Programme Area: Bioenergy

Project: Biomass to Power with CCS

Title: Model and Sub-model Specification and user Documentation

Abstract:

This document (from Work Package 3) provide the specification and user guidance for the the first two, of eight, parameterised technology models that will be used by the Bioenergy Value Chain Modelling (BVCM) project. The two technologies covered in this report are Biodedicated IGCC and Co-fired IGCC both with physical absorption-based carbon capture.

Context:

The Biomass to Power with CCS Phase 1 project consisted of four work packages: WP1: Landscape review of current developments; WP2: High Level Engineering Study (down-selecting from 24 to 8 Biomass to Power with CCS technologies); WP3: Parameterised Sub-System Models development; and WP4: Technology benchmarking and recommendation report. Reports generally follow this coding. We would suggest that you do not read any of the earlier deliverables in isolation as some assumptions in the reports were shown to be invalid. We would recommend that you read the project executive summaries as they provide a good summary of the overall conclusions. This work demonstrated the potential value of Biomass to Power with CCS technologies as a family, but it was clear at the time of the project, that the individual technologies were insufficiently mature to be able to ‘pick a winner’, due to the uncertainties around cost and performance associated with lower Technology Readiness Levels (TRLs).

Biomass to Power with CCS Project

TESBiC: Techno-Economic Study of Biomass to power with CCS

BwCCS. PM 04. D3.4, D3.5, D3.6 [T1,T2]

Deliverable Report:

D3.3: Parameterised sub-system models

D3.4: Model requirements specification and strategy

D3.5: Model and sub-model user documentation

T1: Co-fired IGCC with physical absorption-based carbon capture

T2: Dedicated biomass, BIGCC with physical absorption-based carbon capture

12/12/11

V0.1

Title	Deliverable on parameterised sub-system models, model requirements specification, modelling strategy and model user documentation
Client	Energy Technologies Institute LLP (ETI)
Reference	BwCCS PM04 D3.3, D3.4, D3.5 (T1,T2)
Date	12 December 2011
Version	0.1
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University of Leeds

Distribution

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EXECUTIVE SUMMARY

The Techno-economic Study of Biomass to Power with CCS (TESBIC) project, which has been commissioned by ETI, is concerned with the performance of an overview techno-economic assessment of the current and potential future approaches to the combination of technologies which involve the generation of electricity from biomass materials, and those which involve carbon dioxide capture. The present document forms the deliverable within work package, WP3; and it covers the work on:

D3.3: Parameterised sub-system models

D3.4: Model requirements and specifications and modelling strategy

D3.5: Model and sub-model user documentation

Following the first variation of Contract/Agreement with ETI, the aforementioned deliverables have been applied to two (T1,T2) out of eight technology combinations.

T1 denotes co-fired integrated gasification combined cycle (IGCC) with carbon capture using physical absorption; and

T2 represents dedicated biomass IGCC with carbon capture using physical absorption.

The overall model structure finalised for WP3 employs the “base+delta” modelling framework (see D3.1 and D3.2). This fits the requirements for the capture of information and transfer to ETI and compatibility with the Biomass Value Chain Modelling (BVCM) and ETI’s Energy System Modelling (ESME) projects. The models were developed based on the techno-economic sensitivity data obtained from WP2 and additional available data. The “base+delta” model is readily implementable in MS-Excel™.

This document also provides user documentation of the models and its sub-models developed as part of WP3. This document is intended to enable any potential user to use and understand the models and their application. Data standard validation, parameter estimation and improvement of model robustness were carried out using the Model Development Suite (MoDS). Overall, the models offer evaluation of key techno-economic variables such as CAPEX, OPEX, efficiencies, and emissions as a function of inputs such as co-firing, capacity factor, nameplate capacity and extent of carbon capture.

Within WP3, the next deliverable of the project will focus on utilising the methodology and infrastructure developed in the present deliverable along with the techno-economic sensitivity data from WP2 for the next three technology combinations.

1. MODEL REQUIREMENTS OVERVIEW

The models developed within WP3 should be easily translated into the modelling structures of the Biomass Value Chain Modelling (BVCM) and ETI's Energy System Modelling (ESME) projects. As discussed in the project proposal and the acceptance criteria, WP3 will use the detailed models and results of WP2 and other available data (as shown in Figure 1) to generate meta-models (rather than first principles models) for delivery to the ETI.

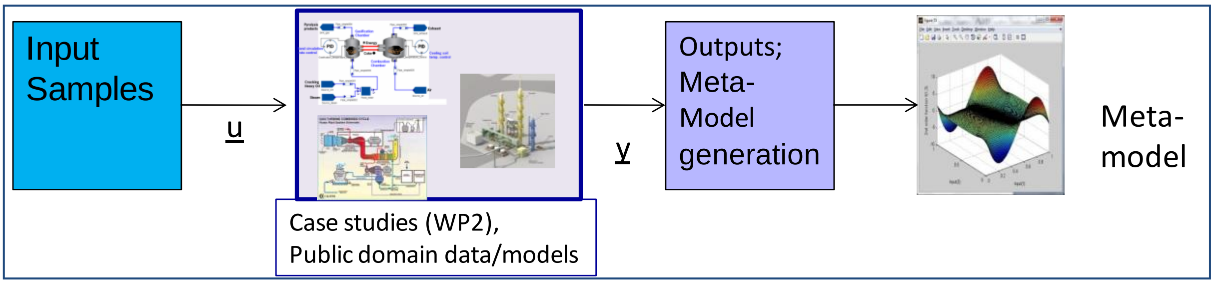

Figure 1: Overview of metamodelling approach.

