Final Technical Report

Evaluation and demonstration of commercialization potential of CCSI tools within gPROMS advanced simulation platform

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Disclaimer

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Abstract

PSE, in the first phase of the CCSI commercialization project, set out to identify market opportunities for the CCSI tools combined with existing gPROMS platform capabilities and develop a clear technical plan for the proposed commercialization activities. PSE completed a detailed technical and commercial assessment of four pre-identified toolkit items:

- *SorbentFit*/*SolventFit*,
- Process Models
- *FOQUS*
- *ALAMO*

In addition, PSE performed a pre-feasibility study in order to identify any additional CCSI toolkit items with significant potential within the *gPROMS* platform. The following tools were also considered for commercialization:

- Uncertainty Quantification module
- Optimization under uncertainty
- Dynamic reduced order models
- iREVEAL

The technical assessment involved the development of prototypes and an implementation plan within the *gPROMS* platform for each tool. The commercial assessment identified and valued opportunities, also taking account of their potential exploitation outside of the carbon capture and storage (CCS) space. In addition, feedback from key stakeholders such as the potential customers and different business units within PSE was taken into account.

The assessment outputs were used to rank and select the tools that met PSE's commercialization criteria. In addition, they informed the development of integration and commercialization plans for the Phase 2 renewal application. Finally, plans for application of the CCSI tools to some advanced energy cases were developed. These plans included identifying suitable industrial partners to carry out required demonstrations.

As a result of the commercialization activities in Phase 1, the following achievements were recorded:

- Further improvement of CCSI tools specifically the Process Models, ALAMO and SorbentFit
- Extension of the scope of application of CCSI tools
- Dissemination of the developed CCSI tools via conferences and journal papers
- Collation of feedback on CCSI tools from key stakeholders
- Assessment of the Strengths, Weaknesses Opportunities and Threats of various CCSI tools
- Training and development of research professors, fellows and students

Although PSE's Phase 2 renewal application was unsuccessful, PSE will continue to support CCSI^2 developments in its Industrial Advisory Board capacity.

Contents

Executive Summary

The objectives of this project were to:

1. Identify opportunities for the commercialization of aspects of the Carbon Capture Simulation Initiative (CCSI) toolkit using the *gPROMS* platform, and
2. Develop and demonstrate a clear technical delivery path towards realizing these opportunities.

To achieve these objectives, Process Systems Enterprise (PSE) performed the following tasks.

Tasks performed

The scope of work for the project comprised 6 main tasks.

- Task 1: Project Management and Planning
- Task 2: Fast track tools – Workshops. WVU and PSE participated in the workshop held in WVU from 27th to 30th October 2015 covering the Process Models, SorbentFit, D-RM Builder and the Advanced Process Control Framework. A workshop was held in CMU on the 5th and 6th of November 2015 which covered FOQUS and ALAMO.
- Task 3: Pre-feasibility screening – the following tools were considered in the screening phase (excluding the fast-track tools):
    - Derivative-Free Optimization (DFO) module
    - The Uncertainty Quantification module
    - Optimization Under Uncertainty (OUU)
    - Dynamic Reduced-Order Model (D-RM)
    - iREVEAL
    - CCSI Superstructure Formulation
    - CCSI Oxy-combustion Models
    - CCSI UT_2-MPZ/Pz Model
    - CCSI CFD Models

  Many tools were incompatible with the gPROMS platform or replicated functionality that already existed. Apart from the four preselected tools, the following tools were selected after the screening process for further consideration:

    - Uncertainty Quantification module
    - Optimization under uncertainty
    - Dynamic Reduced models
    - iREVEAL
- Task 4: Stage gate – Detailed commercialization and integration assessments were carried out on the fast track and the screened tools. Based on the assessments, the tools were ranked and compared with PSE's commercialization criteria. The following tools (or tool components) were considered for commercialization:
    - ALAMO
    - FOQUS Turbine for cloud computing
    - Bayesian Calibration concepts
- Task 5: Taskforces - value proposition and prototyping – Further assessments and tests were carried out on the tools considered for commercialization.
- Task 6: Final assessment and commercialization plan – the assessments carried out in Task 5 provided integration and commercialization requirements which informed the execution of this task.

PSE executed these tasks and delivered the following as described below:

Deliverables

Deliverable #	Task	Description	Planned Completion	Actual Completion
D1.3	1.4	Negotiate commercial distribution licence	Q6	Not concluded - Phase 2 application was unsuccessful
D2.1	2.1	Report - SolventFit/SorbentFit integration requirements	Q1-2	Q3
D2.2	2.2	Report - Process Models integration requirements	Q1-2	Q3
D2.3	2.3	Report - FOQUS integration requirements	Q1-2	Q3
D2.4	2.4	Report - ALAMO integration requirements	Q1-2	Q3
D3.1	3.1 / 3.2	Evidence-based ranking of the CCSI tools with recommendation	Q2	Q3
D4.1	4.1/4.2	Stage gate decision: agree selections to take forward	Q2	Q3
D5.1	5.1.1	Report: implementation plan for each qualifying tool	Q4	Q4
D5.2	5.1.2	Report: commercialization plan for each qualifying tool	Q5	Q4
D5.3	5.1.3	Agreed model developments essential for assessing capabilities	Q5	Q4
D5.4	5.1.3	Minimum 2 prototype or case study applications covering two Advanced Energy Systems, each with dissemination via conference presentation or journal publication	Q5	Q6
D6.1	6.1.2	Agree candidates to take forward to Phase 2	Q6	Q4
D6.2	6.2	Finalize Phase 2 proposal	Q6	Q4

1 Introduction

This report summaries the activities and deliverables of the first phase project titled “Evaluation and demonstration of commercialization potential of CCSI tools within gPROMS advanced simulation platform”.

Section 2 describes the workshop for the four fast track tools and a selection of the rest of CCSI tools along with their preliminary assessments.

Section 3 describes the CCSI fast-track tools discussing what they are, the proposed commercialization product and a SWOT analysis of each tool.

Section 4 discusses the pre-feasibility screening activity of all the CCSI tools and results. This was carried out to determine which additional tools to assess for commercialization.

Section 5 describes the current and proposed integration requirements for the fast-track tools.

Section 6 describes the prototypes developed to assess the utility of the tools for advanced energy applications

Section 7 provides a summary of the stakeholder feedback collected during the project.

Section 8 discusses the assessment and ranking results.

Section 9 provides a description of the CCSI tools/components proposed for commercialization as well as the proposed case studies to demonstrate their application.

Section 10 provides the Project plan proposed for Phase 2.

2 Fast track tools workshops and preliminary assessments

PSE through a series of activities acquired a clear description of each of the four fast track tools. The fast track tools workshop and preliminary tool assessments are described in the following sections:

2.1 Workshops

Firstly, PSE team members met with their counterparts in West Virginia University (WVU) and Carnegie Mellon University (CMU) for workshops in October and November 2015 respectively.

2.1.1 WVU Workshop

WVU and PSE participated in the workshop held in WVU from 27th to 30th October 2015.

During this workshop, presentations and demonstrations were provided for the following process models: bubbling fluidized bed (BFB), moving bed (MB), CO_2 compressor, solids heat exchanger, balance of the plant, integrated systems and solvent system.

The discussions held during the workshop covered:

- The features and benefits of the various tools
- Current applications and potential applications of the models
- Future development work planned as well as preliminary plans for developing suitable prototypes to investigate technical and commercial integration issues.
- A proposal to develop a fixed-bed adsorber model in addition to the existing CCSI models. These models could form the basis of a commercial process model library in gPROMS

In addition, presentations and demonstrations were made by the developers of CCSI Dynamic reduced order model (D-RM) Builder and Advanced Process Control (APC) Framework tools:

- Dr. Jinliang Ma (NETL) presented the D-RM Builder
- Dr. Priyardarshi Mahapatra (NETL) presented the APC Framework
- Dr Stephen Zitney (NETL) led the team

They presented the features, software basis, current and potential applications of the tools.

Furthermore, a demonstration of the *SorbentFit* tool was provided. This was accompanied by a thorough, detailed discussion of the tool, including chemistry, mathematics and computational structure. Opportunities for commercialization of the present *SorbentFit* tool and/or pieces of that tool were discussed. (An additional demonstration and related discussion was provided to PSE senior management during the AIChE Annual meeting in Salt Lake City, UT.)

A demonstration of the *SolventFit* tool was not provided since this tool was still in development at the time of the workshop. However, the chemistry, theory and computational implementation of the tool were discussed.

2.1.2 CMU Workshop

A workshop was held in CMU on the 5th and 6th of November 2015. Both *ALAMO* and *FOQUS* were presented and discussed in some detail. Potential usage of both packages was discussed as well as possible ways of testing the capabilities in relation to potential commercialization.

For *ALAMO* there seems to be a relatively straightforward way to develop some form of integration for testing purposes.

Integration with *FOQUS* was already possible, but there are some usability issues at the time.

2.2 Preliminary assessment and prototypes of fast track CCSI tools

The following summarize the outcome of the preliminary investigations of the fast track CCSI tools.

2.2.1 Process Models

2.2.1.1 Integration of process models in gCCS flowsheet

The first prototype explored the feasibility of employing the CCSI toolset gPROMS model in a carbon capture and storage (CCS) chain flowsheet. PSE had developed previously post-combustion CCS whole chain models including the following units:

- Coal-fired power plant
- Monoethanolamine (MEA) chemical absorption process
- CO_2 compression train
- CO_2 transportation models for storage

The MEA chemical absorption process was replaced with a combination of the BFB and MB models from the CCSI Toolset. A steady-state integration was simulated successfully. Figure 1 displays an integrated model in gPROMS.

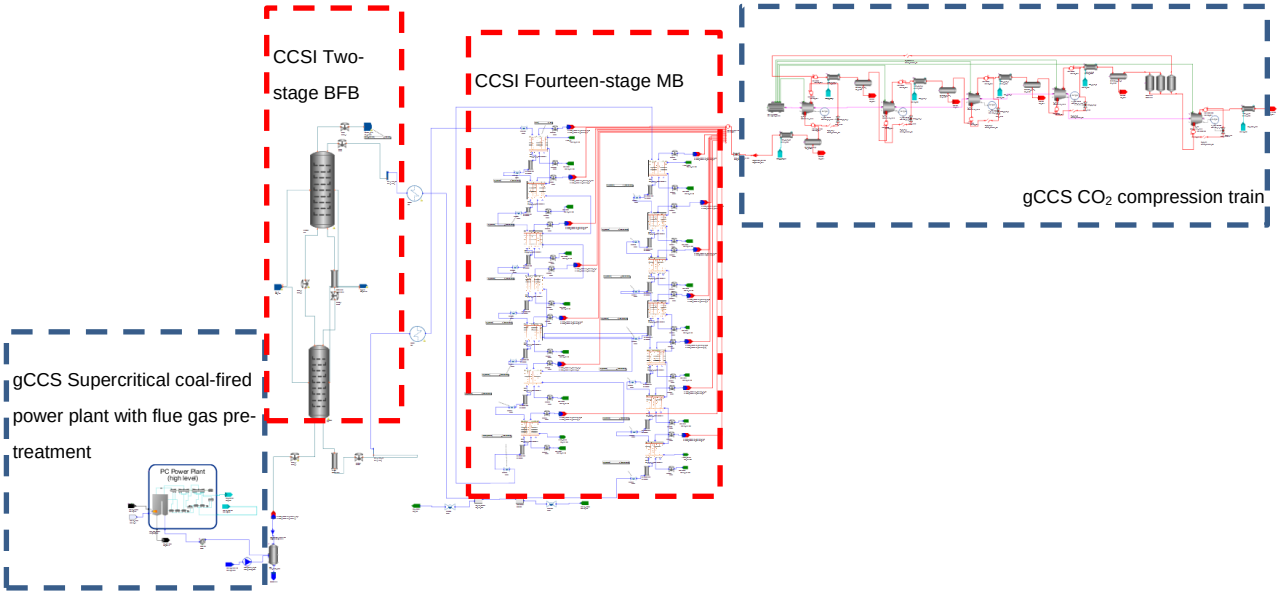

Figure 1 Integrating CCSI Process models with gCCS models

2.2.1.2 Identification of potential applications beyond CO_2 capture

A literature search was conducted to identify potential applications of BFB, MB, Circulating Fluidized Beds (CFB), Dual Fluidized Beds (DFB) and fixed beds. Various potential applications were found including:

- Calcium looping
- Naphtha reforming
- Drying of solids
- Gas separation involving other species

2.2.1.3 Model reduction of the BFB

To carry out further investigations, PSE developed a reduced form of the model. This process requires executing several simulations of the BFB under a range of conditions. However, it was observed that the model failed to initialize for a significant number of conditions deemed to be reasonable for operation. This suggests that some improvement in model robustness may be required.

2.2.2 ALAMO

2.2.2.1 Developing a reduced order model of a physical property package

ALAMO was used to develop a reduced order model of a physical property package for the prediction of steam properties at different temperatures and pressure. For the test a wide range of input values was selected:

Pressure range – 1 bar to 250 bar

Temperature range – 0 °C to 600 °C.

ALAMO was used to predict 11 model outputs which were various forms of mass specific enthalpies, entropies, densities and vapor fractions.

In general, ALAMO was able to predict with a simple subset of bases functions, the model outputs for most vapor or liquid property calls but had not as good results for the total calls (particularly where changes in the temperature and pressure conditions resulted in phase changes). This is shown in Figure 2.

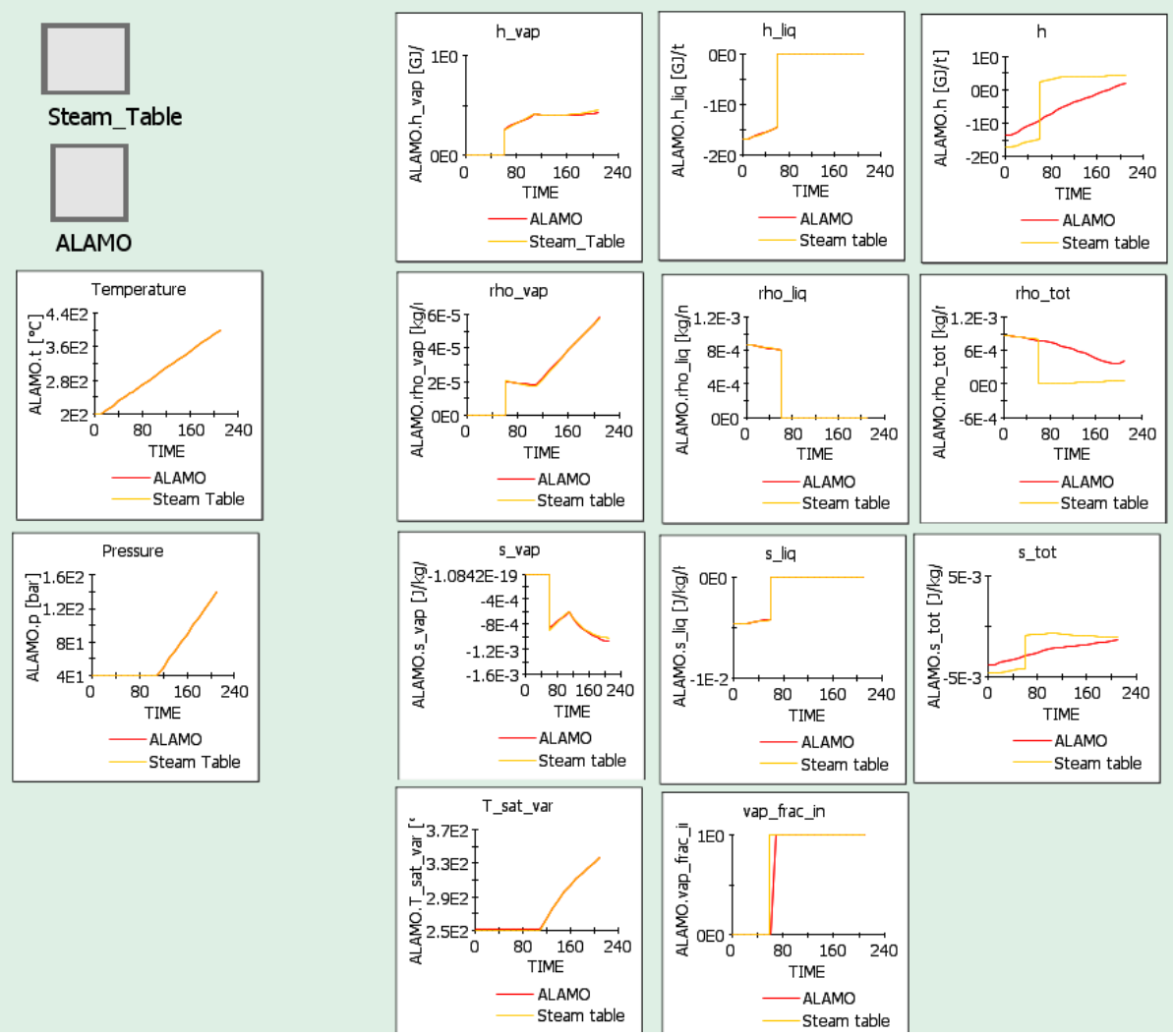

Figure 2 Comparison of ALAMO and physical property package predictions

2.2.2.2 Developing a reduced order model of a tubular reactor

In this case, the outlet temperature, flowrate and composition of the reactor (consisting of a series of tubular reactors) shown in Figure 3 was predicted by ALAMO. A physically reduced model (Continuously Stirred Tank Reactor (CSTR)) was developed to compare results (Figure 4). The ALAMO model consisted of 6 model inputs and 7 model outputs. There were 13000 model equations in the full model.

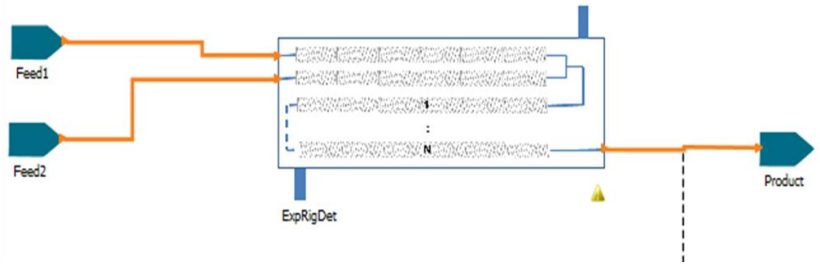

Figure 3 Jacketed reactor model in gPROMS with several tubes

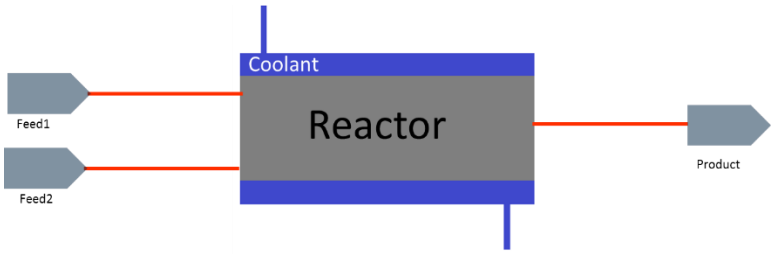

Figure 4 Physically reduced reactor model in gPROMS

Both ALAMO and the physically reduced model give fairly good predictions of the reactor temperature (Figure 5) but ALAMO's predictions are less accurate than the physically reduced models as shown in Figure 6. The predictions of composition of the main product from the detailed model (x_mp2 detailed) are plotted against those from the two reduced models (x_mp2 reduced). The ALAMO predictions do not show the right trend at higher MP2 compositions.

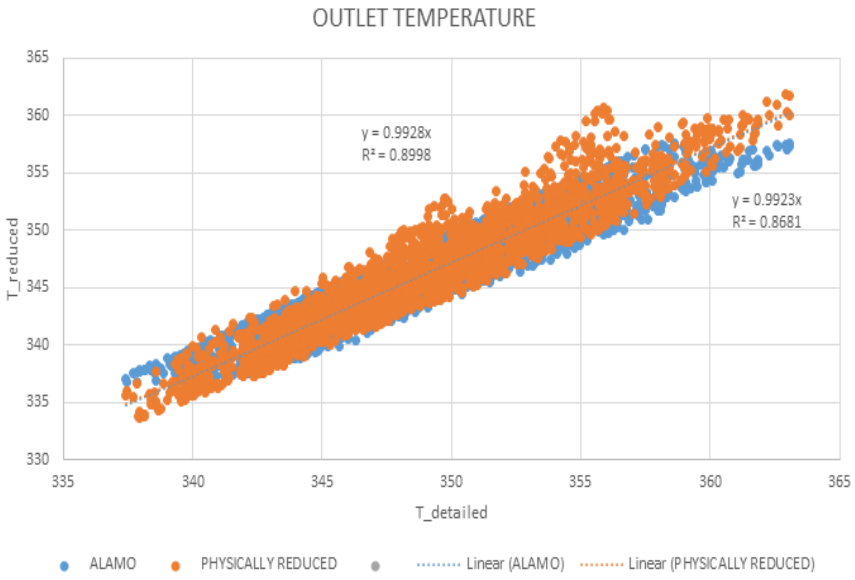

Figure 5 Comparing ALAMO and physically reduced model predictions of outlet temperature with the detailed model predictions

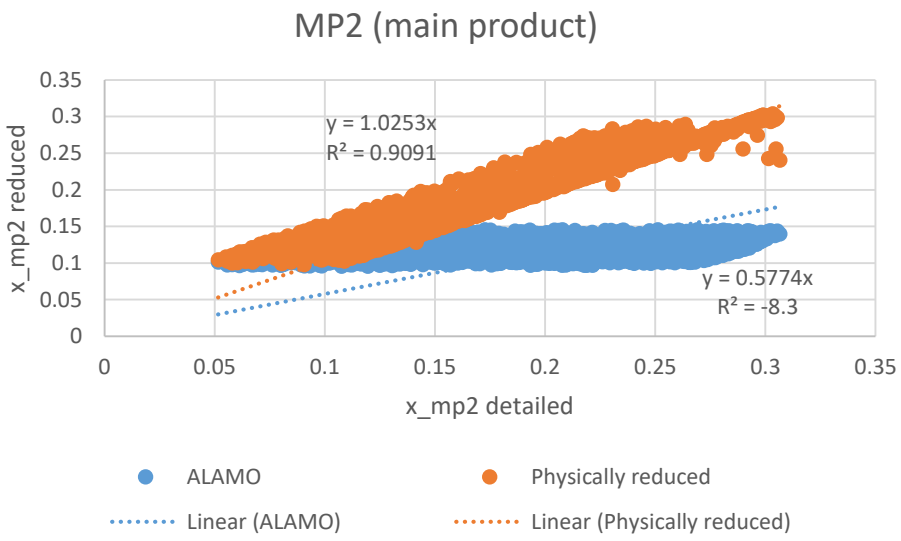

Figure 6 Comparing ALAMO and physically reduced model predictions of product composition with the detailed model predictions

2.2.2.3 Identification of competitors, potential markets and possible applications of ALAMO

A literature survey was conducted to determine this and several competitors were found to offer products that create surrogate models. Only one product, however, (EUREKA) was found to use the same technique as ALAMO. EUREKA, unlike ALAMO, cannot handle constrained regression.

