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Incorporating local surrogates into large-scale deterministic optimisation models for integrated decision-making in complex systems

Michael Short

Senior Lecturer
School of Chemistry and Chemical Engineering
University of Surrey

Modern decision-making and need for integrated platforms

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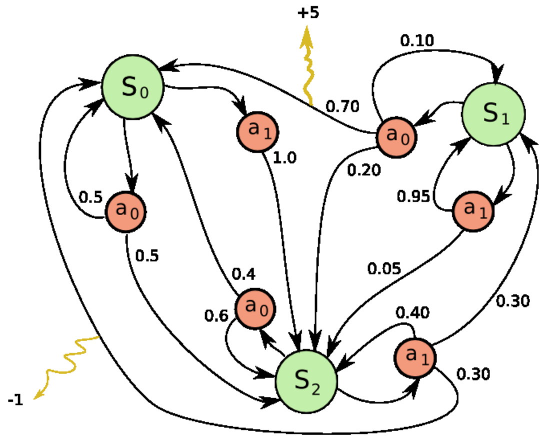
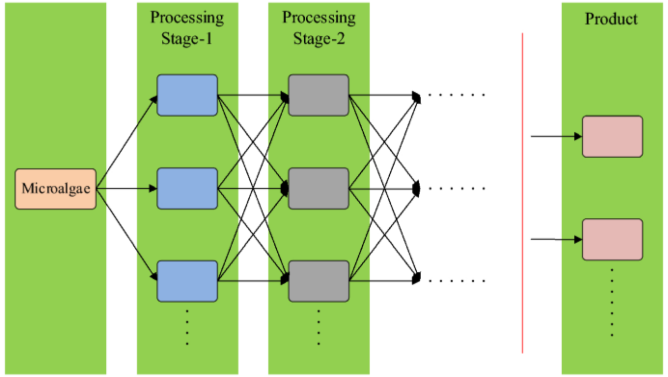
- Strategic, tactical, and operational
- Real-time optimisation
- Considering uncertainty
- Multi-objective
- Large-scale (degrees of freedom)
- Data and machine learning





Short research group @ Surrey

Combining data-driven and first-principles models to develop multi-scale models and software, from molecules to supply chains, to deliver optimal solutions to decision-makers.

Challenges and Opportunities:

Multi-scale and tractability

Ease of use and mathematical complexity

Data-driven and non-mechanistic modelling

Incorporating uncertainty and non-technical aspects

Applications for integrated decision-making and Sustainability

Group research areas:

Sustainable energy systems and bioenergy

Model predictive control and real-time optimisation

Parameter estimation

Flowsheet optimisation

Non-convex multi-scale optimisation

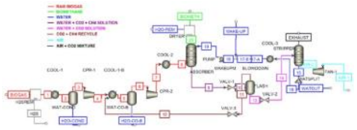
Specialised Decision-support Software

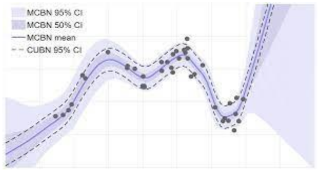
Problem formulation using algebraic models

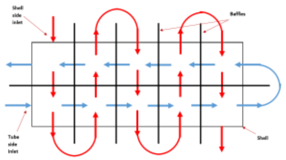
Detailed simulations of individual system components

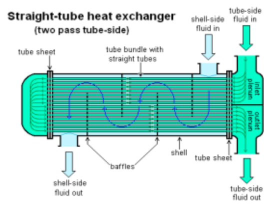
Custom algorithms, decomposition techniques and surrogate modelling

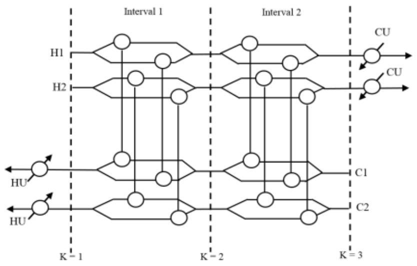
Mixed-integer and Nonlinear programming solvers

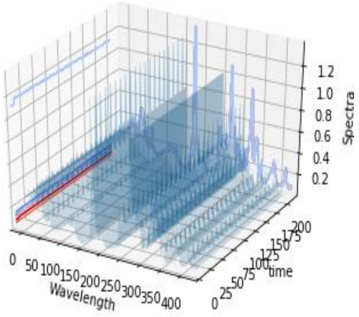


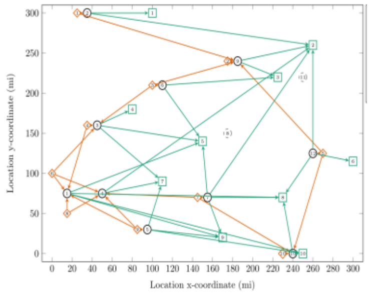












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Solving large-scale (mixed-integer) nonlinear problems

Applications to:
- Design of heat-integrated chemical processes
- Building energy control
- Biogas optimisation and control

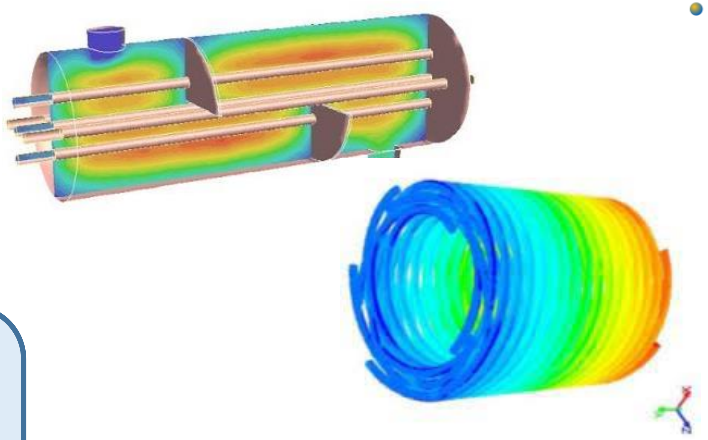
Heat-Integrated Process Synthesis

Network Scale

- **Optimisation model**
- **Modeled using primary design equations**
- **Less accurate and maybe practically infeasible**

- **First-principles based design model (DAE)**
- **Computationally tractable method (Trust-Region)**

Equipment Scale



- **Simulation based model**
- **Modeled using PDE conservation laws**
- **High accuracy but becomes intractable**

DAE - Differential Algebraic Equations
PDE - Partial Differential Equations

HENS superstructures

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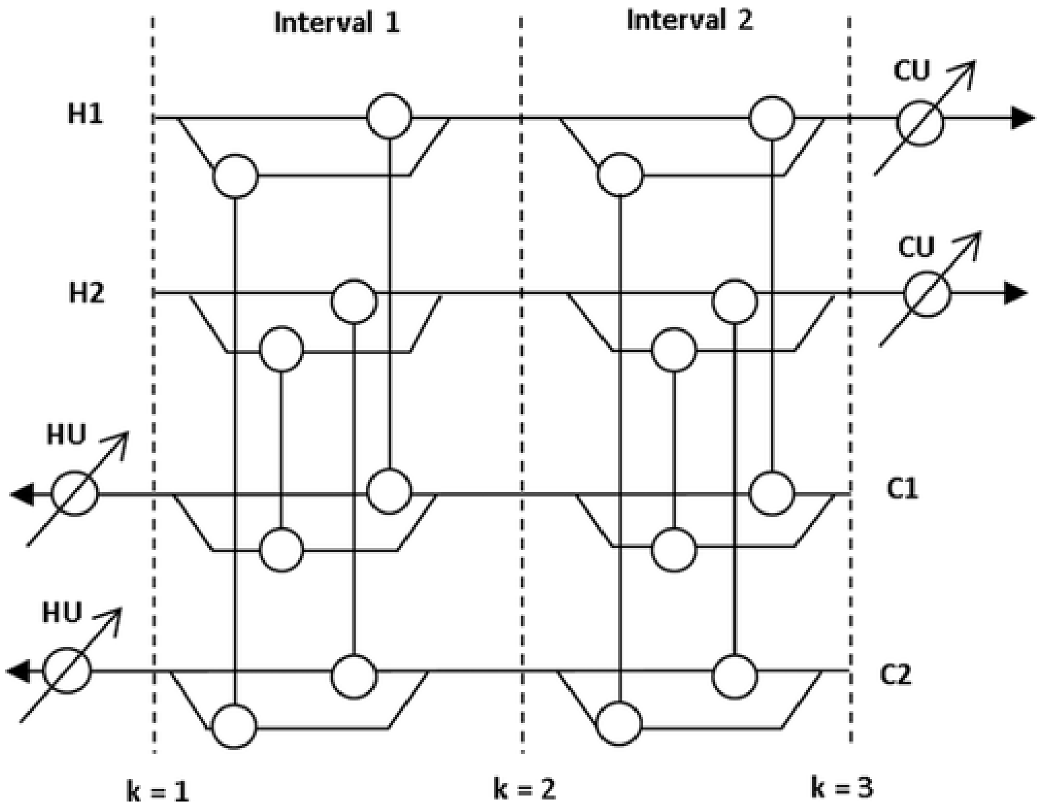
Can use this for mass exchange as well



Yee and Grossmann, 1990, Simultaneous optimization models for heat integration—II. Heat exchanger network synthesis, Computers and Chemical Engineering, 14(10), 1165-1184

$$\min \quad \Big[\sum_{i\in H} CUCqc_i + \sum_{j\in C} HUCqh_j + CF\Big(\sum_{i\in H}\sum_{j\in C}\sum_{k\in K} z_{ij,k} + \sum_{i\in H} zcu_i + \sum_{j\in C} zhu_j\Big)$$

$$+ \sum_{i\in H}\sum_{j\in C}\sum_{k\in K} AC\Big(\frac{q_{i,j,k}}{(U_{i,j,k})(LMTD_{i,j,k})}\Big)^{AE}$$

$$+ \sum_{i\in H} AC\Big(\frac{qc_i}{(U_i)(LMTD_i)}\Big)^{AE} + \sum_{j\in C} AC\Big(\frac{qh_j}{(U_j)(LMTD_j)}\Big)^{AE} +$$

- s.t. Heat balances, temperature constraints, big-M constraints, bounds
- LMTD approximations are commonly used

Heat Exchanger Design Model

AIChE JOURNAL
An Official Publication of the American Institute of Chemical Engineers
AIChE
PROCESS SYSTEMS ENGINEERING

Heat exchanger network synthesis with detailed exchanger designs: Part 1. A discretized differential algebraic equation model for shell and tube heat exchanger design

