List of the Models in the Availability of the Partner Research Groups and their Main Characteristics

1. Introduction

The goal of the present document is the assessment of the plant modelling resources availability among the SP4 (System Analysis sub-project) partners.

The overall objective of H_2-IGCC project is to provide and demonstrate technical solutions which will allow the use of highly efficient and reliable state-of-the-art gas turbines in the next generation of IGCC plants, suitable for combusting undiluted hydrogen-rich syngas derived from coal gasification and pre-combustion CO_2 capture.

Activities to be carried out within SP4 are aimed at evaluating optimum IGCC plant configurations with special emphasis on the power island system components. Guidelines for an optimised full scale integration and operation of gas turbine will be defined. In particular, the compatibility of the combustion technology with the materials and turbo-machinery requirements will be optimised. To minimise operation and maintenance costs, the integration of enhanced lifetime modelling of components within the overall gas turbine control system will also be taken into consideration.

The above implies the implementation of detailed IGCC-CCS plant simulators. Such simulators have to be capable of evaluating aspects concerning the adoption of new materials and coatings, the introduction of improved combustion techniques and the modifications required to existing component models of apparatus and machinery. To meet design specifications related to various gas compositions, including hydrogen-rich undiluted syngas, commercial machine flow function modifications has to be investigated. In order to assess safe and reliable design, structural aspects concerning major GT parts (shafts, bearings, casing, etc.) will be studied. Required modifications will be carefully evaluated taking technical feasibility and costs into consideration.

Plant simulators suitable to explore the possibilities offered by both present state-of-the-art technologies as well as by the proposed improvements in combustion, materials and turbomachinery design will be developed within this project. Therefore plant components models should have the capability of including data and information related to present and future improved technologies.

According to the project work plan, to establish relationships among modifications of commercially available components and overall plant performance, the resulting plant simulators have to be capable of handling both direct (analysis) and inverse (synthesis) problems. Simulators developed for direct problems will be able to carry out part load analysis and set up the plant operating maps. Simulators for inverse problem will be capable to establish sizes, reality and actual status during operations (health functions and indexes to perform diagnosis and optimum operation planning).

A survey of plant component simulation models available at Roma TRE University, Stavanger University and NUON has been carried out. The aim is to select the partner models in a complementary way to share model modifications and new ad hoc required developments.