ALAMO essentially provides a black box model between inputs and outputs. As such, it can be applied to a wide range of potential markets ranging from studies in Engineering to Social science and so on.

2.2.3 FOQUS

2.2.3.1 Testing the performance of flowsheets consisting of gPROMS models connected to other simulations software

A single stage represents one CSTR in gPROMS. A 2 stage case represents a CSTR model in gPROMS connected to an Excel model via FOQUS Flowsheet and this model connected to the second stage CSTR model in gPROMS as shown in Figure 7 and so on. This flowsheet structure was also duplicated with only gPROMS models. The performance (simulation times) of the two set ups are shown in Table 1. The top row show the simulation results from gPROMS-only flowsheets and the bottom show those of the FOQUS flowsheets. There is a clear performance penalty with increasing number of units in the FOQUS much greater than that in gPROMS.

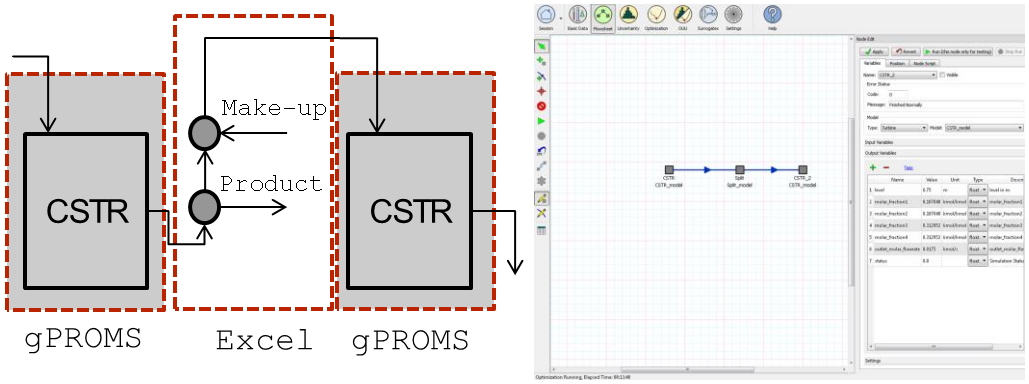

Figure 7 FOQUS flowsheet model set up and FOQUS flowsheet screenshot

Table 1 Performance results for FOQUS flowsheet investigations

Time (s)	**1 stage (1 unit)**	**2 stage (3 units)**	**3 stage (5 units)**	**4 stage (7 units)**
gPROMS	5	5	6	11
FOQUS	15	43	72	110

2.2.3.2 Identification of competitors, potential markets and possible applications of FOQUS

The job queueing service of Turbine on the cloud offers the capability of parallelization of simulations. This would be particularly useful for a number of types of simulations such as sensitivity analysis. The FOQUS Flowsheet functionality could be useful for connecting gPROMS to other tools. However, other tools which provide similar functionality, such as CAPE-OPEN interface, are currently not widespread.

2.2.4 SorbentFit

2.2.4.1 Comparison of Bayesian calibration results in SorbentFit with gPROMS Maximum Likelihood parameter estimation

SorbentFit provides probability and distribution information of parameter values which is considerably more information than what gPROMS Maximum Likelihood parameter estimation would produce. Table 2 shows the time required to carry out a SorbentFit parameter estimation. This was conducted in gPROMS using the Maximum Likelihood approach in about 20 minutes.

Table 2 Time required to carry out a SorbentFit parameter estimation

Preparation Time	30 min
Run Time	30~40hrs
Memory Used	24GB
Cores Used	8

The following sections briefly describe the fast-track tools (detailed description of the tools are provided in the Brochures in Appendix A):

3 Defining the CCSI fast track tools

3.1 Process models

3.1.1 What are the Process models?

The CCSI Process Models include a set of solid/gas system models developed in gPROMS containing the following:

3.1.1.1 gPROMS component models

- Bubbling fluidized bed (BFB) (gas/solid contactor with immersed HX)
    - Adsorber
        - Overflow/Underflow
        - Dynamic/Steady state
    - Regenerator
        - Overflow/Underflow
        - Dynamic/Steady state
- Moving bed (MB) (gas/solid contactor with immersed HX)
    - Overflow/Underflow
    - Dynamic/Steady state
- Ancillary models – hoppers, valves, heaters.

3.1.1.2 gPROMS flowsheet projects

- BFB standalone and MB standalone
    - Overflow/Underflow
    - Dynamic/Steady state
    - 1-stage/2-stage
- Integrated BFB+MB + CO_2 compression and dehydration

The BFB reactor model is one-dimensional (1D) partial differential algebraic equation (PDAE)-based, two phase and non-isothermal, incorporating heat transfer tubes to provide external heating and cooling capability. It can be used to simulate over-flow type configuration where the solids leave the stage by flowing over the weir or the underflow-type configuration where the solids leave from the bottom of the bed. This model can also be modified to use it as a heat exchanger model.

The MB reactor model is also 1D PDAE-based, two-phase and non-isothermal, with heat transfer tubes. When used as a regenerator, an integral heat-recovery system heats the incoming solid sorbent using the steam that is produced by recovering heat from the hot sorbent leaving the regenerator. The reaction kinetics, heat and mass transfer, and the hydrodynamics are considered both in the MB reactor and heat recovery system.

3.1.1.3 Workflow

Other than the input boundaries, the user needs to provide the design inputs for the gas/solid contactors. Output information includes results of the output streams and the transport profiles and other variables typical of process models.

3.1.2 Proposed commercialization product

- Gas/Solid Contactor models (with heat and mass transfer)
- Fixed bed, Bubbling Fluidized bed and Moving bed flowsheet models
- Balance of plant equipment models (transport, etc.)
- Potentially a gas / solid advanced model library for
    - Refining / Petrochemicals
    - Food / Pharmaceuticals
    - Power generation

3.1.3 SWOT Analysis – Process models

3.1.3.1 Strengths

- Steady state and dynamic models
- Models are flexible such that it can be used as an adsorber or regenerator
- Embedded cooler/heater depending on the application
- Flexible configuration- solids can enter/leave at/from the top or bottom

3.1.3.2 Weaknesses

- Currently limited scope of application
- Relatively large BFB/MB models
- Improvements in robustness needed
- No model verification of BFB or MB process models

3.1.3.3 Opportunities

- Extend application to various process industries involving gas/solid fluidized beds
- Apply learnings from uncertainty propagation to other process models

3.1.3.4 Threats

- Similar (in-house) process models developed for Fluid Catalytic Cracking units
- Very complex models that require significant improvement and training

3.2 SorbentFit/SolventFit

3.2.1 What are SorbentFit and SolventFit?

SorbentFit is a chemical kinetic fitting tool. It contains two models pertaining to amine-based CO_2 adsorbents: a lumped-kinetic model and a high-fidelity reaction-diffusion model. Models can be fit to either (dynamic) Thermogravimetric analysis (TGA) or fixed bed datasets.
SolventFit is a fitting tool for high-viscosity CO_2 solvents, based on wetted-wall column data.

Both tools are developed in C++.

SorbentFit can estimate 13 parameters simultaneously. It includes 3 executable files:

- Process simulation with given parameter values
- Parameter estimation using Particle Swarm Optimizer (PSO)
- Parameter estimation using Bayesian Analysis

3.2.1.1 Process simulation

This file simulates the amine sorbent-based carbon capture process with given parameter values

3.2.1.2 Parameter estimation using PSO

The inputs to this code are:

- Configuration file which contains initial guess for all parameters and the bounds for all parameters to be estimated
- Experimental data file

The outputs from this code are:

- Parameter estimation results for each step
- Calculated results for experimental measured variables

3.2.1.3 Parameter estimation using Bayesian Analysis

The inputs to this code are:

- Configuration file which includes bounds, initial guess, and standard deviation for all the 13 parameters to be estimated, observation error and tuning parameters for the prior.
- Experimental data file

The outputs from this code are:

- Parameter estimation results, observation error per data file, likelihood, percentage error per data file
- The acceptance rates of all 13 parameters
- Calculated results for experimental measured variables

3.2.1.4 Workflow

Users must provide formatted data in the form of space- or tab-delimited text files. Configuration files pertaining to the relevant experiment. Configuration files specify the model parameters for which estimation is desired, along with bounds on those parameters. (Default values are provided.) Tolerances and settings for the solver (including the time step used) can also be changed from their default values in the configuration file. A list of formatted data files must also be provided. The user can also change the number of agents used in the particle swarm optimizer (point estimate) or the proposal variances and total number of samples obtained (Bayesian calibration) from their defaults.

Users invoke SorbentFit at the command line. Periodic output is written to the console, with final results written to disk. For the point estimate tool, the final results are the final parameter set along with predictions of the fitted model compared with experiment. For Bayesian calibration, results are a list of sampled parameter sets that represent the posterior distribution for the parameters.

SolventFit is GUI-based, with the relevant configuration taking place in the FOQUS GUI.

3.2.2 Proposed commercialization product

- Provide a generic version of the Bayesian calibration features as a gPROMS parameter estimation entity
- Create suitable Graphics User Interface

3.2.3 SWOT Analysis – SorbentFit

3.2.3.1 Strengths

- Gives probability distribution (allowing for additional metrics such as expected value) of estimated parameters
- Efficient multi-core algorithm

3.2.3.2 Weaknesses

- Takes long time to run
- No GUI
- Expert input required at present
- Output is high dimensional data (needs some training at present)

3.2.3.3 Opportunities

- Bayesian estimation is not available in flowsheet tools

3.2.3.4 Threats

- Free Bayesian estimation tools available

3.3 ALAMO

3.3.1 What is ALAMO?

The Automated Learning of Algebraic MOdels (ALAMO) distribution provides executables and examples for building models from data and/or simulations. ALAMO can work with a pre-existing dataset and/or interface with an executable that provides new data at points specified by ALAMO. The ALAMO downloads from www.minlp.com are zip archives for different operating systems (Windows, Linux and Mac OSX); versions are provided for 64 and 32 bit architectures. Each zip archive comes with an ALAMO executable, the ALAMO manual in PDF, example data files, and example executables that can be used to provide new data.

3.3.1.1 Workflow

Inputs

The user specifies the number of input and output variables in the system of interest, the range of interest for the input variables, the types of functions that ALAMO should consider in building an input-output model, and a data set with measurements of the output variables at the corresponding values of the input variables. Optionally, the user may prepare an executable that can sample the input-output system at will. More information is provided in the ALAMO manual. Additional examples are provided in the distribution—See the examples folder, which includes several ALAMO input files (all with the extension `.alm`).

ALAMO must be called from the command line. For example,

```
alamo example1
```

will run ALAMO on file `example1`. An example input file was provided in the previous section.

Data Output

In addition to providing output on the screen, ALAMO generates a results (listing) file with the extension `.lst`. For instance, running ALAMO on `example1` (or `example1.alm`), will generate a results file named `example1.lst`. This file contains all data used by ALAMO in the calculations, all option files used in the run, and the models obtained by ALAMO. Typically, many models are found and reported. The model that is reported last is the best one found.

3.3.2 Proposed commercialization product

- Integrate product with gPROMS as a separate entity or within Global Sensitivity Analysis tool

3.3.3 SWOT Analysis – ALAMO

3.3.3.1 Strengths

- Wide applicability
- Accounts for synergistic effects between different potential basis functions
- Designed to minimize data points needed
- Constrained regression
- Adaptive sampling (not available yet)

3.3.3.2 Weaknesses

- Lack of installer and GUI
- Basis functions need to be provided manually by user (experience needed)
- Requires GAMS/BARON for complex fitting problems and MATLAB/SNOBFIT for constrained regression
- Complex problems may take considerable computing time due to the sophisticated ALAMO algorithms
- (Explicit directionality from input to output)

3.3.3.3 Opportunities

- Automate process for use in Uncertainty quantification or Sensitivity analysis

3.3.3.4 Threats

- May cannibalize PSE's high-fidelity model libraries
- The Optimization Firm is also planning to commercialize ALAMO independently through other channels (no exclusivity)
- No access to source code

3.4 FOQUS Flowsheet, SimSinter and Turbine

3.4.1 What is FOQUS?

The Framework for Optimization, Quantification of Uncertainty, and Surrogates (FOQUS) serves as a computational platform enabling advanced process systems engineering capabilities to be integrated with commercial process simulation software.

FOQUS consists of several modules (Miller, 2015).

1. **SimSinter** provides a .NET wrapper for Windows-based process simulators such as Aspen Plus ACM, Excel, and the Windows version of gPROMS. It provides a generic interface, and a simple means to define a simulation inputs, outputs and settings. SimSinter has some dynamic simulation support currently for ACM.

SimSinter is used by Turbine to interface with process simulations, and provides COM interface allowing simulations to be accessed in using VBA.

2. **Turbine** is a job queuing system for process simulations supported by SimSinter and for FOQUS flowsheets. Turbine allows simulation jobs to be executed on a single workstation, or in parallel on cloud, cluster, or local network resources.
3. The **FOQUS Flowsheet** is used to link simulations together and connect model variables between simulations. FOQUS enables linking models from different simulation packages. FOQUS flowsheets can be executed in parallel using Turbine to support derivative free optimization (DFO), uncertainty quantification (UQ) and surrogate modelling. The FOQUS flowsheet also provides a graphical interface and platform for analysis tools.
4. The **Automated Learning of Algebraic MOdels (ALAMO)** module can create algebraic surrogate models to support large-scale deterministic optimization, including superstructure optimization to determine process configurations. The ALAMO module is an external product due to background Intellectual Property (IP) issues.
5. The **Derivative-Free Optimization (DFO)** module enables derivative-free (simulation-based) optimization directly on the process models linked together on a FOQUS Flowsheet. Excel can be used to calculate complex objective functions, such as the cost of electricity.
6. The **UQ module** enables the effects of uncertainty to be propagated through the complete system model, sensitivity of the model to be assessed, and the most significant sources of uncertainty identified to enable prioritizing of experimental resources to obtain additional data.
7. The **Optimization Under Uncertainty (OUU)** module combines the capabilities of the DFO and the UQ modules to enable scenario-based optimization, such as optimization over a range of operating scenarios.
8. The **Dynamic Reduced-Order Model (D-RM)** module can be used to create dynamic reduced models from more detailed process models to support advanced model predictive control or enable more rapid evaluation of dynamic operating scenarios.
9. The **iREVEAL** module is an automated tool to create reduced-order models from computational fluid dynamics (CFD) simulations and export them in a form that can be used in process simulators.
10. The **SolventFit** module is an uncertainty quantification tool for the calibration of an Aspen Plus solvent process model. The current state-of-the-art is Maximum Likelihood as found in gPROMS for example. The Maximum Likelihood indicates the optimal value as well as the variance (for an assumed error model, typically normally distributed as in gPROMS). The state of the art estimators do not give the level of uncertainty in model output directly, they typically only supply the covariance matrix. SolventFit allows for predictions with uncertainty bounds by accounting for uncertainty in model parameters and deficiencies in the model form. This yields an improved understanding of the model parameters and results in more complete predictions with uncertainty bounds. This distribution of parameters allows for predictions with uncertainty in the sense that one can generate an output distribution.

This assessment was based on the FOQUS Flowsheet, SimSinter and Turbine capabilities

3.4.1.1 Workflow

Data input

For typical meta-flowsheeting purposes, in addition to the simulation, a SimSinter configuration file is required which defines a simulation input, output, and settings. The simulation and configuration files are uploaded to Turbine. Once simulations are available from Turbine, a flowsheet is defined in the FOQUS flowsheeting tool. Nodes are created and a simulation is assigned to each node. Directed edges between nodes between nodes define how data is transferred from node to node. If cycles are created in the flowsheet FOQUS can determine tear steams and solve the flowsheet iteratively. Once the flowsheet is defined, data analysis tools can be used.

Data Output

After running the results of every flowsheet evaluation are presented in tabular form. Analysis tools also produce text and graphical output in many cases. In the case of optimization, an objective function plot is obtained that displays the objective function value at each iteration. The details such as current iteration, number of samples, successful samples as well as failed samples are displayed in the status bar.

3.4.2 Proposed commercialization product

- Create a separate FOQUS flowsheet interface which is fully integrated with gPROMS – allowing seamless integration of gPROMS model.
- Incorporate Turbine functionality for job sequencing

3.4.3 SWOT Analysis – FOQUS

3.4.3.1 Strengths

- Turbine allows simulation jobs to be executed on a single workstation, or in parallel on cloud, cluster, or local
- User can interface, simulate and optimize gPROMS models with other software
- FOQUS flowsheets can be simulated and optimized

3.4.3.2 Weaknesses

- Time-consuming procedure to load models
- FOQUS is currently not compatible with some gPROMS language syntax

3.4.3.3 Opportunities

- Could complement GSA with cloud computing

3.4.3.4 Threats

- This presents an alternative to the users migrating models to gPROMS
- Simulation times could become impractical for large number of nodes and be seen as a gPROMS flaw

4 Pre-feasibility screening

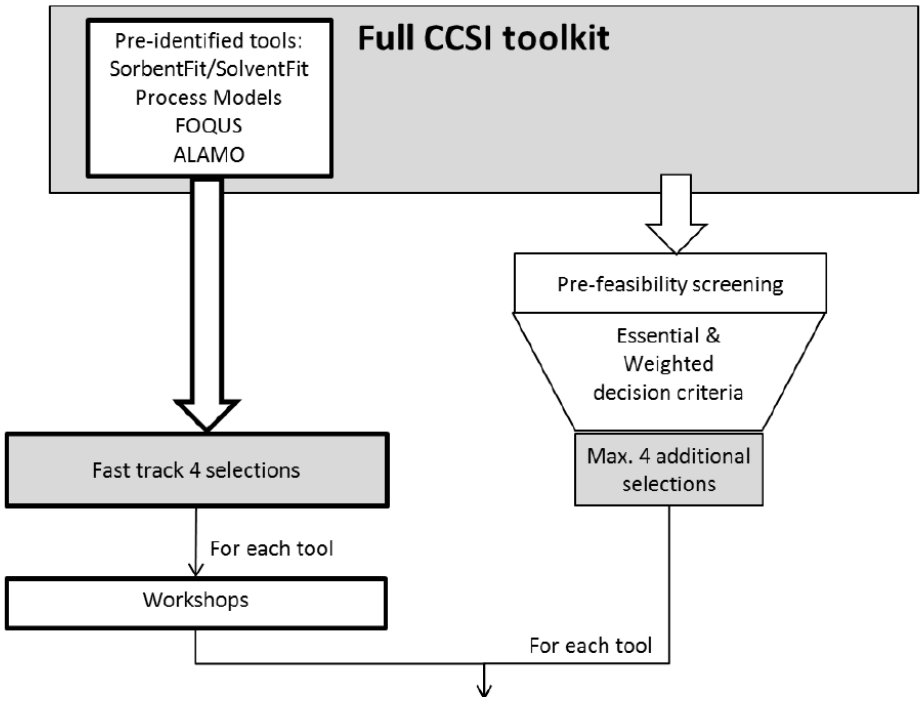

Figure 8 Pre-feasibility screening

Figure 8 shows the process with which PSE has screened tools for commercialization assessments. The four fast track tools were assessed in detail:

- Process Models
- ALAMO
- FOQUS
- SorbentFit / SolventFit

PSE was unable to access SolventFit until mid-May 2016 as it had not been made available for testing and evaluation until then. As a result, PSE is unable to provide a proper assessment of the tool. However, since it is similar to SorbentFit, in principle, some of the conclusions regarding SorbentFit can be assumed to apply to SolventFit as well.

The FOQUS Bundle consists of several CCSI tools including ALAMO and SolventFit. PSE considered the FOQUS Flowsheet, SimSinter and Turbine capabilities as the preselected fast track tools. The other tools available in the FOQUS Bundle are:

4.1 Derivative-Free Optimization (DFO) module

This enables derivative-free (simulation-based) optimization directly on the process models linked together on a FOQUS Flowsheet. Excel can be used to calculate complex objective functions, such as the cost of electricity. Derivative-free optimization does not align with PSE's current product strategy. As a result, this tool was not considered any further.

4.2 The UQ module

This module enables the effects of uncertainty to be propagated through the complete system model, sensitivity of the model to be assessed, and the most significant sources of uncertainty identified to enable prioritizing of experimental resources to obtain additional data. This tool was considered because of its uncertainty quantification and propagation features.

4.3 Optimization Under Uncertainty (OUU)

This module combines the capabilities of the DFO and the UQ modules to enable scenario-based optimization, such as optimization over a range of operating scenarios. This tool was considered because of its application of uncertainty quantification to optimization.

4.4 Dynamic Reduced-Order Model (D-RM)

This module can be used to create dynamic reduced models from more detailed process models to support advanced model predictive control or enable more rapid evaluation of dynamic operating scenarios. This tool, which was reviewed during the WVU workshop, was considered as the model reduction feature was considered useful.

4.5 iREVEAL

This module is an automated tool to create reduced-order models from computational fluid dynamics (CFD) simulations and export them in a form that can be used in process simulators. Again, this model was selected for its model reduction capabilities.

Other CCSI tools considered include:

4.6 CCSI Superstructure Formulation

This tool contains a model formulation to optimize the structure of a carbon capture system. The problem to be solved can be generalized as the minimization problem below,

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0 \\ & x^l \le x \le x^u \end{aligned} \tag{1}$$

Where the aim is to minimize a cost function, $f(x)$ with respect to the degrees of freedom x. These degrees of freedom include continuous decisions of operating conditions and geometry and discrete decisions about process alternatives and flowsheet configuration. The process was optimized on the basis of minimizing the estimated cost of electricity (COE) on a 2007 basis for the power plant with carbon capture and compression. The primary constraint is the requirement that the process achieve a minimum of 90% removal of carbon dioxide from the incoming flue gas stream.

The superstructure optimization model is written in GAMS and can be solved by the BARON software. This software dependency makes this particular tool unattractive to PSE for commercialization.

4.7 CCSI Oxy-combustion Models

The oxy-combustion models package consists of two primary components: A detailed CFD boiler model and a suite of equation-based models of the other components of a complete oxy-combustion power generation system. The first principle-based model contains advanced submodels for the calculation of radiation properties and for the

heterogeneous reactions between coal particle and the gas reactants. The boiler model is applicable to both air-firing and oxy-firing conditions. PSE already provides oxy-combustion models through its gCCS application software.