Saif R. Kazi, Michael Short, Lorenz T. Biegler

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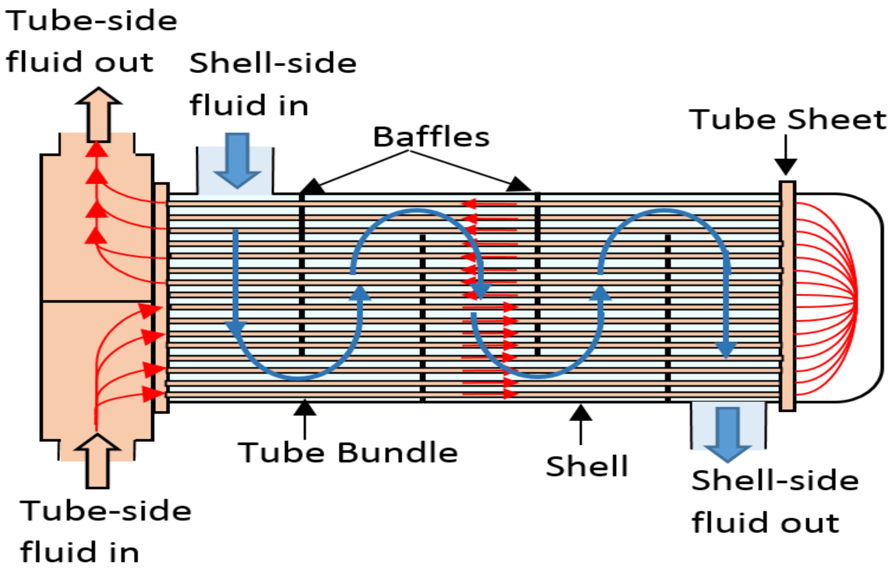
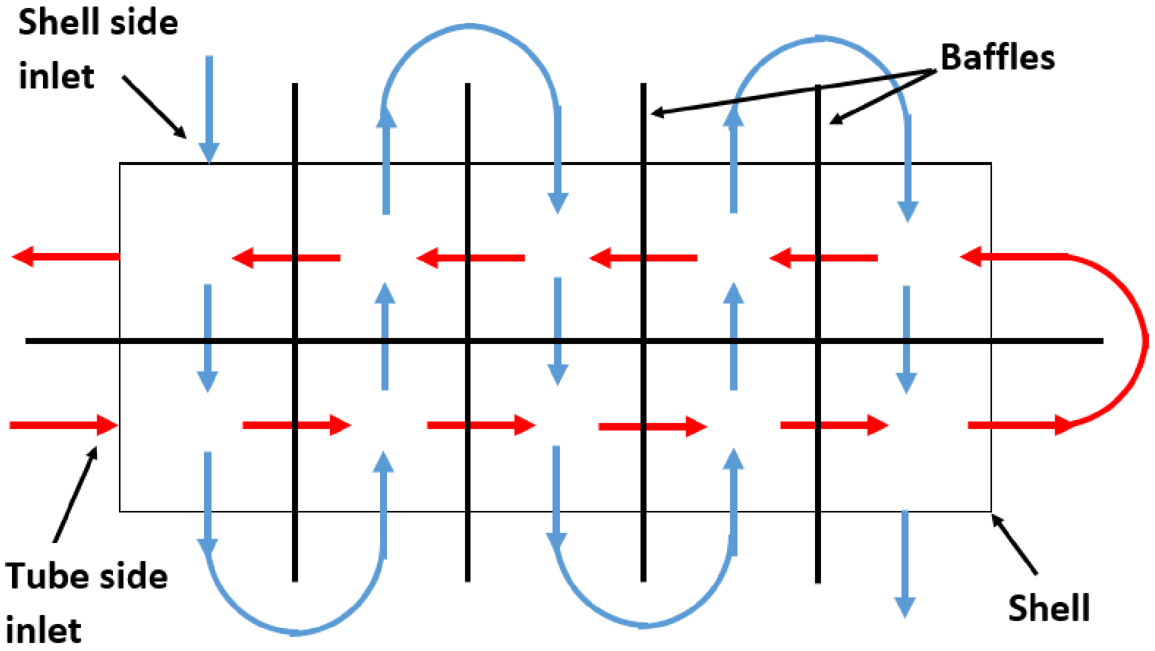


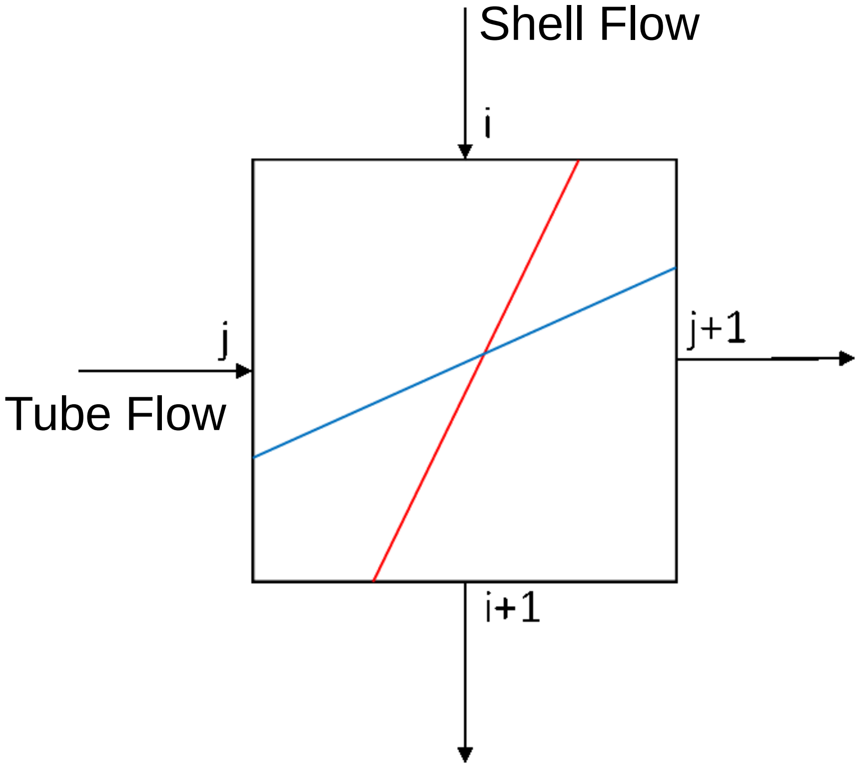


- Represent the shell and tube heat exchanger as a cascade of small elements
- Formulate the mass and energy conservation equations inside each element
- Correlate the exchanger area inside element with design variables like number of tubes etc.

DAE Model

https://doi.org/10.1002/aic.17056

Discrete Element



- 2D Heat Equation

$$\rho C_p \left(u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} \right) = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + q_v$$

- Can be simplified

$$C_h \frac{dT}{dA} + U(T - t) = 0$$

$$C_c \frac{dt}{dA} - U(T - t) = 0$$

C - Heat Capacity, *A* - Heat Exchanger Area

U - Overall Heat Transfer Coefficient

Discrete Algebraic Form

$$C_h \left(\frac{T_{i+1} - T_i}{2} \right) + U\Delta A \left(\frac{T_{i+1} - t_{j+1}}{3} \right) + U\Delta A \left(\frac{T_i - t_j}{6} \right) = 0$$

$$C_c \left(\frac{t_{j+1} - t_j}{2} \right) - U\Delta A \left(\frac{T_{i+1} - t_{j+1}}{3} \right) - U\Delta A \left(\frac{T_i - t_j}{6} \right) = 0$$

Example

AIChE JOURNAL
PROCESS SYSTEMS ENGINEERING
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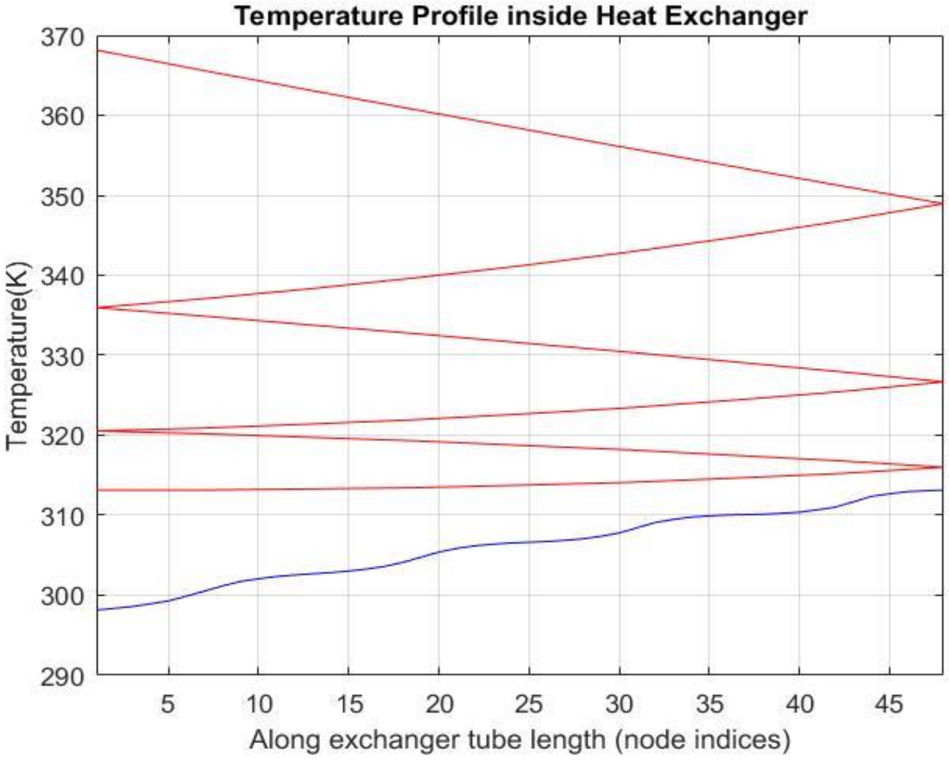
	Mizutani et al. (2003)	Onishi et al. (2013)	LMTD Solution	Discrete Model (fixed L_t)	Discrete Model (variable L_t)
Total Cost($/yr)	5250.00	5134.21	5157.25	5279.28	5169.21
Area Cost($/yr)	2826.00	3175.61	3045.50	3041.44	3077.48
Pumping Cost($/yr)	2424.00	1958.59	2111.75	2237.84	2091.73
Area(m^2)	202	247.22	230.3	229.8	234.4
Duty(kW)	4339	4339	4339	4339	4339
$LMTD(K)$	30.78	31.27	30.78	N/A	N/A
F_t	0.812	0.823	0.823	N/A	N/A
N_{tp}	2	2	8	8	8
$D_s(m)$	0.69	0.79	1.15	1.15	1.18
N_t	832	616	790	790	842
N_b	8	17	4	4	4
$d_o(mm)$	15.9	19.05	25.4	25.4	25.4
$d_i(mm)$	12.6	16.60	21.18	21.18	21.18
$p_t(mm)$	19.88	25.4	31.75	31.75	31.75
$L_t(m)$	4.88	6.706	3.658	3.658	3.49
$v_t(m/s)$	-	1.04	1.03	1.07	1.00
$v_s(m/s)$	-	0.50	0.41	0.41	0.42
$h_t(W/m^2.K)$	6480	4356.7	1951.1	2022.9	1919.3
$h_s(W/m^2.K)$	1829	1880.2	2728.4	2729.8	2761.3
$U(W/m^2.K)$	860	682.2	724.2	725.2	710.8
$\Delta P_t(kPa)$	22.68	15.92	26.85	29.43	25.26
$\Delta P_s(kPa)$	7.49	10.61	8.92	8.93	9.55
Hot fluid allocation	Shell	Shell	Tube	Tube	Tube



