Enhanced Methodology for developing a soft sensor to estimate surface area and zeta potential in advanced manufacturing systems

BUILD-IT2023 Workshop

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Roja Moghadam

Postdoctoral Researcher

Roja.Moghadam@ul.ie

Multiphase Reactor and Intensification Group/ Bernal Institute/ Department of Chemical Sciences
Faculty of Science & Engineering
University of Limerick/ Ireland

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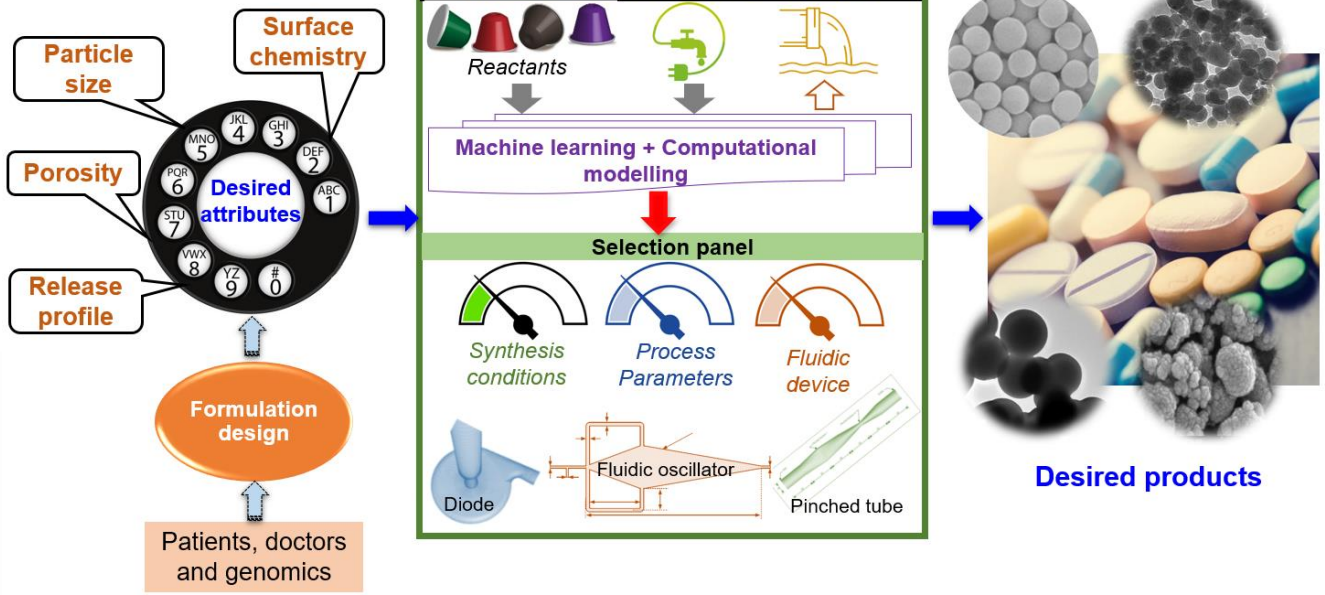
- Brief description and purpose of the project
- Methodology/Result
- Outcome
- Further plan

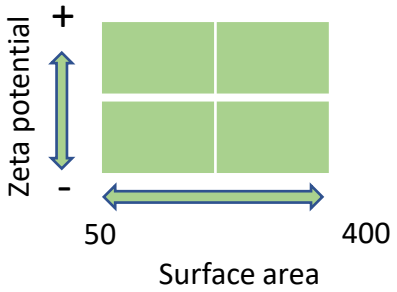
Table-Top Manufacturing of Tailored Nano-silica for Personalised Medicine [SiPM]

Funded by EPSRC-SFI

- The purpose of this work is to develop a distributed tabletop on-demand manufacturing of drug delivery systems at the scale needed for personalized medicine (PM) by combining controlled green synthesis with novel intensified reactors/devices and machine learning tools.
- The aim is to design soft sensors using ML-based strategies to relate online measurements with CQAs of produced BIS for quality assurance:
  - ✓ Design of soft sensor based on physics-informed machine learning (ML) to estimate total surface area and zeta potential using dye adsorption-based conductivity.

Expected outcome





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The University Of Sheffield.