Model Description

The overall model structure finalised for WP3 employs the linear additive "base+delta" modelling framework (see D3.1 and D3.2) based on system-specific data, in order to relate a specified set of "input" conditions to a specified set of "output" variables. This fits the requirements for the capture of information and transfer to ETI and compatibility with BVCM and ESME.

The "base+delta" model is readily implementable in MS-Excel^{TM}, by following these steps:

- Define standard units and reporting structures for model inputs and outputs, including confidence measures for data
- Identify sensible ranges for input variables
- Use WP2 models/data and other data to generate outputs from a sampled range of inputs
    - Prototype meta-model fitting (e.g. through least-squares optimisation)
    - Review meta-model approach and finalise model by model development
    - Produce model library and documentation
- Agree with ETI model storage and transfer protocol

The "base+delta" linear regression is described as:

$$y = y_b + A(x - x_b)$$

where y_b is a *n*-dimensional "base" data point, and x_b is the corresponding *m*-dimensional input. The *n* by *m* matrix A therefore describes how fast the responses change as we perturb the inputs away from the base x_b. Note that the data also give individual uncertainties for the outputs, which is taken into account. In the present work, *n* equals 7 and *m* equals 4, thereby rendering a 7 x 4 matrix A.

Implementation

The base+delta linear regression was performed using CMCL's software, MoDS (Model Development suite) together with Cambridge University, MoDS implements a whole variety of algorithms for improvement of models, including parameter estimation. In the case of the co-fired IGCC and the BIGCC data, the model is the linear regression model, and the parameter to be estimated is the matrix A.

Another facet of MoDS is its ability to check the input data given an appropriate XML schema. Earlier in WP3, such an XML schema was created for the BIGCC data (which ensured the sensible values for the inputs and outputs, and the associated uncertainties).

In terms of implementation, the following steps have been followed:

1) A standardised Excel spreadsheet has been created which contains the base case values, and the parameter estimates (once they have been calculated). This is in the "Model" worksheet. Another worksheet "Raw Data" in the same spreadsheet contains the raw data.
2) The data was extracted from the "Raw Data" worksheet, converted to XML so that the data can be validated using the XML schema (MoDS uses the XML schema to validate the data). This was implemented through a visual basic script (can run only on Windows machines).
3) Another visual basic script then creates the appropriate input files for MoDS.
4) MoDS is run using the data in XML format and the MoDS input file.
5) The parameters are then extracted from the MoDS output, and automatically entered into the "Model" worksheet of the Excel spreadsheet.

2. MODEL DETAILS: CO-FIRED IGCC CASE

For co-fired IGCC with physical absorption, the data was of the form:

- Inputs (4-dimensional vector x)
    - Nameplate capacity (MWe)
    - Operating capacity (MWe)
    - Co-firing (%)
    - Carbon capture extent (%)
- Outputs (6-dimensional vector $y = (y_1, y_2, y_3, y_4, y_5, y_6)^T$))
    - Capital cost (k £/MWe)
    - Non-fuel operating cost (k £/MWhe)
    - Generation efficiency (%)
    - CO_2 emissions (kg CO_2/MWhe)

- SO_2 emissions (kg SO_2/MWhe)
- NO_x emissions (kg NO_x/MWhe)

The detailed model was developed using the IECM (http://www.cmu.edu/epp/iecm/) model from Carnegie Mellon University. Some corrections were made to the predicted CO_2 intensity.

The process flow diagram is illustrated in Figure 2 below.

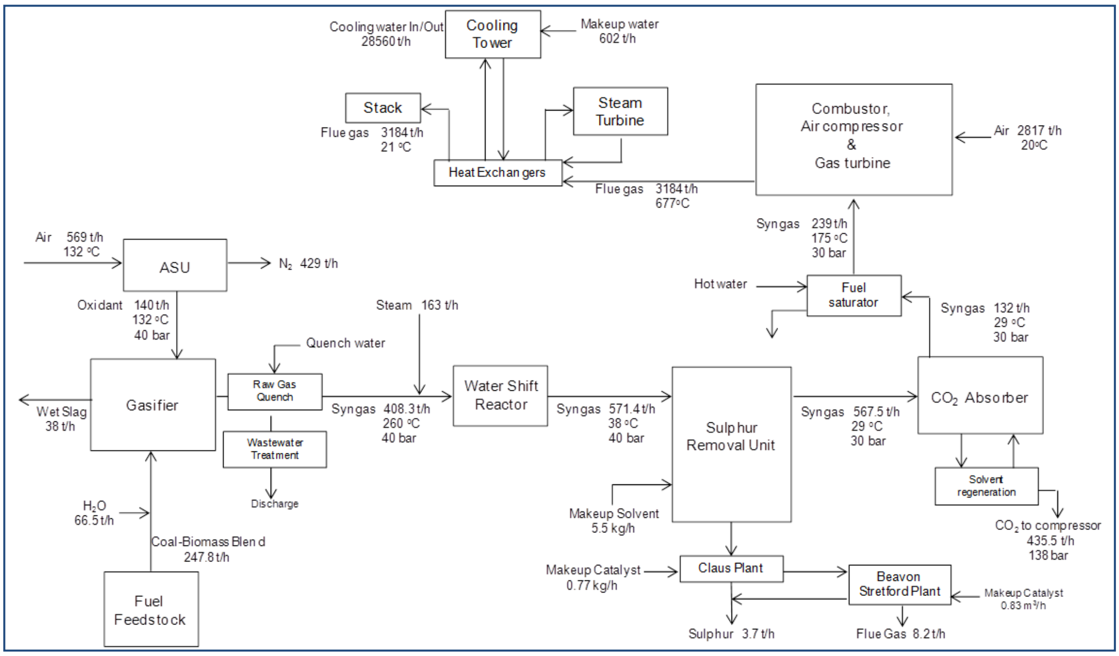

Figure 2. Process flow diagram for IGCC plant

As explained in the WP2 deliverable, the IECM tool contains all the necessary unit operations and so the assumptions in the detailed model are based on those embedded in the tool.