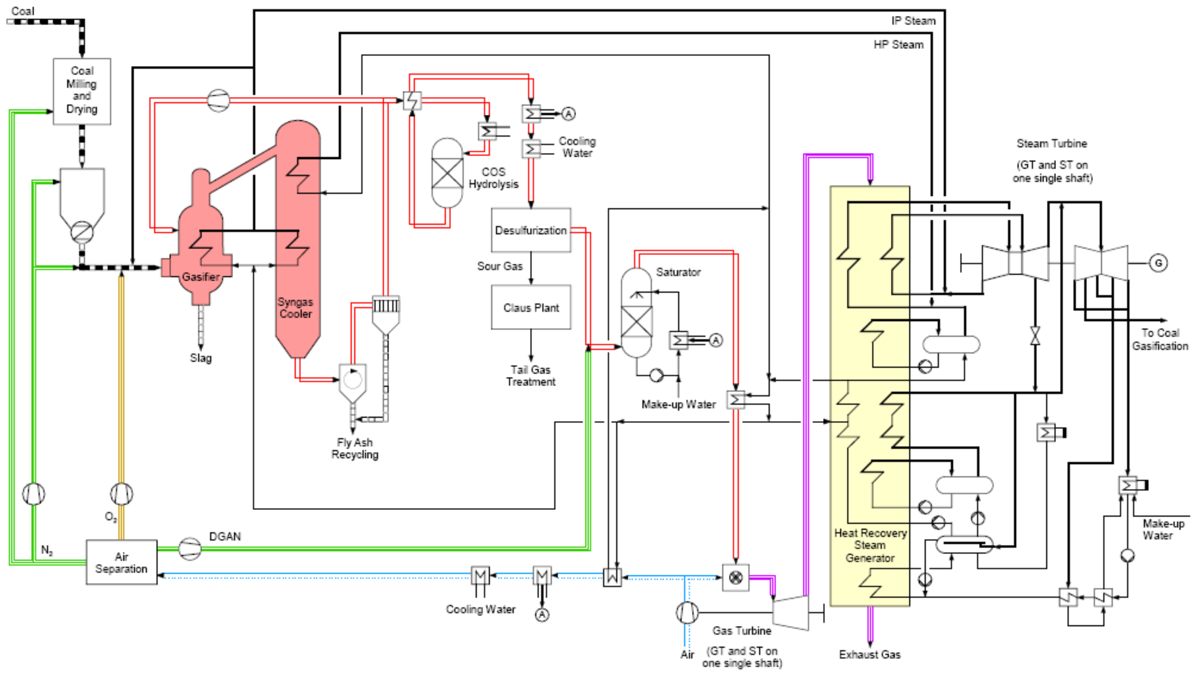

Fig. 1: IGCC Plant schematic layout

2. Component models required to simulate IGCC Plants

IGCC plants are really complex systems constituted by a high number of components usually characterized by a high level of integration.

As an example of a typical IGCC plant in Fig. 1 is given the schematic layout of the Buggenum plant. Three main plant sections can be identified:

- Gasification Island: constituted by the gasifier, the Air Separation Unit (ASU), feedstock treatment apparatuses (mills, driers, dust separators, etc.), process compressors for air, O_2, N_2;

- Syngas Processing Section: which may include syngas coolers (radiative, convective, water or chemical quench), particulate removal devices, sulphur and other contaminants (Nitrogen compounds, Halogen compounds, metals, etc.) removal sections, CO_2 removal apparatuses (shift reactors, CO_2 separation units);

- Power Island: usually arranged as a gas-steam Combined Cycle Unit (CCU).

System modelling to be carried out in SP4 will include all these main sections. As stated in the previous chapter, H_2-IGCC activities are focused on the Power Island. Therefore the Gasification Island and the Syngas Process Section will be treated with a level of detail sufficient to provide with a satisfactory level of accuracy the quantities entering through the Power Island boundary and to allow the assessment of the overall plant performance.

According to H_2-IGCC documents (Proposal for overall project boundary conditions [1], H_2-IGCC baseline conditions [2], H_2-IGCC parameters database [3]) different options will be taken into consideration concerning coal feedstock, gasification technologies, Gas Turbine size and features, etc. Consequently an appropriate library of plant component models is required.

The main component models required to simulate IGCC plants with CO_2 sequestration option are listed below.

Gasification Island

- Process compressors (for air, NO_2, O_2)
- Air Separation Unit (cryogenic)
- Coal drying system (including drier, blower filter etc.)
- Coal mill
- Dust separator
- Gasifier (accounting for different technologies)

Syngas Processing Section

- Syngas cooler (radiative, convective, water quench, gas quench)
- Shift reactor

- Dry and wet particulate removal apparatuses (candle filter, cyclone, scrubber,etc.)
- Syngas saturator
- Heat transfer devices for heat recovery
- CO_2 separation unit apparatuses
- Sulphur recovery unit apparatuses
- Syngas compressor

Power Island

- Gas Turbine (compressor, combustion chamber, expander, balance of the plant components)
- Heat Recovery Steam Generator (economiser, evaporator, superheater, steam drum, deareator, attemperator, HRSG inlet duct, stack, afterburner, feedwater treatment system)
- Steam Turbine
- Feedwater and condensate pumps
- Heat Exchanger devices (condenser, regenerative preheaters)
- Cooling Tower
- Electric generator
- Fan

Other

- Valves
- Pipes
- Fluid lines connecting elements (manifold, junction, etc.)
- Storage vessels (for water, syngas, other process fluids)
- Electric motors
- Pumps, fans and compressors.