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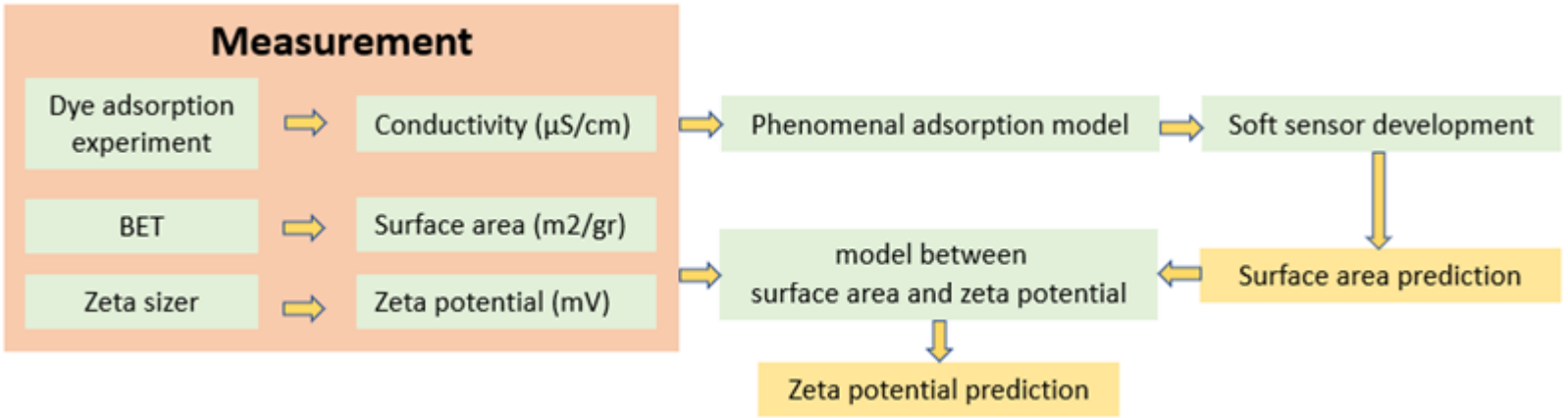
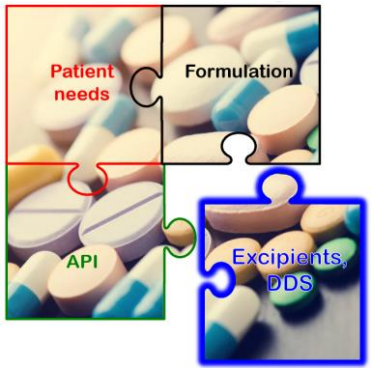
Brief description and purpose of the project:

- The purpose of this work is to design a soft sensor to estimate total surface area using dye adsorption-based conductivity.

Factory-in-a-Box:

(i) Ability to manufacture on-demand,
(ii) Flexible to deliver multiple products with desired properties,
(iii) Sustainable (energy efficient and using mild conditions), and
(iv) Ability to integrate various unit operations using data science tools.