The second module is a collection of equation-based flowsheet optimization models and examples implemented in the General Algebraic Modeling System (GAMS). This software dependency again makes this particular tool unattractive to PSE for commercialization.

4.8 CCSI UT_2-MPZ/Pz Model

This is an Aspen Plus® absorption/stripping model for CO_2 capture from natural gas or coal-fired power plants using the solvent 4 molal 2-methylpiperazine (2MPZ)/4 molal piperazine (PZ). This model can be used for techno-economic assessments, pilot plant data reconciliation, and process design. However, as this tool is based on Aspen PIus®, it is not a feasible option for commercialization in gPROMS.

4.9 CCSI CFD Models

This product bundle contains all the device scale CFD models developed in the course of CCSI project, and they include the coupled reactive gas particle flow model for the 1MWe sorbent-based adsorber, CFD models for the decoupled and coupled bench-scale C2U cases in order to build a hierarchical calibration and validation framework for quantifying the predictive confidence for systems yet to be built, gas-particle subgrid filtered models with and without the presence of heat exchanger tubes to enable geometric upscaling, as well as particle attrition models for predicting particle side degradation. It also contains the solvent-relevant CFD models and modules developed by the CCSI team in an effort to predict the device-scale behaviors for a solvent-based capture system. PSE did not consider these models because they were based on CFD software.

4.10 Summary of screening results

In conclusion, apart from the four preselected tools, the following tools were selected after the screening process for further consideration (it should be noted that they were assessed in less detail based on their perceived relevance and market):

- Uncertainty Quantification module
- Optimization under uncertainty
- Dynamic Reduced models
- iREVEAL

5 Integration requirements for fast track tools

This Section highlights the integration requirements for the fast track tools. Both current and planned (for the commercialized product) integration requirements are discussed.

5.1 Process Models

5.1.1 Current integration requirements

The process models are already implemented in gPROMS hence, they can be used with gPROMS application software in their current state and no additional software is required.

5.1.2 Integration requirements of proposed product

As discussed in Section 3.1.2, the proposed finalized product is a model library developed from the existing models capable of modelling a variety of gas/solid systems. For the finalized commercial product, a number of changes are proposed:

- Improvements in model robustness and speed of execution
- Modification of models to make them more generic in application - for instance, provision of the capability to model other gas/solid systems apart from
- Preparation of model specification dialogs and model report for the entire model library
- Model documentation with associated models including validation results
- Example process flowsheets including cases with model verification against real plant data

5.2 SorbentFit

5.2.1 Current integration requirements

SorbentFit is coded in C++. SorbentFit requires the BOOST C++ library, and the Eigen numerical package. Currently, the best way of integrating SorbentFit and gPROMS is through gPROMS Foreign Process Interface (FPI). FPI provides general mechanism for exchange of info between gPROMS simulations and external software. Communication takes place at discrete time points throughout the duration of the simulation as specified by the gPROMS model. The user is entirely free to determine the frequency and content of the data exchange which may include:

- time-synchronization signals
- values of variables and flags
- Information on the mathematical model used for the simulation and its current state.

Key two tasks are carried out through this interface:

- “GET” info from external package
- “SEND” info to external package

Figure 9 shows the reference architecture for prototyping. Communications between SorbentFit and gPROMS is via the FPI (specifically TextFPI which writes and reads data to/from a text (“IO”) file.

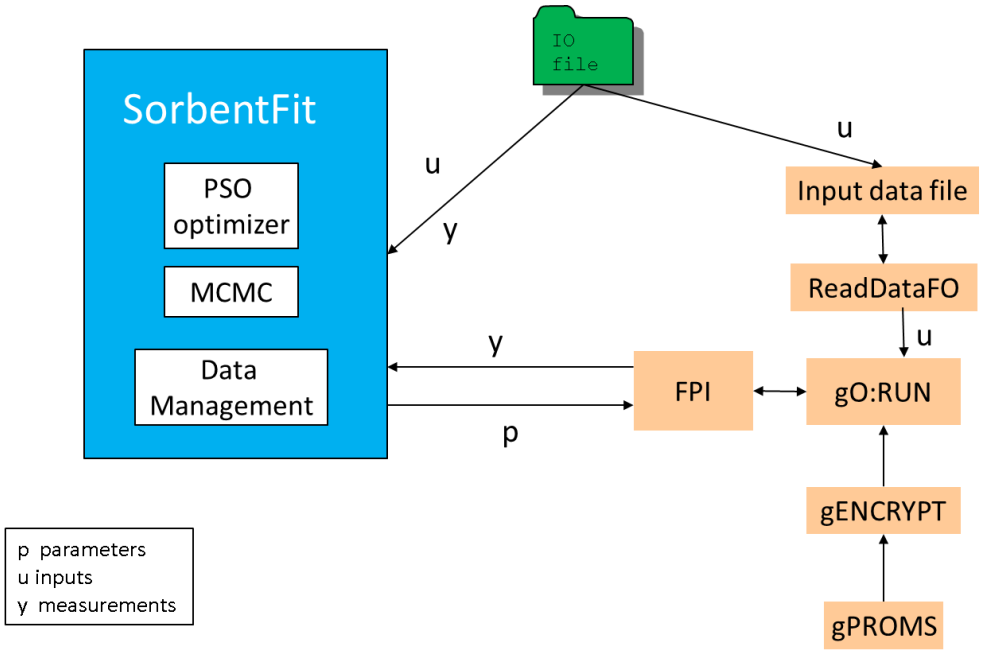

Figure 9 Reference architecture for prototyping

5.2.2 Integration requirements of proposed product

The proposed commercialization product discussed in Section 3.2.2 is a feature capable of parameter estimation using Bayesian calibration methods. This feature shall be provided as a gPROMS parameter estimation entity without the need to integrate with external software. A new graphics user interface (GUI) would need to be developed as well as suitable forms of data visualization.

5.3 ALAMO

5.3.1 Current integration requirements

ALAMO is coded in FORTRAN. ALAMO requires GAMS/BARON for complex fitting problems and MATLAB/SNOBFIT for constrained regression. Currently ALAMO can be integrated with gPROMS via a similar TextFPI interface as SorbentFit.

5.3.2 Integration requirements of proposed product

In Section 3.3.2, it is proposed that ALAMO is provided with gPROMS as a separate entity or within Global Sensitivity Analysis tool with software dependency restricted to only BARON or preferably without any external software dependencies.

5.4 FOQUS

5.4.1 Current integration requirements

FOQUS SimSinter provides a .NET wrapper interface for Windows-based process simulators such as Aspen Plus, ACM, Excel, and the Windows version of gPROMS. FOQUS Flowsheet and Turbine are supported by SimSinter.

The gPROMS model inputs are linked to variables in a gPROMS Foreign Object. Model outputs are defined via SimSinter. A flowsheet node or instance is created in FOQUS flowsheet and simulations are run through the job queuing system, Turbine. This process is illustrated in Figure 10. The process of defining model inputs and outputs was found to be manual and cumbersome.

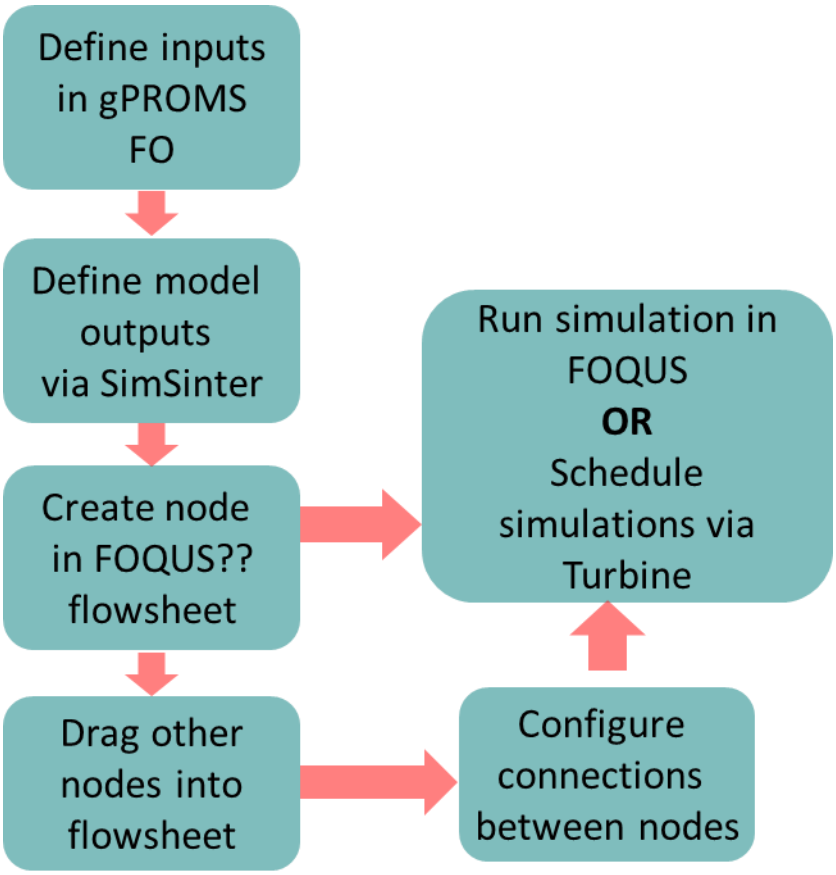

Figure 10 Running a gPROMS simulation in FOQUS

5.4.2 Integration requirements of proposed product

One key objective would be to develop an interface that automates the definition of model inputs and outputs. Another would be to migrate the flowsheeting functionality of FOQUS flowsheet to gPROMS applications.

6 Prototypes developed for advanced energy applications

6.1 Fixed-Bed Reactor Models for CO_2 Adsorption

Towards extending the CCSI toolset process models to cover more adsorption unit operations, a fixed-bed adsorption model was developed. Fixed-bed reactors are more widely applied in industry than moving or bubbling fluidized beds. A number of versions of this model were developed over the course of the project:

- Steady state, single-component, isothermal fixed bed adsorber
- Steady state, single-component, non-isothermal fixed bed adsorber
- Steady state, multi-component, non-isothermal fixed bed adsorber
- Dynamic, multi-component, non-isothermal fixed bed reactor model capable of simulating the cycle sequence for Pressure swing adsorption (PSA)

6.1.1 Complete Mathematical Model of the Fixed Bed Adsorber

The complete dynamic mathematical model consists of three mass balance equations for the bulk gas phase, macropore gas phase and solid phase micropore mass balances, three energy balance equations for the gas phase, solid phase and reactor wall energy balances, as well as of the Ergun momentum balance equation for computing the changing velocity within the reactor bed. The model is one-dimensional, dynamic, and non-isothermal, with axial dispersed plug flow. The CO_2 adsorption is described by the Langmuir adsorption isotherm. Both external and internal (macropore and micropore) resistances to diffusion are considered. The assumptions of the model are:

(1) Radial concentration, temperature and velocity gradients within the bed are negligible.

(2) External mass and heat transfer resistances are expressed with the film model.

(3) The gases follow the ideal gas law within the operating conditions under study (1 bar).

(4) The momentum balance is modeled by the Ergun equation.

(5) Single component (CO_2) adsorption is described by the Langmuir adsorption isotherm.

(6) Constant porosity along the bed.

The balance equations based on the assumptions are presented in Table 3.

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Table 3 Mass, momentum and energy balance equations of the mathematical model of the fixed bed adsorber (Ribeiro et al. 2008).

Mass component balances

Gas phase:

$$\varepsilon \frac{\partial C_{g,i}}{\partial t} = -\frac{\partial \left(v_g C_{g,i}\right)}{\partial z} + \varepsilon \frac{\partial}{\partial z}\left(D_{ax} \frac{\partial C_{g,i}}{\partial z}\right) - \frac{(1-\varepsilon) a_p k_f}{1 + Bi_i}\left(C_{g,i} - \overline{C_{s,i}}\right) \quad (1)$$

Solid phase, macropore:

$$\frac{\partial \overline{C_{s,i}}}{\partial t} = \frac{a_p k_f}{\varepsilon_p (1 + Bi_i)}\left(C_{g,i} - \overline{C_{s,i}}\right) - \frac{\rho_p}{\varepsilon_p} \frac{\partial \overline{q_i}}{\partial t} \quad (2)$$

Solid phase, micropore:

$$\frac{\partial \overline{q_i}}{\partial t} = \frac{15 D_{c,i}}{{r_c}^2}\left(q_i^* - \overline{q_i}\right) \quad (3)$$

Momentum balance (Ergun equation, Ergun 1952):

$$-\frac{\partial P_g}{\partial z} = \frac{150\, \mu (1-\varepsilon)^2 v_g}{\varepsilon^3\, {d_p}^2} - \frac{1.75 (1-\varepsilon) \rho_g |v_g| v_g}{\varepsilon^3\, d_p} \quad (4)$$

Energy balances

Gas phase:

$$\varepsilon C_{g,T} C_{v,g} \frac{\partial T_g}{\partial t} = -v_g C_{g,T} C_{p,g} \frac{\partial T_g}{\partial z} + \frac{\partial}{\partial z}\left(\lambda \frac{\partial T_g}{\partial z}\right) + \varepsilon R_g T_g \frac{\partial C_{g,T}}{\partial t} - (1-\varepsilon) a_p h_f \left(T_g - T_s\right) - \frac{4 h_w}{D_r}\left(T_g - T_w\right) \quad (5)$$

Solid phase:

$$\left[\varepsilon_p \overline{C_{s,T}} C_{v,s} + \rho_p \left(\widehat{C_{p,s}} + C_{v,ads} \sum_i \overline{q_i}\right)\right] \frac{\partial T_s}{\partial t} = \varepsilon_p R_g T_s \frac{\partial \overline{C_{s,T}}}{\partial t} - \frac{\rho_p}{(1-\varepsilon)} \Delta H \frac{\partial \overline{q_i}}{\partial t} + a_p h_f \left(T_g - T_s\right) \quad (6)$$

Reactor wall:

$$\rho_w C_{p,w} \frac{\partial T_w}{\partial t} = a_w h_w \left(T_g - T_w\right) - a_{w1} h_0 \left(T_w - T_\infty\right) = 0 \quad (7)$$

In Eq. (7), a_w is the ratio of the internal surface area to the volume of the reactor wall, a_{w1} is the ratio of the logarithmic mean surface area of the reactor shell to the volume of the reactor wall (Cavenati et al., 2006):

$$a_w = \frac{D_r}{w_{th}(D_r + w_{th})} \quad (8)$$

$$a_{w1} = \frac{1}{(D_r + w_{th}) \ln\left(\frac{D_r + w_{th}}{D_r}\right)} \quad (9)$$

The axial mass dispersion is computed as a function of the Reynolds and Schmidt numbers:

$$\frac{\varepsilon D_{ax,i}}{D_{m,i}} = 20 + 0.5\, Sc_i\, Re \tag{10}$$

where $D_{m,i}$ is the molecular diffusion coefficient calculated using the Wilke correlation :

$$D_{m,i} = \frac{1 - y_{g,i}}{\sum_{j,j\neq i} \frac{y_{g,j}}{D_{ij}}} \tag{11}$$

Additional correlations (Cavenati et al. 2006, Dantas et al. 2011) needed for the model are presented in Table 4 below.

Table 4 Correlations for the estimation of mass and heat transfer parameters

Effective macropore diffusivity (Bosanquet equation):	$\frac{1}{D_{p,i}} = \tau_p \left(\frac{1}{D_{m,i}} + \frac{1}{D_{K,i}} \right)$	(12)
Knudsen diffusion:	$D_{K,i} = 97 r_p \sqrt{\frac{T_g}{MW_i}}$	(13)
Binary molecular diffusivity (Chapman-Enskog equation)* (Bird et al., 2007):	$D_{ij} = \frac{2.33 \times 10^{-2}\, T_g^{3/2}}{P_g\, {M_{ij}}^{1/2}\, {\sigma_{ij}}^{1/2}\, \Omega_{Dij}}$	(14)
Film heat transfer (Nusselt #):	$\frac{h_f d_p}{k_g} = 2.0 + 1.1 {Re_p}^{0.6} Pr^{1/3}$	(15)
Internal convective heat transfer coefficient (Nusselt #):	$\frac{h_w D_r}{k_g} = 12.5 + 0.048 Re$	(16)
External convective heat transfer coefficient:	$\frac{h_0 L}{k_g} = 0.68 + \frac{0.67\, Ra^{1/4}}{\left[1 + \left(\frac{0.492}{Pr}\right)^{9/12}\right]^{4/9}}$	(17)
Axial heat dispersion:	$\frac{\lambda}{k_g} = 7 + 0.5\, \mathrm{Pr}\, Re$	(18)

* Values of σ_{ij} and Ω_{Dij} calculated using the Lennard-Jones parameters (Bird et al., 2007).

The pore tortuosity needed in Eq. (12) is assumed to have a value of 2 (Ribeiro et al. 2008).

The reactor is initialized assuming that it is under equilibrium initially with the gas mixture from which CO_2 is to be separated, but containing no CO_z, at the feed pressure and temperature. The initial and boundary conditions for the mass, momentum and energy balance equations are:

At *t = 0:*

$$\begin{aligned} & C_{g,i}(t=0,z) = y_{gi,initial}\, P_{g,init} / \left(R_g\, T_0\right) \\ & \overline{C_{s,i}}(t=0,z) = y_{gi,initial}\, P_{g,init} / \left(R_g\, T_0\right) \\ & \overline{q_i}(t=0,z) = q_i^* \\ & T_g(t=0,z) = T_s(t=0,z) = T_w(t=0,z) = T_0 \end{aligned} \tag{19a}$$

At *z = 0*:

$$\begin{aligned} & v_{in} C_{in,i} - v_g C_{g,i} = \varepsilon D_{ax} \frac{\partial C_{g,i}}{\partial z} \\ & v_{in} C_{in,T} = v_g C_{g,T} \\ & C_{p,g}\left(v_{in} C_{in,T} T_0 - v_g C_{g,T} T_g\right) = \lambda \frac{\partial T_g}{\partial z} \end{aligned} \tag{19b}$$

At $z = L$:

$$T_g = T_0$$
$$\frac{\partial C_{g,i}}{\partial z} = 0$$
$$\frac{\partial T_g}{\partial t} = 0 \quad (19c)$$
$$P_g = P_{g,exit}$$

The adsorption model used to describe the equilibrium relationship between the adsorbed CO_2 and the gas-phase CO_2 concentration is the pure Langmuir model:

$$q^*_{CO2} = \frac{q_{max}\, K\, P_{CO2}}{1 + K\, P_{CO2}} \quad (20)$$

Here, q^*_{CO2} (mol/kg) is the equilibrium concentration of the adsorbate in the adsorbed phase, q_{max} (mol/kg) is the maximum adsorptive capacity of the solid phase corresponding to the monolayer saturation coverage, K (1/bar) is the Langmuir equilibrium constant, and P_{CO2} (bar) is the partial pressure of CO_2 in the gas phase.

6.1.2 Langmuir isotherm calibration

The Langmuir adsorption sub-model was calibrated within a Bayesian framework developed in SorbentFit. Two scenarios are compared: calibration accounting for parametric uncertainty only and calibration accounting for both parametric uncertainty and model form discrepancy. In the following, the latest posterior parametric distributions for the two scenarios are presented, followed by the associated Langmuir model predictions.

For Bayesian calibration, the equilibrium constant *K* of the Langmuir adsorption model is written as a function of *ΔH* and *ΔS*, while the maximum adsorption capacity of the particles, q_{max}, is written as a function of n_v (Mebane et al. 2013, Bhat et al. 2015):

$$K = \exp\left(\frac{\Delta S}{R}\right)\exp\left(\frac{-\Delta H}{R\, T_g}\right)/P$$
$$q_{max} = \frac{n_v}{\rho_p} \quad (30)$$

Under scenario 1, only the parametric uncertainty in ΔS, *ΔH* and n_v is estimated via Bayesian calibration using the experimental data published by Hauchhum and Mahanta, 2014. For scenario 2, the discrepancy term $\delta(T_g, P_{CO2})$ is added to the Langmuir model that accounts for physical and chemical deficiencies of the model. To include the model form discrepancy, Eq. (30) is rewritten as:

$$K_{new} = K\exp(\delta)$$
$$q_{max} = \frac{n_v}{\rho_p} \quad (31)$$

The discrepancy function, which may be written more generally as $\delta(\zeta, \beta)$, is a Gaussian Process with BSS-ANOVA covariance function:

$$\delta(\zeta, \beta), = \sum_{j=1}^{J}\sum_{l=1}^{L_j^{\delta}} \beta_{j,l}\Phi_{j,l}(\zeta) \quad (32)$$

For the pure Langmuir adsorption model $\zeta = \{T_g, P_{CO2}\}$ is the vector of system conditions. In Eq. (32), $\beta_{j,l}$ are discrepancy function parameters, $\Phi_{j,l}$ are basis functions, j indexes over the J functional components included in the

discrepancy realizations and l indexes over the number of basis functions L_j^{δ} used for the jth functional component (Bhat et al. 2015).

6.1.3 Posteriors

Scenario 1 – Parametric uncertainty. Using Bayesian calibration, the three parameters of the model ΔH, ΔS and n_v are estimated, resulting the univariate and bivariate distributions presented in Figure 11. The univariate posterior distributions of the enthalpy and entropy suggest high uncertainty in these parameters, seen from their wide probability distributions.

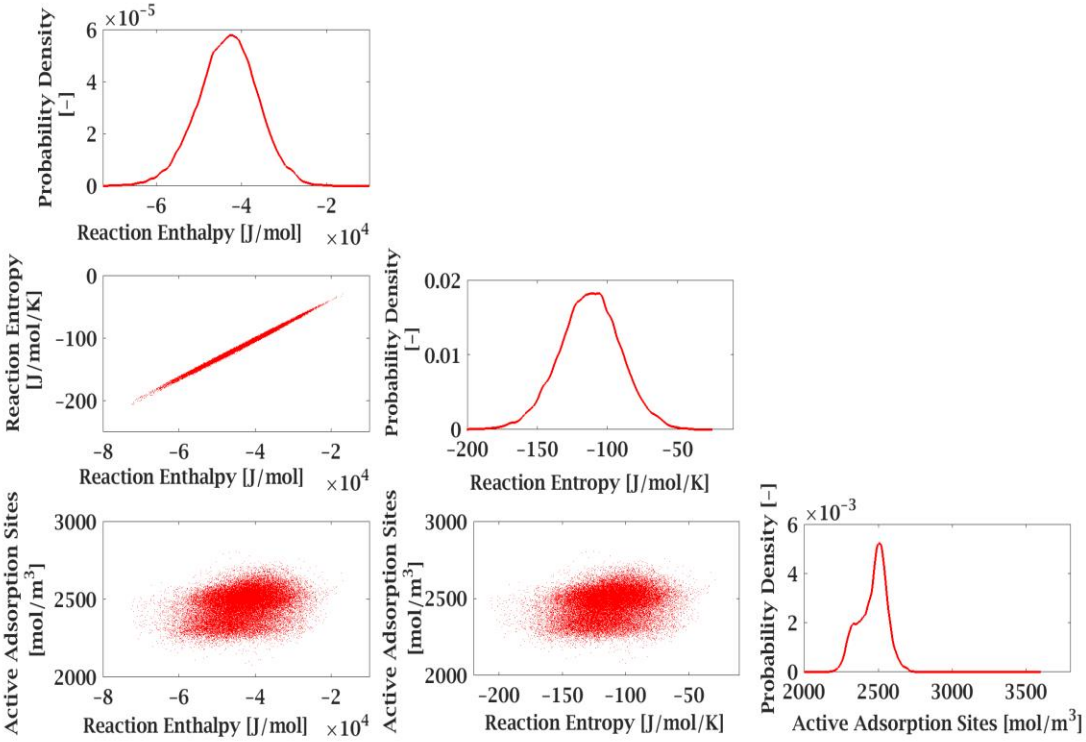


Figure 11 Univariate and bivariate posterior distributions of the adsorption isotherm parameters ΔH, ΔS and n_v for Scenario 1

Scenario 2 – Parametric uncertainty and model form discrepancy. In addition to the three parameters of the adsorption model ΔH, ΔS, n_v, the hyperparameters β of the discrepancy δ are also estimated, resulting the posterior distributions shown in Figure 2. The posterior distributions of the hyperparameters β of δ are not displayed.