3. IGCC plant component models presently available

In the following the list of component models in the availability of SP4 partners is given. Main features of component models are reported.

3.1. Component Models available at ROMA TRE University

The plant physical model is built by adopting a modular approach. Each module represents a plant component or sub-component being characterized by one or more phenomena to perform a defined job.

An equality constraint recursive quadratic programming technique is adopted to achieve a simultaneous optimised solution of the plant model. The method has been described in detail [4] and already applied to solve several problems [5-13]

Models developed at ROMA TRE University can perform the following tasks:

- <u>Cycle thermodynamic analysis and optimisation.</u>

Models treat the component as a black box establishing the conservation equations (mass, energy, momentum and entropy). Work (produced or absorbed) and heat transferred between fluid streams are evaluated accordingly. The behaviour of the component is specified by assigning global performance indexes (such as efficiency, effectiveness, etc.), temperature approaches between fluid streams evolving in the component, suitable functions accounting for losses, and so on. The above quantities or functions are preliminarily assumed according to the state of the art. They have to be verified in the following component selection and sizing phases.

- <u>Component sizing.</u>

On the basis of cycle calculation results, plant components will be sized or selected among those available on the market. The models establish architectures, sizes, geometrical and other quantities related to the plant components. Models include databases (DBs) containing shapes, architectures and related correlations (for example profile cascade features and related losses and deviations, finned tube bundles features and related heat transfer coefficients). Such DBs are adopted to select arrangements on the basis of manufacturer information or default choices. Moreover boundary conditions as well as surface qualities and geometric data are required to set up the model.

Since manufacturers do not furnish all the geometric and architectural quantities part of them are unknown variables. The identification of such unknowns is performed by solving a first level inverse problem where component performance quantities are constraints. Such an inverse problem leads to a “slack” solution due to the fact that the above DBs do not necessarily fit exactly the real machine details. This means that imperfect similarity exists between elements of the real machine or apparatus and the DB shapes and correlations. As a consequence, the characteristic curves of the component fit only one or few points while no agreement exists in the remaining range of operations. Therefore once the plant component has been sized, in order to adapt the DB correlations a vector of Reality Functions (RFs) is included in the model. RFs are introduced to adapt models to the reality of machines and apparatuses. RF coefficients are calculated by solving a minimization problem whose objective function is a RMSE, errors representing differences between measured and calculated quantities. The former can be obtained by carrying out “ad hoc” campaigns or at least collected at acceptance tests. After the sizing is performed and the RFs are determined, the model is capable of replicating N&C behavior of a specific real component.

- Models for part load analysis.

Once components and machinery have been sized (or selected) and their maps have been setup a matching analysis will be carried out to check how above components run together and to calculate plant performance at the design point.

To ensure safe plant operations and to establish control policies minimizing fuel consumption and emissions the part load plant behaviour has to be investigated.

A relevant issue of component modeling is related to the fact that during plant operations component features are continuously changing because of the variation of shapes, surface qualities, dimensions and so on. Such variations are usually connected with phenomena like fouling, erosion, wear etc. This means that going on with operations instant by instant different machines and apparatuses exist. Accordingly characteristic curves of components and performance maps are continuously changing, thus they need to be continuously re-established inside the model if an accurate plant operation management is to be accomplished.

To take the above into account component models contain polynomial Actuality Functions (AFs) which adapt N&C real component models to the continuously changing actual component behaviours. Such functions are established to modify component performance in terms of work transfer or heat transfer, dissipative phenomena and effective flow functions. AFs are evaluated by solving an inverse problem on the basis of actual data collected by the plant monitoring system. Alternatively AFs trends can be given to simulate plant performance deterioration along the time.

RO3 models are in-house developed and included in computer codes written in FORTRAN language, COSMO (Cogeneration Steady State MOdel) for cycle thermodynamic analysis and optimization and CGSPO (Combined Gas-Steam Plant Optimization) for plant sizing and part load analysis. Any required modification or improvement can be easily included in the component model without changing its structure.