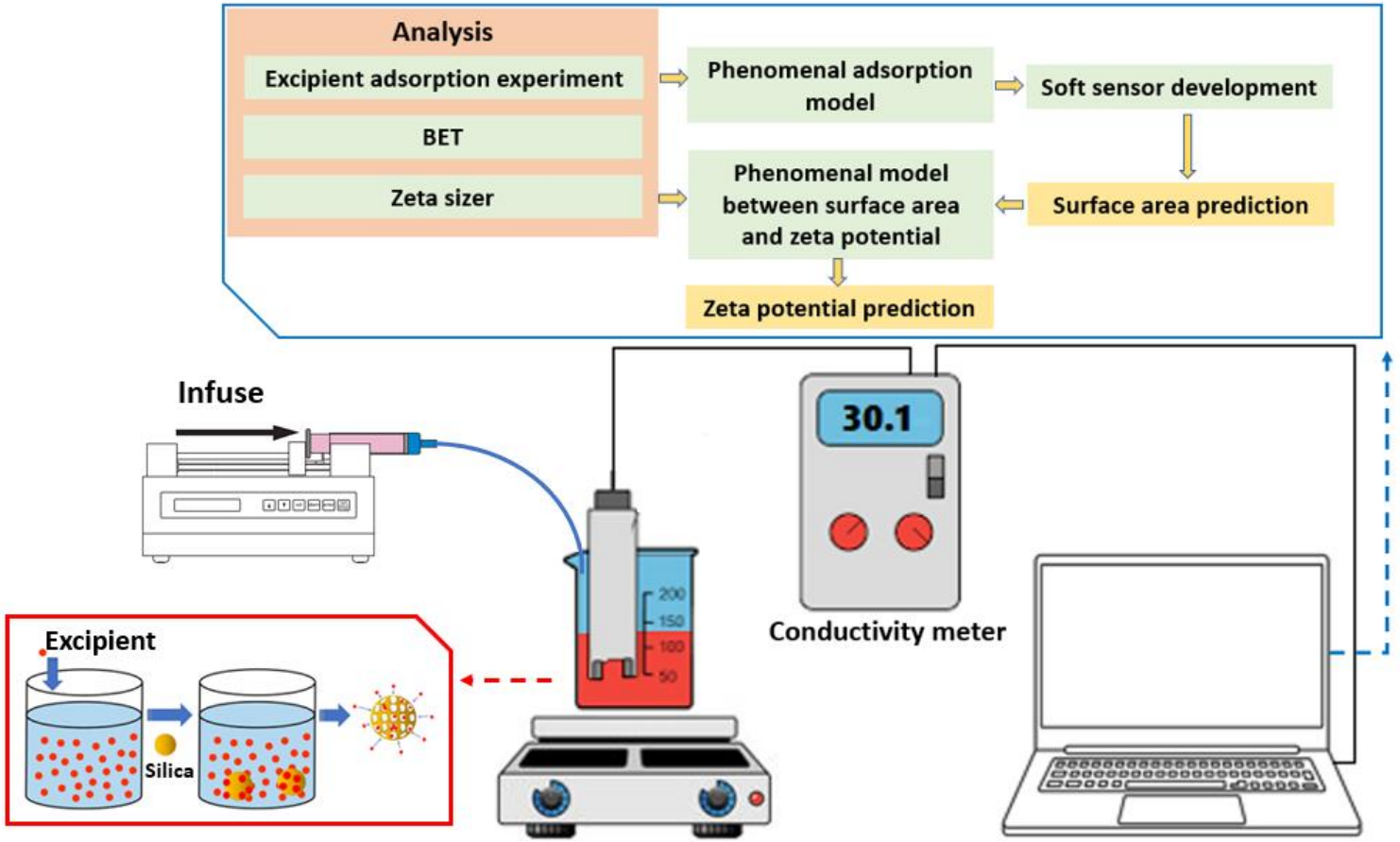




Online prediction instead of time-consuming analysis

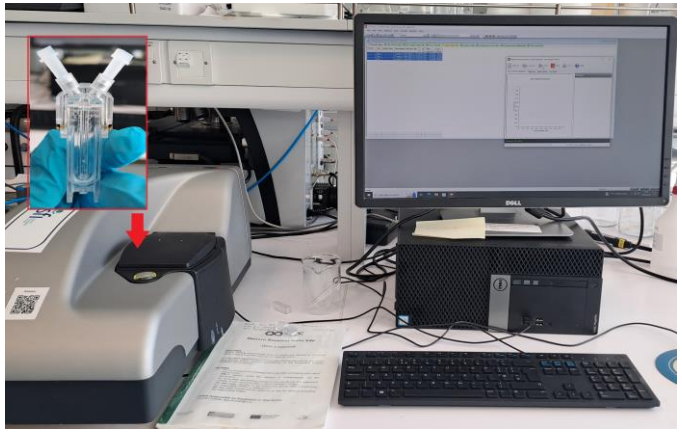
BET analysis is a technique for the measurement of surface area and it is time-consuming and it is not possible to do in in-line system.

Brief description and purpose of the project:



Methodology/Result:

- The experimental data were achieved by BET test by Quantachrome Autosorb, Zeta potential test by zeta sizer, and dye adsorption experiments.
- Some porous silica particles of different grades and Rhodamine B as a water-soluble dye were used in this system.
- As silica slurry is added to the dye solution, the dye in the solution adsorbs on the porous silica particles depending on the surface area and silica-dye interactions.
- The surface area and surface charge are two important attributes in relation to conductivity in the dye adsorption process.
- Finding the physical relations between these parameters is effective to generate artificial data for training the soft sensor.



