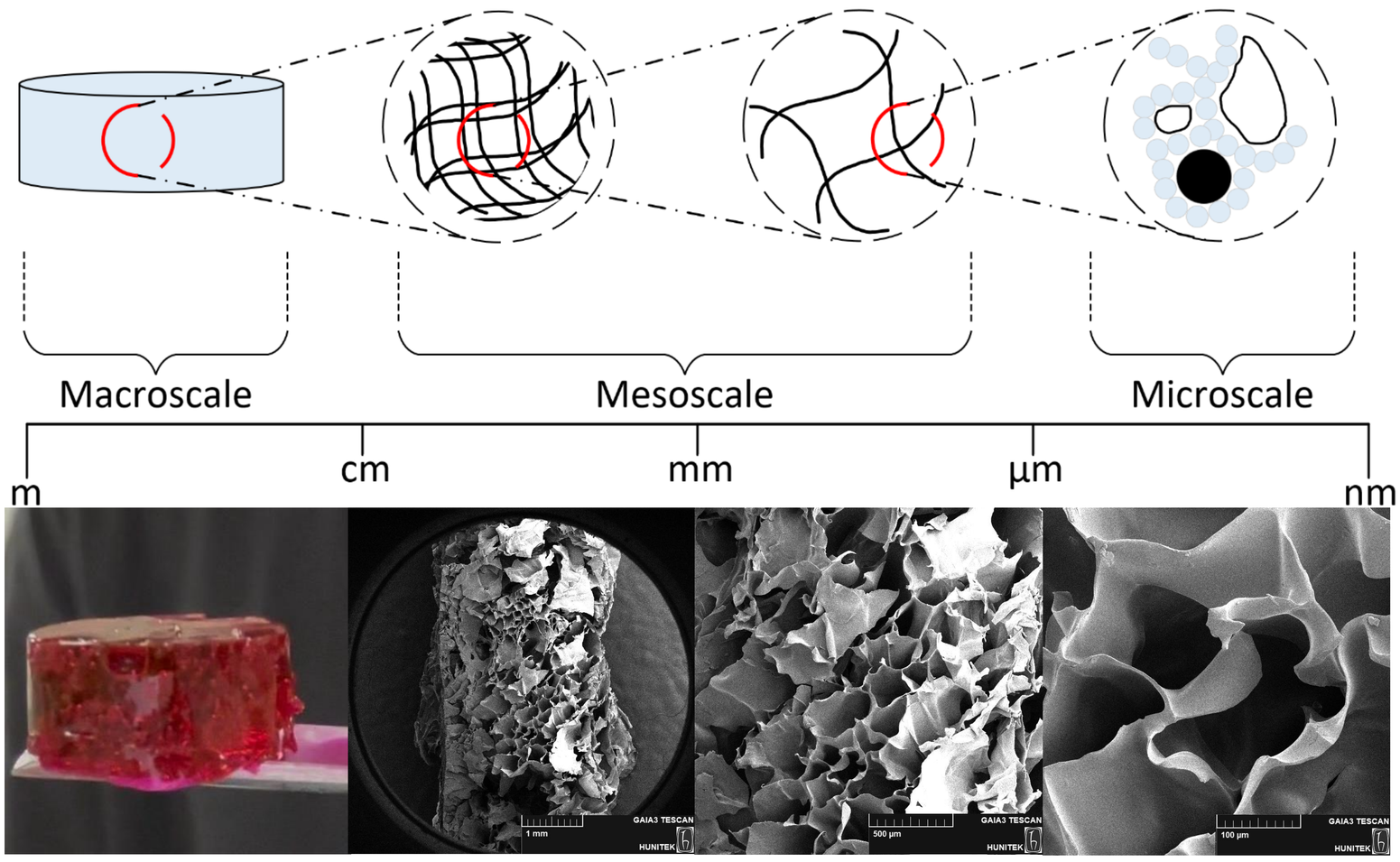

Figure 4. CMC–ODex multi-scale poreous structure

4 Results & Discussion

The PINN framework is applied to florescence imaging data across free aqueous solution (Fig. 3), porous cloth and hydrogel media.