Eleven case studies (1 base and 10 delta) were generated using IECM and used to calibrate the meta-model. A summary of the case study data is in Appendix 1.

3. MODEL DETAILS: BIGCC CASE

Input and output data: This technology does not have co-firing, and so the inputs and outputs are:

- Inputs (3-dimensional vector x)
  - Nameplate capacity (MWe)
  - Operating capacity (MWe)
  - Carbon capture extent (%)
- Outputs (4-dimensional vector $y = (y_1, y_2, y_3, y_4)^T$)
  - Capital cost (k £/MWe)
  - Non-fuel operating cost (k £/MWhe)
  - Generation efficiency (%)
  - CO_2 emissions (kg CO_2/MWhe)

Six data sets were generated by perturbing the inputs (1 base study and 5 delta studies). These were then passed through the MoDS parameter estimation algorithm developed at CMCL Innovations.

The summary of the data sets and results are included in Appendix 2. The combination of a spreadsheet model for pyrolysis based on biomass gasification data and a flowsheeting model based on a variety of publications was used to run the cases 1-6.

The process details are as described in the WP2 report and will not be reproduced here; however, the process flow diagram is in Figure 3 below.

The key data sources for detailed model building were:

i. Excel spreadsheet based calculations were used to predict the component distributions in various pyrolysis products [Peijun, J.; Feng, W.; Chen, B., Production of ultrapure hydrogen from biomass gasification with air. Chemical Engineering Science, 2009, 64, 582–592]; these were used as input to a flowsheet gasification Gibbs reactor model.

ii. The process flowsheet configurations, e.g. heat and water recovery strategy and utility network design, and operating conditions are based on these papers: Sadhukhan J, Ng KS, Shah N, Simons HJ. (2009) 'Heat Integration Strategy for Economic Production of Combined Heat and Power from Biomass Waste'. ENERGY FUELS, 23, pp. 5106-5120. Sadhukhan J, Zhao YR, Shah N, Brandon NP. (2010) 'Performance analysis of integrated biomass gasification fuel cell (BGFC) and biomass gasification combined cycle (BGCC) systems'. CHEMICAL ENGINEERING SCIENCE, 65 (6), pp. 1942-1954.

iii. The solvent consumption in the Selexol process is determined using equilibrium (Henry's Law) analyses, as described by Henni, Tontiwachwuthikul and Chakma, "Solubilities of Carbon Dioxide in Polyethylene Glycol Ethers", 2005, 23, THE CANADIAN JOURNAL OF CHEMICAL ENGINEERING.

iv. The percentages for the total direct capital (TDC) and total indirect capital (TIC) in terms of Inside Battery Limit (ISBL) capital cost were assumed as in the WP2 report and on the work: Ng KS, Sadhukhan J. (2011) Process integration and economic analysis of bio-oil platform for the production of methanol and combined heat and power. BIOMASS BIOENERGY, 35 (3), pp. 1153-1169.

v. The Gas Turbine and Combined Cycle data was extracted from: "The power of Technology, Experience and Innovation by GE", http://www.filter.ee/extensions/filter/brochures/113-27620.pdf (accessed December 2011).

As explained in WP2, the main sources of uncertainty will be in the operational performance of the gasifier; few wood chip gasifiers have been built and operated at this scale, and there is a low level of information in the public domain. This should be an area of future focus for uncertainty reduction.

The actual meta-model delivered to the ETI and associated user information is documented in the next Section.