Stream	$T_{in}(K)$	$T_{out}(K)$	$\dot{m}(kg/s)$	$\mu(Pa.s)$	$\rho(kg/m^3)$	$C_p(kJ/kg.K)$	$k(W/m.K)$
1	368.15	313.75	27.78	3.4e-04	750	2.840	0.19
2	298.15	313.15	68.88	8.0e-04	995	4.200	0.59

a_{cost}=123, b_{cost}=0.59, c_{cost}=1310

NLP model for packed columns

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Mass transfer equations:

$$\frac{dM}{dz} = N_{total}$$

Pratt's correlation for mass transfer coefficient

$$L_{r,l,k}\frac{dx_{r,l,k}}{dz} = Flux_{r,l,k,tt}$$

$$G_{r,l,k}\frac{dy_{r,l,k}}{dz} = Flux_{r,l,k,tt}$$

$$ky_{r,l,k} = \frac{G'_{r,l,k}}{\epsilon_{r,l,k}}.a_G.\left(\frac{de_{r,l,k}.G'_{r,l,k}}{\epsilon_{r,l,k}.\mu_{r,l,k}}\right)^{-0.25}.Sc^{-0.667}\omega e^{\beta L_p}$$

Henry's coefficient is a function of temperature

$$Flux_{r,l,k,ii,jj} = ky_{r,l,k}.ai_{r,l,k}.A_{r,l,k}.\left(Cr_{r,l,k,ii,jj} - He.Cl_{r,l,k,ii,jj}\right)$$

Solved for every exchanger selected by MINLP simultaneously

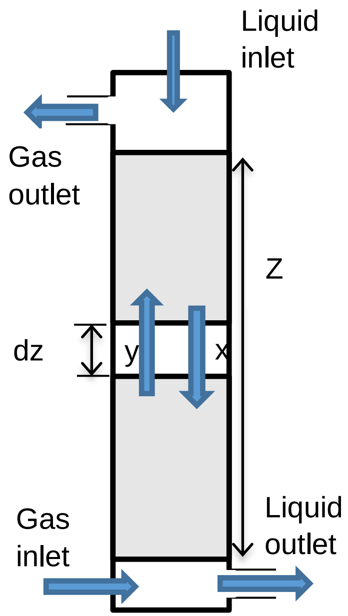
Flooding equations:

$$FloodPoint_{r,l,k} = \frac{249.089}{0.3048} * 0.12 * \left(0.3048 * PackFact_{r,l,k}\right)^{0.7}$$

$$Pdrop_{r,l,k} = (94\cdot\left(\frac{ReL_{r,l,k}^{1.11}}{ReG_{r,l,k}^{1.8}} + 4.4\right)\cdot 6\cdot\left(1 - \frac{\epsilon_{r,l,k}}{de_{r,l,k} * \epsilon_{r,l,k}^{3}}\right).\rho_r.{G'_{r,l,k}}^2$$

$$G_{r,l,k} = A_{r,l,k}.G'_{r,l,k} \qquad ReL_{r,l,k} = \frac{\rho_l.L'_{r,l,k}}{\mu_l.ai_{r,l,k}} \qquad FloodPoint_{r,l,k} \geq Pdrop_{r,l,k}$$

$$L_{r,l,k} = A_{r,l,k}.L'_{r,l,k} \qquad ReR_{r,l,k} = \frac{\rho_r.G'_{r,l,k}}{\mu_r.ai_{r,l,k}} \qquad A_{r,l,k} = \frac{\pi}{4}.\left(D_{r,l,k}\right)^2$$



Trust Region Filter Optimisation

- TRF is useful for rigorous optimisation with reduced/surrogate model
- High-fidelity 'truth' exchanger models may be too expensive
- Deriving reduced models (RMs):
  - Solutions must match truth model
  - Must recognise the same optimum (same KKT conditions satisfied)
  - Must be stable – objectives remain bounded and sufficient improvement

- Idea is to have an optimisation problem with certain parts as "black box" and certain as "glass box" models

$$
\begin{aligned}
\min_{z,w} \quad & f(z, w, t(w)) \\
\text{s.t.} \quad & h(z, w, t(w)) = 0 \\
& g(z, w, t(w)) \leq 0
\end{aligned}
$$

Trust Region Filter Optimisation

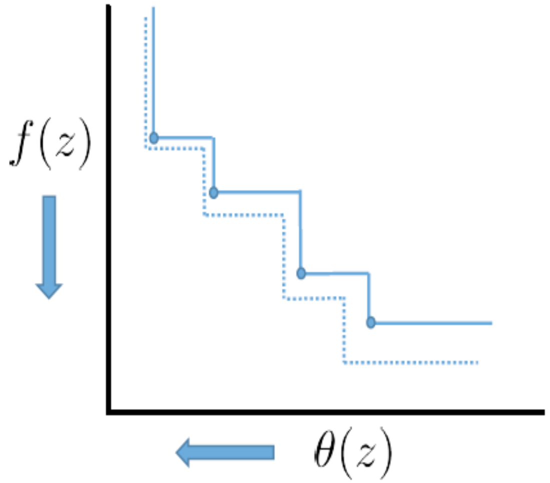
$$\min_{x} \quad f(x)$$
$$\text{s.t.} \quad h(x) = 0$$
$$y = r_k(w)$$
$$g(x) \leq 0$$
$$\|x - x_k\| \leq \bar{\Delta}_k$$

$$x^T = [z^T, w^T, y^T]$$

(TRSP)

$$s_k := x^*_{s,k} - x_k$$ step

$$\theta(x_k) = \|y_k - t(w_k)\|$$ infeasibility



$$r_k(w) = \tilde{r}(w) + (t(w_k) - \tilde{r}(w_k)) + (\nabla t(w_k) - \nabla \tilde{r}(w_k))^T (w - w_k)$$

$\hat{r}(w)$ can be any model (shortcut-based, sampling based or constant)

Process synthesis framework

Integer Cuts

MINLP Stagewise Superstructure

Lower Bound

Topology and initialisation

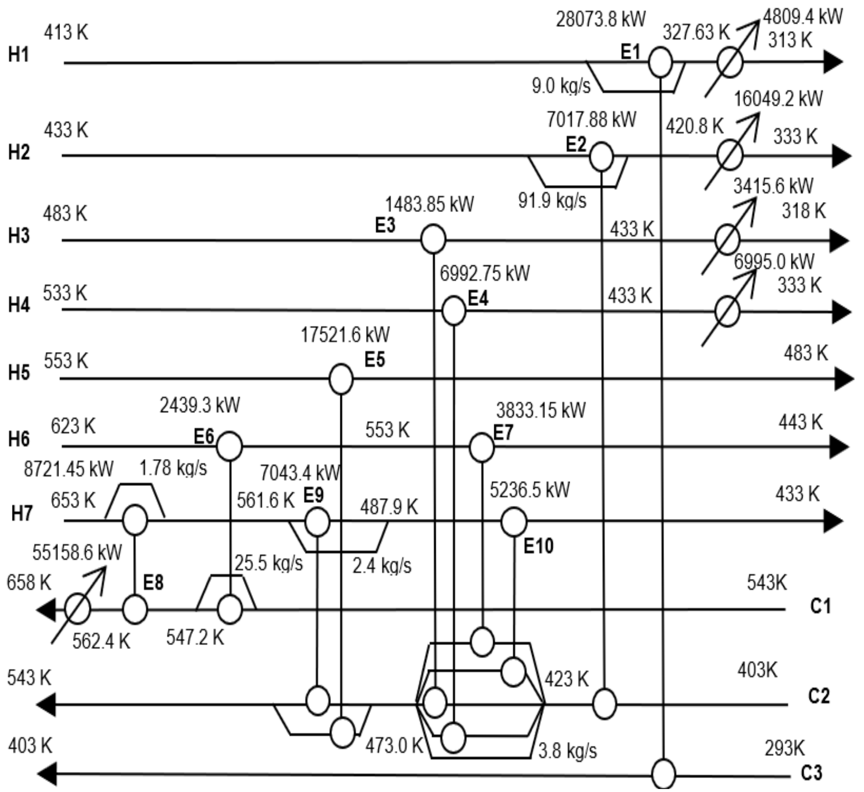
NLP network formulation with reduced models

Inputs to truth models

Updates to reduced models

DAE exchanger models ("truth" models)

Trust Region Filter Optimisation



Upper Bound

Computers & Chemical Engineering
Volume 153, October 2021, 107447

A trust region framework for heat exchanger network synthesis with detailed individual heat exchanger designs

Saif R. Kazi [a], Michael Short [b], Lorenz T. Biegler [a]

CHAMENS results

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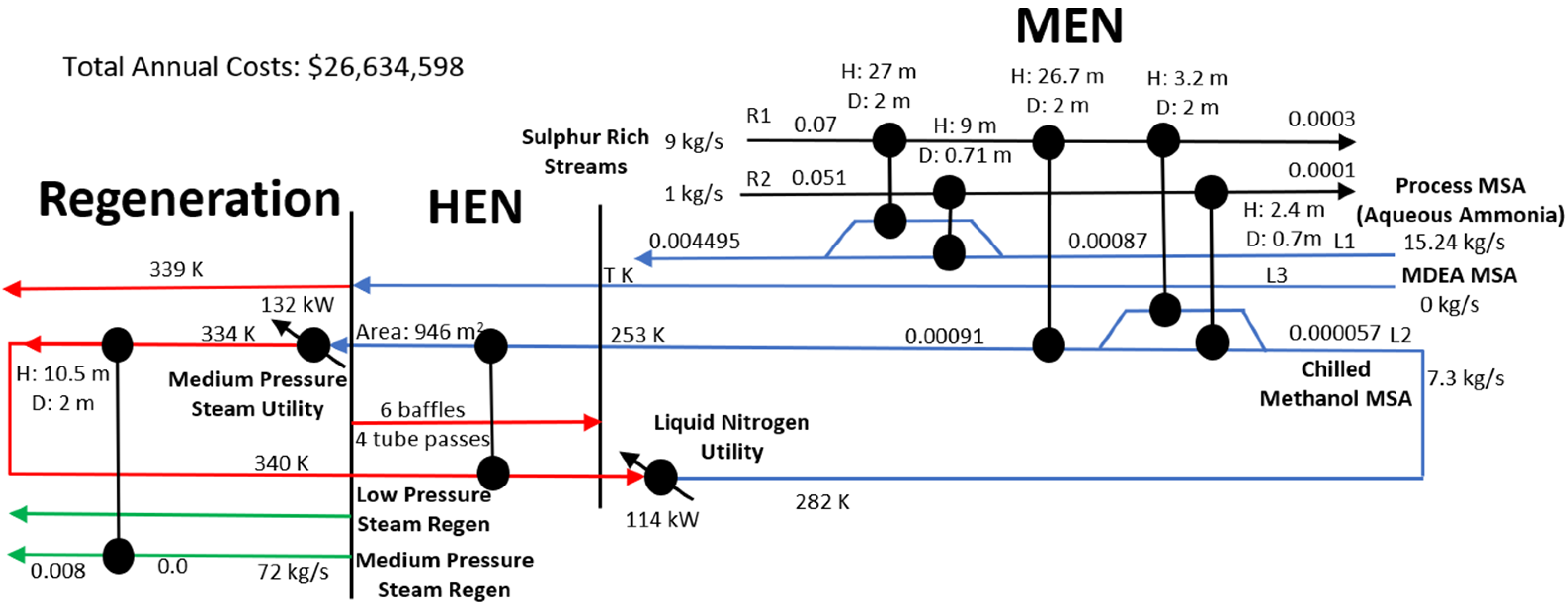
Total Annual Costs: $26,634,598