By comparing the two sets of posterior distributions, it becomes obvious that accounting for the model form discrepancy leads to less uncertainty in both ΔH and ΔS – in Figure 12, the probability distributions of these parameters are significantly narrower.

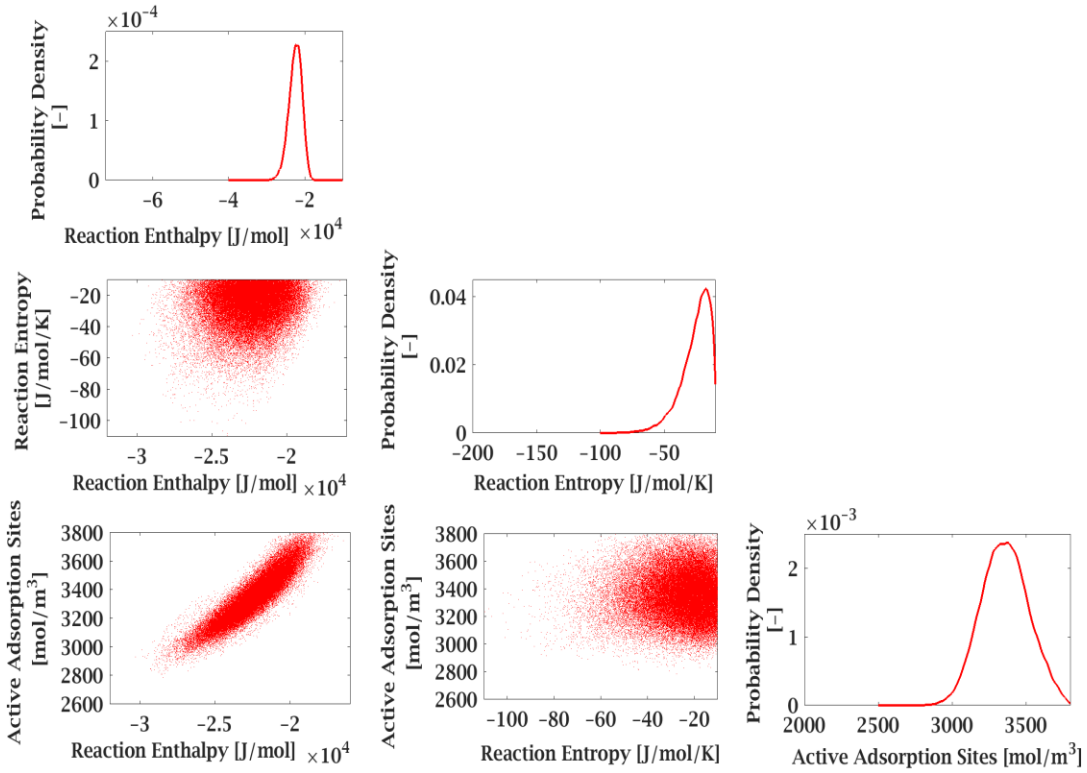


Figure 12 Univariate and bivariate posterior distributions of the adsorption isotherm parameters ΔH, ΔS and n_v for Scenario 2

6.1.3.1 Langmuir model predictions with quantified parameter uncertainty and discrepancy

Predictions of the Langmuir model under scenario 1, using 150 samples from the posterior distributions of ΔS, ΔH and n_v are shown in Figure 13 (a)-(d), for four different temperatures. The high uncertainties observed in the posterior distributions of ΔH and ΔS (Figure 11) are reflected in the predictions from the Langmuir model as well, indicated by the wide band of the posterior Langmuir model realizations.

The predictions resulting from the propagation of the posteriors due to both parameter uncertainty and model form discrepancy are presented in Figure 14 (a)-(d). First thing to note is that the inclusion of the stochastic discrepancy function within the small-scale sorbent model leads to a significantly better fit of the model output to the data. Based on the improved fit when both parameter uncertainty and discrepancy are considered, it is clear that the pure Langmuir model does not best describe the system. The discrepancy function accounts for the deficiencies of the model, but for a fix that is based on physics, a model that includes adsorption of multiple species on multiple sites should be considered.

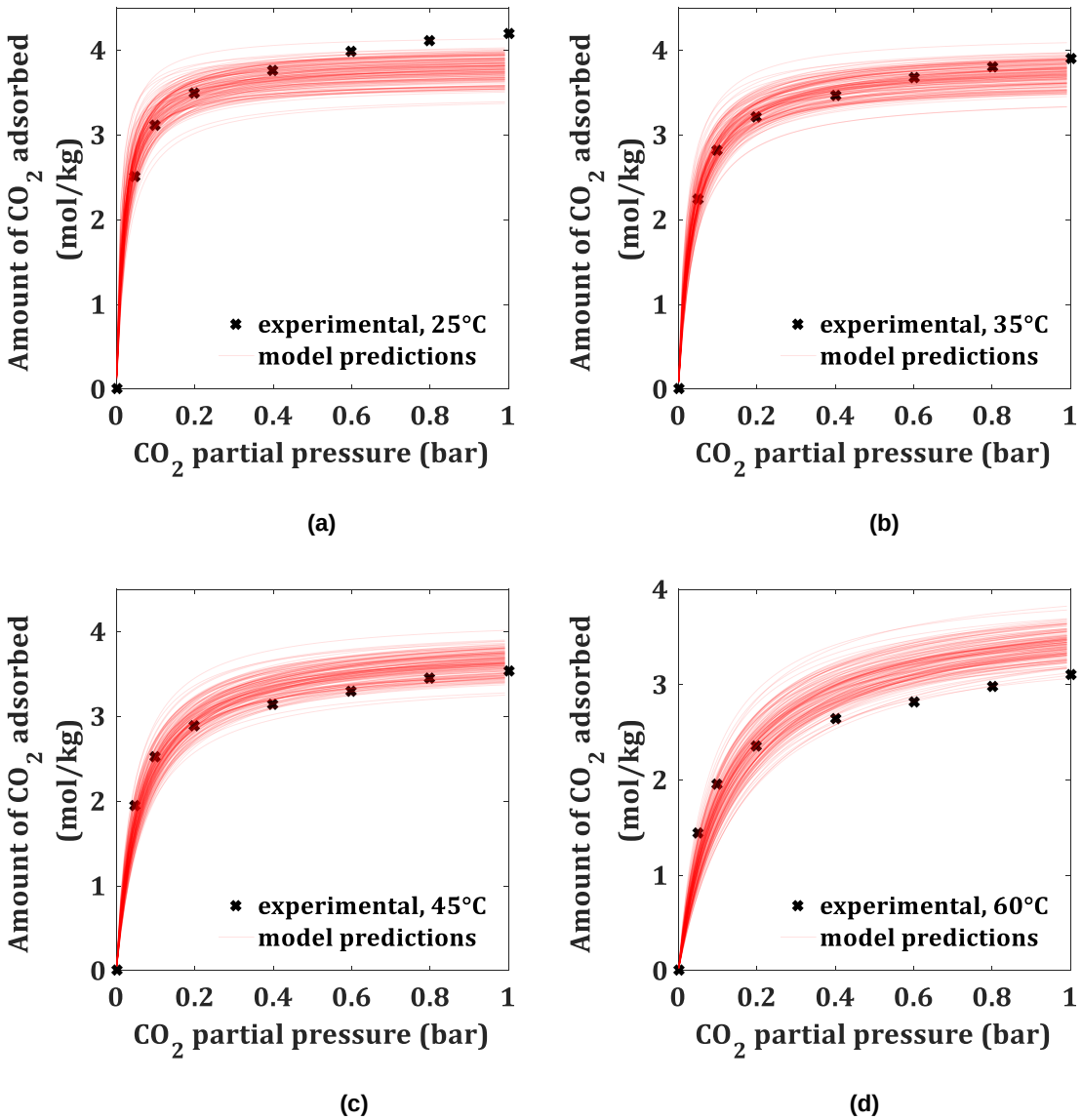


Figure 13 Parameter uncertainty. Experimental amount of CO_2 adsorbed vs. model predictions as a function of CO_2 partial pressure, at (a) **25°C,** (b) **35°C,** (c) **45°C and** (d) **60°C.**

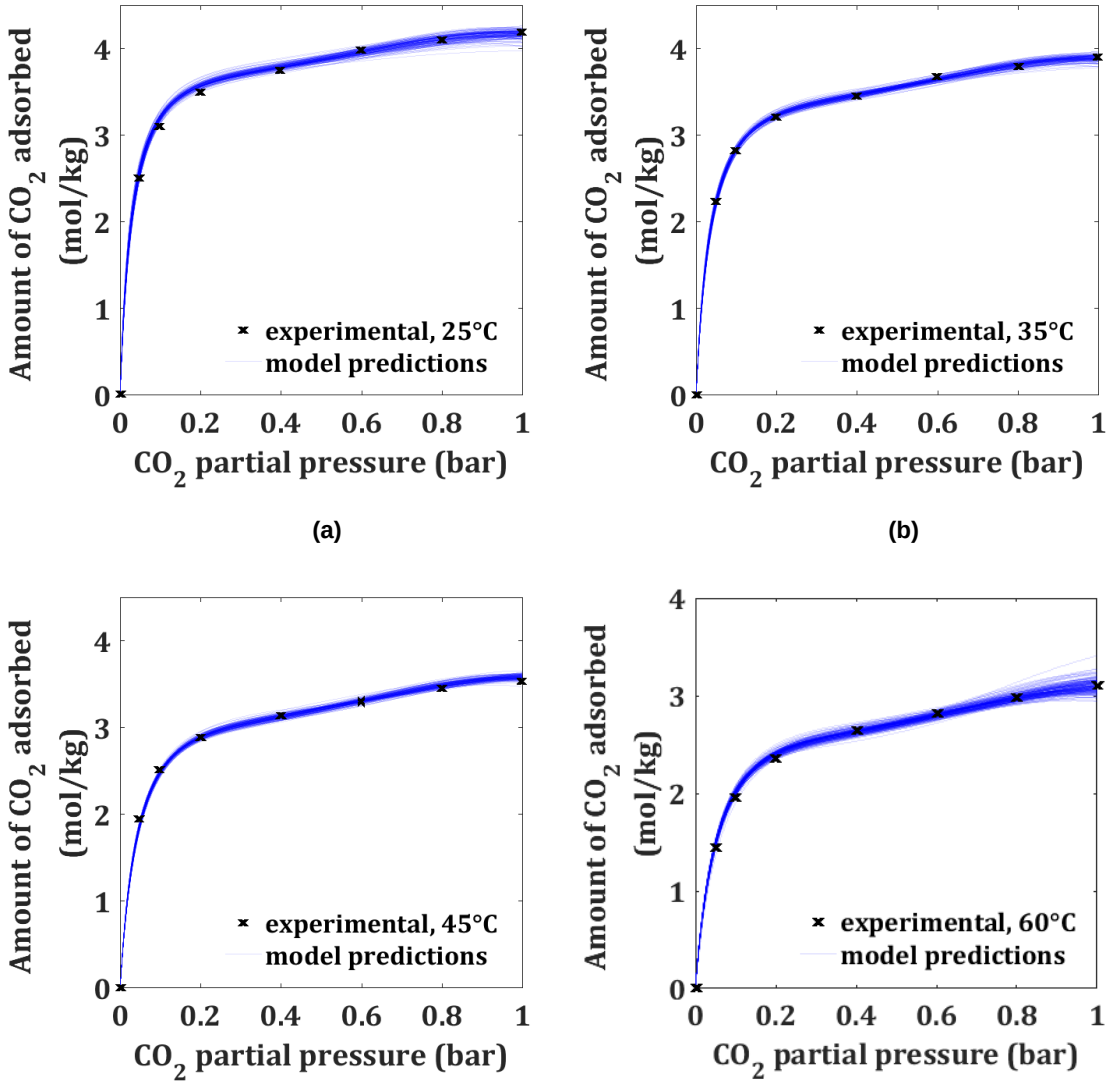
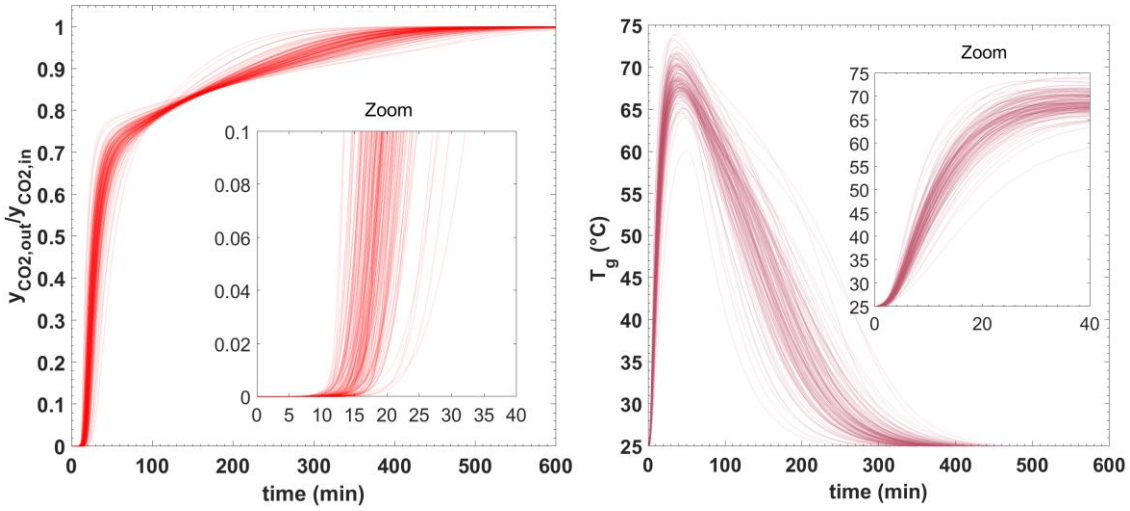


Figure 14 Parameter uncertainty with discrepancy. Experimental amount of CO_2 adsorbed vs. model with discrepancy predictions as a function of CO_2 partial pressure, at (a) **25°C,** (b) **35°C,** (c) **45°C and** (d) **60°C.**

6.1.4 Uncertainty propagation and upscaling using the reduced mathematical model

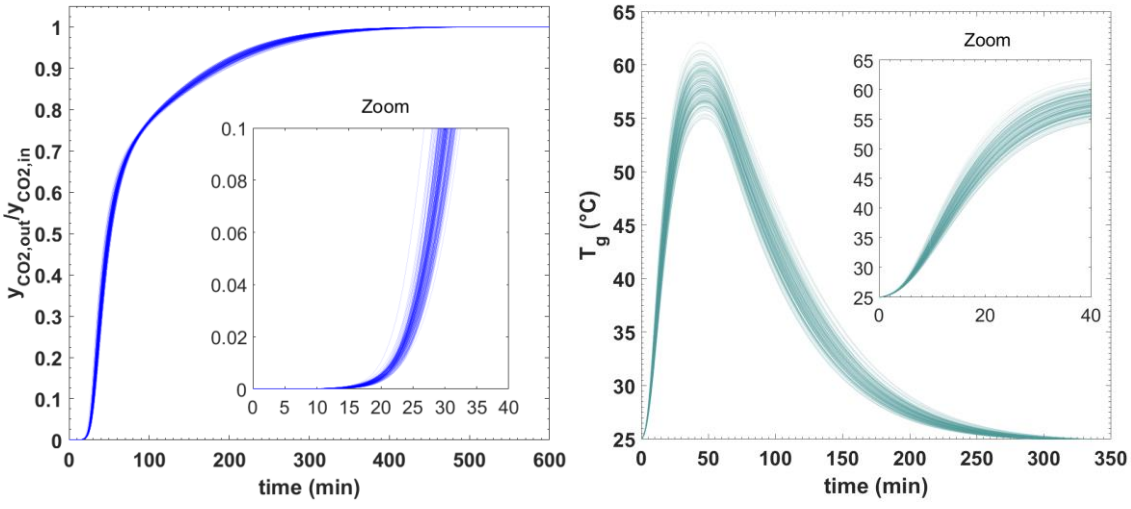
Having quantified and propagated the uncertainty in the Langmuir adsorption model, results of upscaling the uncertainty from model parameters and discrepancy to the CO_2 fixed bed capture process are presented. We again compare the two scenarios – parametric uncertainty only and parameter uncertainty with model form discrepancy. Upscaling the uncertainty from the adsorption sub-model parameters results in distribution of the process model's predictions of variables of interest such as breakthrough curve and gas temperature profile.



(a) **(b)**

Figure 15 Parameter uncertainty. Results from upscaling posterior distributions of the equilibrium model parameters to the fixed bed CO_2 adsorption model. (a) **Distribution of the breakthrough curves.** (b) **Distribution of the gas-phase temperature.**

150 posterior samples are propagated from the joint distribution of the Langmuir model parameters to the CO_2 fixed bed capture process. Figure 15 represents the distribution of the breakthrough curve (Figure 15 (a)) and that of the gas-phase temperature (Figure 15 (b)), under scenario 1. There is substantial uncertainty in the process model predictions, noticeable in the wide distributions of the breakthrough curve and the temperature profiles. However, this is not surprising given the high uncertainty in the Langmuir model parameters when considering parametric uncertainty only. In contrast, when the model form discrepancy is accounted for, under scenario 2, the uncertainty is reduced, resulting in narrower distributions for the breakthrough curve and gas-phase temperature. Not only are the distribution bands narrower for both predictions, but they are also less dispersed.



(a) **(b)**

Figure 16 Parameter uncertainty with model form discrepancy. Results from upscaling posterior distributions of the equilibrium model parameters to the fixed bed CO_2 adsorption model. (a) **Distribution of the breakthrough curves.** (b) **Distribution of the gas-phase temperature.**

6.2 Fixed-Bed Reactor Models for H_2 Purification

The fixed bed reactor model can be used to simulate an adsorber or a regenerator for gas phase systems. To study the general behavior of the system, the separation of H_2 from a 5-component gas mixture ($H_2/CO_2/CH_4/CO/N_2$) by adsorption is simulated. Operating conditions, adsorbent properties, adsorption equilibrium and kinetic data needed to run the model are obtained from Ribeiro et al., 2008.

Further, parameter uncertainty and model form discrepancy in the pure Langmuir model was propagated through a simpler, single component adsorption, 1D dynamic, non-isothermal, and adiabatic plug flow fixed bed reactor model. The adsorbent bed is comprised of Zeolite 13X particles, whose properties and adsorption isotherm data are acquired from Hauchhum and Mahanta, 2014.

6.2.1 Purification of H_2 using a layered activated carbon/zeolite (AC/Zeo) reactor bed

The complete mathematical model capable of simulating a PSA cycle was described in detail in the report sent by WVU in September. The model is implemented in gPROMS Model Builder 4.2.0. The axial domain for the concentration of gas components, $C_{g,i}$, and gas-phase temperature, T_g, is discretized using second-order centered finite difference method (CFDM), while the axial domain for all other variables is discretized using first-order forward finite difference method (FFDM). The system of ordinary differential and algebraic equations is integrated over time using the DASOLV integrator.

Initial and inlet mole fractions, transport parameters, Langmuir isotherm parameters and other parameters needed for the simulation are read in from foreign objects, using Excel FOs.

6.2.1.1 Model testing – Validation against published results

The simulation is set up as adiabatic and it is initialized considering that the column is filled with H_2 at the feed temperature and pressure. The adsorption of the contaminants from the feed gas stream is simulated for a duration of 40 s, which corresponds to the feed step of the PSA process modeled by Ribeiro et al. (2008). The reactor bed considered is a layered activated carbon/zeolite (AC/Zeo) reactor bed.

The performance of the model is assessed by comparing the temperature and methane concertation profiles obtained from simulating the adsorption of the contaminants from the feed gas stream with results of Ribeiro et al. (2008) reported at the end of the feed step of the first PSA cycle. The results are presented in Figure 17 (a) and (b). It can be observed that the results match quite well. A similar trend can be observed in the CH_4 concentration profile.

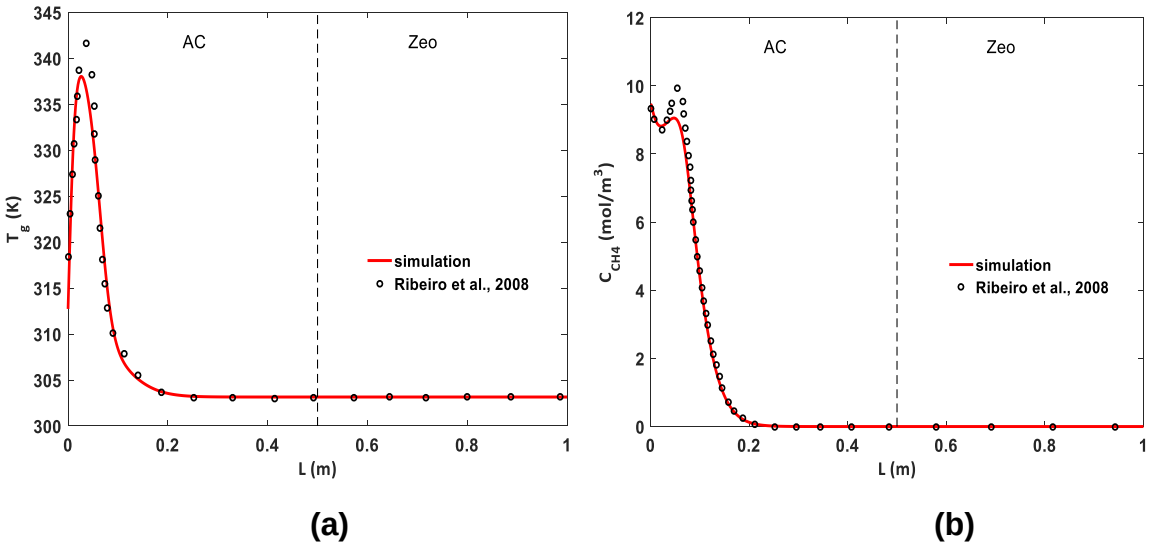


Figure 17**. (a)** Gas temperature profile and **(b)** methane gas concentration profile at the end of the feed step (simulation time t = 40 s), as a function of bed length. Simulation results compared to results published by Ribeiro et al. (2008)

6.2.1.2 Purification of H_2 by PSA, using an activated carbon (AC) reactor bed

For the simulation of the PSA cycle, a single AC reactor bed is considered instead of the layered bed. The PSA cycle is composed of 8 steps: a feed step (1), two pressure equalization – depressurization steps (2) and (3), a blowdown step (4), a purge step with hydrogen (5), two pressure equalization – pressurization steps with hydrogen (6) and (7), and a final pressurization step with hydrogen (8). The duration of each cycle step is set to be equal to the duration of the steps used by Ribeiro et al. (2008) (Figure 18).