In the following existing main plant component models for thermodynamic analysis, sizing and part load analysis available at ROMA TRE for IGCC plants simulations are listed and briefly described. Circuital elements required to connect among them plant components such as mechanical shafts, pipes, junctions, valves, etc. are available but not reported in the list.

GAS TURBINE

- **Weather Hood**
  The model performs preliminary calculations aimed at establishing design quantities for GT weather hood and simulates the part load behaviour relating pressure losses with the actual air mass flow.

- **Air Filter**
  The model carries out preliminary calculations to establish design quantities for filters placed inside the GT inlet duct. Part load behaviour is modelled by relating pressure losses and filtration efficiency to the actual air mass flow.

- **Evaporative Cooler**
  Models carry out preliminary calculations aimed at defining reference design quantities (pressure loss and efficiency) and simulate the part load behaviour giving exit pressure, temperature and relative humidity.

- **Coil**
  The model is based on efficiency-Number of Transfer Unit (ε-NTU) approach. The heat transfer surface and pressure loss are evaluated on the basis of design requirements by using databases containing manufacturers' data. The model can be used to arrange anti-icing systems and non adiabatic inlet air cooling systems fed by an external chiller.

- **Compressor**
  The model performs a row-by-row compressor sizing. It accounts for VIGV, OGV and air extractions for gas expander cooling and other purposes. Various

options have been introduced in relation to data available from manufacturers (inlet mass flow, speed, pressure ratio, efficiency, number of stage, through flow section shape and dimensions, stage loading, blade profile features, etc.). The sizing section produces data files directly readable by the compressor part-load model. It evaluates thermodynamic and fluid dynamic quantities at the exit of each row (which is the entrance to the next row) by applying energy, continuity, momentum conservation equations and empirical correlations for losses, deflection and flow deviation suitably modified by introducing reality functions. The overall machine part load performance is calculated by stacking the contribution of the various rows.

- **Combustion Chamber**
  The sizing section reads the reference data corresponding to turbo-gas combustion chamber and performs calculations aimed at establishing global design quantities required for off design analysis. The part load model applies energy, mass and momentum conservation to give exit temperature, composition and pressure. Chemical reactions are assumed to be at equilibrium. The model accounts for water or steam injection for NO_x reduction or power augmentation. Efficiency, emissions and pressure losses are evaluated by using empirical correlations to be selected according to the kind of combustion chamber to be simulated.

- **Expander**
  A row-by-row formulation has been adapted to model gas expanders. Thermodynamic and fluid dynamic quantities at the exit of each row are evaluated by applying energy, continuity, momentum conservation equations. Empirical correlations are introduced for losses and flow deviations. The overall machine performance is calculated by stacking the contribution of the various rows. Different sizing options are offered in order to utilise all data available from manufacturers. Aspects related to blade cooling and to variable setting stator vanes are taken into consideration. Blade cooling is modelled by using suitable relationships giving cooling effectiveness as a function of cooling mass flow ratio at design point. Ducts connecting the coolant extraction points to the delivery points are modelled by introducing equivalent orifice openings. Actual coolant mass flows are evaluated as a function of the above equivalent orifice openings and pressure drops between extraction points (along the compressor path or at compressor exit) and delivery points in correspondence at each cooled row. Mixing between hot gas and coolant is assumed to take place at row exit.

- **Ducts connecting GT components**
  The model relates the inlet and outlet flow quantities (pressure, temperature, velocity) to the duct geometry. The model is used to simulate compressor exit diffuser, transition piece between combustion chamber and expander and turbine exhaust diffuser.

STEAM GENERATION

- **Steam generator 1 (fired)**
  The model simulate an industrial multi-fuel boiler. It evaluates the thermal load related with each fuel supplied, the overall thermal load, the electric power consumption, the combustion efficiency and its correction with respect to fouling. Performance curve of the N&C components are stored into a database included in the model.