Optimal model-based decision-making software for complex nonlinear systems

KIPET – Kinetic Parameter Estimation Toolkit

In collaboration with Carnegie Mellon University, Syngenta, Dow, and Eli Lilly and Company

Open-source software for fast kinetic parameter estimation and chemometrics from spectroscopic data and other sources using nonlinear programming for real-time monitoring and control

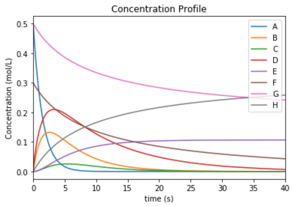
$$\min \sum_{i=1}^{ntp}\sum_{l=1}^{nwp}\left(d_{i,l}-\sum_{k=1}^{nc} c_k(t_i)s_k(\lambda_l)\right)^2/\delta^2+\sum_{i=1}^{ntp}\sum_{k=1}^{nc}\left(c_k(t_i)-z_k(t_i)\right)^2/\sigma_k^2$$

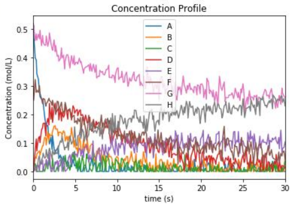
$$\text{s.t.} \quad \sum_{m=0}^{K}\dot{l}_m(\tau)z_{jm}-h_j f(z_{jm},\theta)=0, j=1..ne, m=1..K$$

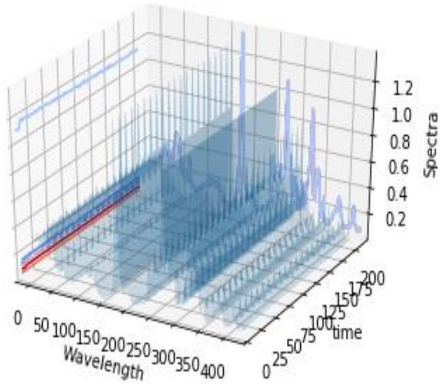
$$z^K(t_i)=\sum_{m=0}^{K} l_m(\tau)z_{jm}, \tau=(t_i-tp_{j-1})/(tp_j-tp_{j-1})$$

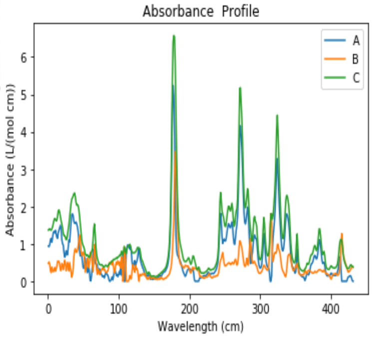
$$C\geq 0, S\geq 0$$

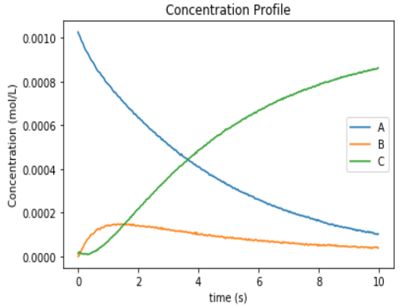
GitHub









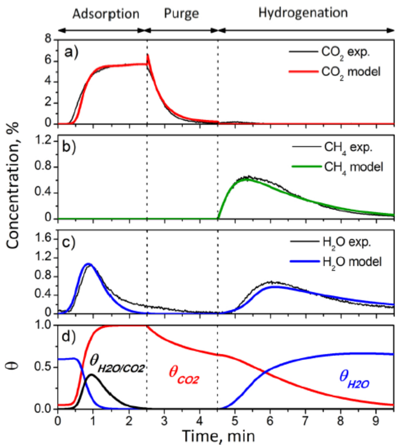


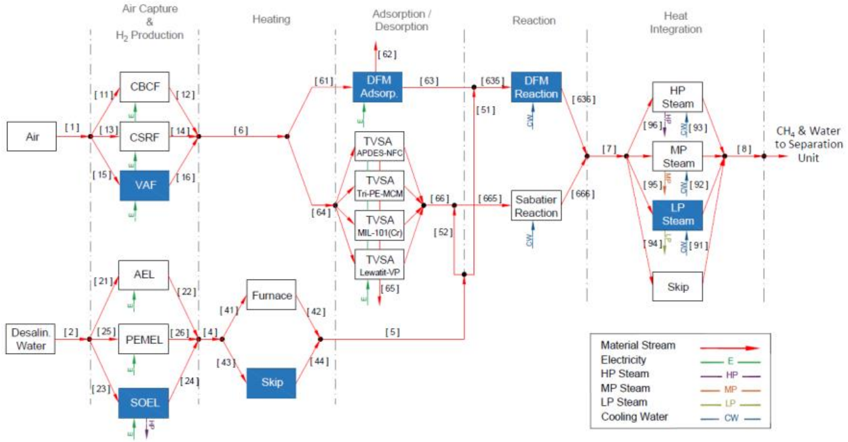
Techno-Economic Analysis of Dual Function Material for DAC

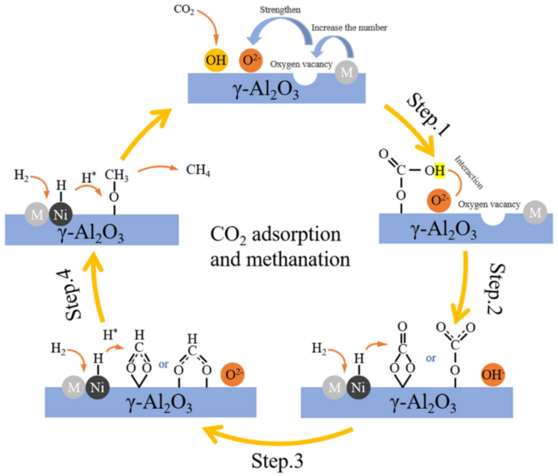
Using kinetic modelling and superstructure approaches to assess DFMs as a potential DAC

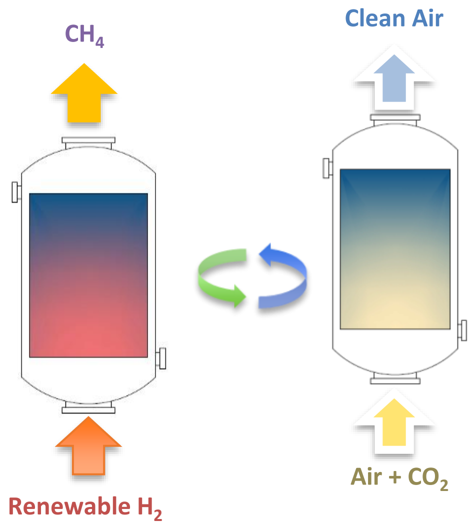
Funding from the EPSRC Adventurous Energy programme

Engineering and Physical Sciences Research Council









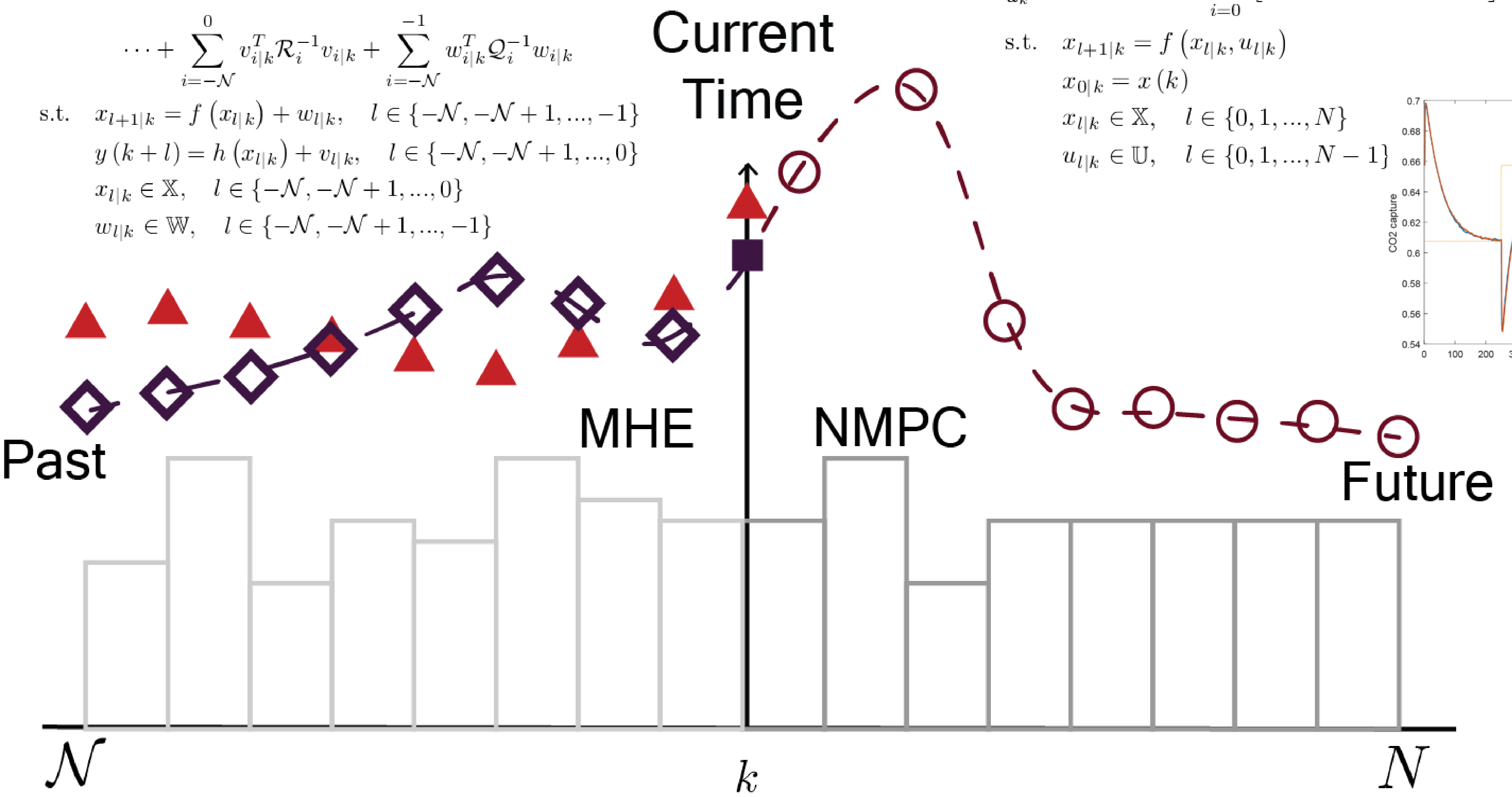
ADVENT-AI: OPTIMISATION OF BUILDING HEATING AND VENTILATION USING ARTIFICIAL INTELLIGENCE