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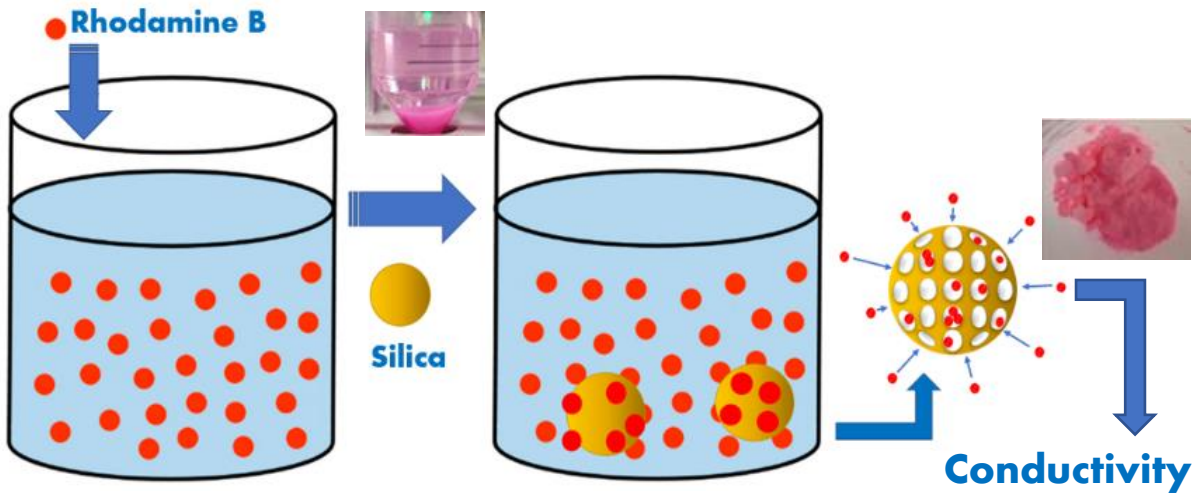
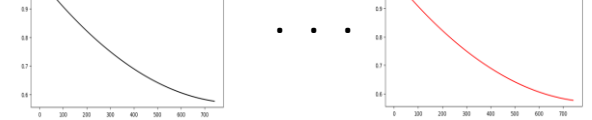
Methodology/Result:



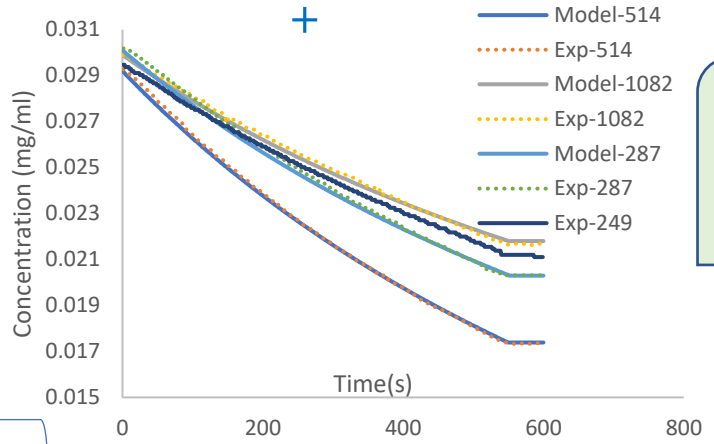
Conductivity measurement



Dye adsorption model

$$C_D = C_{D0}\tau^{(k_{SL}s\,m_f q_F \tau - 1)} \frac{e^{-k_{SL}s\,m_f\left(q_F + \frac{1}{P_1 \alpha_{sF} q_F \rho_s}\right)t}}{(t+\tau)^{(k_{SL}s\,m_f q_F \tau - 1)}}$$

Artificial conductivity profiles generation with different surface areas



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Dye adsorption model & Simulation for conductivity profile generation