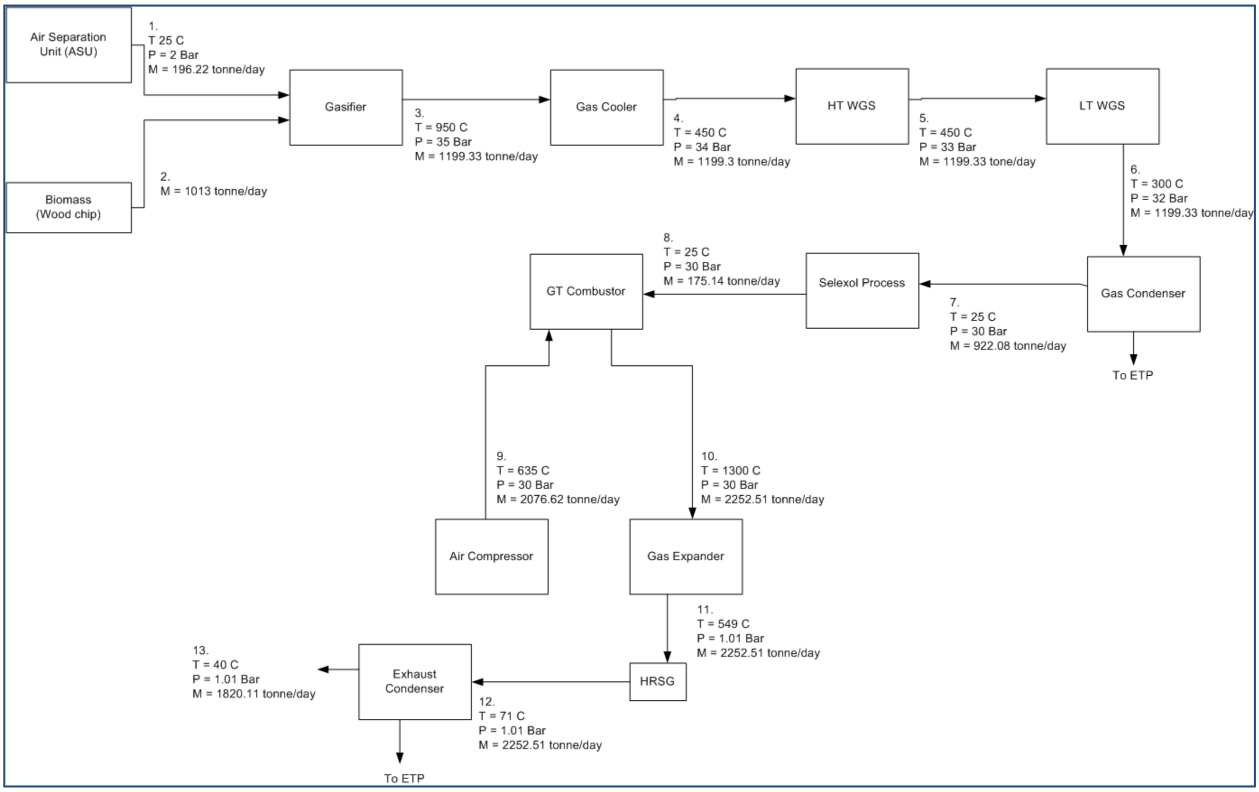

Figure 3. Process flow diagram for BIGCC

4. MODEL OVERVIEW, APPLICATION RANGE AND USER-DOCUMENTATION: CO-FIRED IGCC

A sample model has been developed in Microsoft Excel™. Lastly, we note that in the case of the IGCC technology, the applicable operation ranges of this model are presented in Table 2.

Table 1: Operating range of Co-fired IGCC with CCS (*: of actual capacity)

	Lower bound	Upper bound
Nameplate capacity (MWe)	300	700
Capacity Factor* (%)	60	100
Co-firing extent	0	50
CO2 capture extent (%)	50	98

A screenshot of a sample model for co-fired IGCC case (in the format delivered to the ETI) is shown in **Error! Reference source not found.** 4 with some explanations provided below.

The required user inputs are highlighted in yellow. These are the plant nameplate capacity, its operating capacity and the extent of CO_2 capture. In order to use this model, the user must provide these inputs within the operating ranges specified in Table 2.

The model outputs are highlighted in blue. These are the plant capital cost, the non-fuel operating cost, the plant efficiency and the CO_2 emissions. These inputs and outputs can then be entered into the BVCM technology database and the ESME data sheets