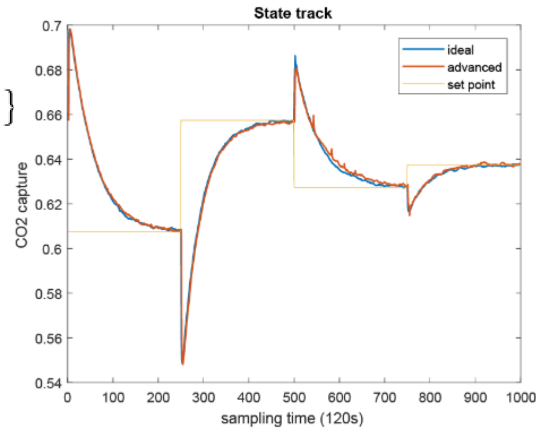
$$\mathcal{M}\left(\Pi_{-\mathcal{N}|k-1}, \hat{x}_{-\mathcal{N}|k-1}, y(k), \ldots, y(k-\mathcal{N})\right):$$

$$\begin{aligned}
\min_{x_{-N}, \boldsymbol{w}_k} \quad & \Phi_{-N}\left(x_{-\mathcal{N}|k}, \hat{x}_{-\mathcal{N}|k-1}, \Pi_{-\mathcal{N}|k-1}\right) + \cdots \\
& \cdots + \sum_{i=-\mathcal{N}}^{0} v_{i|k}^T \mathcal{R}_i^{-1} v_{i|k} + \sum_{i=-\mathcal{N}}^{-1} w_{i|k}^T \mathcal{Q}_i^{-1} w_{i|k} \\
\text{s.t.} \quad & x_{l+1|k} = f\left(x_{l|k}\right) + w_{l|k}, \quad l \in \{-\mathcal{N}, -\mathcal{N}+1, \ldots, -1\} \\
& y(k+l) = h\left(x_{l|k}\right) + v_{l|k}, \quad l \in \{-\mathcal{N}, -\mathcal{N}+1, \ldots, 0\} \\
& x_{l|k} \in \mathbb{X}, \quad l \in \{-\mathcal{N}, -\mathcal{N}+1, \ldots, 0\} \\
& w_{l|k} \in \mathbb{W}, \quad l \in \{-\mathcal{N}, -\mathcal{N}+1, \ldots, -1\}
\end{aligned}$$

$$\mathcal{P}\left(x(k)\right):$$

$$\begin{aligned}
\min_{\boldsymbol{u}_k} \quad & \varphi_N\left(x_{N|k}\right) + \sum_{i=0}^{N-1}\left[x_{i|k}^T Q x_{i|k} + u_{i|k}^T R u_{i|k}\right] \\
\text{s.t.} \quad & x_{l+1|k} = f\left(x_{l|k}, u_{l|k}\right) \\
& x_{0|k} = x(k) \\
& x_{l|k} \in \mathbb{X}, \quad l \in \{0, 1, \ldots, N\} \\
& u_{l|k} \in \mathbb{U}, \quad l \in \{0, 1, \ldots, N-1\}
\end{aligned}$$





ADVENT-AI - HOW IT WORKS

Immediate savings

Once installed, the solution immediately begins resulting in savings through smart energy management via a smart thermostat (based on current thermal comfort and occupancy)

Model improvement

Over time, the model learns the thermal properties of the space as well as the occupancy patterns (e.g., in just 2 weeks, model can predict occupancy with 80% accuracy in initial studies)

Increasing returns

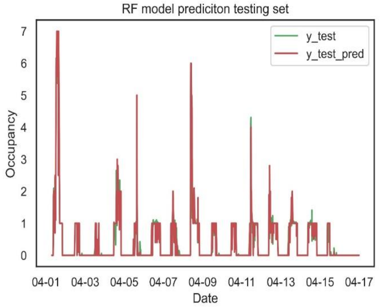
A combination of artificial intelligence and first-principles models is used to increase performance over time, taking advantage of dynamics within the space to save energy, reduce bills, and lower carbon emissions, while maintaining thermal comfort

SMART MODEL PREDICTIVE CONTROL SYSTEM

Historical occupancy data

Real-time occupancy data

ML models for predicting occupancy



Historical thermal performance data

Building layout & properties

Historical weather data

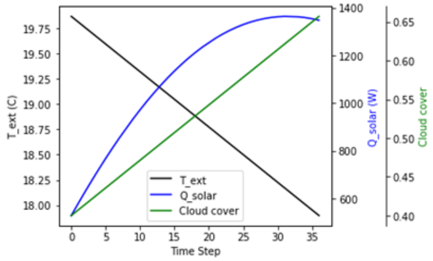
Hybrid thermal model of a building

Model Predictive Control for thermal comfort & energy use minimisation

$T_{setpoint}$
RH
ACH

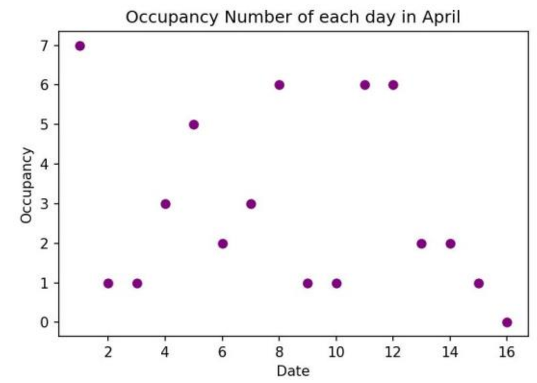
Thermal comfort settings

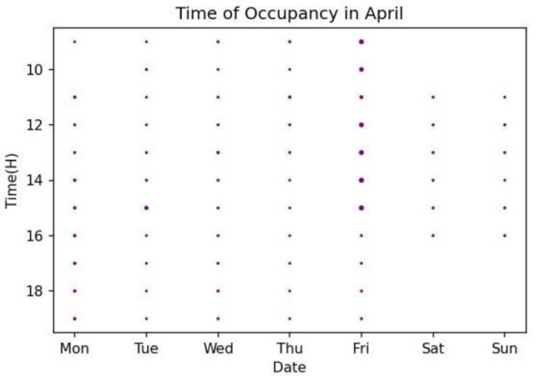
Weather forecast

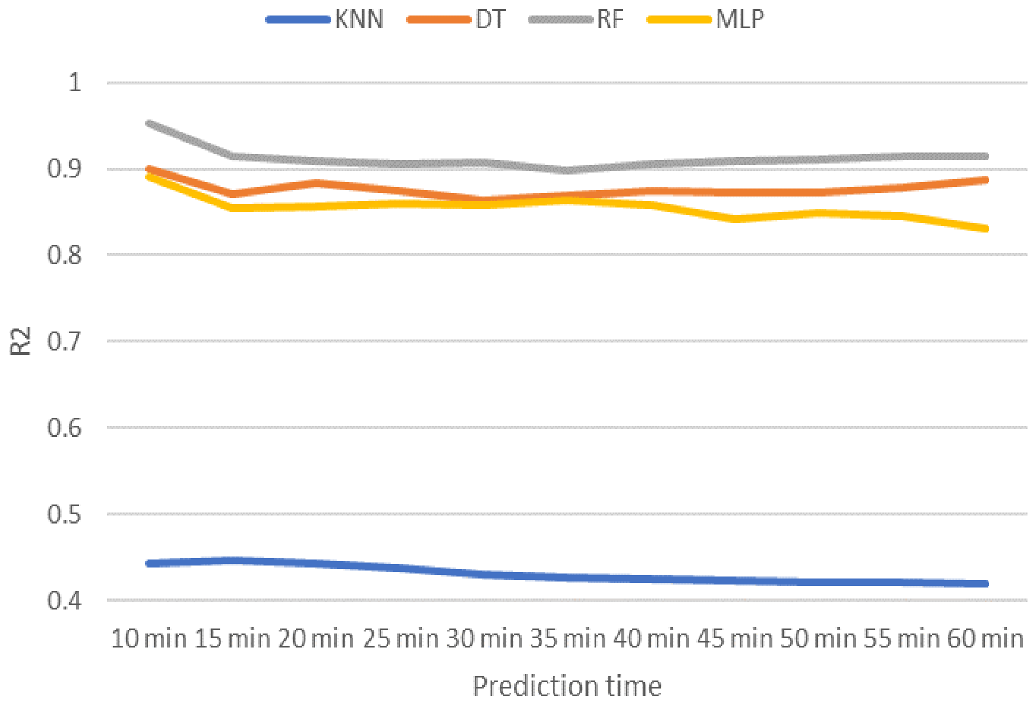


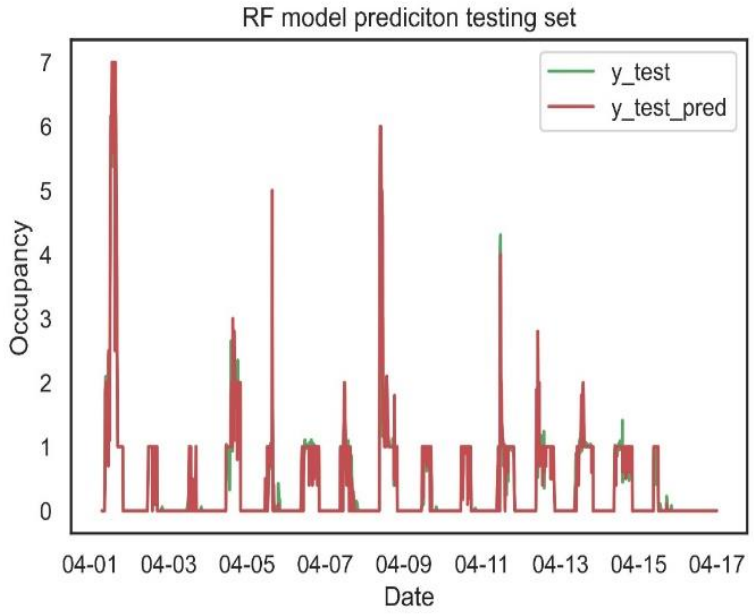
OCCUPANCY MODEL

A rigorous assessment of different machine learning models was used to determine the occupancy prediction model based on data from DIREK Ltd.









R^2 for the occupancy prediction models with different number of outputs in 5 min frequency.

