Grant Agreement No.: 604656

Project acronym: NanoSim

Project title: A Multiscale Simulation-Based Design Platform for Cost-Effective CO_2 Capture Processes using Nano-Structured Materials (NanoSim)

Funding scheme: Collaborative Project

Thematic Priority: NMP

THEME: [NMP.2013.1.4-1] Development of an integrated multi-scale modelling environment for nanomaterials and systems by design

Starting date of project: 1st of January, 2014

Duration: 48 months

WP N°	Del. N°	Title	Contributors	Version	Lead beneficiary	Nature	Dissemin. level	Delivery date from Annex I	Actual delivery date dd/mm/yyyy
8	D8.1	Optimal usage of the phenomenological models for industrial use	Authors: •Shareq Mohd Nazir •Olav Bolland	1.0	NTNU	R	PU	31/12/2015	31/12/2015

Abstract

The objective of the work carried out under Task 8.1 (as per DOW for Project NanoSim) was to link 1D Phenomenological Model of CLR to the full scale power plant simulations in Thermoflow Suite. Version V.0 of 1D Phenomenological Model was developed using Matlab as a part of work carried out under Work Package 6. The water gas shift process and the CO_2 capture process with chemical absorption was simulated using Aspen Hysys. For CO_2 capture using Selexol process (physical solvent), a simplified model is present in Thermoflow Suite. The combined cycle power plant has been simulated using Thermoflex component of Thermoflow Suite. A systematic methodology has been established to connect the three process models, through the exchange of data between them on MS Excel platform. This helps the entire power generation unit to be simulated under steady state conditions and hence exposing the models for industrial use.

Optimal Usage of the Phenomenological Models for Industrial Use

A gas based combined cycle power plant consists of gas and steam turbines producing electrical work. In the process high amount of fuel is consumed. The idea of Chemical Looping Reforming (CLR) followed by CO_2 Capture is to provide carbon free fuel to the power plant, to reduce greenhouse gas emissions into atmosphere. CLR in itself acts as air separation unit and also converts and reforms Natural Gas. The water gas shift process can produce hydrogen rich fuel post CLR process.

Two of the most important parameters that decide the success of the power generation process is the net electrical efficiency and net power output. These two parameters are heavily dependent on the composition and flowrate of fuel consumed in the gas turbine system. Hence, the upstream processes needs to be tuned to provide the required fuel in gas turbine. Modeling and simulating these process systems will involve parameter interaction at every step in the process as it is shown in Figure 1.

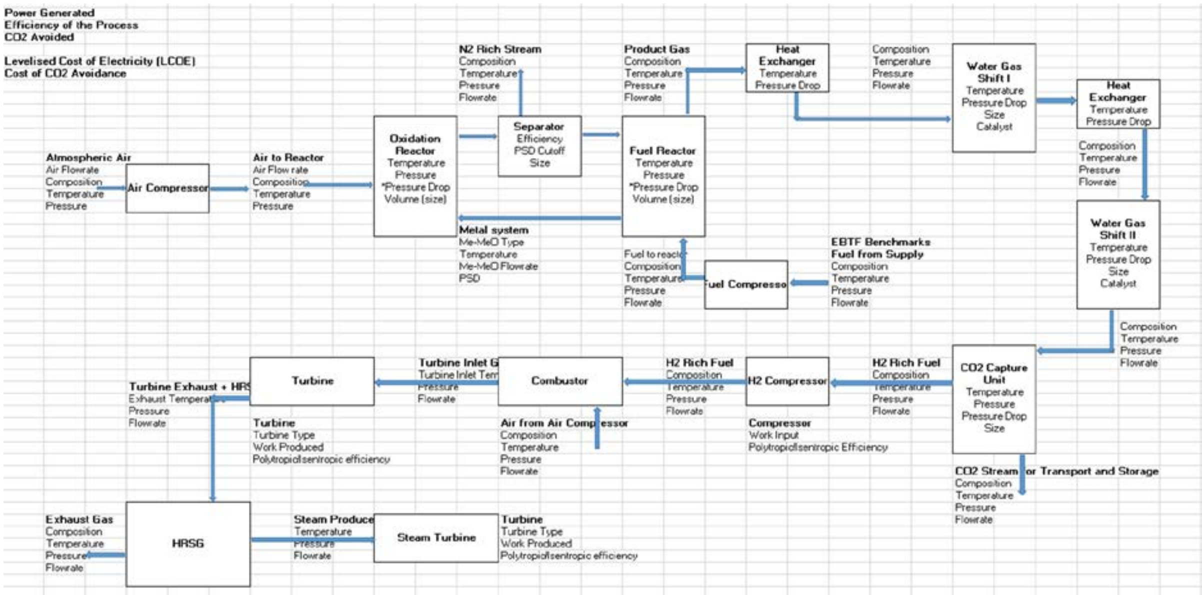

Figure 1: Schematic depicting interaction of parameters between different processes and operations in a combined cycle power generation process

The power plant simulations were carried out using the Thermoflex package in Thermflow suite. Standard available gas and steam turbines models were used as per the guidelines given in the European Benchmarking Taskforce (EBTF) Report. F - class gas turbine system was preferred in this case as the fuel being used is rich in Hydrogen. The amount of fuel consumed in the gas turbine system is estimated from the power plant model in Thermoflex based on the composition of fuel.

