

# Status of ClaRaCCS: Modelling and Simulation of Coal-Fired Power Plants with CO<sub>2</sub> Capture

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## Abstract

Within the DYNCAP project, the Modelica library ClaRaCCS is being developed. This library will provide a framework to model both steam power plants and carbon capture units in an integrated manner. The current status of the library is presented. The structure of the library and the general model design is outlined. Its user-friendly handling as well as its high flexibility in the modelling of individual complex scenarios are demonstrated by the concrete modelling of a furnace. The scenario of a closed steam cycle coupled to a carbon capture cycle based on an amine gas treatment is described and simulation results are briefly discussed.

*Keywords: power plant; Clausius-Rankine cycle; CO<sub>2</sub> capture; CCS; amine gas treatment; transient simulation; library*

## 1 Introduction

The ongoing climate change is a serious ecological and economical challenge in the next decades. The Intergovernmental Panel on Climate Change (IPCC) recommends a reduction of CO<sub>2</sub> emissions to below 80% until 2050 compared to 1990 [1]. Although the proportion of renewable energies is growing significantly, fossil fuels such as coal will remain central to the world's energy supply during the next decades.

It is therefore necessary to evaluate power plant technologies appropriate for a significant reduction of CO<sub>2</sub> emissions in the short term. One already available technological solution is the capture of CO<sub>2</sub> from flue gases of fossil-fuelled power plants and its storage (CCS). This technology has to be embedded into

a future energy mix with a large percentage of renewable and fluctuating energies, such as wind and solar power. Hence, the need for a flexible operation of conventional fossil-fuelled power plants under rapid, large and frequent load changes arises.

The evaluation of such variable operation scenarios requires a thorough investigation of future power plant dynamics. This shall result in recommendations for the design and operation of power plants, that meet certain objectives regarding efficiency, technical limitations and ecological standards. A valuable tool to tackle this challenging task is computer simulation.

As a part of COORETEC [2], an initiative of the German Federal Ministry of Economics and Technology, the project DYNCAP [3] aims at studying the dynamic behaviour of steam-power processes with CO<sub>2</sub> capture in order to provide balancing energy. The project started in March 2011 and will be finished in September 2014. One major outcome of the project is the Modelica library ClaRaCCS (Clausius-Rankine with CO<sub>2</sub> Capture and Storage). The goal of the library is to provide models for the analysis of complex power plants with CO<sub>2</sub> capture in both static and dynamic operation mode. After completion of the DYNCAP project, the library will be freely available under the Modelica license. The current development is performed using Dymola [4], however the final version of the library is intended to work with SimulationX [5] as well.

This paper gives an introduction to ClaRaCCS and presents the current status of development. The paper is organised as follows: Section 2 summarises the technical fundamentals for conventional steam power plants as well as carbon capture processes modelled in the library. In Section 3 general properties of the li-

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brary are introduced: Starting from the general library structure the guiding principles, that underlie the models in ClaRaCCS, are explained. The treatment of media data as well as validation of models will also be outlined. The described properties will then be illustrated by a concrete modelling example in section 4, where the model of a furnace is described. Section 5 demonstrates the current status of ClaRaCCS by giving an example of use: the model of a coal-fired power plant with attached carbon capture unit is presented. The results of a simulation scenario are shown, where throttling of the carbon capture unit is used in order to meet the demand for a short term increase of the generator power output of the plant. Finally, section 6 gives a summary and outlines future steps of development.

## 2 Technical Background

The processes covered in ClaRaCCS are conventional hard-coal-fired power plants and their derivatives for CO<sub>2</sub> capture, the Post-Combustion Capture process (PCC) and the Oxyfuel process (further information in [6]). Lignite-fired power plants and gas-fired combined cycle power plants are not part of the project DYNCAP, but may be included in the future.

Because the model implementation of the Oxyfuel process is still work in progress the respective section will only give a short overview. The section of the PCC process will introduce a little more of this technology because it is part of the simulation example given in section 5.

### 2.1 Conventional Hard-Coal-Fired Power Plants

State-of-the-art conventional hard-coal-fired power plants burn pulverised coal in the steam generator with air. The heat is transferred to a steam cycle that converts it to electric energy. The general simplified process scheme of the power plant is shown in figure 1. Mills pulverise and dry the raw hard-coal. The raw flue gas contains, additionally to nitrogen, CO<sub>2</sub>, oxygen and water, also certain amounts of nitrogen oxides, fly ash (dust) and sulphur oxides. Therefore the flue gas treatment comprises a denitrification system, an electrostatic precipitator and a wet desulphurisation unit.

