P08

Physics-Informed Neural Networks for Enhanced Flow Reactor Modeling and Parameter Estimation

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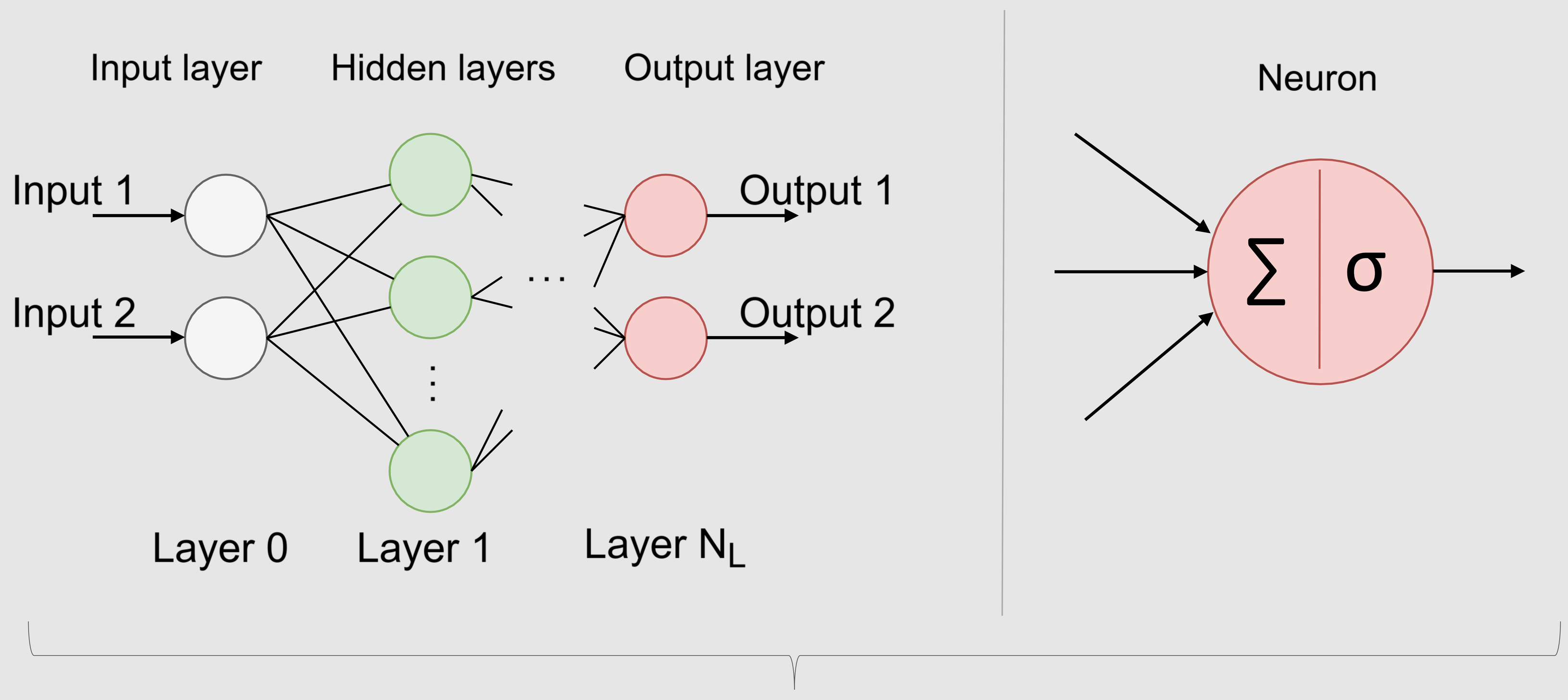
1 Neural Networks (NN)

- inspired by the **structure** and **functioning** of the **human brain**
- recognize patterns, classify information, make predictions - **predict time-series**
- **interconnected nodes** ("neurons") which are organized into **layers**
- **universal approximation theorem:** shallow NN with parameters Θ sufficient to approximate any continuous function



input ↘ bias values

$$\mathcal{N}(\mathbf{x},\Theta) = \sigma\left(\mathbf{W}^{N_L-1}\sigma\left(\ldots\sigma(\mathbf{W}^0\mathbf{x}+\mathbf{b}^0)\right)+\mathbf{b}^{N_L-1}\right)$$

learnable weights from one layer to the next — nonlinear activation function

2 Physics-informed NN (PINN)

- **integrate physical laws into the training process** of the NN and **guide the learning** of the NN parameters Θ
- **extend the loss function** used for training by the residuals of the **incorporated equations**
- weight each part of the loss and find a **balance in learning the data** and the **incorporated physical equations**
- Obtain **physical parameters** Γ **as a side-product** of the training process