#N records available for training

Soft sensor output

Conductivity Profile => Surface area

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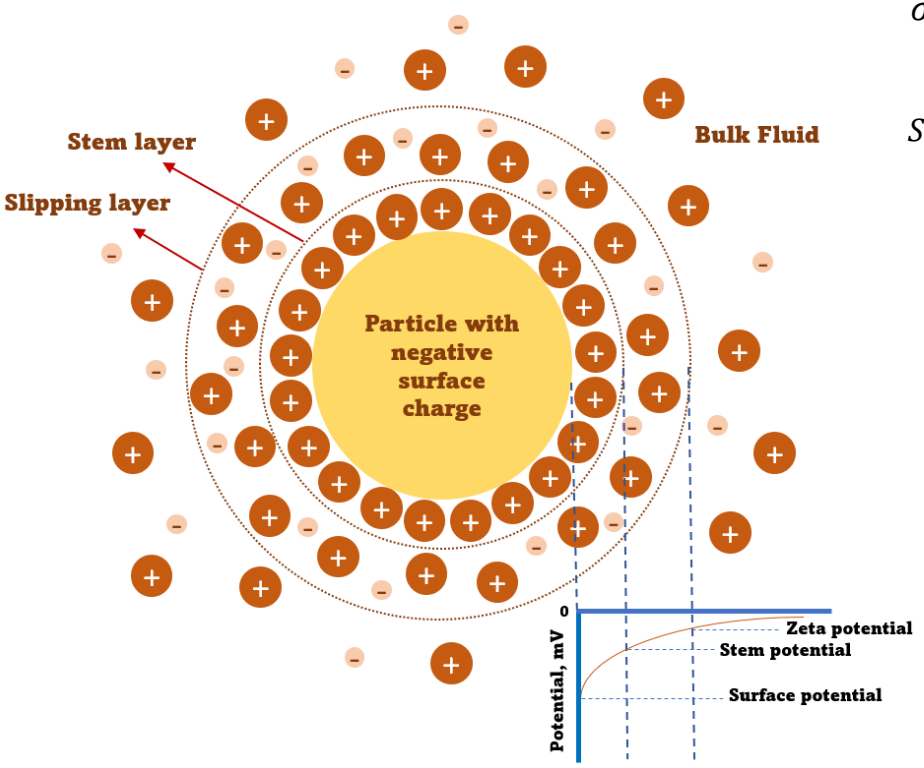
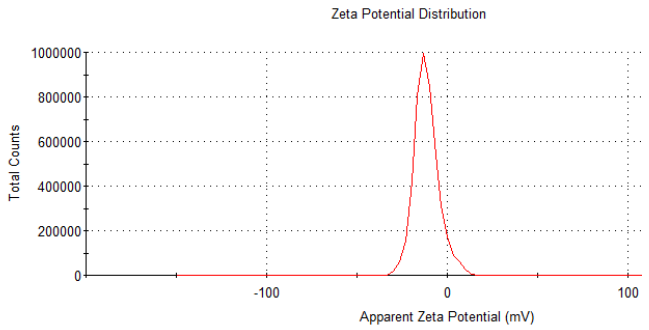
Methodology/Result:

