Computationally efficient surrogate based multi-objective optimisation for PSA for Carbon capture

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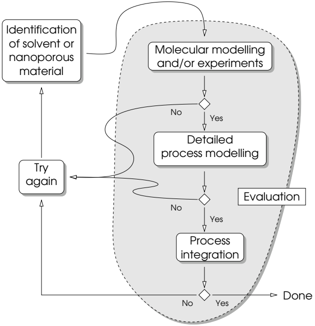
Topic

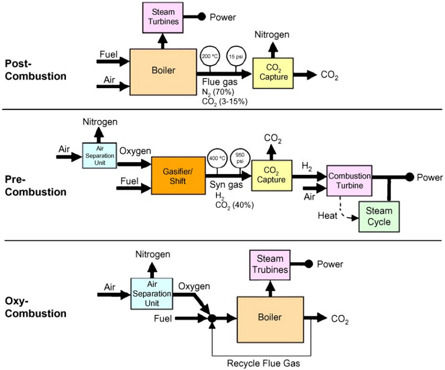
Efficient carbon capture



- reduce efficiency loss due to carbon capture.
- combined materials and process design.
- evaluation based on experiments, detailed modelling and process simulation and optimisation.

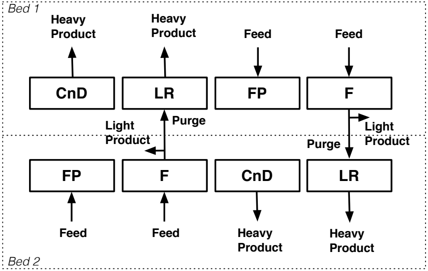
EPSRC EP/G062129/1

Integrating carbon capture



- The project considered both pre- and post-combustion capture.
- This talk concentrates on post-combustion alone.

Pressure Swing Adsorption (PSA)



Four step cycle:

FP: Feed pressurisation

F: Feed (adsorption)

CnD: Countercurrent depressurisation

LR: Light reflux (desorption)

Modelling I

Component mass balances (axial dispersed plug flow model):

$$\frac{dc_i}{dt} + \frac{1-\epsilon_b}{\epsilon_b}\frac{d\bar{Q}_i}{dt} + \frac{\partial(uc_i)}{\partial z} + \frac{\partial J_i}{\partial z} = 0$$

$$\frac{d\bar{Q}_i}{dt} = \epsilon_p \frac{dc_i^m}{dt} + (1-\epsilon_p)\frac{d\bar{q}_i}{dt} = k_i^p \frac{A_p}{V_p}(c_i - c_i^m)$$

Energy balance for the adsorbate in the gas phase:

$$\epsilon_b \frac{d\hat{U}_f}{dt} = -(1-\epsilon_b)\frac{\partial \hat{U}_p}{\partial t} - \epsilon_b \frac{\partial(\hat{H}_f u)}{\partial z} - \frac{\partial J_T}{\partial z} - \sum_{i=1}^{N_c} \frac{\partial(J_i \hat{H}_i)}{\partial z} - h_w \frac{A_c}{V_c}(T_f - T_w)$$

Modelling II

Energy balance for the adsorbate in the solid phase:

$$\frac{\partial \hat{U}_p}{\partial t} = \epsilon_p \frac{d\hat{U}_{p,f}}{dt} + (1-\epsilon_p)\frac{d\hat{U}_{p,s}}{dt} = h_p \frac{A_p}{V_p}(T_f - T_p)$$

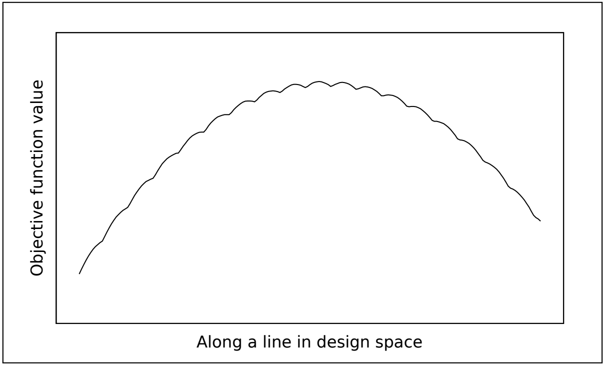
Energy balance in the bed wall:

$$\rho_w C_{p,w} \frac{\partial T_w}{\partial t} = -h_w \frac{A_c}{V_w}(T_w - T_f) - U\alpha_{wl}(T_w - T_\infty)$$

and so on.

As simulation must reach *cyclic steady state*,
$\Rightarrow$ computational effort is significant.

Behaviour of objective function



⇒ motivates use of surrogate modelling (response surface modelling, meta-modelling, . . .).