ROLLING HORIZON MPC

$$\int_{t_0}^{t_0+PH}\left[\alpha\frac{\dot{Q}_{heater}(t)}{Q_{heater}^{max}}+(1-\alpha)H\left(N_{occupants}(t)-0.5\right)\frac{\left(T(t)-T_{setpoit}\right)^2}{\Delta T^2}\right]dt\rightarrow\min_{\dot{Q}_{heater}(t)}$$

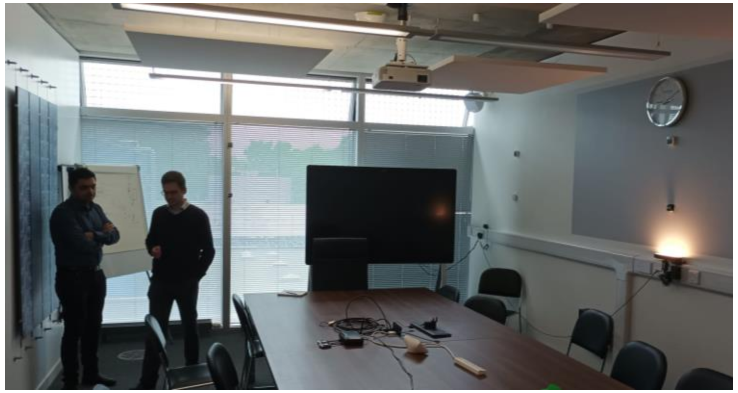
$$s.t.\quad T(t)\geq T_{setback}(t),\qquad \forall t$$

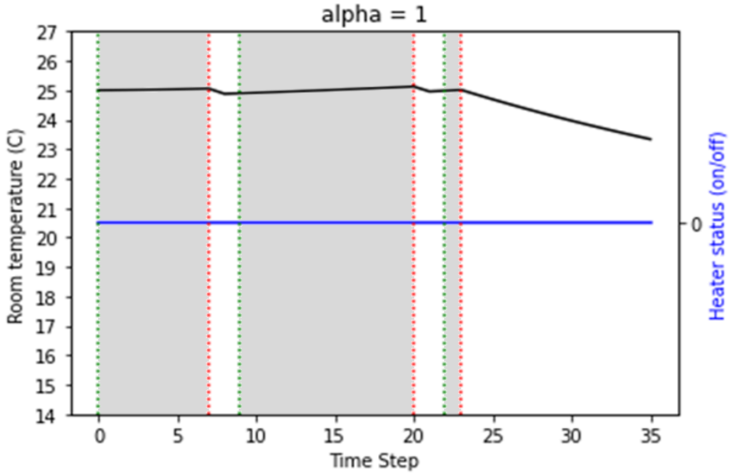
$$0\leq\dot{Q}_{heater}(t)\leq\dot{Q}_{heater}^{max}$$

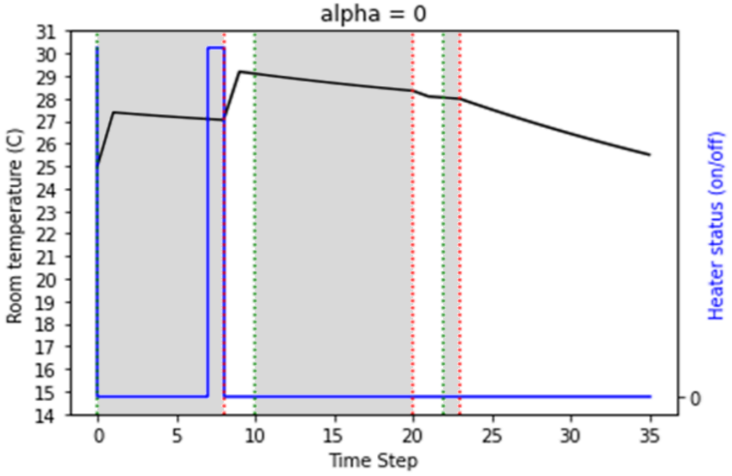
$$\frac{dQ}{dt}=\dot{Q}_{heater}(t)+\dot{Q}_{solar}(t)-\dot{Q}_{diffusion}(t,T,T_{ext})-\dot{Q}_{convection}(t,T,T_{ext})+\dot{Q}_{occupants}(t)+\dot{Q}_{equipment}(t)$$

$$T(t_0)=T_{measured}(t_0)$$

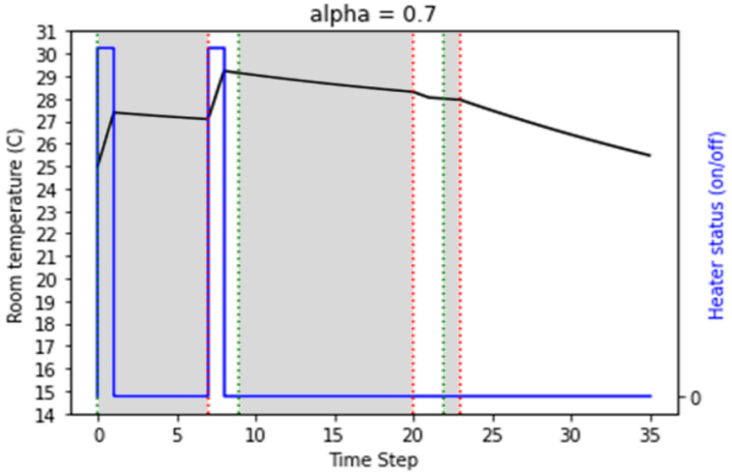
CASE STUDY: A MEETING ROOM







- Temperature set point is 28°C with a tolerance of ±1°C
- Thermal comfort is ensured when the space is predicted to be occupied (greyed intervals)
- Parameter α sets relative priorities of thermal comfort and energy saving:
  - α = 0: thermal comfort only
  - α = 1: energy saving only
  - 0 < α < 1: trade-off between the two objectives



AI4AD

UNIVERSITY OF SURREY

Artificial Intelligence Enabling Future Optimal Flexible Biogas Production for Net Zero

Funded by UKRI AI for Net-Zero

May 2023 – April 2025

University of Surrey
University of Southampton
The University of Nottingham
The University of Manchester (MANCHESTER 1824)
UKRI Engineering and Physical Sciences Research Council

Project Overview

AI4AD

DEPARTMENT OF CHEMICAL AND PROCESS ENGINEERING
UNIVERSITY OF SURREY

In this project, we will develop new tools to increase flexibility and profitability of anaerobic digestion for biogas production in the UK. We will link the various feedstocks (and their combinations) to the microbial populations and productivity of the biodigester, along with developing whole-systems AD site optimisation. We plan to do this by developing decision-making tools including:

- **Uncertainty-aware Hybrid Machine Learning Biodigester Digital Twin**
- **Optimisation-based system models of feedstock procurement and operation for real-time whole-site optimisation**

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Artificial Intelligence Enabling Future Optimal Flexible Biogas Production for Net Zero

DEPARTMENT OF CHEMICAL AND PROCESS ENGINEERING
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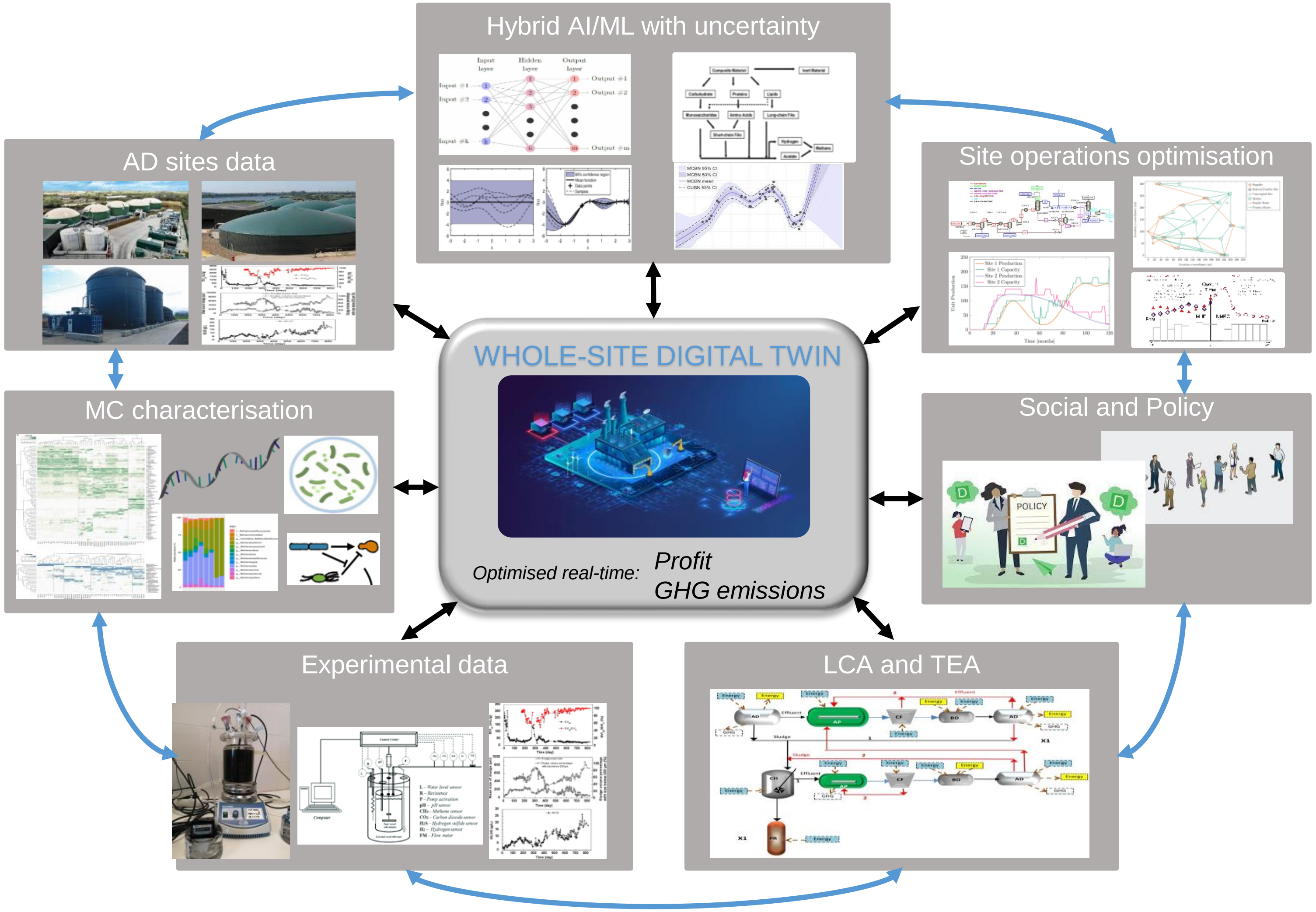

UNIVERSITY OF SURREY
University of Southampton
The University of Nottingham
MANCHESTER 1824 The University of Manchester
UKRI Engineering and Physical Sciences Research Council
ADBA Anaerobic Digestion and Bioresources Association
PSE A Siemens Business
SLR global leaders in environmental and advisory solutions
Ixora Energy
futurebiogas