The water gas shift process (WGSP) and the CO_2 capture process with chemical absorption was simulated using Aspen Hysys. In case of using physical solvents for CO_2 capture, the simplified model for Selexol process available in the Thermoflex package of Thermfow suite is used. The process model is fine tuned to generate the required flow rate of the Hydrogen rich fuel in the gas turbine system. This way, the flow rate of reformed gas entering the water gas shift process is estimated. The estimated flow rate of the reformed gas acts as an input to the 1D Phenomenological Model of CLR. Flow rates of Natural Gas, Air, circulating metal/metal oxide and the Nitrogen stream is estimated accordingly. The resulting composition of the reformed gas and flow rate is then fed to the WGSP and CO_2 Capture Process in Aspen Hysys. The Aspen Hysys process model then evaluates the composition of Hydrogen rich fuel to be consumed in the gas turbine. Simultaneously, the flow rate and composition of the Nitrogen stream is used in the gas turbine model in Thermoflex. The Nitrogen stream acts as a diluent in the gas turbine system. The process is also highly heat integrated with different process integration options to utilize the heat generated during reforming and water gas shift reaction steps. Finally, the power plant model in Thermoflex is run with the new set of data, and the fuel consumed is again estimated. This new value of fuel consumed is used to estimate the flow rate of reformed gas followed by estimation of flow rates of different streams from the 1D Phenomenological Model. This systematic method of exchanging data between the models converges when the difference in new and previous estimated values of flow rates of fuel consumed in the gas turbine has very low relative error. The linking approach is shown schematically in Figure 2.

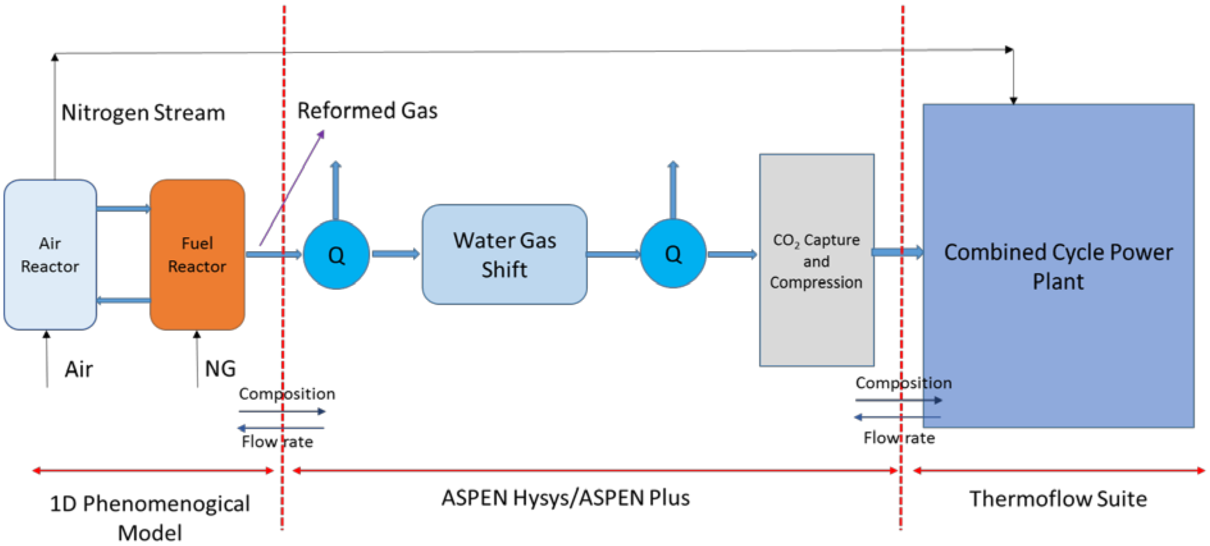

Figure 2: Linking approach for different process models

A test case was run to establish the linking approach between the version V.0 of the 1D Phenomenological Model, the WGSP and CO_2 capture process model in Aspen Hysys, and the power plant model in Thermoflex (Thermoflow suite). This linking approach of different models was used to generate the net electrical efficiencies of the process, by using the CLR model in Aspen Plus, Selexol process and power plant model from Thermoflex. Four different test cases were run. The first case had zero degree of heat integration and all the heat of reforming and shift reactions was transferred to cooling water. The next test case runs were carried out by integrating the heat of reforming and shift reaction to generate low pressure steam, which is then used in steam turbine to generate power. In these three cases, the effect of pressure conditions in the CLR process on the overall efficiency of the process was evaluated. Table 1 shows the results for net electrical efficiencies of the power plant with CLR and compares it with standard Natural Gas Combined Cycle (NGCC) plants with and without CO_2 capture (values for which have been taken from EBTF Report). The future work will involve process integration and optimization.

Cases	1 – CLR No Heat Integration	2 – CLR 20 atm + Heat Integration	3 – CLR 5 atm + Heat Integration	4 – CLR 30 atm + Heat Integration	NGCC with Post Combustion MEA Absorption	Base Case NGCC without CO2 capture*
Net Efficiency (LHV)	45.41	48.15	46.73	48.10	49.9	58.3

Table 1: Comparison of efficiencies of different combined cycle processes