G Fiandaca, ESF & S Brandani (2009), Engineering Optimization 41(9):833-854.

Topic

Surrogate model

- a fast approximation of model's response $y(x) : \mathbb{R}^p \to \mathbb{R}$ where $\mathcal{X} \subset \mathbb{R}^p$ is the space with p design variables.
- suitable for black box optimisation models as the surrogate model is non-intrusive.
- based on training data: a set of known design points.

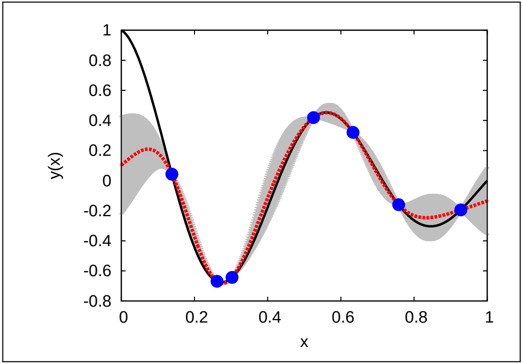
Most surrogates have form

$$\hat{y}(x) = \sum_{k=1}^{q} \beta_k h_k(x) + \epsilon(x)$$

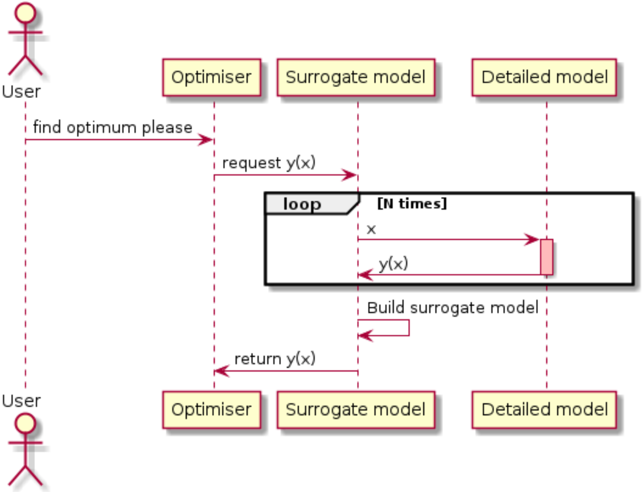
with regressors $h_i(\cdot)$ and a residual random process, $\epsilon(\cdot)$.

Kriging

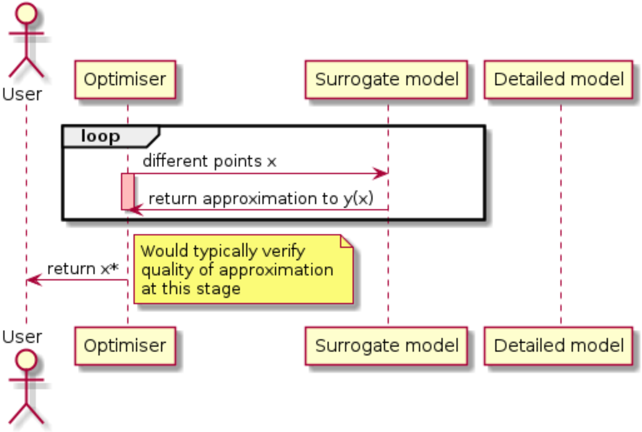
A statistical interpolating approach used for approximating deterministic models.



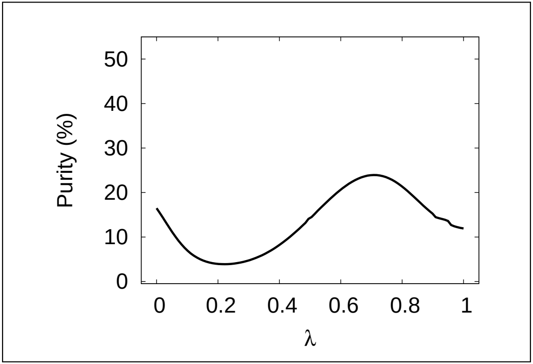
Surrogate Based Optimisation I



Surrogate Based Optimisation II



Optimiser

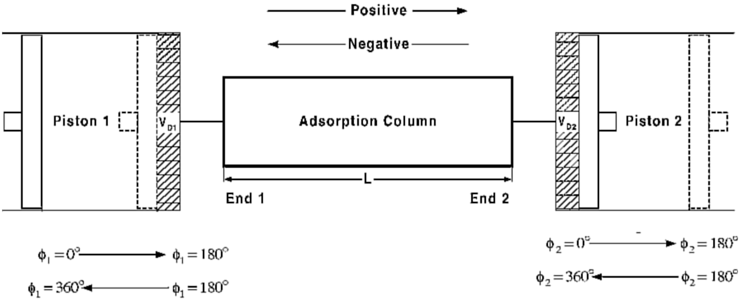


We use evolutionary stochastic methods to cater for multi-modality of objective function.