- Predictions show satisfactory agreement with experimental values: At 20°C literature range, D_{exp} = 2.91–4.36×10^{-10} m^2/s with PINN predicting D_{pinn} = 6×10^{-11} - 6×10^{-10} m^2/s. spanning one order of magnitude.
- Predicted diffusion coefficients reduces significantly in the cloth medium, which is physically consistent.
- Concentration fields (Fig. 3) show small % error (C) between measured (A) and PINN prediction (B) for all experimental conditions <2.7% mean error.

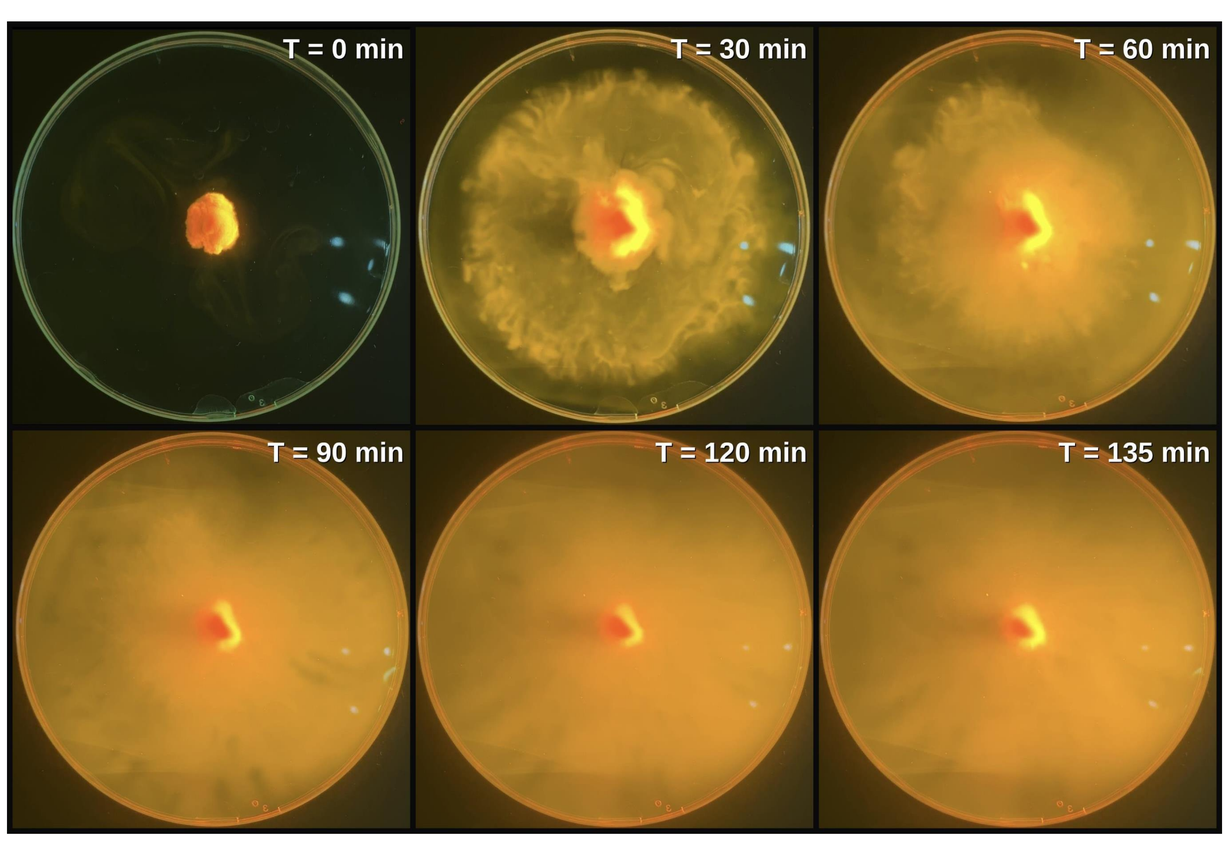

Figure 5. CMC-ODex gel in aqueous solution release of prodye

5 References

[1] Raissi et al., 2017. Physics informed deep learning (part i). arXiv:1711.10561.