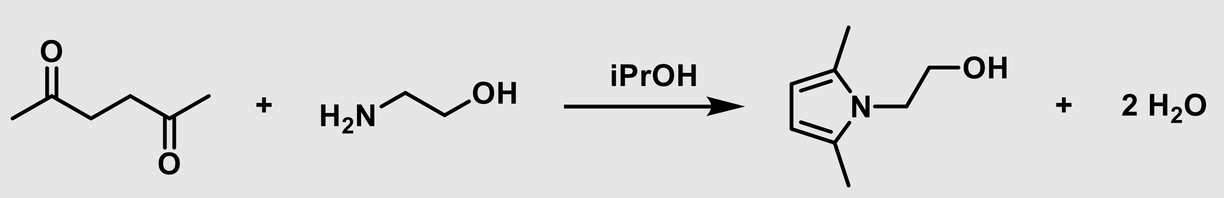
loss due to physical laws

$$\mathcal{L}_{PINN}(\Theta,\Gamma) = \lambda_D\mathcal{L}_D(\Theta) + \lambda_P\mathcal{L}_P(\Theta,\Gamma) + \lambda_R\mathcal{L}_R(\Theta)$$

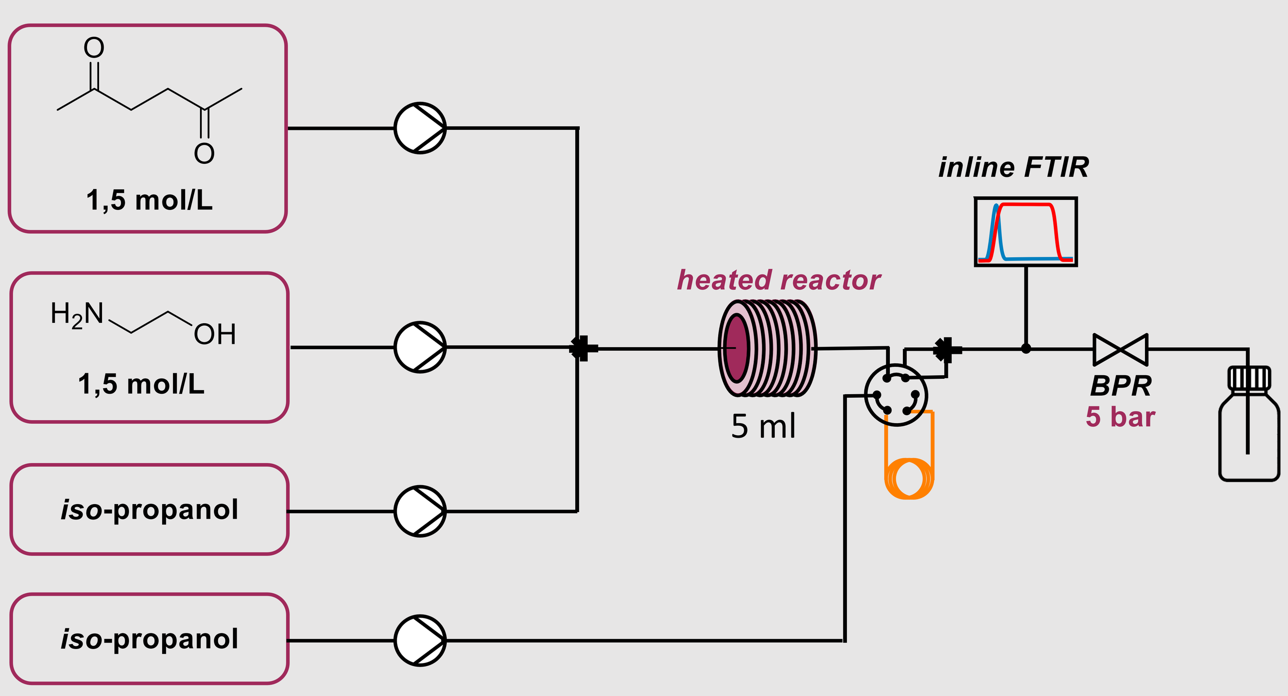
loss due to data — regularization

3 Example: Paal Knorr Reaction (PKR)

- Paal Knorr reaction of **2,5-hexanedione with ethanolamine** in isopropanol **forms pyrrole as product**



- flow reactor setup with a 5 ml **heated reactor**, an **inline FTIR** at the outlet, and individual **actuation of the flow rates**



4 Modeling and Parameter Identification

- **integration** of the **axial dispersion model** into a **shallow Neural Network**