Topic

1. The challenge
2. Surrogate modelling
3. Case studies
4. Conclusion

Case study 1: Dual Piston PSA



DP-PSA: Decision variables

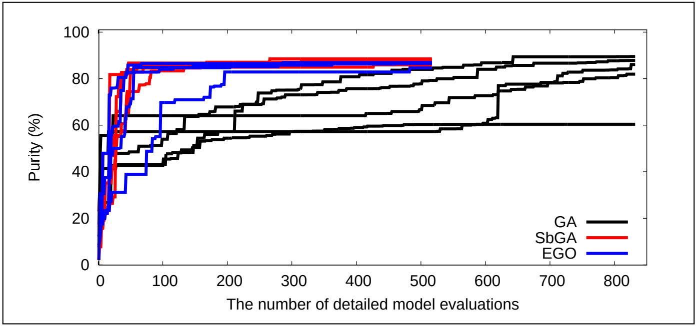
	Variables	a	b	
t_c	Cycle time	1	20	s
T_b	Bed temperature	15	70	°C
V_{p1}	Volume of piston chamber 1	$0.5V_0$	$15V_0$	m^3
V_{p2}	Volume of piston chamber 2	$0.5V_0$	$15V_0$	m^3
ϕ_{p1}	Offset angle of piston 1	0	2π	radians
ϕ_{p2}	Offset angle of piston 2	0	2π	radians

DP-PSA: Objective Function

Purity of CO_2 (%) in piston chamber 1 at CSS:

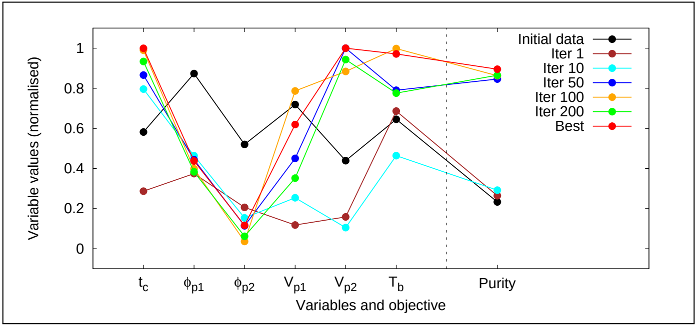
$$100 \times \frac{\int_{t_c} u y_{CO_2,p1}\, dt}{\int_{t_c} u \sum_{j=\{CO_2,N_2\}} y_{j,p1}\, dt}$$

DP-PSA: Objective Function Evolution

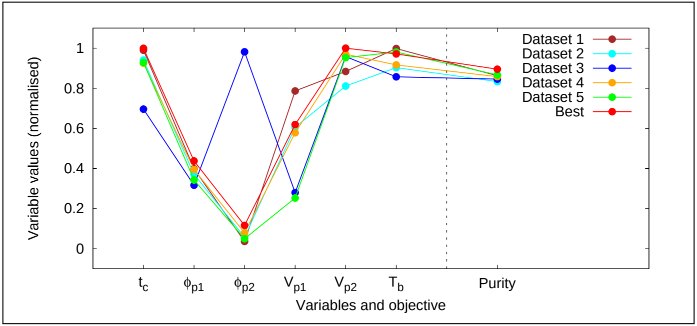


J Beck, D Friedrich, S Brandani, S Guillas & ESF (2012), Proc. ESCAPE-22.

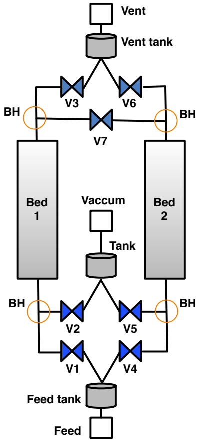
DP-PSA: Design Evolution



DP-PSA: Diversity

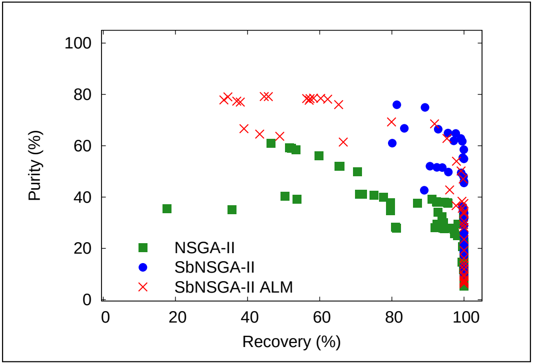


Case study 2: 6 step, 2 bed PSA

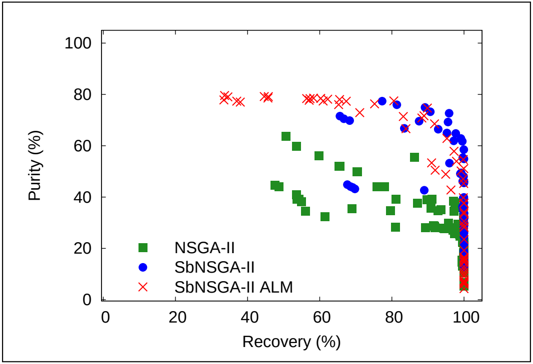


- 6 design variables.
- 3 objective functions: recovery, purity and power (but will illustrate 2).
- computational effort large: 30-60 minutes per objective function evaluation.