AI4AD

Overview

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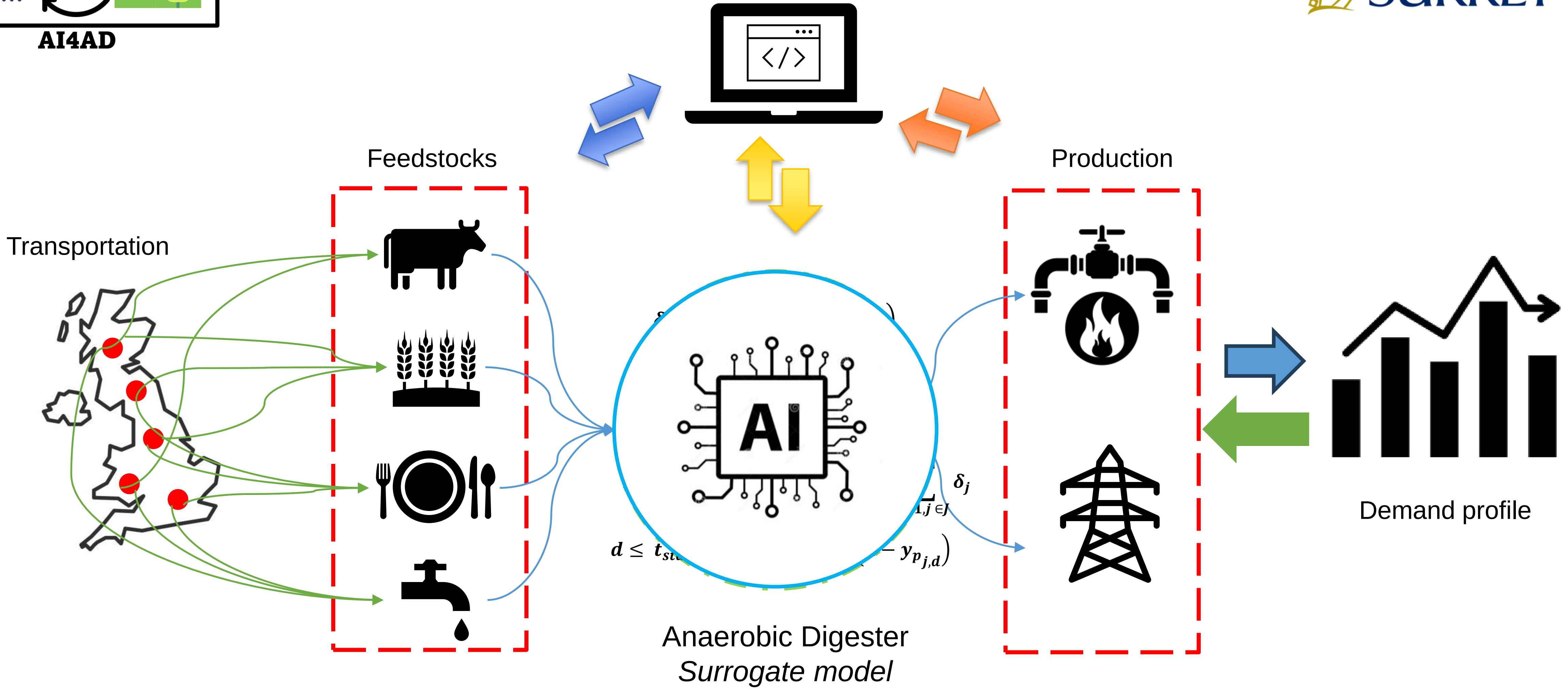

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Demand-oriented feed scheduling

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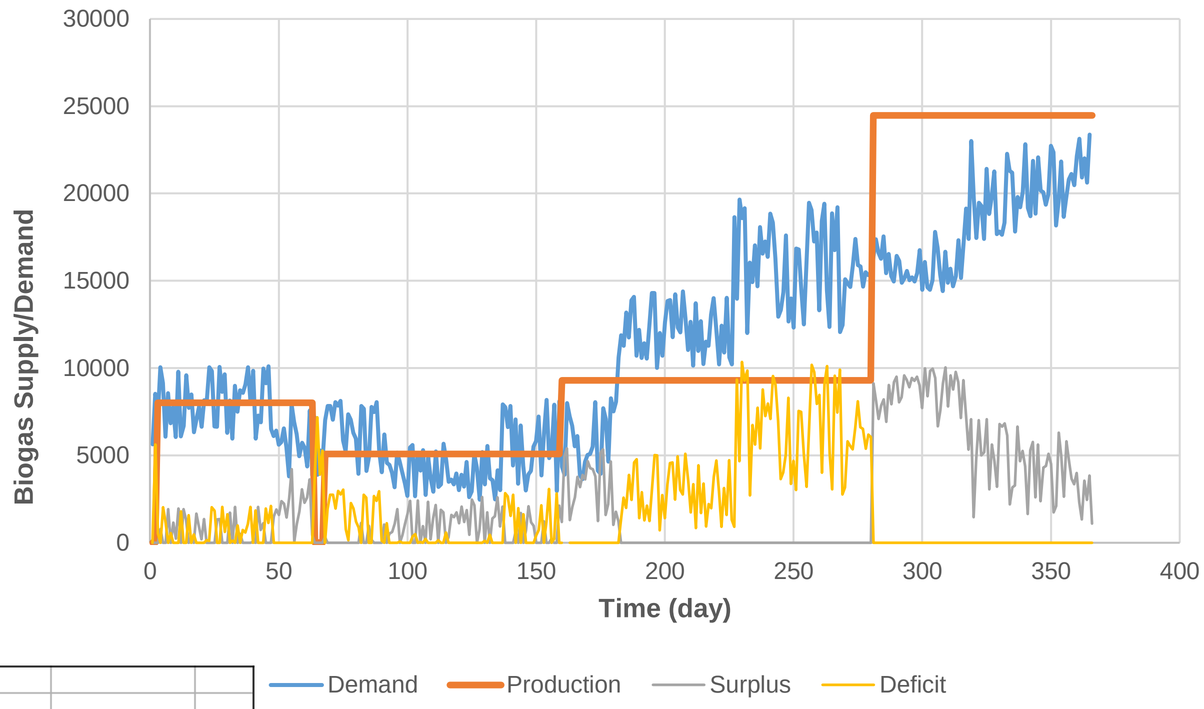
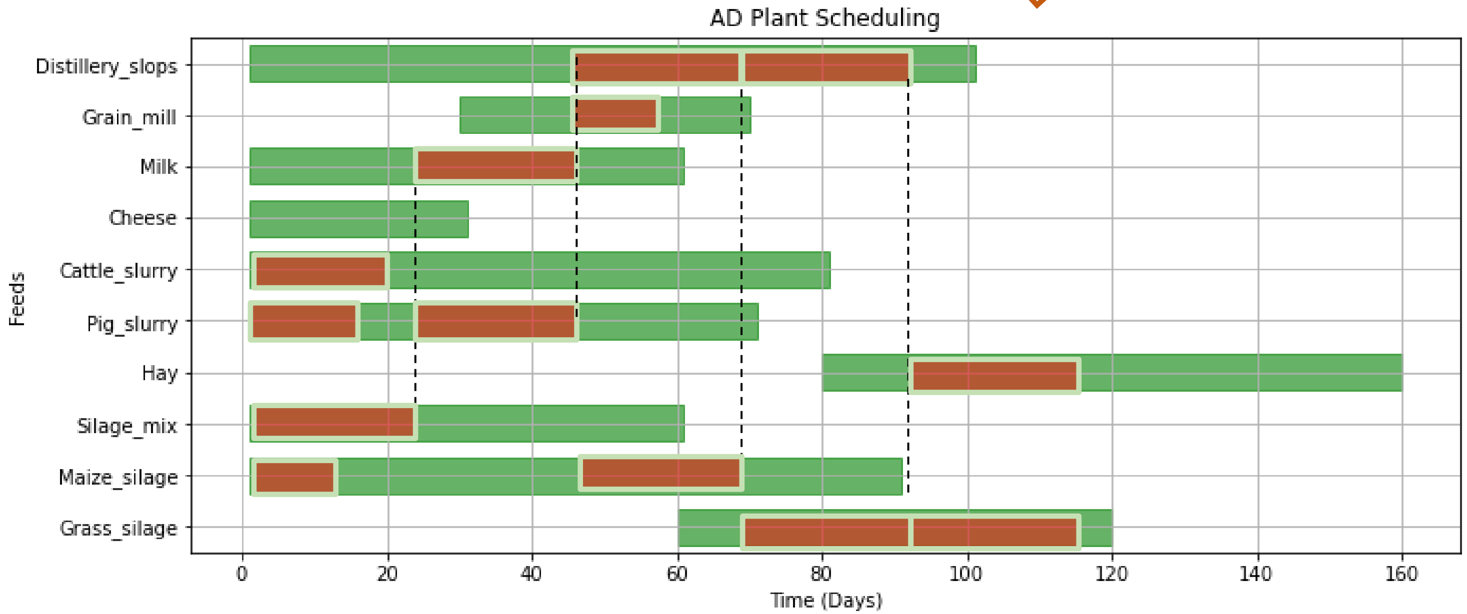
- A surrogate model is formulated to estimate the Co-Digestion effect.
- TBMP, EBMP, biomethane yield, C/N ratio, Total Solid (TS), Volatile Solid (VS), etc. considered.
- Considers storage losses.

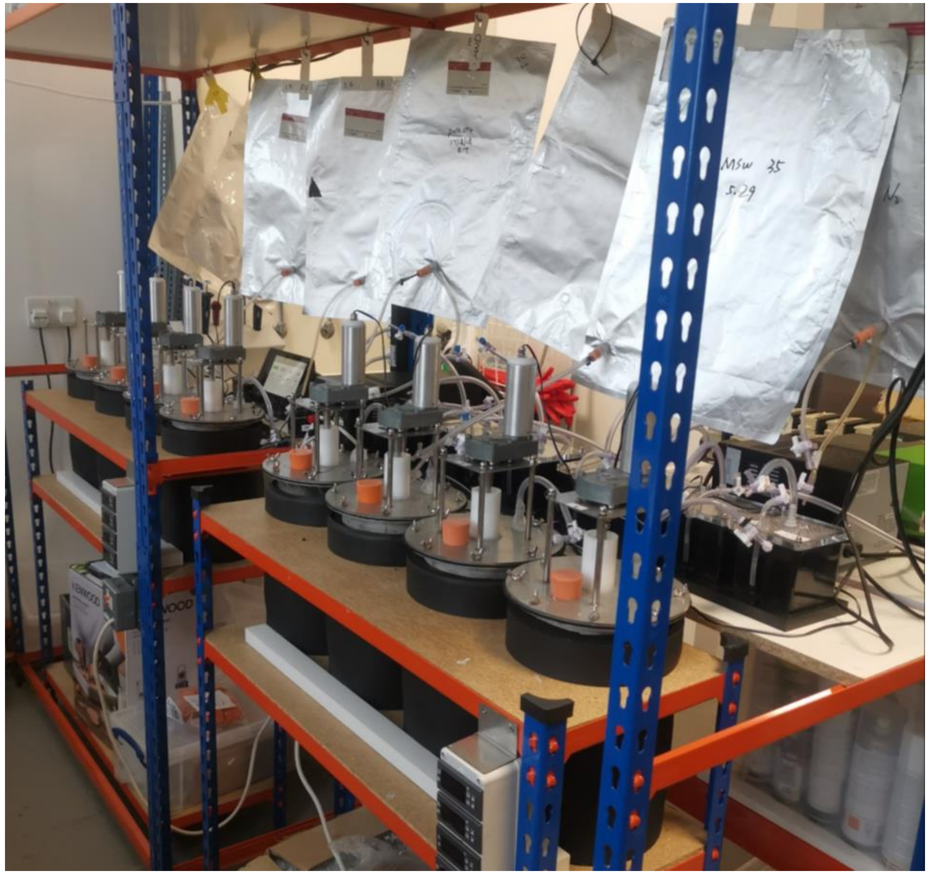
Demand profile





Feed selection

Semi-continuous anaerobic digestion



- To study the effects of **feedstock, SRT, temperature and trace elements**
- To investigate **robustness and resilience of microbes** when encountering perturbations of operating conditions including the change in feedstock and extreme operational conditions
- To explore **new organic wastes as feedstock** to improve the acquisition of feedstock and reduce the reliance on energy crops
- To feed **lab-scale AD data/samples** to microbial study and process modelling teams and experimentally validate models in a quicker and easier manner

- **Biogas production**
  - Yield (m^3/ton VS feed)
  - Productivity ($m^3/(m^3.d)$)
  - Biogas compositions (CH_4, CO_2, H_2, H_2S, N_2O)
- **Digestate properties**
  - pH
  - Conductivity
  - ORP
  - FOS/TAC
  - TS and VS
  - VFAs and COD
  - Ammonia (TAN)
  - Nutrients and trace elements
  - Organic polymers (Cellulose, Proteins, Fats)