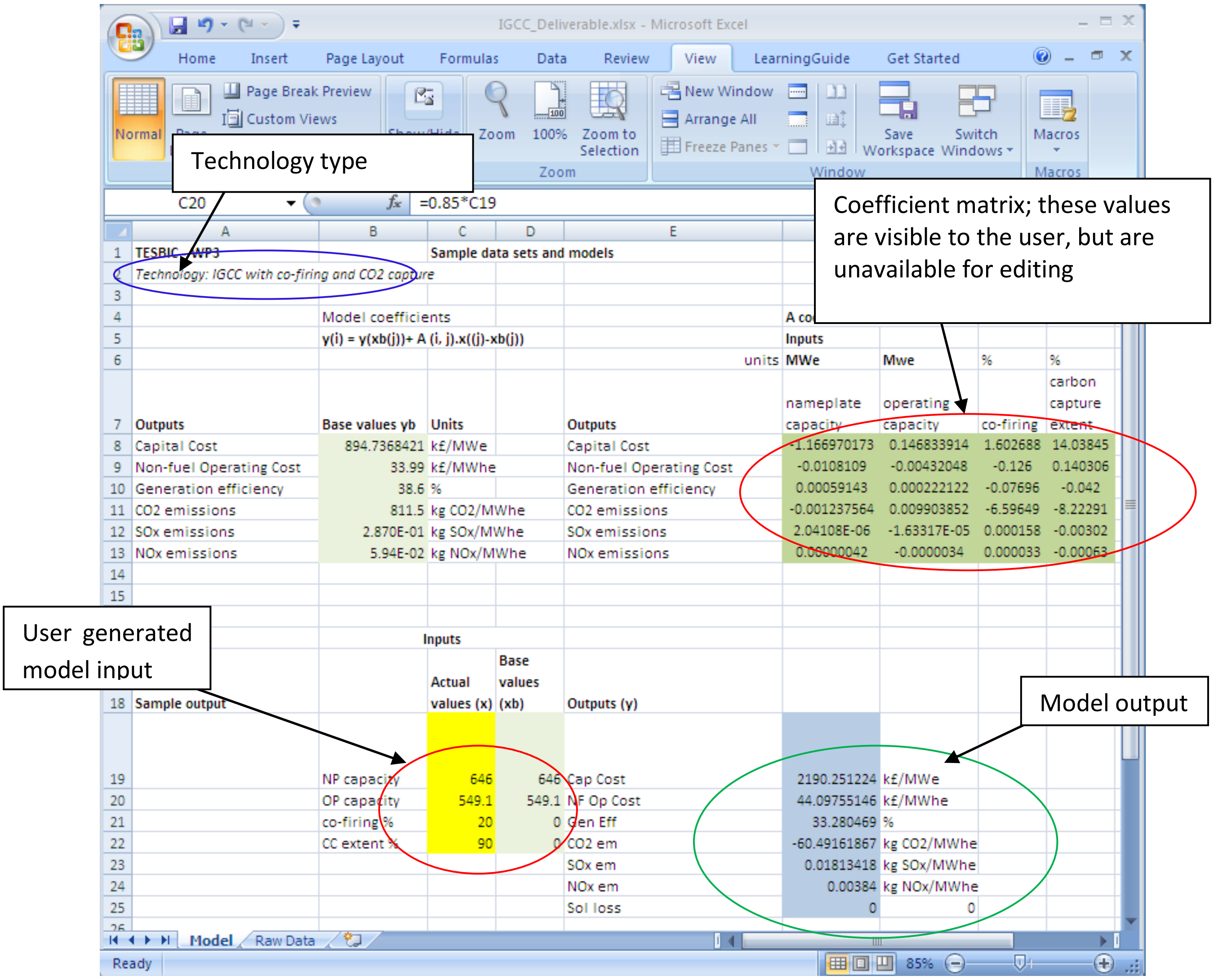

Figure 4: Screenshot of IGCC + co-firing model. Required user inputs are highlighted in yellow, model parameters are highlighted in green and model outputs are highlighted in blue. Only the cells corresponding to user inputs are editable, all other cells are protected

Model Fidelity

In this section, we present an analysis of the fidelity of the proposed IGCC with co-firing model. As can be observed from 5, the proposed model gives a quantitatively reliable description of the data available from WP2. Thus, this model is considered suitable for data generation for the BVCM and ESME teams.

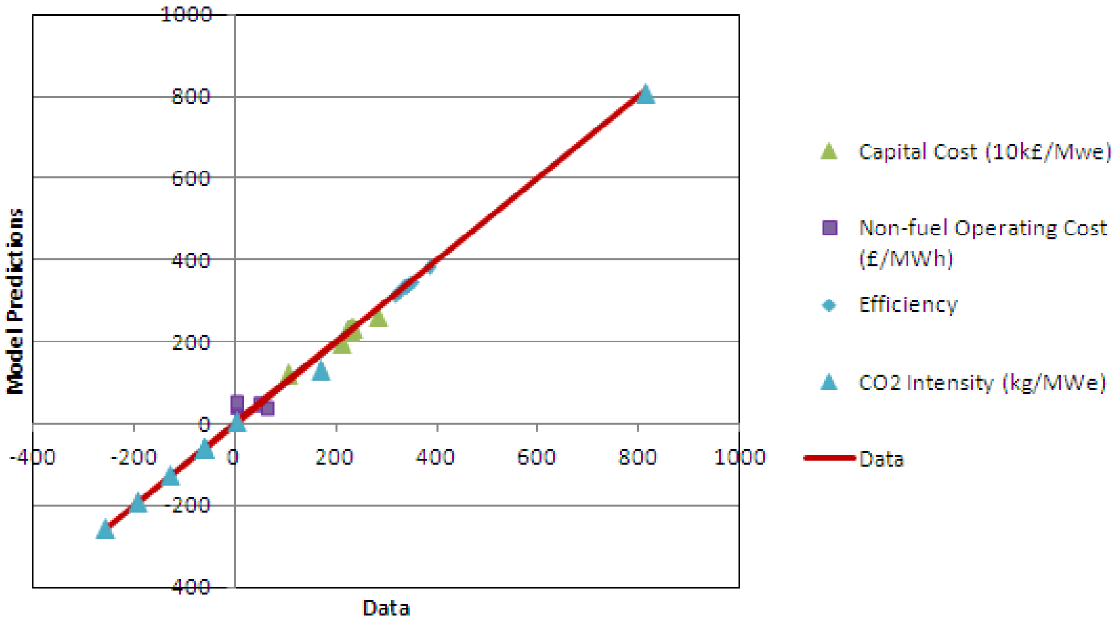

Figure 5: Deviation of IGCC+co-firing model outputs from "experimental data"

5. MODEL OVERVIEW, APPLICATION RANGE AND USER-DOCUMENTATION: BIGCC

A sample model has been developed in Microsoft Excel™.

We note that in the case of the BIGCC technology, the applicable operation ranges of this model are presented in Table 2.

Table 2: Operating range of BIGCC model

	Lower bound	Upper bound
Nameplate capacity (MWe)	20	80
Capacity Factor (%)	60	100
CO2 capture extent (%)	50	95

The models will be delivered to the ETI in this format. A screenshot of a sample model for BIGCC is shown in **Error! Reference source not found.**6 with some explanations.