The PSA cycle starts with the feed step, considering that the reactor is filled with hydrogen at the feed temperature and feed pressure. During the purge and the three pressurization steps, the inlet gas stream is pure hydrogen.

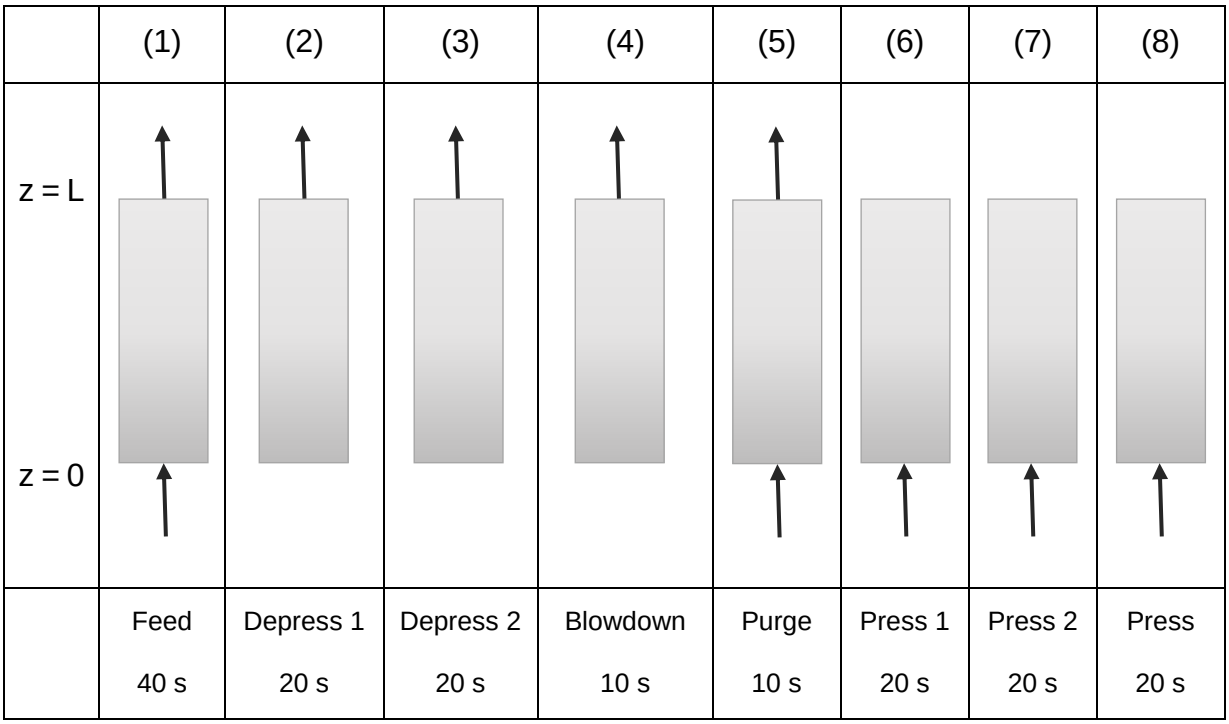


Figure 18 Schematic diagram of the cycle sequence used for the PSA simulation.

Next, results from the simulation of a PSA cycle are summarized (without having reached a cyclic steady state).

To illustrate the system behavior, the outlet system pressure during one PSA cycle is presented in Figure 19. From comparing the simulation results with the data published by Ribeiro et al. (2008), it can be seen that the model correctly simulates the 8 steps of the PSA cycle.

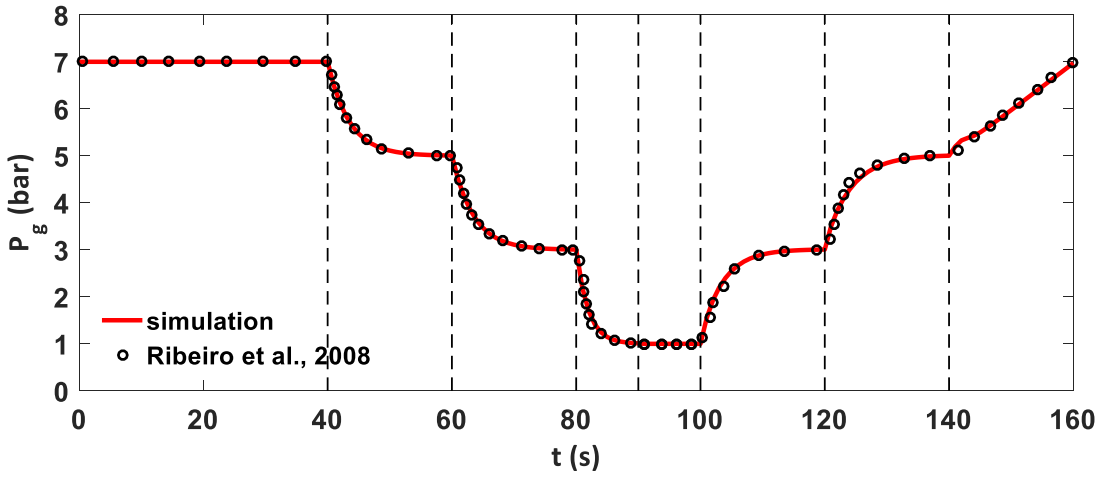


Figure 19 Pressure at the reactor outlet – comparison between simulation results and results published by Ribeiro et al. (2008)

Further, Figure 20 depicts the molar flow rate of the gas stream at the reactor outlet during one PSA cycle. At the end of the feed step (t = 40 s), the molar fractions of impurities is of order 10^{-6}, thus the eluted gas is considered to be pure H_2.

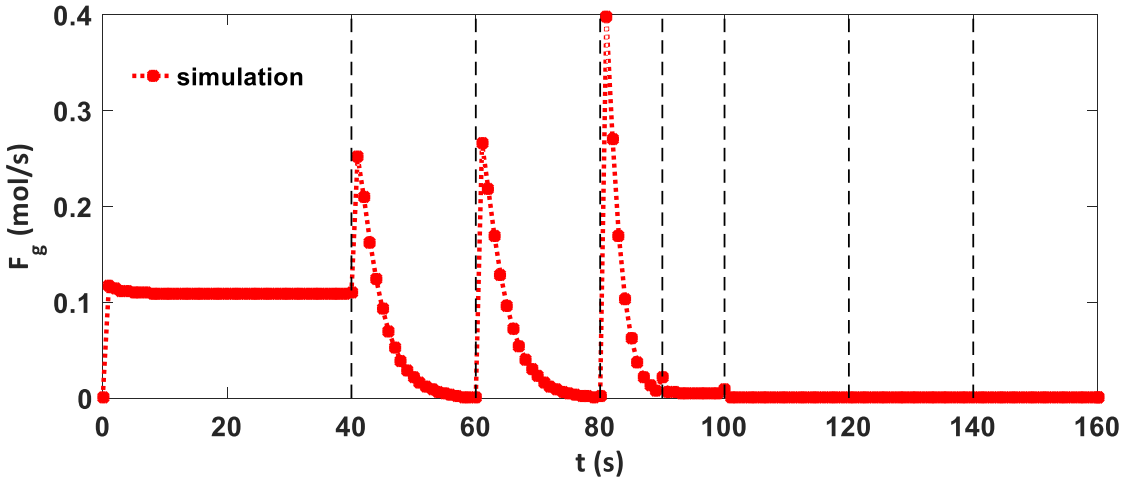


Figure 20 Total molar flow rate at the reactor outlet.

6.3 Outputs

Ostace A, Bhattacharyya D, Kocan K, Mebane D, Lawal, A, Schmal, P, “Dynamic Modeling with Uncertainty Quantification of a Fixed Bed Adsorption Process”, Manuscript under preparation, To be submitted to AICHE Journal by August, 2017

Ostace A, Bhattacharyya D, Kocan K, Mebane D, “Data-driven model building of zeolite adsorption processes with uncertainty quantification and propagation to dynamic simulations of CO_2 adsorption”, To be presented at the AICHE Annual Meeting, Minneapolis, MN, Oct 29-Nov 3, 2017

Ostace A, Bhattacharyya D, Kocan K, Mebane D, “Dynamic Modeling with Uncertainty Quantification of Solid Sorbent Based CO_2 Capture Processes”, Paper 71g, AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016

Mebane D, Li K, Mahapatra P, Bhat S, Kress JD, Miller DC. “Dynamic Discrepancy Reduced Modeling: Overview and Applications”, Paper 266b, AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016

6.4 ALAMO - Developing a reduced order model of an Air Separation Unit

ALAMO was used to develop a reduced-order model of an Air Separation Unit. An Air Separation Unit (ASU) model in gPROMS is illustrated in Figure 21.

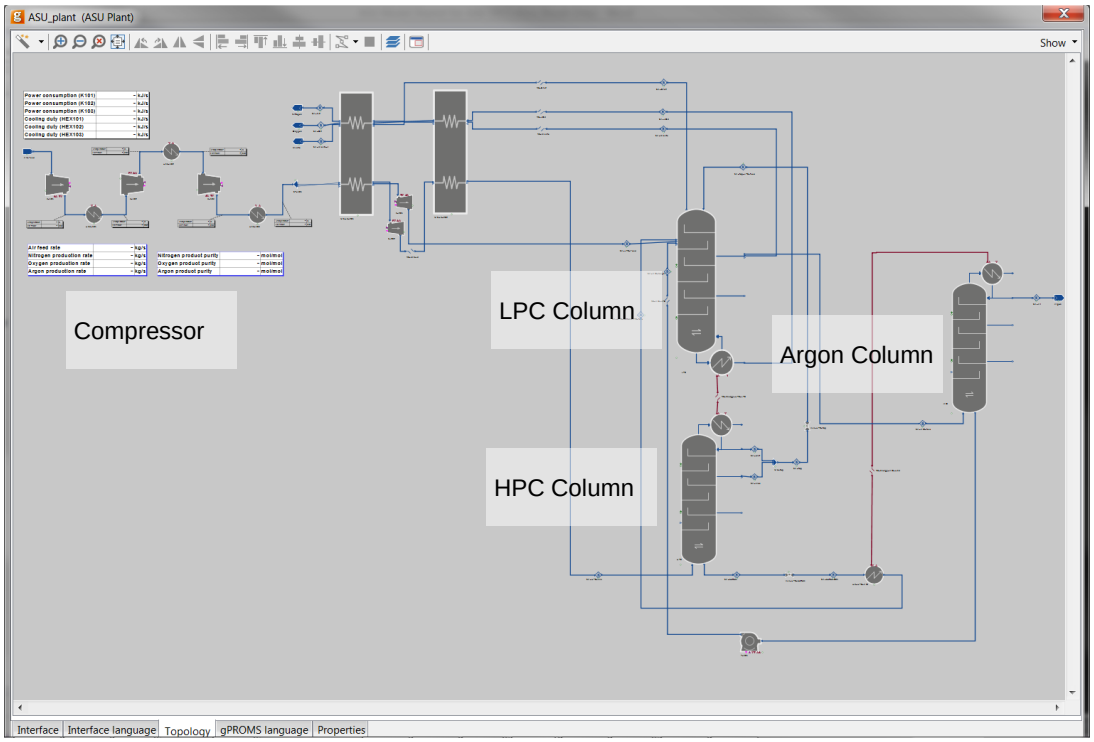


Figure 21 ASU Plant model in gPROMS

The Global System Analysis feature in gPROMS was used to collect the data set from the detailed model required to develop the corresponding ALAMO model. Two cases were considered – one with two inputs to the reduced ALAMO model and the other with 5 inputs. The following input specifications were used:

Case 1

Inputs:

- Air feed flowrate: 95-101 kg/s
- Side vapor draw from LPC column to Argon column: 600 – 800 kmol/hr

Case 2

Inputs:

- Air feed flowrate: 95-110 kg/s
- HPC Column reflux ratio: 1.2 – 2 kg/kg
- Outlet pressure of compressor 3: 6.2 – 6.4 bar
- Side vapor draw from LPC column to Argon column: 600 – 1000 kmol/hr
- Side vapor draw from LPC column to waste: 8000 – 9500 kmol/hr

Outputs:

- Argon purity
- Argon flowrate
- Nitrogen purity
- Nitrogen flowrate
- Oxygen purity
- Oxygen flowrate
- Objective (annualized air compression cost)
- Waste nitrogen purity
- Waste flowrate

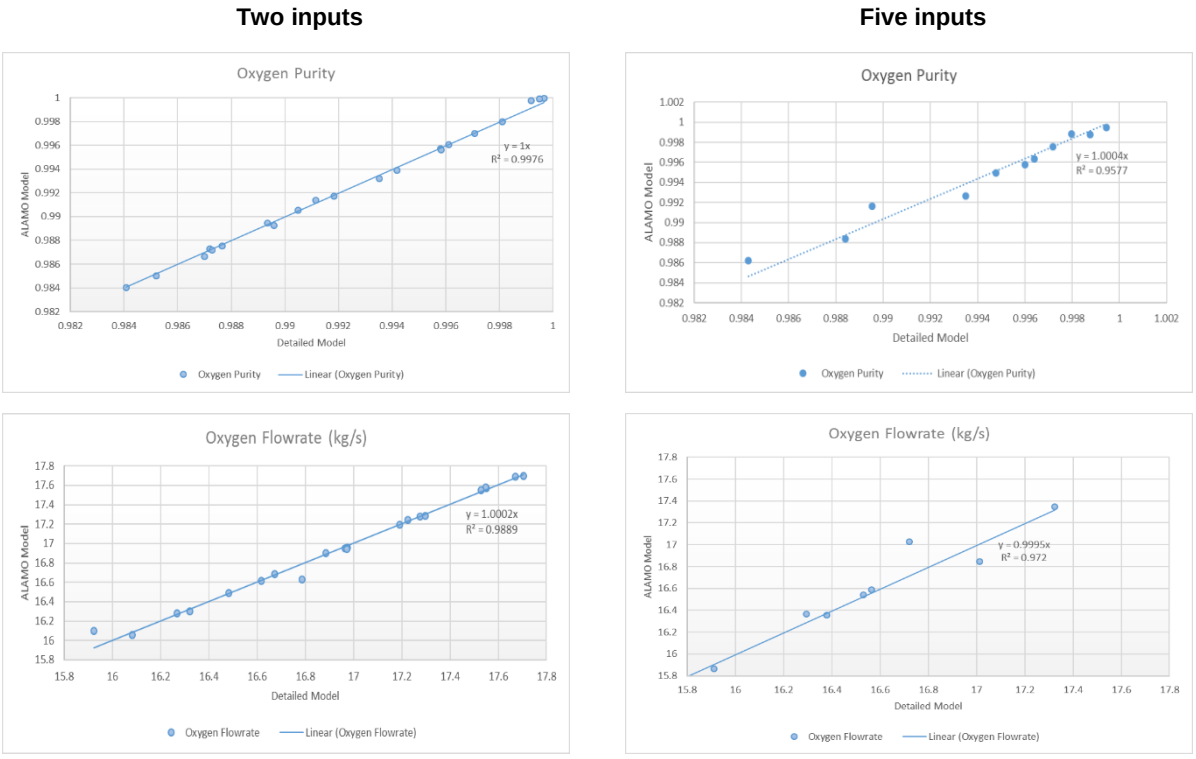


Figure 22 Oxygen purity and flowrates predicted by two- and five-input ALAMO models

As expected there is a reduction in accuracy of predictions from the ALAMO model with increased number of inputs as shown in Figure 22. However, the accuracy of predictions is still acceptable.

6.5 Outputs

Schmal, P.,A. Chowdhury, A. Lawal, M. Kılınç and N. V. Sahinidis, Model reduction for complex systems analysis, AIChE Spring National Meeting, San Antonio, Texas, March 2017

7 Stakeholder feedback

Feedback from Industry advisory board members was obtained from IAB meetings and monthly IAB conference calls which typically included technical presentations of developments in components of the CCSI toolkit. Interviews were also arranged with members to discuss their experience with the CCSI toolkit.

A CCSI project showcase was organized within PSE to present the CCSI tools and the results of the investigations carried out during Phase 1 of the project. The following groups were presented to:

- Global Consulting Group which provides consulting services to the following industries:
    - Chemicals and Petrochemicals
    - Formulated Products
    - Energy and Environment
    - Oil and Gas
- Chemicals, Petrochemicals and Refining Group which provides software solutions to Downstream oil and gas, Power generation and CCS as well as Waste water treatment industries
- Formulated Products Group which provides software and consulting services to the Pharmaceutical and Food processing industries.
- Oil and Gas Group which provides software and consulting services for Upstream oil and gas production as well as Depressurisation studies

7.1 Potential customers

The following is a summary of observations made from feedback from potential customers from the Industry advisory board members and a select potential customers of the CCSI toolkit:

- The CCSI tools represent cutting-edge and innovative solutions in their various fields and provided a good combination of both fundamental and empirical modelling approaches.
- The FOQUS framework presented new methodologies for technology development. These new methodologies often were associated with new workflows which may be challenging to proliferate and commercialize. Demonstrating the added benefit of using the tools was deemed critical
- Various component tools in their current form appear to have limited scope. However, many tools provided potential benefits for a wide range of applications beyond carbon capture and storage (CCS).
- For the various tools considered and for Bayesian calibration in particular, the need to clearly articulate and present the benefits of using this approach over the simpler approaches was identified as critical to the success of its commercialization.
- FOQUS ability to use with commercial simulators is a plus
- Many potential users were concerned about the provision of long-term support

7.2 Internal Showcase feedback

The following are a few comments from the CCSI project showcase organized within PSE:

- Few customers have unit operations applicable to Process Models
- Dynamic Reduced Order Models could be valuable (if it is accurate)
- Uncertainty Quantification, iREVEAL conflict with existing capabilities
- FOQUS Flowsheet (no need to link gPROMS simulations other computer programs)

- SorbentFit (Bayesian Calibration, specifically) is of particular interest to Pharmaceutical clients.
- Unclear about potential applications of the Process models.
- Cloud computing of particular interest
- Surrogate modelling with ALAMO has general applicability

8 Assessment results and ranking

8.1 Assessment Criteria

To determine whether a software tool can be commercialized successfully, different aspects need to be considered ranging from technical functionality criteria (such as how well it performs a certain task) and usability criteria (such as how easy it is to use), all the way to commercial criteria (such as the size of the potential market). Failure to meet any one of these criteria significantly reduces the chance of a successful commercialization.

We have developed a criteria tool matrix to help judge the extent to which each of the tools is viable for commercialization. The matrix uses the following criteria described in Table 5:

Table 5 Explanation of assessment criteria

Criteria	Explanation	Factors considered
General applicability	Can this tool be used for general purpose or is it specific	Market size and attractiveness
User-friendliness	How easy is it to understand and are the features intuitive?	Customer investment, Ease of use, Scalability
Impact on customer workflows	How consistent is it with existing customer workflows	Addresses real problem, Ease of use, investment required from customer
Alignment with platform	How well does it align with PSE's gPROMS platform and products (current and/or roadmap)	Positioning, Ease of implementation, competitive differentiation
Perceived estimated market	How large a market do we expect to have for this at this point	Market size and attractiveness
Technical Advance Level	How advanced is the tool from a technical point of view	Addresses real problem, Competitive differentiation, ability of others replicating offering
Technical Readiness Level	How ready is it technically	Time to market, Ease of implementation
Commercial Readiness Level	How ready is it commercially	Time to market, Ease of sale, value proposition, address real problems
Required development	How much work would be required to implement the commercialized product	Time to market, Ease of implementation, Positioning
Support / maintenance required	How much support and maintenance would be required	Ease of implementation, Positioning

The scoring scale ranges from 1 to 10, where 1 implies a poor performance against the commercialization criterion.

8.2 Assessment results

Scores of the short-listed CCSI tools are presented in Table 6. The scores for each tool were estimated based on the following:

1. Assessments carried out investigating the technical integration requirements described in Sections 3, 4, 5 and 6 .
2. The CCSI tool brochures prepared described in Appendix A
3. The feedback obtained from the CCSI Project Showcase and Industrial Advisory Board members discussed in Section 7

Table 6 Assessment of CCSI tools

		FOQUS Flowsheet and SimSinter	FOQUS Turbine	ALAMO	UQ module	Optimization Under Uncertainty	Dynamic Reduced Models	iREVEAL	Process Models	SorbentFit	Bayesian Calibration concepts
1	General applicability	2	7	6	3	3	4	1	4	1	7
2	User-friendliness	3	5	7	2	4	3	5	4	3	4
3	Impact on customer workflows	3	6	8	3	5	3	6	4	4	4
4	Alignment with platform	3	6	7	5	6	6	6	6	5	7
5	Perceived estimated market	3	8	7	4	4	4	4	4	2	8
6	Technical Advance Level	6	7	6	7	8	4	6	4	8	8
7	Technical Readiness Level	4	5	7	4	5	5	6	7	4	5
8	Commercial Readiness Level	3	7	7	3	4	4	5	5	3	5
9	Required development	3	5	7	3	5	4	5	5	4	5
10	Support / maintenance required	2	5	7	4	5	6	5	6	4	6
	TOTAL	**32**	**61**	**69**	**36**	**49**	**44**	**48**	**50**	**37**	**59**

A total score of 50 was considered the cut off for assessing whether a tool was worth commercializing or not. This corresponds to an average score of 5.