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Tools: Microbial ecology and systems microbiology

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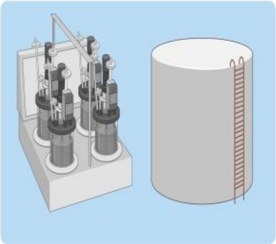
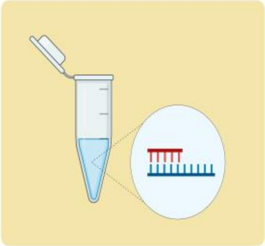
Simplified workflow

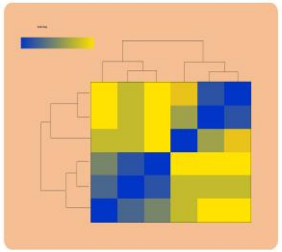


Lab reactor and full-scale samples

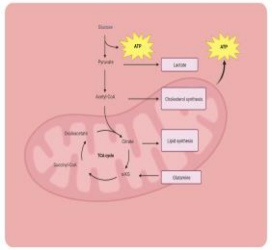


DNA and RNA extraction

Molecular analysis
- Metagenomics
- Metatranscriptomics
- Metabolomics
- RT-qPCR



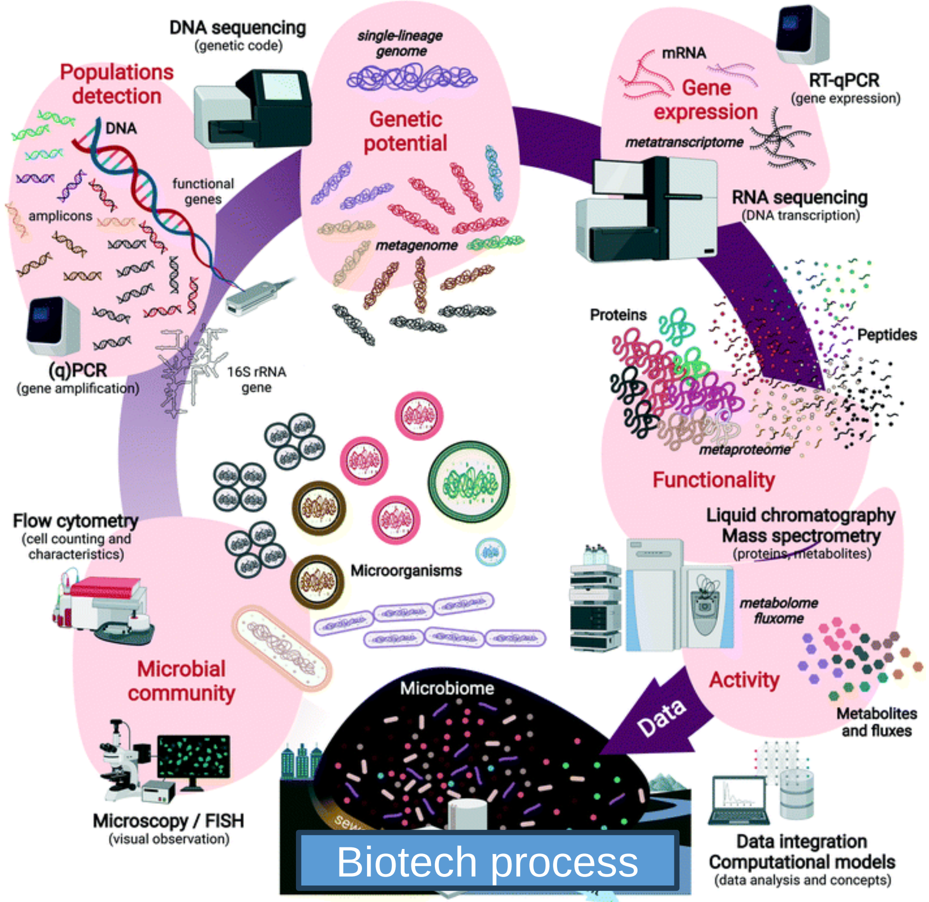
Data analysis (bioinformatics)
- Microbial community
- Gene expression
- Functionality



- Genome-scale metabolic network model
- Metabolites and fluxes

Design and control

Molecular microbiology analysis



Artificial Intelligence Enabling Future Optimal Flexible Biogas Production for Net Zero

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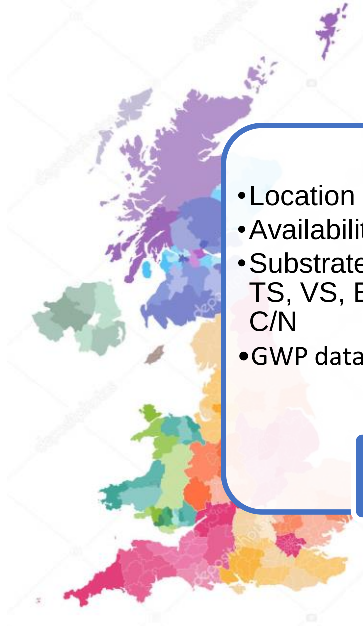
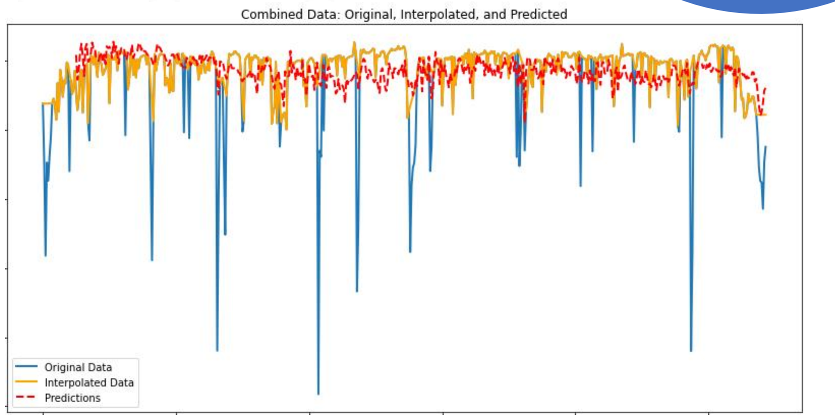


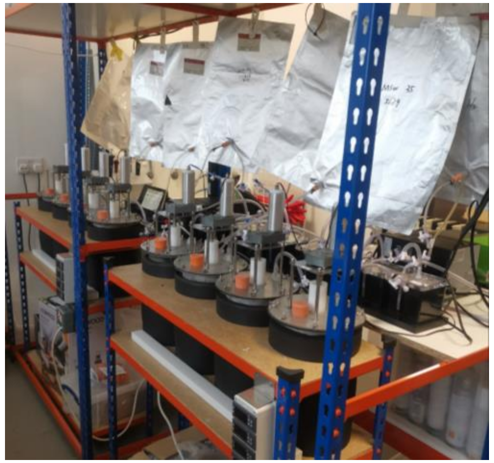
Feed data

- Location
- Availability period
- Substrate Characteristics: TS, VS, EBMP, TBMP, k, C/N
- GWP data α_c, γ_c



CoD function

- Takes combinations of feeds (A,B), (A,C), (B,C),…
- Calculates the optimal fraction leading to maximum BMP of the blend

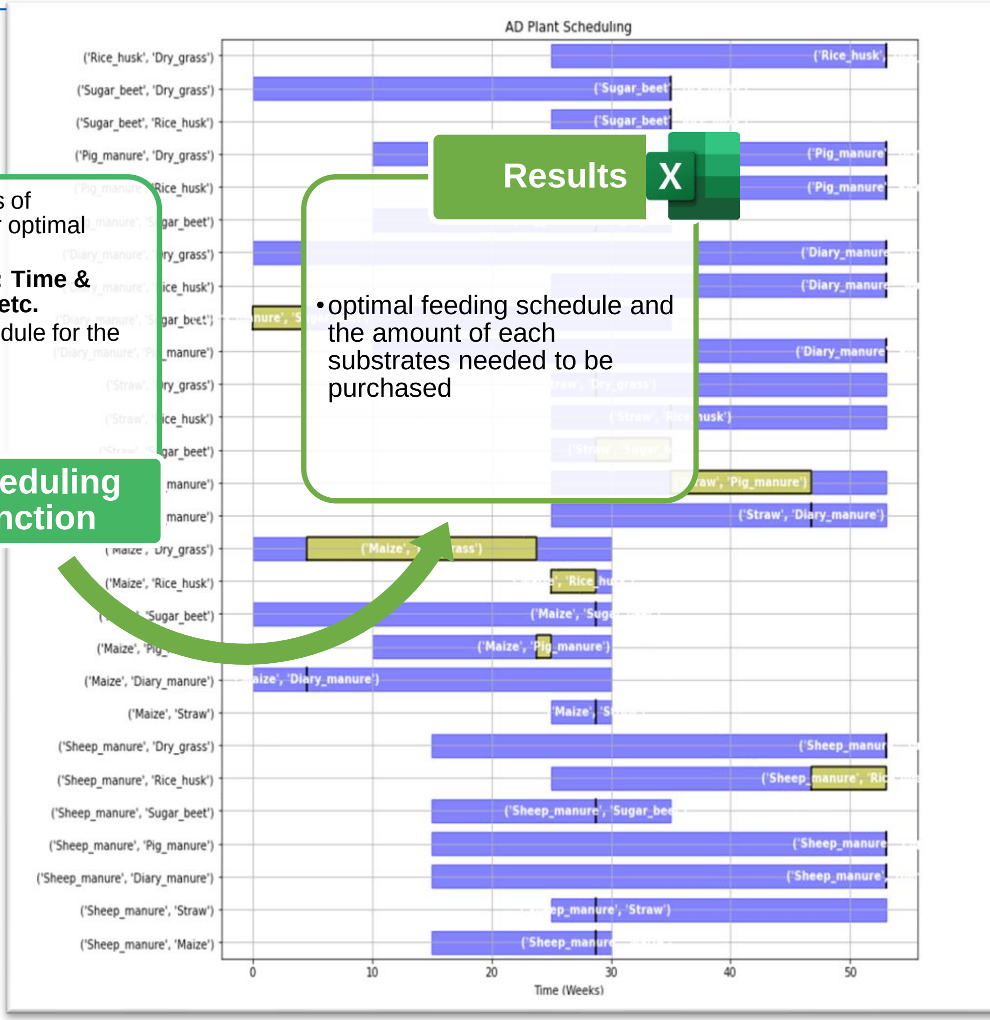


Scheduling function

- Takes combinations of substrates and their optimal blend and yield
- Takes, **Availability: Time & quantity, storage, etc.**
- Calculates the schedule for the **Optimal economic performance**

Results

- optimal feeding schedule and the amount of each substrates needed to be purchased



<u>None of this would be possible without my wonderful team:</u>

Dr Ishanki De Mel, Rob Steven, Anamika Kushwah, Ruosi Zhang, Qingyuan Wang, Meshkat Dolat, Floris Bierkens, Gul Hameed, Dr Amin Zarei, Rohit Murali, Dr Benaissa Dekhici and others!

Dr Michael Short

m.short@surrey.ac.uk

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@mchlshort

michael-short13

mchlshort

YouTube @michaelshortoptimisation