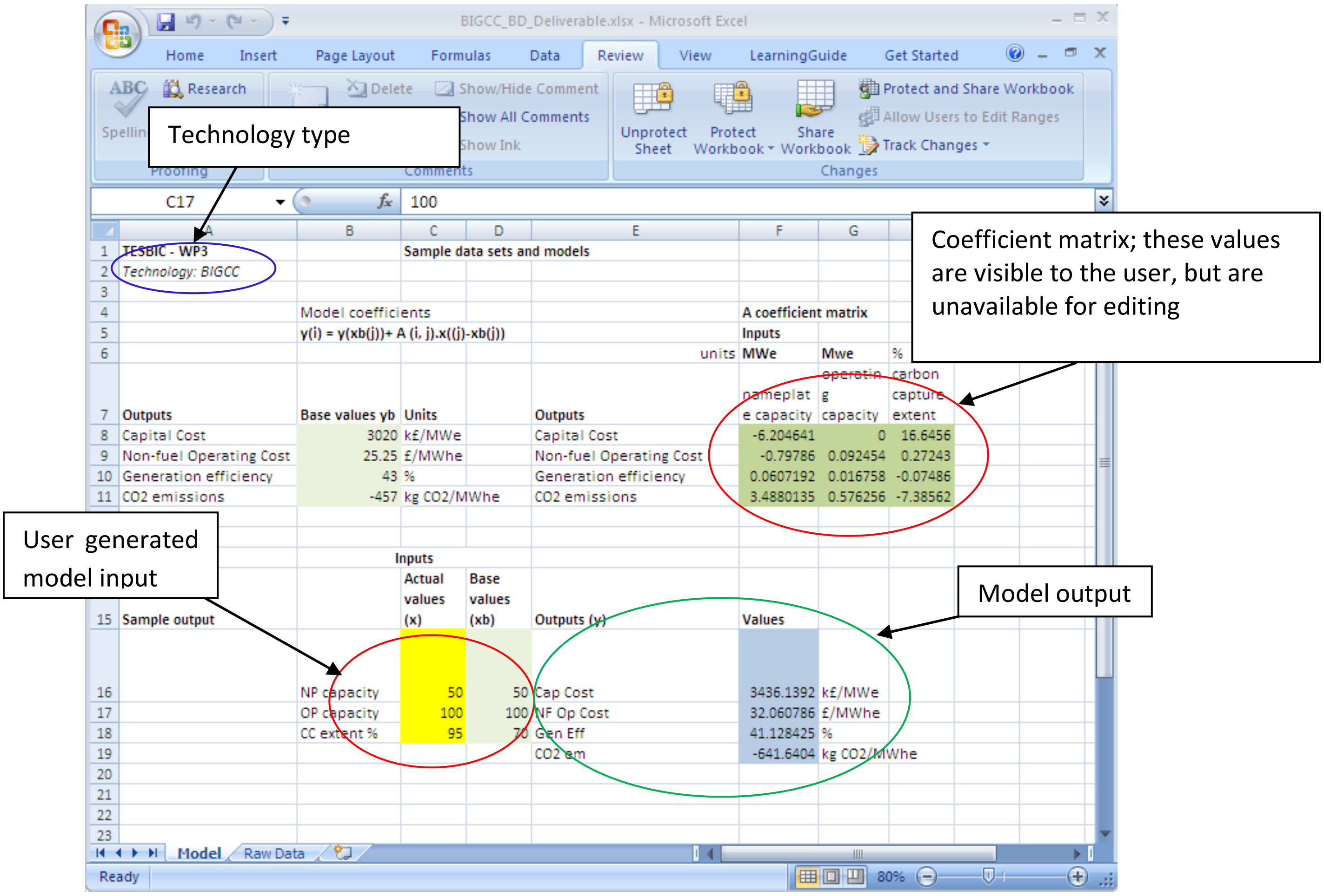

Figure 6: Screenshot of BIGCC model. Required user inputs are highlighted in yellow, model parameters are highlighted in green and model outputs are highlighted in blue. Only the cells corresponding to user inputs are editable, all other cells are protected.

A screen shot of the BIGCC model is presented in Figure6. The model has been implemented in MS Excel ™ and the worksheet has been password protected.

The required user inputs are highlighted in yellow. These are the plant nameplate capacity, its operating capacity and the extent of CO_2 capture. In the case of BIGCC, there is no “co-firing” variable. In order to use this model, the user must provide these inputs within the operating ranges specified in Table 2.

The model outputs are highlighted in blue. These are the plant capital cost, the non-fuel operating cost, the plant efficiency and the CO_2 emissions. These inputs and outputs can then be entered into the BVCM technology database and the ESME data sheets

Model Fidelity

In this section, we present an analysis of the fidelity of the proposed BIGCC model. As can be observed from Figure 7, the proposed model gives a quantitatively reliable description of the data available from WP2. Thus, this model is considered suitable for data generation for the BVCM and ESME teams.