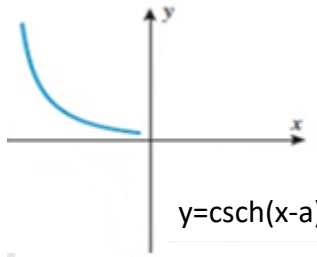


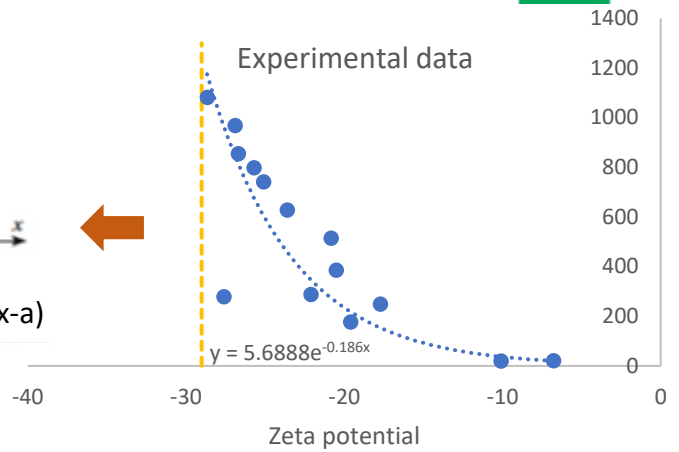


surface charge density $\sigma = F\frac{C_M V}{m\, S_{BET}}$

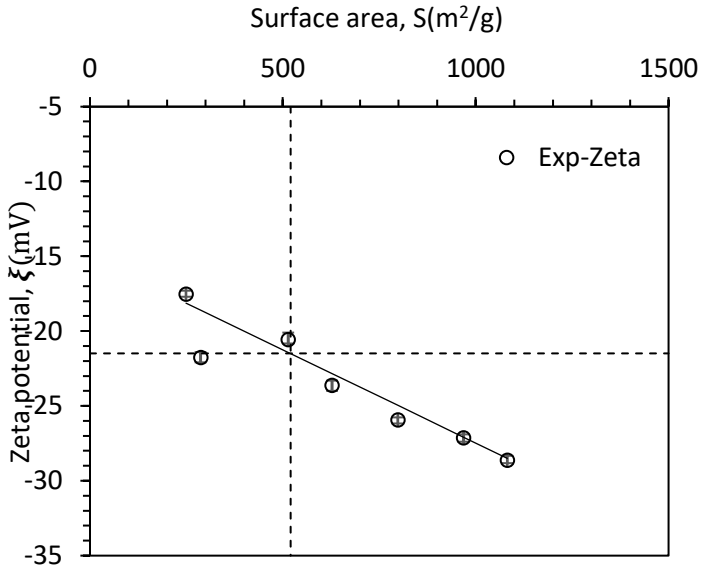
$$\sigma = \sqrt{8\, c\, N\, \epsilon_r\, \epsilon_0\, K_B\, T}\, \sinh\left(\frac{e\psi_0}{2\, K_B T}\right)$$

$$S_{BET} = \frac{1}{C_4 \sinh(C_1 \xi)}$$





$$S = C_3\, e^{[-C_1(\xi - \xi_0)]}$$

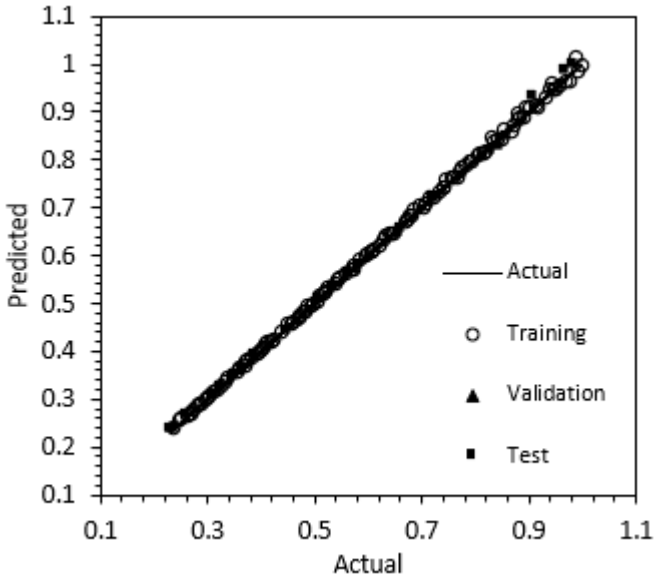


$$\xi = -21.5 - \left(\frac{S - 520}{80.32}\right)$$

Soft sensor design:

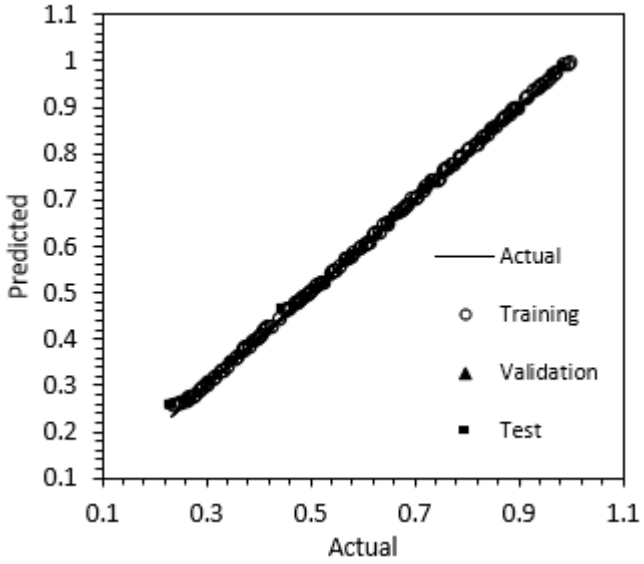
Conductivity profiles as features or input variables and surface area as output variable were used for developing and training the ANN, random forest (RF), and X-gradient boosting (XGB) models.

