MACHINE LEARNING OPTIMISATION OF FLOW IN ALKALINE WATER ELECTROLYSER

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GREEN HYDROGEN PRODUCTION

- UK hydrogen strategy: replace 20% of natural gas usage with low-carbon hydrogen by 2030[1].

- Alkaline water electrolysers (AWE) split water into hydrogen and oxygen bubbles via electrolysis.

- Reduced cell efficiency due to ohmic losses from bubbles in gas-liquid flow:
  - Bubble coverage of electrode
  - Reduced conductivity of electrolyte solution

- Improved understanding of flow in AWE is key to increase efficiency and reduce production cost of green hydrogen.

MULTI-PHYSICS MODELLING OF ALKALINE WATER ELECTROLYSERS

USER INPUTS

- Geometry
- Operating conditions
- Model parameters
- Physical constants

Open-source C++ toolkit: combines existing and in-house solvers

MULTIPHASE FLOW
ELECTROCHEMISTRY
HEAT TRANSFER
POPULATION BALANCE

INDUSTRIAL OUTPUTS

- Cell efficiency
- Hydrogen production
- Temperature field
- Bubble distribution
- Gas purity

RESULTS

- Automated tuning of simulation parameters leads to more accurate predictions.
- Simulation predictions used to inform electrolyser design and operation.
- Further insights provided into flow physics: uncovered average bubble diameter and coalescence rate.

H₂ distribution on cathode at 1000 Am². Dark areas represent high gas volume fraction, and lead to increased electrical resistance and reduced efficiency.

Illustrative Bayesian optimisation with Gaussian processes for 1D function.

ML OPTIMISATION

- Surrogate model trained on sim output
- Acquisition function selects next simulation parameters by optimising over surrogate model

- Uncertain bubble diameters and unknown coalescence rates in electrolyte solutions.
- Bayesian optimisation and surrogate modelling with Gaussian processes (GP).
- Minimise objective function: gas distribution error.
- Find optimal simulation input: bubble diameter \( d_b \) and coalescence coefficient \( C_1 \).

Default settings:

\[ d_b = 100 \mu m, C_1 = 1 \]

Optimised settings:

\[ d_b = 70 \mu m, C_1 = 105 \]

Contour plot of bubble parameter objective function. Sampling points are displayed in black and optimal point in red.