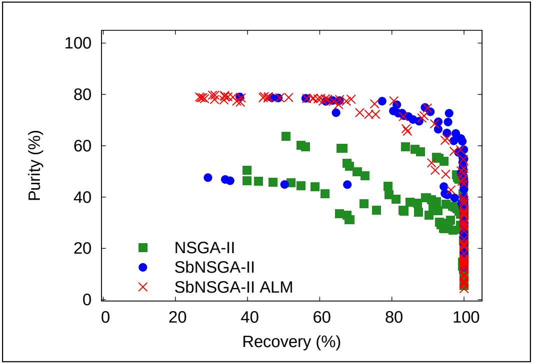
Pareto front: $n = 64$



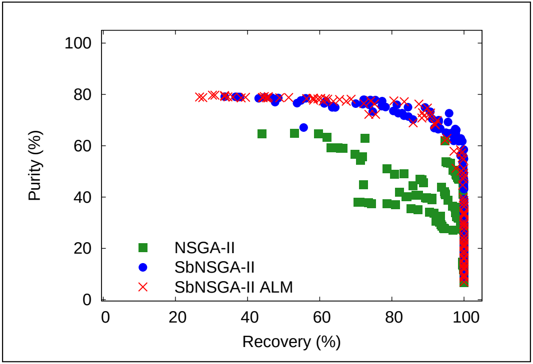
Pareto front: $n = 96$



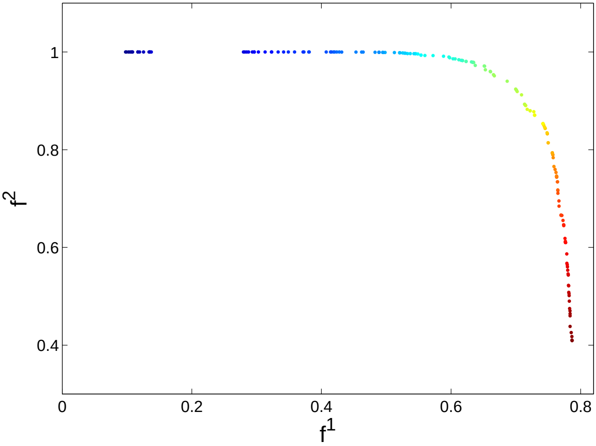
Pareto front: $n = 176$



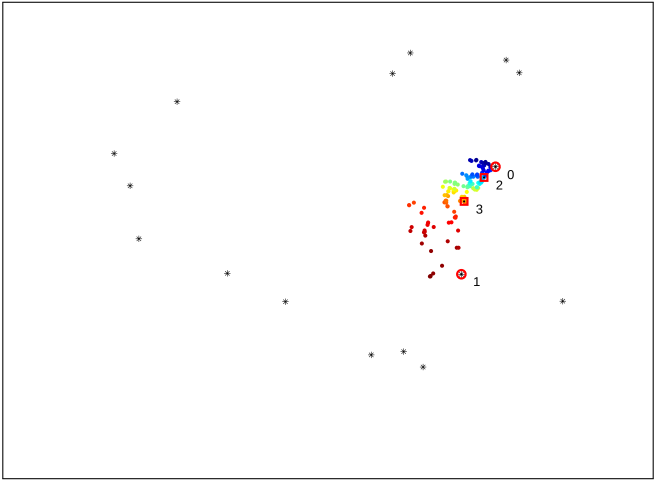
Pareto front: $n = 256$



Visualisation I



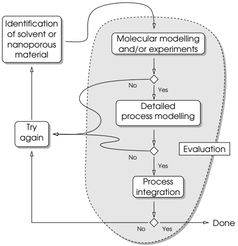
Visualisation II



A Žilinskas, ESF, J Beck & A Varoneckas (2015), J of Chemometrics **142**:151-158.

Topic

Summary



- surrogate modelling effective in optimal design.
- suitable for multi-objective optimisation.
- now considering discrete functions and uncertainty.

Acknowledgements

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http://www.ucl.ac.uk/~ucecesf/