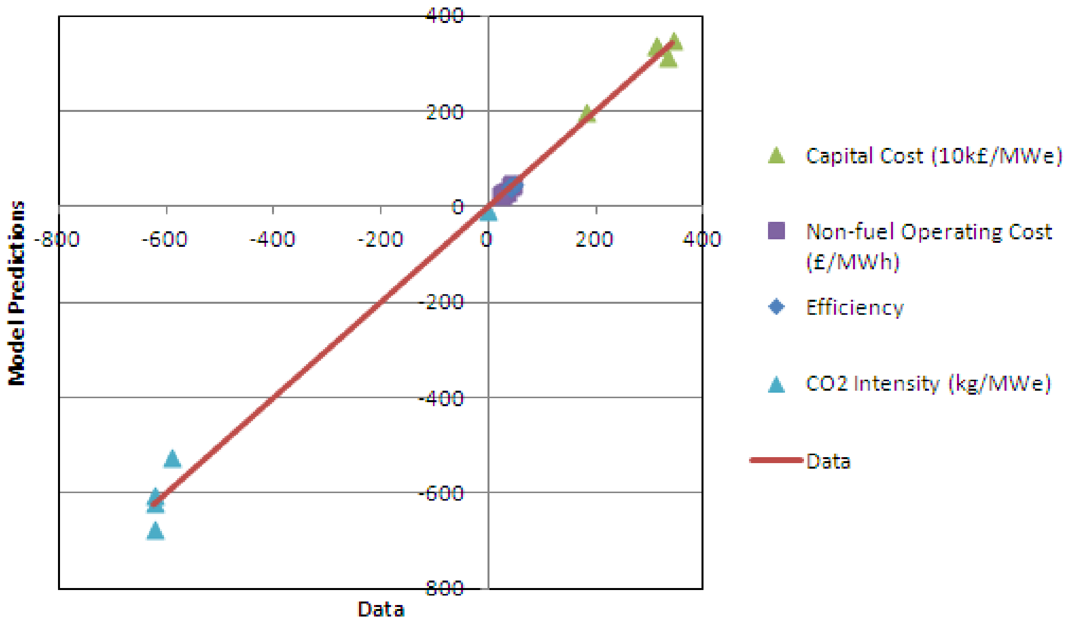

Figure 7; Deviation of BIGCC model outputs from "experimental data"

6. SUMMARY

This document has presented the modelling requirements specification and modelling strategy, as well as associated model parameterisation and user documentation for two out of eight technology combinations within the TESBiC project. Co-fired IGCC with physical absorption-based carbon capture and dedicated biomass/BIGCC with physical absorption-based carbon capture were the two technologies studied here.

APPENDIX 1: SUMMARY OF RAW DATA (DETAILED MODEL OUTPUTS) FOR CO-FIRED IGCC

Case	Data name	Value	Units
1- Base	Nameplate capacity	646	MWe
	Operating capacity	549.1	MWe
	co-firing %	0	%
	CO2 Capture extent %	0	%
	Capital Cost	894.7368421	k£/MWe
	Non-fuel Operating Cost	33.99	£/MWhe
	Generation efficiency	38.6	%
	CO2 emissions	811.5	kg CO2/MWhe
	SOx emissions	0.287	kg SOx/MWhe
	NOx emissions	0.05943	kg NOx/MWhe
2-delta	Nameplate capacity	646	MWe
	Operating capacity	549.1	MWe
	co-firing %	0	%
	CO2 Capture extent %	98	%
	Capital Cost	2191.073171	k£/MWe
	Non-fuel Operating Cost	47.74	£/MWhe
	Generation efficiency	34.58	%
	CO2 emissions	0.05697	kg CO2/MWhe
	SOx emissions	0.00002509	kg SOx/MWhe
	NOx emissions	0.000060886	kg NOx/MWhe
3-delta	Nameplate capacity	646	MWe
	Operating capacity	549.1	MWe
	co-firing %	10	%
	CO2 Capture extent %	98	%
	Capital Cost	2240.485967	k£/MWe
	Non-fuel Operating Cost	46.48	£/MWhe
	Generation efficiency	33.61	%
	CO2 emissions	-64.948727	kg CO2/MWhe
	SOx emissions	4	kg SOx/MWhe
	NOx emissions	0.000061146	kg NOx/MWhe

Case	Data name	Value	Units
1- Base	Nameplate capacity	646	MWe
	Operating capacity	549.1	MWe
	co-firing %	0	%
	CO2 Capture extent %	0	%
	Capital Cost	894.7368421	k£/MWe
	Non-fuel Operating Cost	33.99	£/MWhe
	Generation efficiency	38.6	%
	CO2 emissions	811.5	kg CO2/MWhe
	SOx emissions	0.287	kg SOx/MWhe
	NOx emissions	0.05943	kg NOx/MWhe
2-delta	Nameplate capacity	646	MWe
	Operating capacity	549.1	MWe
	co-firing %	0	%
	CO2 Capture extent %	98	%
	Capital Cost	2191.073171	k£/MWe
	Non-fuel Operating Cost	47.74	£/MWhe
	Generation efficiency	34.58	%
	CO2 emissions	0.05697	kg CO2/MWhe
	SOx emissions	0.00002509	kg SOx/MWhe
	NOx emissions	0.000060886	kg NOx/MWhe
3-delta	Nameplate capacity	646	MWe
	Operating capacity	549.1	MWe
	co-firing %	10	%
	CO2 Capture extent %	98	%
	Capital Cost	2240.485967	k£/MWe
	Non-fuel Operating Cost	46.48	£/MWhe
	Generation efficiency	33.61	%
	CO2 emissions	-64.948727	kg CO2/MWhe
	SOx emissions	4	kg SOx/MWhe
	NOx emissions	0.000061146	kg NOx/MWhe