- **Steam generator 2 (fired)**
  Another approach allows the modelling of a steam generator by assembling the elemental component modules: combustion chamber, radiative SH bundles, convective SH bundles, economizer bundles, air preheater, fans. The routine connects and groups thermal powers exchanged by each elemental component, calculates the overall loss, evaluates efficiency and impose the steam generator operational constraints.

- **Heat Recovery Steam Generator (HRSG)**
  The HRSG model is obtained by assembling the elemental component modules: economizers, vaporizers, superheaters bundles, drums, circulation pumps and so on. Models of tube bundles are based on ε-NTU approach. Features of finned and bare tube bundles architectures are stored in databases included in the model. The routine connects and groups thermal powers exchanged by each elemental component, calculates the overall loss, evaluates efficiency and impose the steam generator operational constraints.

STEAM POWER PLANT

- **Steam Turbine (1)**
  The model is capable to carry out computations for back pressure or condensing industrial steam turbines with steam extractions. Willan curves connecting steam consumption, power production and steam extraction are available in a database imbedded in the model.

- **Steam Turbine (2)**
  The module evaluates the expansion of a constant steam mass flow through a group of turbine stages. The model is based on a modified Stodola ellipse approach. Two regulation options are available: partial admission and throttling. The model uses generalised efficiency curves.

- **Partial admission regulation stage**
  The module evaluate the expansion of a steam mass flow through a partial admission regulation stage. The model accounts for throttled flows through partially close admission sectors. Stage efficiency is evaluated as a function of expansion ratio and of the number of admission sectors fully and partially opened.

- **Steam/water surface heat exchangers**
  The model can be used to simulate feed water pre-heaters and condensers. To accounts for phase changes of the fluid on one side or on both sides the model is a multi-zone one (i.e. De-superheating, condensing, and sub-cooling sections). The extension of each zone represents a fraction (fixed or variable depending on the architecture of the heat exchanger under consideration) of the overall heat transfer surface. Each zone is modelled by using ε-NTU (effectiveness - Number of Transfer Units) approach.

- **Deareator**
  The model equations express mass and energy conservation. Constraints are provided in the model so that the liquid temperature is in the equilibrium with the pressure.

- **Storage Vessel**
  The model simulates atmospheric as well as pressurized tanks.

- **Pump**
  The model simulates constant as well as variable speed pumps. The model simulates the part load behaviour by using characteristics curves (head and efficiency versus volumetric flow at different speeds). Reference generalized characteristic curves are stored in the model database and are selected according to design quantities.

- **Attemperator**
  This subroutine simulates a pressure reduction valve with an attemperator.

GASIFICATION ISLAND

- **Gassifier**
  A two-stage equilibrium model has been developed for entrained flow gasifiers. Solid–gas reactions and gas-phase reactions are separated and considered at equilibrium. The model allows the evaluation of the effects of the temperature, O2 to coal ratio, water to coal ration on carbon conversion, syngas composition and heating value.

- **Process compressors, fans and pumps**
  Models perform preliminary calculations to establish design quantities. Part load behaviour is simulated by using characteristics curves (head and efficiency versus volumetric flow at different speeds). Reference generalized characteristic curves are stored in the model database.

SYNGAS PROCESSING UNIT

- **Heat Exchanger**
  Models for heat transfer devices based on ε-NTU approach required to simulate heat transfer processes between fluid streams in syngas process unit are available.

3.2. Component Models available at University of Stavanger

Component models available at University of Stavanger are developed and implemented into the commercial software IPSEpro.

Models presently available allow steady state simulations of the following plant components.