Python 3.7 platform was applied to construct the purposed soft sensor models. The sklearn library was used to split randomly train(70% of dataset), validate (15% of the dataset) and test data (15% of dataset). To design a robust model, it was considered to evaluate the extrapolation performance of trained model by some unseen data outside of training range.



X-gradient boosting

(R-square: 0.9984, MAE: 0.0060)

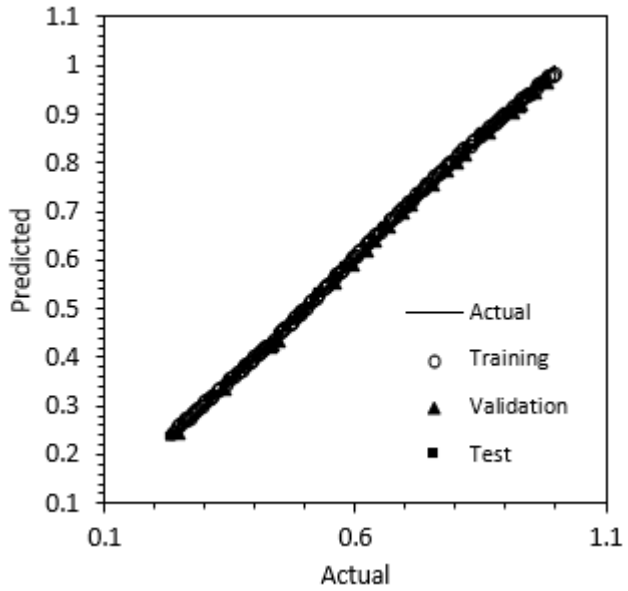


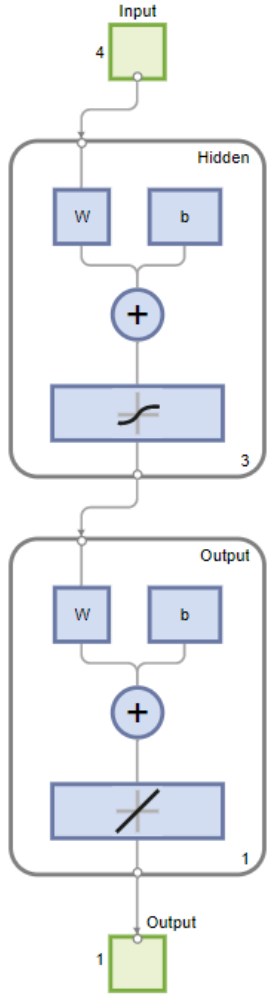
Random forest

(R-square: 0.9988, MAE: 0.0052)

ANN

(R-square: 0.9998, MAE: 0.0022)





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Outcome:

ACS Publications
Most Trusted. Most Cited. Most Read.

I&EC research
Industrial & Engineering Chemistry Research

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Article

A Novel Machine Learning-based Method for Estimation of Surface Area of Porous Silica Particles

Roja P. Moghadam, Chinmay A. Shukla and Vivek V. Ranade*
Multiphase Reactors and Process Intensification Group
Bernal Institute, University of Limerick, Ireland
* Corresponding author: Vivek.Ranade@ul.ie

Abstract

This work reports a novel and quick method to estimate the surface area of porous materials. Conventionally surface area measurement requires the BET method/ N_2 adsorption experiment which is time-consuming. In this work, we have developed a method based on machine learning (ML) and the adsorption of a conductive dye on porous materials. The rate and quantity of dye adsorption, which is characterized by dynamic measurement of conductivity, provide an indirect measure of surface area and zeta potential. An ML-based soft sensor is developed to relate the measured conductivity profiles with surface area and zeta potential. A phenomenological model on dye adsorption is also developed, validated, and used to augment experimental data for training the soft sensor. The developed method was tested for porous silica particles with a range of surface areas (250-1100 m^2/g) and zeta potential (-17mV: -29mV). The developed soft sensor was able to estimate surface area and zeta potential quite well. The developed approach and method reduce overall measurement time for surface area from several hours to a few minutes. The method can potentially be implemented in continuous plants producing porous materials like silica.

Further plan:

- Design of soft sensor for synthesized Bio-inspired silica
- Design of adaptive soft sensor for in-line prediction of surface area
- Development of digital twins by data integration and using ML and CFD models

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Thank you!

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