In Table 6, the fast track tools are highlighted in blue. ALAMO was assessed as the top ranking tool for commercialization. The following factors were considered especially favorable:

- ALAMO can be applied to a wide range of problems – generating surrogate models from theoretically any model or directly from a set of data
- There are clear synergies with ongoing and planned developments of PSE's platform
- There has been positive feedback from the Industrial Advisory Board members on its prospects
- ALAMO can positively impact the customer's workflow improving the speed and/or feasibility of tasks such as sensitivity analysis and uncertainty quantification.

Some alternative versions of the tools are presented as well. Two of these alternatives are presented (highlighted in green in Table 6):

1. Bayesian Calibration concepts which describes the parameter estimation capability using Bayesian Analysis which could be applied to any model. Figure 23 shows the improvement in assessment scores with the Bayesian calibration concept alternative particularly in the "General applicability" and "Perceived estimated

market" criteria where SorbentFit performed poorly due to its restricted application. PSE believes Bayesian calibration could provide additional parameter estimation capabilities in the future.

2. FOQUS Turbine which is a component of the FOQUS (Flowsheet, SimSinter and Turbine) option described in Section 3.4. FOQUS Flowsheet and SimSinter could be used to connect gPROMS simulations to other simulation software in a flowsheet environment. This tool was found to score poorly for "Alignment with platform", "support / maintenance required" and "Perceived estimated market" criteria. There have been tools which have aimed to provide similar functionality as FOQUS Flowsheet and SimSinter such as the CAPE OPEN interface but have experienced limited success. The Turbine functionality in FOQUS provides the prospect of running simulations on the cloud which is attractive to PSE and aligns with current developments.

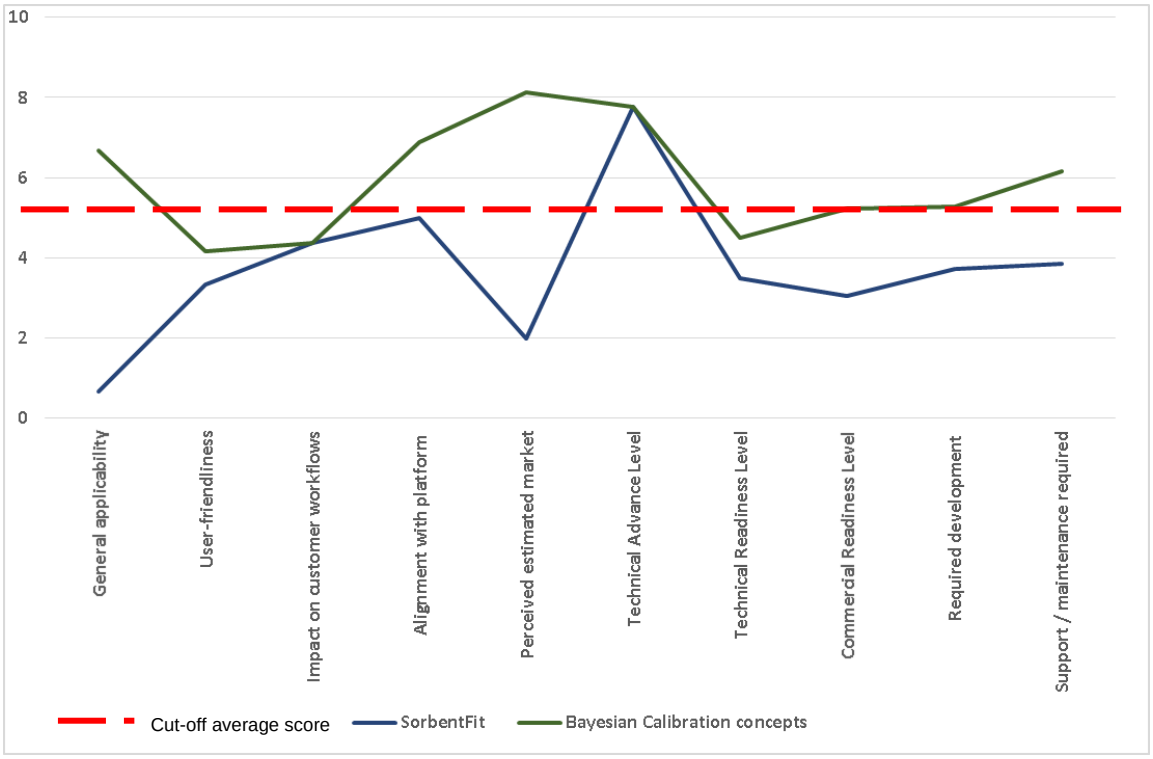


Figure 23 Comparison of assessment scores for SorbentFit and alternative concept

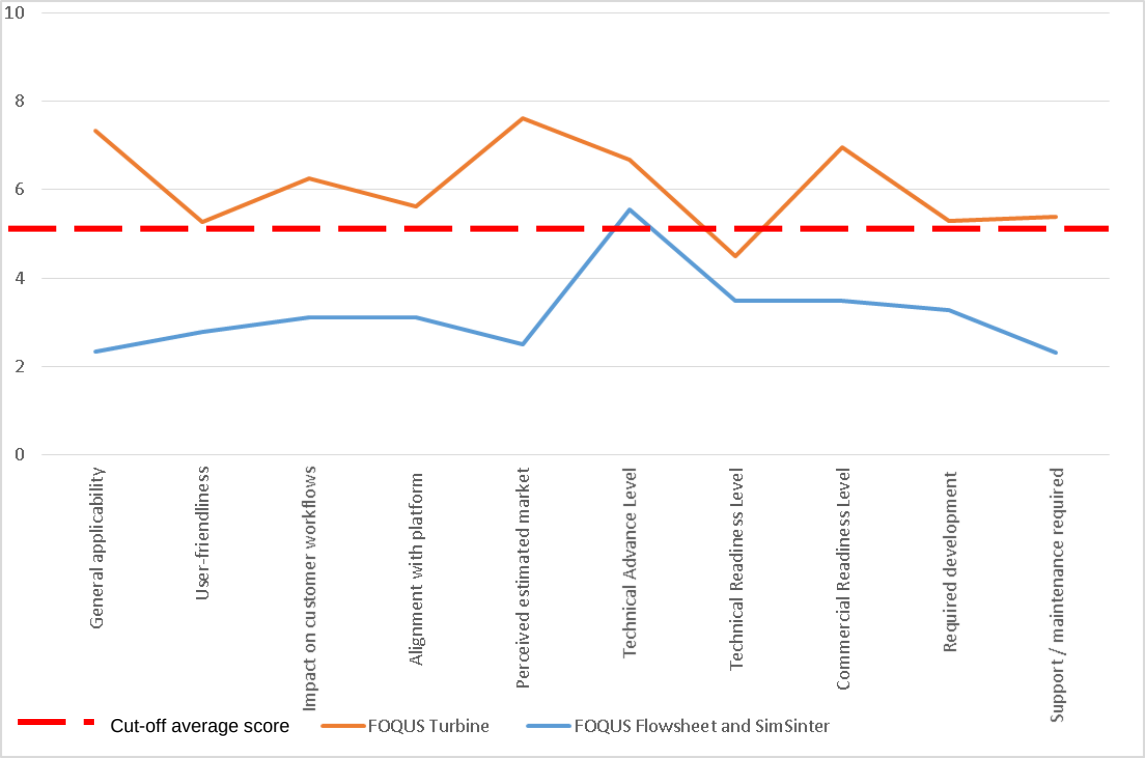


Figure 24 Comparison of assessment scores for FOQUS Flowsheet/SimSinter and FOQUS Turbine alternative

8.3 CCSI Tool Ranking

Based on the assessment results in Table 6, the following ranking was concluded:

1. ALAMO
2. FOQUS (Turbine functionality)
3. Bayesian calibration concepts
4. Process Models
5. Optimization under uncertainty
6. iREVEAL
7. Dynamic reduced models
8. SorbentFit
9. Uncertainty Quantification module
10. FOQUS (Flowsheet and SimSinter functionality)

A stage gate meeting was held on the 10th June 2016 to conclude on which tools to consider for commercialization.

For each tool, an overview of the tools capabilities was first presented. Subsequently, the tools current features were compared to the possible commercialization product conceived by the respective taskforce. A summary of the investigations carried out by each taskforce was then presented. Next, PSE's assessment was discussed – first PSE's SWOT analysis (based on the market research and investigations carried out by the taskforces) for each tool was presented followed by the assessment of the tool based on PSE's product assessment model.

An overview of the non-fast track tools features, advantages and benefits was presented.

The following summarizes the assessments of the fast track tools based on the discussions:

1. Process Models – these gPROMS models were found to just meet the average assessment threshold score. However, a significant threat to commercialization was the presence of a similar process model library that had been recently developed in PSE (for a Fluid Catalytic Cracking project).
2. ALAMO – this tool was deemed to have the potential to be applied to a wide range of applications and to also complement some of the recent developments in Global Sensitivity Analysis (GSA) in PSE. ALAMO received the highest average assessment score amongst the products.
3. SorbenFit / SolventFit – SolventFit could not be properly assessed due to the late availability of the tool on FOQUS. SorbentFit in its current state was found to be limited in application. It was agreed that applying Bayesian calibration concepts to general parameter estimation problems could be a more viable product commercially.
4. FOQUS Flowsheet, SimSinter and Turbine – FOQUS Flowsheet had low scores on PSE's product assessment model particularly because of the limitations in general applicability and the perceived market size for the product. FOQUS Turbine's capability to run several simulations in parallel on the cloud was considered significantly beneficial and complementary to current GSA developments.
5. Although many non-fast track tools showed some promising features, it was concluded that the fast track tools had covered PSE's key areas of interest.

In conclusion, the following tools are being considered for commercialization:

1. ALAMO
2. FOQUS Turbine for cloud computing
3. Bayesian Calibration concepts

9 Proposed commercial products

9.1 ALAMO (C16038 CCSI Project Toolset, FOQUS Module – Feb. 5, 2016)

9.1.1 Background – Complimentary gPROMS feature

Most process simulators provide simulation results that are essentially point calculations. PSE recently developed Global System Analysis (GSA) feature, available on its gPROMS platform, which gives users the ability to explore global behavior of a system model via two complementary analysis methods. The two types of analysis currently available are uncertainty analysis and sensitivity analysis.

Sensitivity analysis is the study of how uncertainty in the output of a model can be apportioned to different sources of uncertainty in the system model inputs. Uncertainty analysis is the quantization of uncertainty in the system model outputs resulting from variations in the model inputs. Practitioners have different engineering questions which are answered by one or both of these activities. In terms of workflows, there is a constant cycle between uncertainty and sensitivity analyses. Regarding computational approaches, these two techniques may share common elements or require completely different (specialized) strategies given that they are computationally intensive. What unites these techniques is the input/output structure (factors and responses) and the uncertainty/variability adopted by factors. The concept is illustrated in Figure 25.

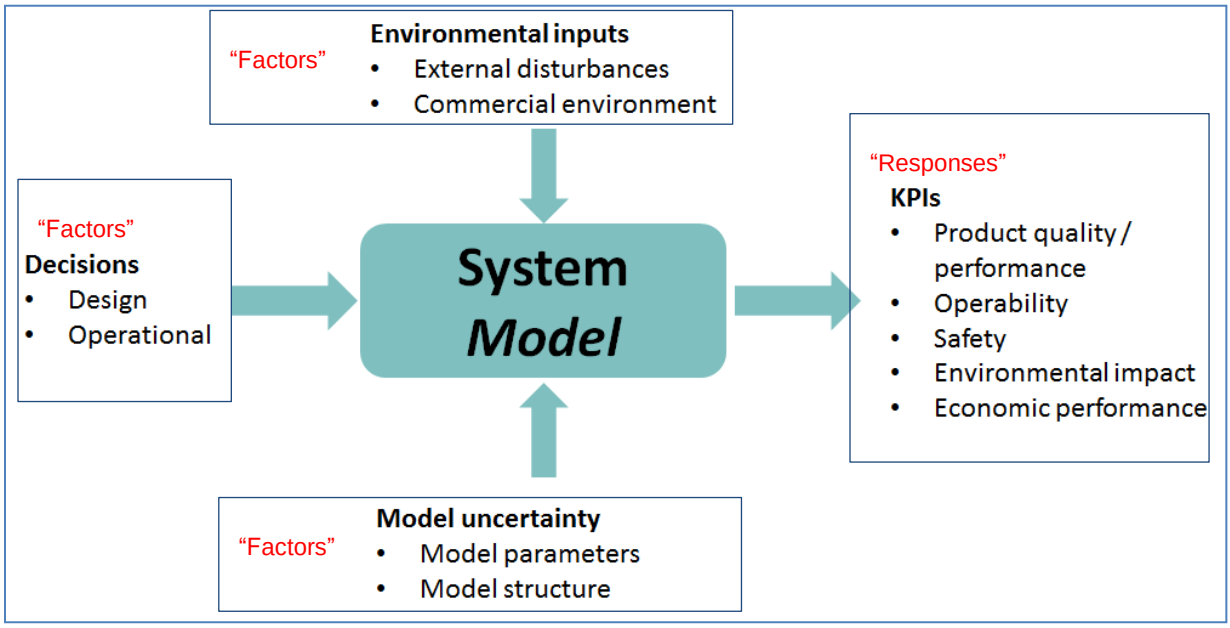


Figure 25. Global system analysis factors and responses

Factors are user specified inputs which could be deterministic or probabilistic. The output ("Responses") could be either steady-state or dynamic depending on the type of system model utilized. Sensitivity and Uncertainty analyses involve potentially tens of thousands of simulations which may be impractical with large system models.

9.1.2 Commercialization objective

In Phase 2, PSE proposes to incorporate ALAMO algorithms in its GSA feature allowing its users develop surrogate models. With accurate surrogate models, sensitivity and uncertainty analyses can be carried out with reduced order models in a fraction of the time. In general, two benefits for our customers are envisaged:

1. Surrogate models of reduced complexity can be generated from detailed models allowing the user run computationally expensive simulations such as optimizations or sensitivity analyses.
2. Algebraic models could be developed to represent the relationship between sets of data for which no process model exists. In industrial applications, it is often the case that users cannot build the right process models from experimental data because they do not know how to or have the computational power to handle suitable models. In addition, users may not have the time to build process models and may only be interested in representing relationships between certain inputs and outputs. ALAMO can offer relatively simple algebraic relations for this purpose.

In addition, GSA features in gPROMS provide a suitable framework for implementing the sampling steps required in the use of ALAMO.

9.1.3 Competitive landscape

A number of regression software that could be used to generate surrogate models. However, most existing tools are too simplistic and lack advanced modelling capability. The software closest to ALAMO in terms of capabilities is Eureqa (from Nutonian). However, Eureqa relies on genetic search, whereas ALAMO utilizes deterministic optimization algorithms and, as a result, often finds better models than Eureqa over short time spans. Moreover, ALAMO has the distinct advantage that it offers constrained regression and adaptive sampling techniques for large datasets.

9.1.4 Proposal

It is proposed that ALAMO is provided with gPROMS platform thus making it available for use with the entire suite of gPROMS application software. PSE aims to implement ALAMO such that it fits within its Global System Analysis tool without any external software dependencies. The following have been identified as areas where improvements in ALAMO user workflows. These would be achieved by automating manual steps or improving the current algorithms used:

1. ALAMO basis function selection: In the current incarnation of ALAMO, the user must specify the types of basis functions to be used by the software.
2. ALAMO algorithm selection: Various algorithms are currently available for fitting purposes. Currently, a default algorithm is used and is only changed if found to perform poorly.
3. ALAMO adaptive sampling on large data sets: Adaptive sampling can optimize the size of data sets used for fitting.

9.2 Bayesian calibration (C16036 CCSI Project Toolset, SorbentFit Module – Feb. 5, 2016)

9.2.1 Background – Complimentary gPROMS feature

A detailed gPROMS process model is constructed from equations describing the physical and chemical phenomena that take place in the system. These equations usually involve parameters that can be adjusted to make the model predictions match observed reality. Examples of model parameters include reaction kinetic constants, heat transfer coefficients, distillation stage efficiencies, constants within physical property correlations, and so on. The more accurate these parameters are, the closer the model response is to reality.

The process of fitting these parameters to laboratory or plant data is called Parameter Estimation. gPROMS contains powerful, state-of-the art Parameter Estimation capabilities that have been applied successfully to a wide range of problems. Key features are:

- Multiple parameters occurring in dynamic or steady-state models may be estimated simultaneously. Nonlinear models of arbitrary size and complexity – including multi-unit flowsheets – may be used.
- Data from both dynamic and steady-state experiments may be used.
- The results of the estimation are subjected to extensive statistical analysis.

Parameter Estimation in gPROMS is based on the Maximum Likelihood formulation which provides simultaneous estimation of parameters in both:

- the physical model of the process
- the variance model of the measuring instruments - the Sensor, which can be:
    - constant variance (e.g. a thermocouple with an accuracy of +/- 1K)
    - Constant relative variance (e.g. a composition analyser with an error of +/- 2%)
    - Heteroscedastic variance, combining both of the above.

When solving a Maximum Likelihood Parameter Estimation problem, gPROMS attempts to determine values for the uncertain physical and variance model parameters that maximise the probability that the mathematical model will predict the measurement values obtained from the experiments. Assuming independent, normally distributed measurement errors, with zero means and standard deviations, this maximum likelihood goal can be captured through the following objective function:

9.2.2 Commercialization objective

PSE aims to develop additional parameter estimation capabilities in gPROMS based on the Bayesian calibration approach based on the current CCSI SorbentFit implementation.

Current parameter estimation methods such as Maximum Likelihood estimation (described above) do not calculate the full probability density function of the likelihood of the parameters and hence have no basis to quantify the uncertainty in the parameters. In addition, these methods assume independent, normally distributed measurement errors.

For the purpose of prediction, the Bayesian approach generates a posterior predictive distribution that represents the current estimate of the value of the response variable, taking into account both the uncertainty about the parameters and model residual variability. Predictions are expressed as probability distributions, thereby conveying significantly more information than point estimates in regard to uncertainty.

9.2.3 Competitive landscape

Bayesian calibration methods are currently not available on commercially available process simulation tools. There are, however, free Bayesian estimation tools available.

9.2.4 Proposal

The proposed commercialization product is a feature capable of parameter estimation using Bayesian calibration methods. This feature shall be provided as a gPROMS parameter estimation entity without the need to integrate with external software.

SorbentFit is a chemical kinetic fitting tool. It contains two models pertaining to amine-based CO2 adsorbents: a lumped-kinetic model and a high-fidelity reaction-diffusion model. Models can be fit to either (dynamic) Thermogravimetric analysis (TGA) or fixed bed datasets. As such, SorbentFit is restricted to parameter estimation applications for this specific application. The proposed product will not have these restrictions but will be customizable and thus applicable to virtually any parameter estimation problem. There are also various opportunities to automate steps in the Markov Chain Monte Carlo (MCMC) routines currently implemented providing improvements in:

1. Tuning
2. Convergence
3. Generating suitable Prior distributions
4. Identifying the Burn-in point
5. Parallelization of simulations

PSE believes that the considerable simulation times encountered with Bayesian calibration methods could be significantly reduced through these improvements.

9.3 Job queuing on the cloud (C16038 CCSI Project Toolset, FOQUS Module – Feb. 5, 2016)

9.3.1 Background – Complimentary gPROMS feature

The execution of GSA (described in Section 9.1.1) involves potentially tens of thousands of simulations. PSE has currently implemented a GSA Manager as part of a framework for parallelized execution of these simulations on multicore processors. The GSA Manager schedules jobs for a number of specified GSA workers. This is illustrated in Figure 26. PSE is currently extending this capability to parallelized execution on multiprocessor clusters.

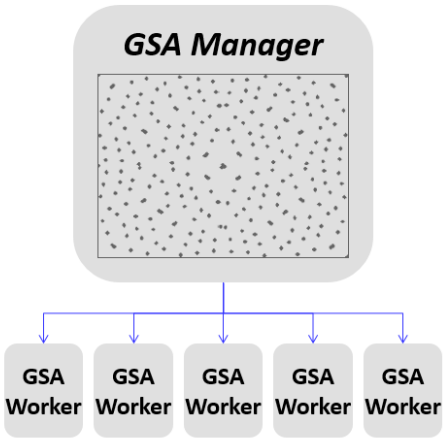


Figure 26 GSA Manager parallelization concept

9.3.2 Commercialization objective

We aim to employ the FOQUS Turbine framework for scheduling simulation jobs to extend GSA parallelized execution beyond multiprocessor clusters to the cloud. Rapid growth in the use of engineering simulation tools – and in the demand for high performance computing (HPC) – is driving interest in parallelization on the cloud. This development is seen as complimentary to the other two products as parallelization can deliver significant performance improvements in their use.

9.3.3 Competitive landscape

Schlumberger's OLGA simulation software currently has an implementation with job scheduling on the cloud. This tool is used specifically for multiphase flow assurance studies in the oil and gas industry. There are no known applications of this feature on competing general process modelling software at present.

9.3.4 Proposal

The proposed commercialization product is an additional feature that enables the parallelized execution of gPROMS GSA simulations on the cloud. The current implementation of FOQUS Turbine currently interfaces with gPROMS via SimSinter. Investigations reveal that the current methodology for setting up a functional interface between Turbine and gPROMS could be more user-friendly. In addition, the overheads of the interface negatively impacted simulation performance speeds. As a result, a redesign of such an interface is planned.