GAS TURBINE

- Compressor
- Inlet duct
- Intercooler
- Inter Cooler Return Duct
- Compressor Exit Diffuser
- Combustor
- Expander
- Turbine Inlet duct

- Turbine Exhaust Diffuser
- Connecting Shaft
- Recuperator
- After cooler
- Humidifier
- Supplementary firing
- Heat Exchanger interconnection ducts
- Exhaust gas condenser

STEAM GENERATION (HRSG)

The Heat recovery steam generator models

- Superheater
- Evaporator
- Economiser
- Stack
- Drum

STEAM POWER PLANT

- Steam Turbine
- Steam Condenser
- Dearator
- Feedwater pump
- Cooling tower
- Condenser

GASIFICATION ISLAND

- Gasifier (based on chemical equilibrium)
- Fuel Drier
- Steam Reformer
- CO_2 Scrubber
- Gas Cleaning Line

3.3. Component Models available at NUON

Libraries of plant component models included in various commercial computer codes are available at NUON.

Apart from commercial computer code other code is also used, in particular *Enssim* software. Some of the characteristics of *Enssim* can be found below.

Enssim is a software package designed to study energy systems or chemical process systems related to energy production or production of fuels. Examples of systems analysed using *Enssim* include**:**

- Conventional CCU and pulverised coal power stations;
- Quite a number of total IGCC schemes (from coal milling system up to machine condenser of the CCU part);
- Cryogenic CO2 capture;
- CO-shift and Methanation units;
- Heat pump systems.

Contrary to all other software packages described in this report, *Enssim* is not a stand-alone application but rather a comprehensive thermodynamic and flowsheeting tool running under Delphi as the 4th generation programming language. Advantages of Delphi compared to other programming languages include:

- Extreme speed of compilation, which is a boost for programming productivity;
- The possibility to write very neat and very readable code which is important when the code must be transferred to other people.

A user of *Enssim* simply programs his flowsheet in a so-called Delphi-unit in a way that resembles Matlab programming. Although *Enssim* has been programmed fully object-oriented, simple standard Pascal (Delphi) will suffice for standard use of *Enssim* and no knowledge of object-oriented programming is required.

Enssim differentiates between design calculation and rating (off-design and part load) calculations. Simple design calculations are written by the user in the Delphi unit representing his or her flowsheet. It is easy to implement iteration loops in the code.

Off-design calculations are done in a totally different way. Here, the flowsheet is seen as a quasi-dynamic system. There is no need to carry out dimensioning calculations to determine mass and thermal inertia for equipment and piping which would be required for a true dynamic simulation program. Mass and thermal inertia are determined at the end of the design phase and will be such that stiffness of the system, leading to oscillations in the calculations, is removed as far as possible. To carry out rating calculations, the user must input (program) PI-controller settings viz.

set point, proportional band and reset time. This simple programming is done in the Delphi flowsheet unit. It is possible to change set points during the course of the calculations using scroll bars. Advantage of this way of calculation is that is user really gets a feel for the behaviour of the system; a disadvantage is that required calculations times are larger than in the case static methods are being used.

Thermodynamic properties are based on:

- IPC-97 steam tables for water/steam;
- Lee-Kesler-Plöcker (LKP) thermodyamics for mixtures of gas compounds;
- Very accurate thermodynamics for a number of coolants (e.g. NH_3, R123a, etc).

Enssim allows for determining dewpoint and bubblepoint of gas mixtures. In case these mixtures do not contain water, two-phase liquid and gas compositions are determined using k-values. In case the mixture contains water, normally only water will condense but the user has the possibility to let *Enssim* determine the dissolution of gaseous compounds in the water like CO_2, NH_3, H_2 etc along with the pH-value of the condensate. In these cases reaction equilibria between acids and bases (weak and strong) are accounted for.

Exergy calculations are possible in *Enssim* by using Exergy functions for the various media types.

In *Enssim*, mixtures can contain condensed (solid or liquid) fuels or ashes. In this case the mixture is called a dirty mixture. The user is not faced with additional programming if he or she wants to calculate with condensed fuels.

Customisation of a given problem is very straightforward because the flowsheet is directly programmed in a neat and efficient programming language that offers all modern programming tools. The object-oriented structure of *Enssim* further eases customisation considerably.

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