WP AC5: OPTIMAL REDUCED ORDER MODELS FOR CCS

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PROJECT OVERVIEW

The complexity of process models accurately simulating PCC systems prohibits their direct inclusion into a system wide assessment. Here, we will produce robust, accurate reduced order models (ROMs) for PCC technologies using solvents and solid adsorbents to bridge this gap and represent the dynamic operation and performance of the capture technologies under operating conditions within the larger energy system model.

KEY OBJECTIVES:

- **Analyze input relevance using Global Sensitivity Analysis (GSA)**
- **Develop model order reduction technique based on GSA**
- **Trial application to solvent based PCC**
- **Provide validated approach to the project partners**

RESEARCH HIGHLIGHTS

A Gaussian Process (GP) surrogate predicts outputs as a normal distribution dependent on the input

$$y(x) \sim N[\mu(x), \sigma^2(x)]$$

The GP learns to mimic the training data starting from the assumption that similar inputs produce similar outputs. Mathematically, the output covariance is measured by the similarity kernel $k(x, X)$ between x and X:

$$Cov[\mu(x), \mu(X)] = k(x, X)$$

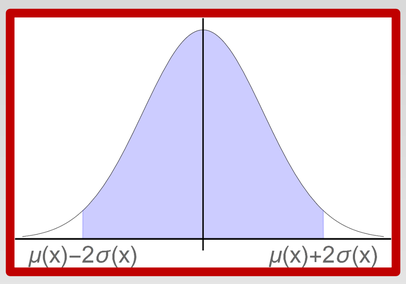

Fig. 1:

An anisotropic similarity kernel (ARD) detects inputs of differing relevance.

Optimally combining inputs according to Global Sensitivity Analysis (GSA) aligns the kernel axes with degrees of relevance.

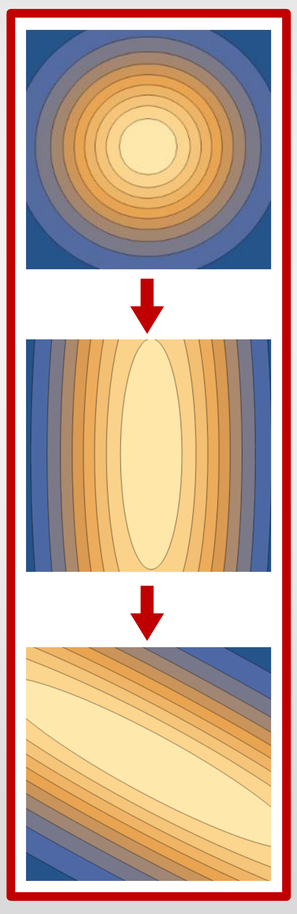
Fig. 2:

EMERGING FINDINGS

The technique has been applied to MEA based PCC for a 453 MWe NGCC power plant. CO_2 capture level is the model output, depending on 5 inputs listed in Fig. 3. Combining inputs using GSA successfully shifts all relevance to the first few inputs.

Cumulative Sobol' indices show how much of the output variance is explained by successively adding inputs in order of relevance.

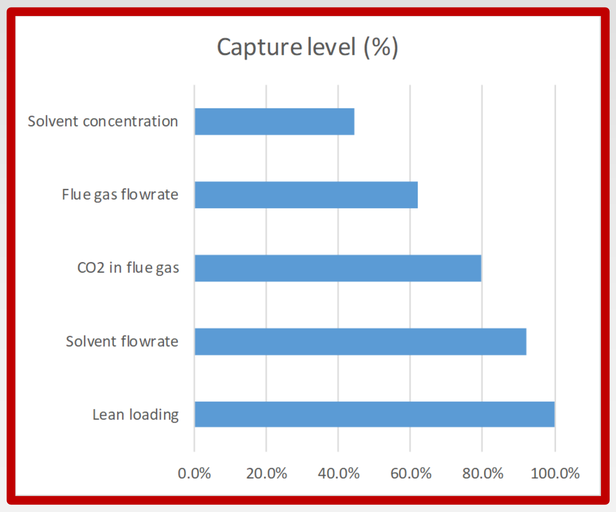

Fig. 3:

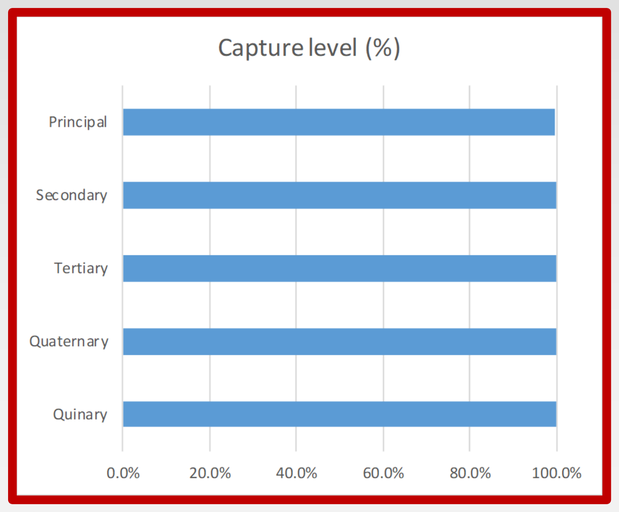

Fig. 4:

After combining inputs, 99% of the output variance is already captured in the principal input.

This results in a GP taking few inputs which simply and efficiently predicts outputs as a normal distribution. This is shown as a 95% confidence interval $(\mu \pm 2\sigma)$ in Fig. 5, scattered with independent test data.

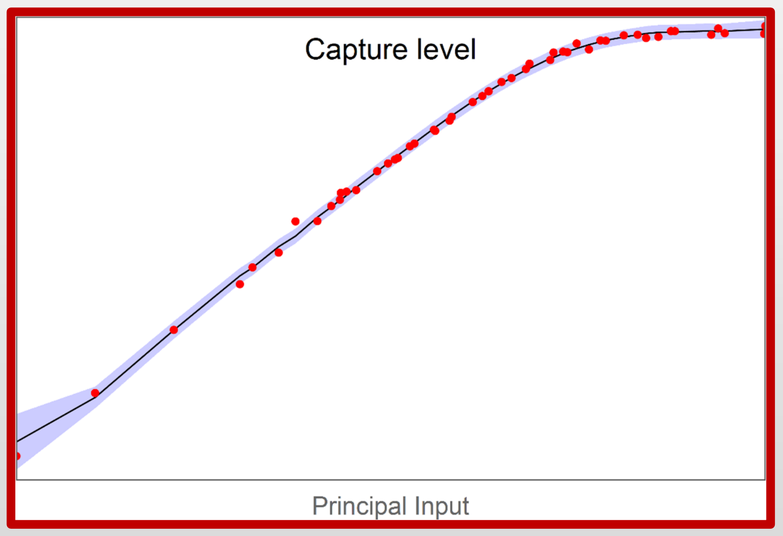

Fig. 5:

Principal Input ≈ 0.7 Solvent concentration – 0.4 Flue gas flowrate – 0.4 CO_2 in flue gas

NEXT STEPS

Publication:

- Novel ROM optimization theory in Brown S.F. and Milton R.A. (in press)
- Complete ROM software (in Python) freely available on GitHub at https://github.com/C-O-M-M-A/rom-comma

Application to other systems:

- Solid sorbent
- Chemical looping

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