9.4 Case Studies involving the application of the products to the development and scale-up of multiple advanced energy systems

PSE proposed to carry out two case studies in collaboration with project partners. In the first year, before the CCSI tools have been fully implemented, conventional modelling methods will be applied to each case study. Case study 1 will be based on a "known" technology/case (from literature, publicized projects). This task will be undertaken primarily by West Virginia University under the supervision of PSE. It will be aimed at demonstrating the workflow, thus delivering key marketing and training resources that will accompany the product when it is launched. A number of applications are being considered:

- Design of Gas turbine – fuel cell hybrid technologies
- Optimization of Air separation unit systems
- Design and scale up of chemical looping (combustion or gasification) process
- Natural gas to liquids technology
- Coal to liquids technology

Case study 2 will focus on a "live industrial" case, the Allam Cycle, and will be carried out jointly with an industrial partner. This case will demonstrate the value of the uncertainty quantification approach and provide crucial insight into:

(a) how uncertainties and sensitivities in the underlying physics/chemistry impact process design parameters (e.g. size and type of CO_2 compression and pumping equipment, water separation equipment, pre and post combustion sulfur removal systems, high effectiveness recuperators and combustor) and, therefore, CapEx and OpEx for any given technology

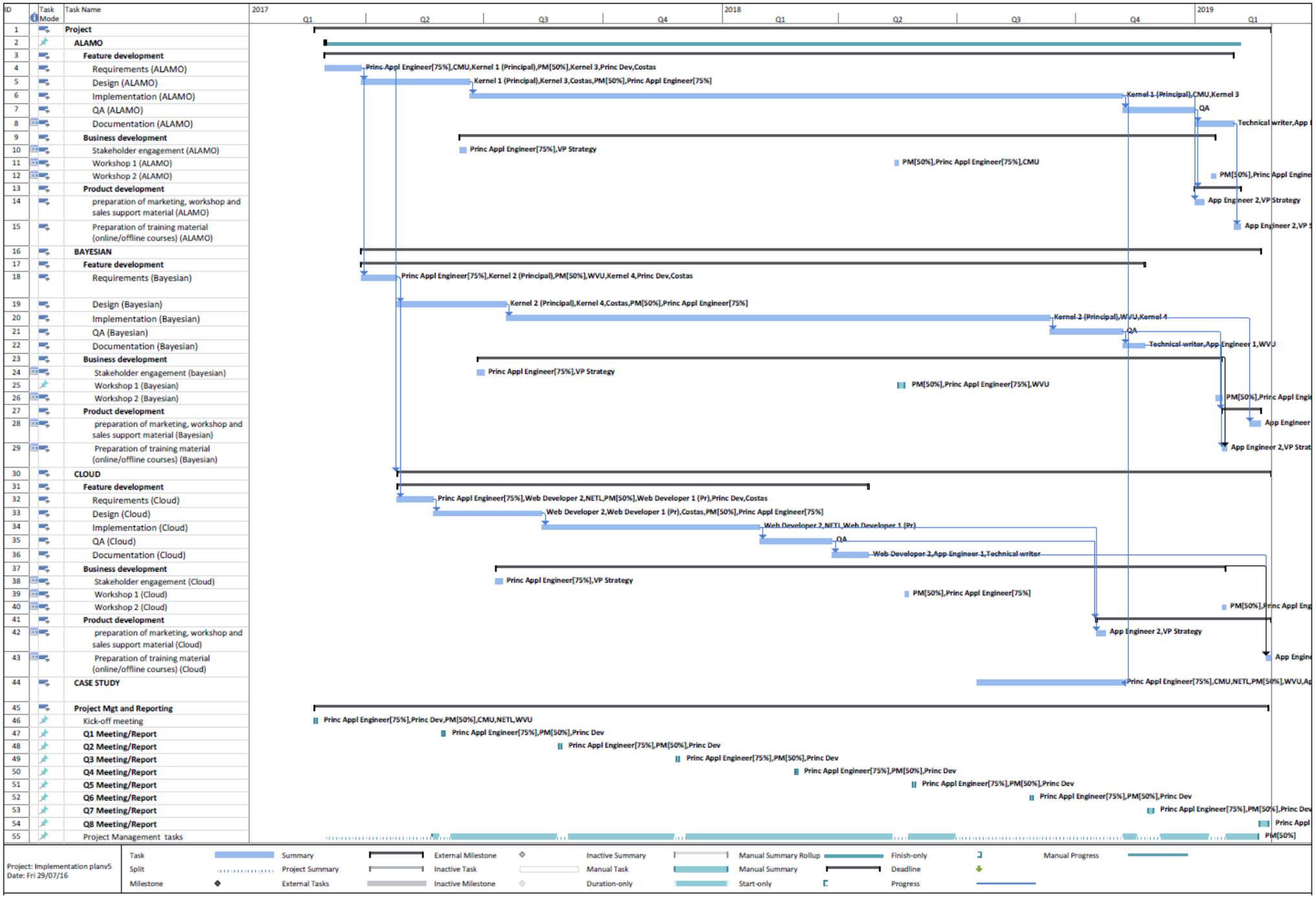
(b) where to carry out targeted experimentation (e.g. an acid gas removal process test and a reaction kinetics test of combustion) to reduce that level of uncertainty and tighten the distribution of CapEx/Opex,

(c) testing the capabilities of Bayesian analysis using selected empirical data sets.

(d) due to the highly recycled and non-linear behavior of the Allam Cycle, testing the improvements to simulation time accelerated by implementation of parallel processing through FOQUS/Turbine.

In first quarter of the project, the team will define the Allam Cycle case to be developed. From the second to the fourth quarter of the project, the process models of the Allam Cycle will be built and validated in gPROMS for both gas and coal-fueled systems. In year two of the project, CCSI tools will be applied to the case study once they are available for use. There may be a number of iterations involved at this stage to improve both the case study models and the CCSI tools. Finally, the results will be reported.

10 Project Plan proposed for Phase 2



The project plan covers the implementation and commercialization activities proposed for Phase 2 and is subdivided based on key deliverables/activities indicated by the following headings:

- “ALAMO”: corresponding to the implementation and commercialization activities of the ALAMO (C16038 CCSI Project Toolset, FOQUS Module – Feb. 5, 2016) product development
- “BAYESIAN”: corresponding to the implementation and commercialization activities of the Bayesian calibration (C16036 CCSI Project Toolset, SorbentFit Module – Feb. 5, 2016) product development
- “CLOUD”: corresponding to the implementation and commercialization activities of the Job queuing on the cloud (C16038 CCSI Project Toolset, FOQUS Module – Feb. 5, 2016) product development. This development will be completed earlier than the other two products as its application should enhance their performance.
- “CASE STUDY”: corresponding to the case studies which show the application of the developed tools for the development and/or scale-up of multiple advanced energy systems.
- “PROJECT MGT AND REPORTING”: corresponding to the project management and reporting activities scheduled throughout the project. This includes the kick-off meeting, quarterly reports and updates as well as day-to-day project management tasks

For each of the three proposed products, the following main activities are proposed:

- Feature development activities
- Business development activities
- Product development activities

10.1 Feature development

This is the main activity of the project and will span most quarters. These are the development steps required to incorporate the proposed features in gPROMS. In general the following steps are required:

- Requirements– this involves meetings between the CCSI tool developers, PSE Consultants, Application Engineers and Software Developers and potential users to establish the technical specification of the proposed product.
- Design – based on the developed requirements, the Software development team, with advice/guidance from the CCSI tool developers will design the new gPROMS features that will be implemented to create the feature.
- Implementation – in this phase, the software developers implement the required code in the gPROMS platform to create the new feature
- Quality Assurance (QA) – as with all PSE developed software products, the new feature will be undergo rigorous and comprehensive testing to ensure they are user friendly, robust and meet all the required quality standards
- Documentation – in this phase, the implemented code is documented for internal purposes.

10.2 Business development

The following steps are planned to ensure the products are relevant to customers’ present and future requirements

10.2.1 Stakeholder engagement

In the second quarter of the project, a workshop will be set up with potential users of the products sourced from the Industry advisory board and other PSE clients. This way, PSE can present the initial developments to stakeholders. This workshop would seek to inform the stakeholders of PSE’s developments, capture their requirements of the users

in detail and ensure that the developments aligns with these requirements. Relevant case studies of applications involving the development and/or scale-up of CCS advanced energy systems would be determined and planned in these meetings.

10.2.2 Workshops

Workshops will be held between the sixth and eighth quarters to review the development of the developed tools and also allow stakeholders carry out assessments of the identified case studies. Two sets of case studies are planned. One set in the sixth quarter which analyses the progress of the product development and assesses the alignment with the user requirements. The second set will be carried out in the eighth quarter where, in addition, the results of the selected case studies will be analyzed and assessed.

10.3 Product development

Once the CCSI tools have been implemented in gPROMS as features, a number of activities would be carried out to ensure it remains a viable product

10.3.1 Marketing

In this phase, marketing material will be prepared; feedback from stakeholder engagement will be collated and actioned; and various channels of communication with potential customers will be explored and utilized.

10.3.2 Sales support

PSE Application engineers will engage with the PSE Sales team with the aim of improving sales of the developed gPROMS features. For instance, PSE Application Engineers can set up evaluations with interested clients in order to boost sales.

10.3.3 Training material

Applications Engineers will develop training materials to guide users on the use of these tools.

10.4 Contributions of the sub-recipients and DOE Federally Funded Research and Development Centers (FFRDCs)

10.4.1 Carnegie Mellon University (CMU)

Prof. Nikolaos V. Sahinidis has been a contributor to the CCSI project, developer of *ALAMO* as well as a variety of other modeling and simulation tools. His proposed role in Phase 2 will be to provide advice and support in the implementation of ALAMO in gPROMS.

10.4.2 West Virginia University (WVU)

Dr David Mebane is a key member of the Basic Data team on the CCSI project: Dr. Mebane and his group are the principal developers of SorbentFit, one of two key Basic Data products in the CCSI project. It is proposed that his role in Phase 2 will be to provide advice and support in the implementation of Bayesian calibration concepts.

Dr. Debangsu Bhattacharyya has served and has been serving as a PI and co-PI on a number of DOE/NETL funded projects with expertise in Process Modeling. It is proposed that Dr. Bhattacharyya's role in Phase 2 will be the development of example applications of the developed modelling tools. In addition, Dr. Bhattacharyya will supervise the definition, execution and reporting of the case studies for the development and/or scale-up of advanced energy systems.

10.4.3 Lawrence Berkeley National Laboratory (DOE FFDRC)

Josh Boverhof was involved in the development of the FOQUS Turbine features that enabled job queueing of parallelized simulations on the cloud. His proposed role in Phase 2 will be to provide advice and support in the implementation of the job queueing on the cloud features in gPROMS.

10.5 Project term

The proposed Phase 2 project term is two (2) years. The project plan presented is based on an assumed start date of February 2017.

10.6 Project Management and Reporting

10.6.1 Project Monitoring and Control

The Project Manager will be responsible for ensuring the project progresses according to plan. This will involve measuring and monitoring progress as well as initiating control measures to address issues and/or delays. This applies to the progress of the main recipient (PSE) and sub-recipients.

10.6.2 Project Reporting and communications

There will be quarterly progress reports and meetings with NETL to communicate the progress of the project with respect to the proposed plan. These reports include the Quarterly Research Performance Progress Reports and the financial reports for the main and sub-recipients.

In addition, the application of the computational tools and models will be documented in detail in peer reviewed journal articles describing both the energy technology and the computational tools. The articles will include data to demonstrate the accuracy and predictive capability of the models.

10.6.3 Project Risk Management

The project manager will identify the key Risks associated with the project and communicate this as a Risk Register in the Project management plan of the proposal. Both qualitative and quantitative risk analyses will be carried out on the identified risks and the appropriate risk responses will be planned. During the course of the project, the project manager will monitor and where applicable control risks.

10.7 Long-term support

The products PSE proposes to develop in this project will be deployed as parts of PSE's gPROMS platform. As such, these tools will benefit from being served by the main PSE gPROMS technical support team.

11 Notation

a_p	particle specific area, m^{-1}
a_w	ratio of the internal surface area to the volume of the reactor wall, m^{-1}
a_{w1}	ratio of the logarithmic mean surface area of the reactor shell to the volume of the reactor wall, m^{-1}
Bi_i	mass Biot number of component *i*, $Bi_i = a_p k_f {r_p}^2/(15\varepsilon_p D_{p,i})$, dimensionless
$C_{g,i}$	gas phase concentration of component *i*, mol/m^3
$C_{g,i,feed}$	inlet gas phase concentration, mol/m^3
$C_{p,g}$	gas mixture molar specific heat at constant pressure, kJ/mol/K
$C_{g,T}$	total bulk gas phase concentration, mol/m^3
$C_{p,s}$	particle specific heat, kJ/kg/K
$\overline{C_{s,i}}$	average concentration of component *i* in the macropores, mol/m^3
$\overline{C_{s,T}}$	average total gas concentration in the macropores, mol/m^3
$C_{v,g}$	gas mixture molar specific heat at constant volume, kJ/mol/K
$D_{\mu,i}$	micropore diffusivity of component *i*, m^2/s
D_{ij}	binary molecular diffusivity, m^2/s
$D_{K,i}$	Kundsen diffusivity of component *i*, m^2/s
$D_{m,i}$	molecular diffusion coefficient of component *i* in the gas mixture, m^2/s
$D_{p,i}$	macropore diffusivity of component *i*, m^2/s
d_p	particle diameter, m
D_r	internal diameter of reactor, m
ΔH	heat of adsorption of component *i*, kJ/mol
h_0	heat transfer coefficient between reactor wall and ambient, $kW/m^2/K$
h_f	film heat transfer coefficient between gas and solid particle, $kW/m^2/K$
h_{gw}	film heat transfer coefficient between gas and reactor wall, $kW/m^2/K$
k_{fi}	film mass transfer coefficient, m/s
k_g	gas thermal conductivity, kW/m/K
k_i	LDF mass transfer coefficient, 1/s
K	Langmuir equilibrium constant, 1/bar
L	reactor length, m

M_{ij}	a function of the molecular weights of components *i* and *j*, mol/g
MW_i	molecular weight of component *i*, kg/kmol
n_v	adsorption site density, mol/m^3
P_g	pressure, bar
$P_{p,i}$	partial pressure of component *i*, bar
$P_{g,init}$	initial pressure drop through the reactor bed given by the Ergun equation, bar
Pr	Prandtl number, $\mathrm{Pr} = \mu C_{p,g}/k_g$, dimensionless
$\overline{q_i}$	particle averaged adsorbed concentration (loading), mol/kg
q_i^*	adsorbed concentration in equilibrium with $C_{g,i}$, mol/kg
q_{max}	saturation adsorption capacity in the multisite Langmuir isotherm, mol/kg
Ra	Rayleigh number, dimensionless
Re	particle Reynolds number, $Re = \rho_g d_p v_{g0}/\mu$, dimensionless
r_c	“microparticle” radius, m
R_g	ideal gas constant, kJ/mol/K
r_p	particle radius, m
ΔS	adsorption entropy of component *i*, kJ/mol/K
Sc_i	Schmidt number, $Sc_i = \mu/(\rho_g D_{m,i})$, dimensionless
t	time, s
T_0	inlet and initial temperature, K
T_∞	ambient temperature, K
T_g	bulk gas temperature, K
T_s	solid temperature, K
T_w	reactor wall temperature, K
v_g	superficial velocity, m/s
w_{th}	reactor wall thickness, m
$y_{g,i}$	gas mole fraction of component *i*
$y_{gi,in}$	inlet mole fraction of component *i*
$y_{gi,initial}$	initial mole fraction of component *i*
z	axial position, m

Greek letters

β_i	orthogonal basis functions
δ	discrepancy function, dimensionless
ε	bed porosity, dimensionless
ε_p	particle porosity, dimensionless
λ	heat axial dispersion coefficient, W/m/K
μ	bulk gas mixture viscosity, kg/m/s
ρ_g	bulk gas mixture density, kg/m^3
ρ_p	particle density, kg/m^3
σ_{ij}	the Lennard-Jones parameter (collision molecular diameter), Å
τ_p	pore tortuosity
Φ_i	eigenfunctions
Ω_{Dij}	collision integral, dimensionless

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Appendix A – Brochures of Fast track tools

Subject	**CCSI Tool Commercialization Brochure (Process Models)**
From	Debangsu Bhattacharyya
To	Adekola Lawal (on behalf of PSE)
Date	3rd March 2016
Doc ID	PSE-RD-R-US-NETL-20160225

Proposed Content

Please describe the content of the tool.

Solid-Gas System Models:

In this class, currently two hydrodynamics have been considered- bubbling fluidized bed and moving bed. The models include both steady-state and dynamic modes to support process design as well as process control. The models capture sufficient detail to provide accurate and predictive results while remaining computationally tractable. They consist of a system of partial differential algebraic equations (PDAEs), which capture the hydrodynamic behavior, interactions of the gas and solids, the heat and mass transfer phenomena, and the kinetics of the adsorption and desorption reactions.

The BFB reactor model is one-dimensional (1D) PDAE-based, two phase and non-isothermal, incorporating heat transfer tubes to provide external heating and cooling capability. It can be used to simulate over-flow type configuration where the solids leave the stage by flowing over the weir or the underflow-type configuration where the solids leave from the bottom of the bed. This model can also be modified to use it as a heat exchanger model.

The MB reactor model is also 1D PDAE-based, two-phase and non-isothermal, with heat transfer tubes. When used as a regenerator, an integral heat-recovery system heats the incoming solid sorbent using the steam that is produced by recovering heat from the hot sorbent leaving the regenerator. The reaction kinetics, heat and mass transfer, and the hydrodynamics are considered both in the MB reactor and heat recovery system.

Solvent System Models:

Solvent system models for MEA-based CO_2 capture system have been developed by practically using all available experimental data for properties, and WWC data. Both the steady-state and dynamic models have been validated with the data from the National Carbon Capture Centre.

CO_2 Compressor Model:

Process models of both inline and integral gear type multistage compressors with interstage coolers and knock-out drums as appropriate have been developed for compressing CO_2 from near-atmospheric pressure to a pipeline pressure of 2216 psia. For applicability in cases with wide variations in Mach numbers, nondimensional performance curves in terms of the impeller exit flow coefficient and polytropic head coefficient have been generated by using data obtained from a commercial vendor. A model of a triethylene glycol absorber has been developed and used to satisfy the desired water content in the compressed CO_2 for pipeline transport.

Integrated System Model:

An integrated process that includes solid sorbent based adsorber, regenerator, heat exchanger, CO_2 compression system, and balance of the plants has been developed in gPROMS.

Workflow

- Briefly itemize the workflow for obtaining typical solutions from your tool.
- Outline the list of inputs, describe the steps involved in inputting data, processing, and generating outputs.
- Please provide a description of the typical outputs.

These models are ready to be run in gPROMS except the solvent model. Other than the input boundaries, the user needs to provide the design inputs for the contactors. Output information includes results of the output streams and the transport profiles and other variables typical of process models.

Application/Relevance to PSE Verticals

- Please list the current and potential applications of the tool.

Currently the models have been developed specifically for CO_2 capture applications. But, the solids models can be used for any solid-gas applications. The models are dynamic and there is hardly any dynamic model for solids systems in the available commercial process modelling software. The model can be used for systems where either physical adsorption, chemical reaction, or both adsorption and reaction take(s) place. The models can currently be used for bubbling bed and moving bed applications. In Phase I, models for fixed bed systems are being developed. In Phase II, models for circulating fluidized beds, transport reactor, and pneumatic transport system can be developed leading to a suite of dynamic models for solid-gas contactors. CO_2 compressor system modelling approach can be generically extended to other compressors. Solvent system models are very generic and can be merged with existing gPROMS AML-GLC model with added features.

- Include a list of the industrial sectors where this tool may be used and for which specific processes.

Fluidized beds are widely used for varieties of applications including petroleum and petrochemicals, food industry, pharmaceutical industry, metallurgical applications, power plants (such as circulating fluidized bed combustors), gasifiers, new chemical looping processes, and variety other processes as recorded in open literature and standard text books. Other than the typical applications of the steady-state models for design and optimization, the dynamic models are of high importance for processes with complex dynamics and control challenges and those where the plant throughput needs to be adjusted very frequently and those that are subjected to large and frequent disturbances. The models can also be very useful for optimizing start up and shut down of such processes as significant equipment damage occurs during those times. Fixed solid beds have many other applications. Moving bed systems are also widely used in petroleum industry and also in other sectors such as agricultural sector for drying of grain, mineral processing such as drying and metallurgical applications. Some of the PSE's current gSOLIDS clientele can be potential users. PSE already has wealth of information on applications of typical tower models and compressor models.

- What will the tool be used for (e.g. process design, process control, parameter estimation, optimization, etc)?

The models can be used for all of the above as well as for studying effects of inputs on process transients, startup, and shutdown.

- Which clients have indicated interest / used this tool?

GE is working with us on the solvent model. ADA-ES, Inc. has used the bubbling fluidized bed model. We are currently working with another industry that is interested in the moving bed models. However, it should be noted that as part of CCSI we mainly worked with the industry that are interested in CO_2 capture applications, which are not many. If we look beyond CO_2 capture applications, there are many industries with such applications.

- What types of feedback did your clients give (user-friendliness, potential applications, etc)?

Researchers from GE spent some time in our lab to feel comfortable with the CCSI models, tools, and approaches. For other industries that we have worked with, they neither have Aspen Custom Modeler nor gPROMS and therefore the studies that they were interested in were mainly conducted by us.

Competition

- Which tools (that you are aware of) can carry out similar tasks?

I am not aware of any commercial software with capabilities for dynamic models of fluidized bed systems. (Does the current/upcoming version of gSOLIDS has these capabilities?)

- Which tool is considered the market-leading tool in the area (apart from yours!)?

See above.

Features and Advantages + SWOT Analysis

- What is unique about this tool?

As mentioned before, dynamic models of solids systems are currently not available in the literature.

- How does it compare to the competition?
    - Think about features such as the accuracy, user friendliness, the range of potential applications, workflow, speed of simulation etc.

See above.

- What will you consider are the advantages of the tool?

Dynamic model of fluidized and moving beds, flexibility in terms of applications (adsorption, reaction, adsorption-reaction, solids heat exchanger), embedded heat exchanger model, flow configuration (currently only overflow-type configuration has a dynamic model, but for the steady-state version both overflow-type and underflow-type configurations do exist; dynamic mode of the under-flow type configuration can be developed in Phase II), models of additional contactor types (such as circulating fluidized bed and transport reactors) can be developed in Phase II by modifying the existing framework.

- Describe some examples / case studies which demonstrate the benefits of this tool

Published papers as well as manuscripts under preparation demonstrate the benefits of the tool from the design, parameter estimation, and optimization as well as control perspective.

- What are the limitations of the tool? (What can it not be used for)

Currently, these models have been developed for CO_2 capture applications and therefore, number of things are hardcoded. For generically applying these to any solids systems, certain sections of the code need to be rewritten. Plus, the codes need to be modified to improve their user friendliness. In addition, the models are available for only bubbling bed and moving beds.

- List at least two ways you think the tool could be improved. What benefits would be obtained from these improvements?

Several things can help in improving the values obtained from these models such as:

    - Making the models generic for any solids applications
    - Developing dynamic model of underflow-type bubbling beds
    - Developing models of the circulating fluidized beds and transport reactors

- Developing models of the pneumatic transport system
- In other words, a dynamic library for solids systems in gPROMS for most common types of hydrodynamics, configurations, and applications can be very useful
- If there is a specific industry with strong potential applications where some specialized development would be helpful, that can be done in Phase II. For example, if petroleum/petrochemical industry is identified to be a potential customer, models need to support generation of pseudo-components/key components and their properties requiring additional correlations/models to be developed.

Requirements

- Describe the tools requirements. For instance,
  - Multi/single core
  - Memory
  - CPU
  - Software requirements (OS, other software components it may require)

No special software are currently needed outside of gPROMS and its typical bundle with Multiflash.

Other comments

- Include any additional information that you feel is relevant and does not fit in the above categories.