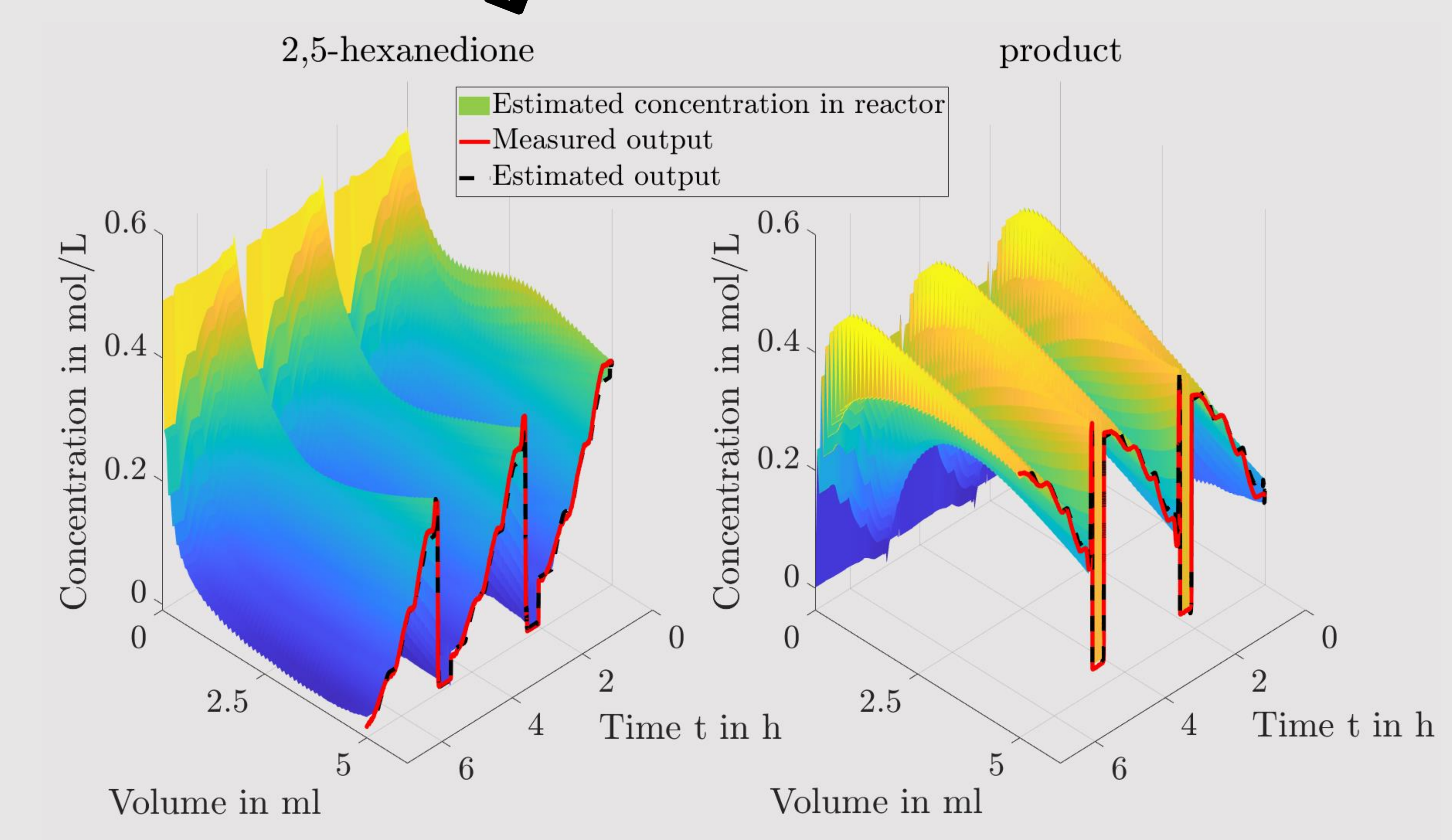
$$\frac{\partial C_i(z,t)}{\partial t} = D\frac{\partial^2 C_i(z,t)}{\partial z^2} - q(t)\frac{\partial C_i(z,t)}{\partial z} + r_i(\ldots)$$

- reaction rates r_i follow the **Arrhenius equation** for which the **reaction parameters** A, E_a **are unknown**

$$r_i = C_{hexa.}(t)C_{ethyl.}(t)\,A\,e^{\frac{-E_a}{R\,T(t)}}$$

- train the PINN **using experimental data**, the Adam optimization algorithm, and a **balanced cost function between** penalizing deviations in the data and the incorporated axial dispersion model

space-time insight — reaction parameters A, E_a



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