4-delta	Nameplate capacity	646	MWe
	Operating capacity	549.1	MWe
	co-firing %	20	%
	CO2 Capture extent %	98	%
	Capital Cost	2246.158778	k£/MWe
	Non-fuel Operating Cost	2.334175073	£/MWhe
	Generation efficiency	33.01	%
	CO2 emissions	-129.954424	kg CO2/MWhe
	SOx emissions	0.00002176	kg SOx/MWhe
	NOx emissions	0.000061231	kg NOx/MWhe
5-delta	Nameplate capacity	646	MWe
	Operating capacity	549.1	MWe
	co-firing %	30	%
	CO2 Capture extent %	98	%
	Capital Cost	2291.591296	k£/MWe
	Non-fuel Operating Cost	2.236714378	£/MWhe
	Generation efficiency	32.17	%
	CO2 emissions	-194.960121	kg CO2/MWhe
	SOx emissions	0.00002	kg SOx/MWhe
	NOx emissions	0.000061438	kg NOx/MWhe
6-delta	Nameplate capacity	646	MWe
	Operating capacity	549.1	MWe
	co-firing %	40	%
	CO2 Capture extent %	98	%
	Capital Cost	2334.868096	k£/MWe
	Non-fuel Operating Cost	2.134661668	£/MWhe
	Generation efficiency	31.4	%
	CO2 emissions	-259.965818	kg CO2/MWhe
	SOx emissions	0.00001779	kg SOx/MWhe
	NOx emissions	0.000061642	kg NOx/MWhe

7-delta	Nameplate capacity	646	MWe
	Operating capacity	549.1	MWe
	co-firing %	10	%
	CO2 Capture extent %	75	%
	Capital Cost	2092.285263	k£/MWe
	Non-fuel Operating Cost	2.36793004	£/MWhe
	Generation efficiency	34.92	%
	CO2 emissions	166.3375	kg CO2/MWhe
	SOx emissions	0.00002284	kg SOx/MWhe
	NOx emissions	0.000056963	kg NOx/MWhe
8-delta	Nameplate capacity	646	MWe
	Operating capacity	646	MWe
	co-firing %	10	%
	CO2 Capture extent %	98	%
	Capital Cost	2245.187418	k£/MWe
	Non-fuel Operating Cost	2.434454066	£/MWhe
	Generation efficiency	33.61	%
	CO2 emissions	-64.948727	kg CO2/MWhe
	SOx emissions	0.00002372	kg SOx/MWhe
	NOx emissions	0.000061146	kg NOx/MWhe
9-delta	Nameplate capacity	646	MWe
	Operating capacity	323	MWe
	co-firing %	10	%
	CO2 Capture extent %	98	%
	Capital Cost	2229.515916	k£/MWe
	Non-fuel Operating Cost	2.434373961	£/MWhe
	Generation efficiency	33.61	%
	CO2 emissions	-64.948727	kg CO2/MWhe
	SOx emissions	0.00002372	kg SOx/MWhe
	NOx emissions	0.000061146	kg NOx/MWhe

10-delta	Nameplate capacity	323	MWe
	Operating capacity	274.55	MWe
	co-firing %	10	%
	CO2 Capture extent %	98	%
	Capital Cost	2812.70936	k£/MWe
	Non-fuel Operating Cost	2.445016875	£/MWhe
	Generation efficiency	33.41	%
	CO2 emissions	-64.948727	kg CO2/MWhe
	SOx emissions	0.00002385	kg SOx/MWhe
	NOx emissions	0.000061483	kg NOx/MWhe
11-delta	Nameplate capacity	323	MWe
	Operating capacity	274.55	MWe
	co-firing %	0	%
	CO2 Capture extent %	0	%
	Capital Cost	1041.795666	k£/MWe
	Non-fuel Operating Cost	62.56965944	£/MWhe
	Generation efficiency	38.4	%
	CO2 emissions	811.5	kg CO2/MWhe
	SOx emissions	0.287	kg SOx/MWhe
	NOx emissions	0.05943	kg NOx/MWhe

APPENDIX 2: SUMMARY OF RAW DATA (DETAILED MODEL OUTPUTS) FOR BIGCC CASE

Case	Inputs	Value	Units	Outputs	Value	Units
1	Size	50	Mwe	Cap Cost	3020	k£/MWe
	OpCap	100	%	Op Cost (non fuel)	25.25	£/MWh
	CC extent	70	%	Efficiency	43	%
				CO2 intensity	-457	kgCO2/MWh
2	Size	50	Mwe	Cap Cost	3120	k£/MWe
	OpCap	100	%	Op Cost (non fuel)	35.5	£/MWh
	CC extent	90	%	Efficiency	41	%
				CO2 intensity	-622	kgCO2/MWh
3	Size	30	Mwe	Cap Cost	3333.3333	k£/MWe
	OpCap	100	%	Op Cost (non fuel)	42.5	£/MWh
	CC extent	70	%	Efficiency	41.4	%
				CO2 intensity	-588	kgCO2/MWh
4	Size	30	Mwe	Cap Cost	3433.3333	k£/MWe
	OpCap	100	%	Op Cost (non fuel)	44.583333	£/MWh
	CC extent	90	%	Efficiency	40.7	%
				CO2 intensity	-623	kgCO2/MWh
5	Size	50	Mwe	Cap Cost	3120	k£/MWe
	OpCap	70	%	Op Cost (non fuel)	27.925	£/MWh
	CC extent	90	%	Efficiency	41	%
				CO2 intensity	-622	kgCO2/MWh
6	Size	30	Mwe	Cap Cost	1833.3333	k£/MWe
	OpCap	100	%	Op Cost (non fuel)	22.916667	£/MWh
	CC extent	0	%	Efficiency	47	%
				CO2 intensity	0	kgCO2/MWh