Subject	**CCSI Tool Commercialization Brochure (SorbentFit)**
From	David Mebane
To	Adekola Lawal (on behalf of PSE)
Date	25th February 2016
Doc ID	PSE-RD-R-US-NETL-20160225

Proposed Content

- Please describe the content of the tool.

SorbentFit is a chemical kinetic fitting tool. It contains two models pertaining to amine-based CO2 adsorbents: a lumped-kinetic model and a high-fidelity reaction-diffusion model. Models can be fit to either (dynamic) TGA or fixed bed datasets.

SolventFit is a fitting tool for high-viscosity CO2 solvents, based on wetted-wall column data.

- Include a list of models/software tools, model documentation and example process flowsheets.

The models included with SorbentFit are just the two mentioned above; there is also a user manual that presents the models in detail and describes what kind of information the software provides, as well as how to use it.

SolventFit contains only the wetted-wall column model.

- This section should describe what the user gets when they download this CCSI tool.

SorbentFit is delivered either as source code (for OSX and Linux) or as a set of executables (Windows). There are separate executables for point estimates and for Bayesian calibration, and for each version of the model (lumped or high-fidelity), as well as for each experiment (TGA or fixed bed). The package includes a sample set of TGA data and configuration files that can be used to test the software.

SolventFit is integrated with the FOQUS uncertainty quantification tool.

Workflow

- Briefly itemize the workflow for obtaining typical solutions from your tool.
- Outline the list of inputs, describe the steps involved in inputting data, processing, and generating outputs.
- Please provide a description of the typical outputs.

Users must provide formatted data in the form of space- or tab-delimited text files. Configuration files pertaining to the relevant experiment. Configuration files specify the model parameters for which estimation is desired, along with bounds on those parameters. (Default values are provided.) Tolerances and settings for the solver (including the time step used) can also be changed from their default values in the configuration file. A list of formatted data files must also be provided. The user can also change the number of agents used in the particle swarm optimizer (point estimate) or the proposal variances and total number of samples obtained (Bayesian calibration) from their defaults.

Users invoke SorbentFit at the command line. Periodic output is written to the console, with final results written to disk. For the point estimate tool, the final results are the final parameter set along with predictions of the fitted model compared with experiment. For Bayesian calibration, results are a list of sampled parameter sets that represent the posterior distribution for the parameters.

SolventFit is GUI-based, with the relevant configuration taking place in the FOQUS GUI.

Application/Relevance to PSE Verticals

- Please list the current and potential applications of the tool.

Currently the tool can be applied to a number of solid sorbent systems, especially amine-based CO2 sorbents. The real value contained in the tool, however, is a more general application of the methodology of Bayesian calibration and uncertainty propagation contained in SorbentFit and associated process models. CCSI tools demonstrate how the uncertainty quantified at the bench / lab scale can be utilized in process design and optimization for an amine sorbent-based carbon capture process. The opportunity is to extend these capabilities in a general way to a large number of different applications.

Model discrepancy is a methodology embedded in SorbentFit that could be used to automatically generate efficient, probabilistic models of chemical processes. The potential here is to have a tool that takes a minimum of information from the user – a set of inputs, outputs and basic model forms – and builds a model to fit the lab-scale data, while simultaneously quantifying uncertainty in a way that can be easily propagated to larger-scale models.

SolventFit's approach to calibration is slightly different, and could be better for complex, user-defined models. The tool obtains a set of data from the model and first builds a fast response surface for that data. The response surface is then used in calibration, which yields a posterior distribution of parameters.

Both tools can be used to generate design of experiments at the bench scale that will tend to decrease uncertainty at larger process scales.

- Include a list of the industrial sectors where this tool may be used and for which specific processes.

Separations, catalytic reactions, distillation, gasification, etc. – any situation in which lab and bench scale data must be used to make predictions about large process-scale behavior.

- What will the tool be used for (e.g. process design, process control, parameter estimation, optimization, etc)?

It is best for process design and parameter estimation – indeed, in the linkage of these two things.

- Which clients have indicated interest / used this tool?

GE is using SolventFit.

- What types of feedback did your clients give (user-friendliness, potential applications, etc)?
-

Competition

- Which tools (that you are aware of) can carry out similar tasks?

There are many tools that estimate parameters, including the suite of parameter estimation tools in gPROMS, Aspen and the open-source ChemKin. *However, there is no commercial implementation of Bayesian calibration and uncertainty propagation capabilities that I am aware of.*

- Which tool is considered the market-leading tool in the area (apart from yours!)?

Various open-source tools (including one developed in our lab) provide Bayesian calibration for specific problems / experiments. Again, there is no general, commercial capability available.

Features and Advantages + SWOT Analysis

- What is unique about this tool?

Bayesian calibration uses experimental data to create input distributions of parameters for uncertainty propagation.

- How does it compare to the competition?
    - Think about features such as the accuracy, user friendliness, the range of potential applications, workflow, speed of simulation etc.

Other tools are available (e.g. Sandia's DAKOTA; LLNL's PSUADE) which enable the propagation of uncertainty from a limited set of user-defined distributions. Results generated in this way can be *fundamentally different* from the results obtained when using a distribution that is consistent with experimental data as is generated by Bayesian calibration.

gPROMS's own parameter estimation tool generates an estimate of uncertainty that can be compared with Bayesian calibration of a version of the underlying model linearized in its parameters. This can yield important information but will fail to capture nonlinear effects, including multi-modality (the existence of more than one distinct "mode" of the model that is consistent with the data).

- What will you consider are the advantages of the tool?

These tools will increase confidence in critical business decisions related to process scale-up, enabling faster time-to-market.

- Describe some examples / case studies which demonstrate the benefits of this tool

The solid sorbent core CCSI case; the GE solvent process case; the ADA-ES solid sorbent case; other case studies (especially involving discrepancy and automated model-building) that are currently in progress.

- What are the limitations of the tool? (What can it not be used for)

These tools will generally require more user input and will run longer than existing tools for parameter estimation. However, there are methods by which much automation and acceleration (especially by parallelization) can be introduced: adaptive tuning, automated termination / burn-in recognition, paralellized sampling through sequential Monte Carlo.

- List at least two ways you think the tool could be improved. What benefits would be obtained from these improvements?

Adaptive tuning would take the task of modifying the tuning parameters from the Monte Carlo sampler out of the hands of the user, and is relatively easy to implement. Automated termination and burn-in would likewise remove some of the current requirements for operator expertise – these would be more difficult than adaptive tuning but still feasible. Sequential Monte Carlo is an embarrassingly parallel method for efficiently sampling on the parameter space that solves a number of problems in the mixing of the more common Markov chain variety (which is what is implemented in SorbentFit and SolventFit). Implementation of s-MC is also straightforward.

Requirements

- Describe the tools requirements. For instance,
    - Multi/single core
    - Memory
    - CPU
    - Software requirements (OS, other software components it may require)

SorbentFit is muilti-core, shared memory. SolventFit is serial. Neither application has significant memory requirements. SorbentFit requires the BOOST C++ library, and the Eigen numerical package. SolventFit requires R and python.

Other comments

- Include any additional information that you feel is relevant and does not fit in the above categories.

Subject	**CCSI Tool Commercialization Brochure (ALAMO)**
To	Adekola Lawal (on behalf of PSE)
From	Nick Sahinidis
Date	2nd March 2016

Proposed Content

The **Automated Learning of Algebraic MOdels (ALAMO)** distribution provides executables and examples for building models from data and/or simulations. ALAMO can work with a pre-existing dataset and/or interface with an executable that provides new data at points specified by ALAMO. The ALAMO downloads from www.minlp.com are zip archives for different operating systems (Windows, Linux and Mac OSX); versions are provided for 64 and 32 bit architectures. Each zip archive comes with an ALAMO executable, the ALAMO manual in PDF, example data files, and example executables that can be used to provide new data.

Workflow

- **Data input**

An example input file for ALAMO is provided below

```
! Example 1 with data from z = x^2
ninputs 1
noutputs 1
xmin -5
xmax 5
ndata 11
logfcns 1
expfcns 1
sinfcns 1
cosfcns 1
monomialpower 1 2 3
BEGIN_DATA
-5 25
-4 16
-3 9
-2 4
```

-1 1

0 0

1 1

2 4

3 9

4 16

5 25

END_DATA

In the above file, the user specifies the number of input and output variables in the system of interest, the range of interest for the input variables, the types of functions that ALAMO should consider in building an input-output model, and a data set with measurements of the output variables at the corresponding values of the input variables. Optionally, the user may prepare an executable that can sample the input-output system at will. More information is provided in the ALAMO manual. Additional examples are provided in the distribution—See the examples folder, which includes several ALAMO input files (all with the extension .alm).

- **Data Processing**

ALAMO must be called from the command line. For example,

alamo example1

will run ALAMO on file example1. An example input file was provided in the previous section.

- **Data Output**

In addition to providing output on the screen, ALAMO generates a results (listing) file with the extension .lst. For instance, running ALAMO on example1 (or example1.alm), will generate a results file named example1.lst. This file contains all data used by ALAMO in the calculations, all option files used in the run, and the models obtained by ALAMO. Typically, many models are found and reported. The model that is reported last is the best one found.

For the above example, here's the ALAMO screen output:

```
*******************************************************************************
 ALAMO version 2016.2.23. Built: LNX-64 Tue Feb 23 22:25:54 EST 2016

 If you use this software, please cite:
 Cozad, A., N. V. Sahinidis and D. C. Miller,
```

```
Automatic Learning of Algebraic Models for Optimization,
AIChE Journal, 60, 2211-2227, 2014.

ALAMO is powered by the BARON software from http://www.minlp.com/
********************************************************************************
Licensee: Nick Sahinidis at The Optimization Firm, LLC., niksah@gmail.com.
********************************************************************************
Reading input data
Checking input consistency and initializing data structures
Warning: eliminating basis log(x)

Step 0: Initializing data set
User provided an initial data set of 11 data points
We will sample no more data points at this stage
********************************************************************************
Iteration 1 (Approx. elapsed time 0.30E-02 s)

Step 1: Model building using BIC

Model building for variable z
z = x**2.0

Calculating quality metrics on observed data set.

Quality metrics for output z
-----------------------------
RMSE:               0.00
R2:                1.00
R2 cross validation:  1.00
Model size:         1
BIC:              -0.100E+31
Cp:               -9.00
AICc:              -0.100E+31
```

HQC: -0.100E+31

MSE: 0.00

Convex penalty: 10.0

RIC: 3.89

Total execution time 0.40E-02 s

Times breakdown

OLR time: 0.0 s in 11 ordinary linear regression problem(s)

MIP time: 0.0 s in 0 quadratic integer problem(s)

Simulation time: 0.0 s to simulate 0 point(s)

All other time: 0.40E-02 s in 1 iteration(s)

Normal termination

****

The listing file produced by this run is 144 lines long.

Application/Relevance to PSE Verticals

Potential applications of ALAMO include:

1. ALAMO can be used to develop surrogate (reduced-order/algebraic) models of black-box systems, such as thermodynamics packages and detailed process simulations. Such an application can be done once or offered as a tool to be used on an as-needed basis.
2. ALAMO can be used for parameter estimation from any set of collected/simulated data. The tool is domain-independent and can therefore be used for building models from data in the financial sector as well as chemical processes, the automotive industry, the social sciences, etc. etc.

Interest in using ALAMO has been expressed by several companies, including Dow, Eastman Chemical, and Air Liquide. The feedback has been very positive regarding the package's unique abilities (automatic consideration of nonlinear compositions of input variables, constrained regression, safe extrapolation, adaptive sampling). Criticism has been expressed regarding the lack of an installer and a GUI.

Competition

There is a huge number of regression software that would compete with ALAMO. However, most existing tools are too simplistic and lack advanced modelling capability. There are many companies offering regression modelling through neural networks, for example. Companies such as Datadvance, for instance, offer nice GUIs but not much algorithmically. The software closest to ALAMO in terms of capabilities is Eureqa (from Newtonian). Eureka implements a form of regression, known as symbolic regression, which is more general than the one currently implemented in ALAMO. However, Eureka relies on genetic search, whereas ALAMO utilizes deterministic optimization algorithms and, as a result, often finds better models than Eureka. Moreover, ALAMO has the distinct advantage that it offers constrained regression and adaptive sampling techniques for large datasets (these two features are discussed below); a future version of ALAMO will provide full symbolic regression capabilities based on deterministic optimization algorithms. Eureqa has been in existence for a few years, which is long enough to capture

a large fraction of regression modellers interested in nonlinear and symbolic regression. See http://www.nutonian.com/products/eureqa/

Features and Advantages + SWOT Analysis

ALAMO is unique in several ways

1. ALAMO returns the simplest regression model possible that fits the data well. As a result, humans can inspect ALAMO's models and confirm the physical correctness of these models before using them.
2. ALAMO is designed to minimize the number of data points required. This is important in the context of applications where the experiments are costly and data availability becomes an issue.
3. ALAMO is the only regression software that permits the user to do *constrained regression*, i.e., to enforce constraints on the response surface. This, for instance, would allow a user to ensure that a model of concentration will always provide concentrations that are not negative. Similarly, a mole fraction can be guaranteed to be always between 0 and 1. No other regression software offers this feature.
4. ALAMO provides an adaptive-sampling mechanism. A huge dataset does not have to be fed into ALAMO directly. Instead, the modeller can provide a small subset, have ALAMO build an initial model in terms of this small dataset, and then rely on ALAMO to sample more points from the huge dataset only if more points are required to improve model quality. This adaptive-sampling process results in unique numerical stability and scalability advantages.

SWOT analysis:

The ALAMO technology has been published in detail in the open literature. Hence, in principle, competitors could adapt the technology. One key consideration here is that ALAMO's technology requires a global MINLP solver in order to solve ALAMO's optimization subproblems. The Optimization Firm, LLC (www.minlp.com) owns the intellectual property rights of ALAMO as well as the BARON solver, which is currently considered as the best global MINLP solver available. By bundling the two packages together, ALAMO will have an edge against any potential competitor that takes a similar algorithmic approach.

Current limitations:

1. The most obvious limitation are the lack of an installer, the lack of a user-friendly GUI, and the lack of a detailed user manual (the current one is only 20 pages).
2. Given the sophistication of the algorithms employed, the current ALAMO system may require considerable computing time for certain problems, depending on the nature and complexity of the functions involved. As a result, some experimentation with algorithmic options may be required for certain applications. There is ongoing work by ALAMO's developers to identify a set of algorithmic options that will work well for most users.
3. ALAMO currently requires GAMS/BARON for large/complex fitting problems. In addition, it requires MATLAB/SNOBFIT for its constrained regression capability. There is ongoing work by The Optimization Firm to do away with both of these requirements.

- **Requirements**

The code runs on Windows (32 and 64 bit), Linux (32 and 64 bit) and OSX (64 bit). While the code itself does not have parallel capabilities, parallelism can be exploited in two ways:

1. The simulator called by ALAMO can run multiple simulation points in parallel; this feature can be currently controlled via an ALAMO algorithmic option.

2. BARON can automatically exploit multiple cores while solving ALAMO's optimization subproblems; this feature is controllable by a BARON algorithmic option.

Other comments

The source code of ALAMO is not available through the CCSI toolset. The Optimization Firm, LLC (TOF) owns the intellectual property rights to this source. TOF is owned by Professor Sahinidis and has been distributing commercially the BARON solver for over 15 years now. While TOF has expressed its willingness to make ALAMO available through the CCSI, it is also planning to commercialize ALAMO independently and may choose to work with additional distribution channels through non-exclusive arrangements.

Subject	**CCSI Tool Commercialization Brochure (FOQUS)**
To	Adekola Lawal (on behalf of PSE)
From	Nick Sahinidis
Date	2nd March 2016

Proposed Content

The Framework for Optimization, Quantification of Uncertainty, and Surrogates (FOQUS) serves as a computational platform enabling advanced process systems engineering capabilities to be integrated with commercial process simulation software.

FOQUS consists of several modules.

1. **SimSinter** provides a .NET wrapper for Windows-based process simulators such as Aspen Plus ACM, Excel, and the Windows version of gPROMS. It provides a generic interface, and a simple means to define a simulation inputs, outputs and settings. SimSinter has some dynamic simulation support currently for ACM. SimSinter is used by Turbine to interface with process simulations, and provides COM interface allowing simulations to be accessed in using VBA.
2. **Turbine** is a job queuing system for process simulations supported by SimSinter and for FOQUS flowsheets. Turbine allows simulation jobs to be executed on a single workstation, or in parallel on cloud, cluster, or local network resources.
3. The **FOQUS Flowsheet** is used to link simulations together and connect model variables between simulations. FOQUS enables linking models from different simulation packages. FOQUS flowsheets can be executed in parallel using Turbine to support derivative free optimization (DFO), uncertainty quantification (UQ) and surrogate modelling. The FOQUS flowsheet also provides a graphical interface and platform for analysis tools.
4. The **Automated Learning of Algebraic MOdels (ALAMO)** module can create algebraic surrogate models to support large-scale deterministic optimization, including superstructure optimization to determine process configurations. The ALAMO module is an external product due to background Intellectual Property (IP) issues.
5. The **Derivative-Free Optimization (DFO)** module enables derivative-free (simulation-based) optimization directly on the process models linked together on a FOQUS Flowsheet. Excel can be used to calculate complex objective functions, such as the cost of electricity.
6. The **UQ module** enables the effects of uncertainty to be propagated through the complete system model, sensitivity of the model to be assessed, and the most significant sources of uncertainty identified to enable prioritizing of experimental resources to obtain additional data.
7. The **Optimization Under Uncertainty (OUU)** module combines the capabilities of the DFO and the UQ modules to enable scenario-based optimization, such as optimization over a range of operating scenarios.
8. The **Dynamic Reduced-Order Model (D-RM)** module can be used to create dynamic reduced models from more detailed process models to support advanced model predictive control or enable more rapid evaluation of dynamic operating scenarios.
9. The **iREVEAL** module is an automated tool to create reduced-order models from computational fluid dynamics (CFD) simulations and export them in a form that can be used in process simulators.

10. The **SolventFit** module is an uncertainty quantification tool for the calibration of an Aspen Plus solvent process model. The current state-of-the-art is a regression that yields single best fit point estimates of some parameters. This shows neither the level of uncertainty in each parameter, nor the level of uncertainty in model output, such as equivalent work. SolventFit allows for predictions with uncertainty bounds by accounting for uncertainty in model parameters and deficiencies in the model form. This yields an improved understanding of the model parameters and results in more complete predictions with uncertainty bounds. This distribution of parameters allows for predictions with uncertainty.

Workflow

- **Data input**

For typical meta-flowsheeting purposes, in addition to the simulation, a SimSinter configuration file is required which defines a simulation input, output, and settings. The simulation and configuration files are uploaded to Turbine. Once simulations are available from Turbine, a flowsheet is defined in the FOQUS flowsheeting tool. Nodes are created and a simulation is assigned to each node. Directed edges between nodes between nodes define how data is transferred from node to node. If cycles are created in the flowsheet FOQUS can determine tear steams and solve the flowsheet iteratively. Once the flowsheet is defined, data analysis tools can be used.

- **Data Processing**

Data processing in FOQUS depends on the tools that the user wants to use. For example, in the case of optimization, user will follow the following steps:

i. Define the variables as decision, fixed or sample. Define the lower and upper bounds of the variables. Define the level value (starting value) of the variables.

ii. Define objective function, constraints, select the solver and solver options.

- **Data Output**

After running the results of every flowsheet evaluation are presented in tabular form. Analysis tools also produce text and graphical output in many cases. In the case of optimization, an objective function plot is obtained that displays the objective function value at each iteration. The details such as current iteration, number of samples, successful samples as well as failed samples are displayed in the status bar.

Application/Relevance to PSE Verticals

Applications of FOQUS:

1. The primary function of FOQUS is to connect multiple components of a flowsheet separately and manage the input and output between those components. This will have two major benefits:
    a. gPROMS can be easily coupled with external simulations developed for specific purposes in Excel, FORTRAN or Aspen.
    b. Issues such as unit conversion between the simulation can be easily handled by FOQUS as it has the capability that lets user define the ‘node script’ i.e. the simulation itself.
2. The initialization procedure of gPROMS can benefit significantly from the reduced-order models developed from ALAMO and D-RM.
3. FOQUS provides gPROMS access to the turbine gateway that allows job queuing and enables these jobs to be run in parallel using cloud- or cluster-based computing platforms.
4. Inbuilt derivative-free optimization solvers will help in treating the simulation or part of the simulation as a black box to provide an optimum input.

FOQUS can be used to synthesize, design, and optimize a complete chemical process system while considering uncertainty. It enables users to effectively screen potential process alternatives in the context of a complete industrial process so that trade-offs can be appropriately evaluated. With the use of FOQUS, a user can analyze techno-economic performance of the process and its dependency on process design and synthesis. A key aspect of FOQUS is that it bridges this gap by supporting a superstructure-based approach to determine the optimal process configuration and equipment interconnections.

Competition

Tools that are similar to FOQUS are modeFRONTIER, Optimus, and pSeven. modeFrontier is probably the leader in this area.

Features and Advantages + SWOT Analysis

Tools that are similar to FOQUS are modeFRONTIER, Optimus, and pSeven. These tools support derivative-free optimization and design of experiments, on linked external simulation software. Although FOQUS is relatively new and unpolished, there are two important advantages FOQUS has: 1) it is able to handle cycles in the flowsheet relatively easily with very little work form the user, 2) it supports connection to chemical engineering process simulators such as Aspen and gPROMS. FOQUS is designed for chemical engineering problems, while competitors are focused more on the aircraft and automotive industries.

Potential limitations may include limitations of DFO or the amount of time required to run very large numbers of simulations. Some problems such as large OUU problems are not really practical without a large cluster of computers.

In FOQUS, simulations can be connected in a meta-flowsheet, which enables parts of a process to be modelled using the most appropriate software and combines them into a single large model, possibly including recycle streams. For example, in studying a carbon capture system for a coal fired power plant: a power plant may be modelled in Thermoflex; a solvent-based carbon capture system may be modelled in Aspen Plus; and a compression system may be modelled in gPROMS. To optimize the entire system, these models can be combined into a single large model. The resulting meta-flowsheet can be used for simulation-based optimization, uncertainty quantification (UQ), or generation of surrogate models. Information extracted from the simulations can also be used to construct a heat integration optimization problem to determine the best way to use excess heat in the process. Heat integration can be combined with simulation-based optimization.

Examples depend on the feature of the tool that the user is trying to use. The detailed procedure and sample cases are provided in the manual.

Requirements

The CPU and memory requirements of FOQUS really depend mainly of the types of process simulations being run. Comparted to the simulation the requirements for FOQUS itself are minimal. FOQUS will run on any platform supported by Python and Qt. SimSinter and Turbine require Windows, and were designed specifically to support Windows based process simulators. The FOQUS flowsheet tool can be run in Linux while running simulations on a remote instance of Turbine.