The steam cycle comprises a super-heater and a re-heater. Power plants currently under construction have a live steam (high pressure) pressure of about 285 bar and a live steam temperature of about 600 °C. The

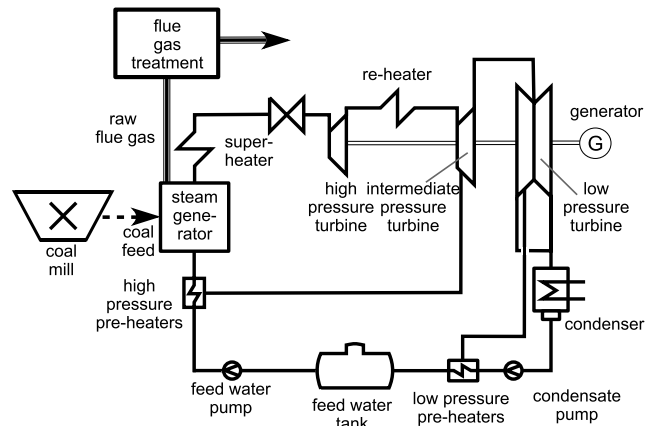


Figure 1: Simplified process scheme of a conventional power plant.

re-heated steam is in the range of 60 bar and 620 °C. Feed water is pre-heated with steam in the low pressure range and the high pressure range. Up to nine feed water pre-heaters are implemented, each with a steam tapping from the turbines or crossover sections. The turbines are all coupled with the same shaft and running at constant speed in normal operation as they are directly coupled with the electric net by the generator.

The overall efficiency of such a power plant is approx. 46 %.

### 2.2 Post-Combustion Capture Process

In a PCC CO<sub>2</sub> is separated from the flue gas of a conventional coal-fired steam power plant by a chemical absorption-desorption process. The reduction of the CO<sub>2</sub> emissions is accompanied by a significant loss in the electrical power output and a related net efficiency penalty of 8-12 %-pts. As reference the solvent Monoethanolamine (MEA) is used with a solvent mass fraction of 30 % MEA and a targeted CO<sub>2</sub> capture rate of 90 %.

Figure 2 shows the schematic PCC process. The flue gas of the boiler passes through the flue gas treatment, where it is cleaned, and then enters the absorber column at the bottom, in which the CO<sub>2</sub> is absorbed by a counter current solution flow. The treated gas is released to the atmosphere, while the rich (CO<sub>2</sub>-loaded) solution leaves the absorber at the bottom. Downstream the absorber, the rich solution is pumped through the rich-lean heat exchanger, heated up and enters the desorber column at the top. In the desorber the absorbed CO<sub>2</sub> is stripped from the rich solution. The required heat duty is provided by a reboiler in which steam from the power plant is condensed. From

the bottom of the desorber, the lean solution is pumped to the entrance of the absorber, passing the rich-lean heat exchanger where it is cooled and pre-heats the rich solution. The captured  $\text{CO}_2$ , nearly pure, is compressed and pumped to the storage. A detailed explanation of the process can be found in [7]. An overview of this process is given in [8].

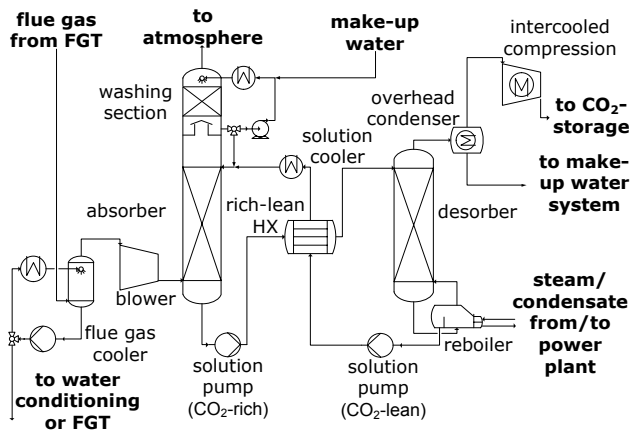


Figure 2: Flow sheet of the PCC process, cf. [7].

The main task of the PCC is the reduction of the  $\text{CO}_2$ -emissions by a certain value. The  $\text{CO}_2$  capture rate depends on the circulated solution flow rate and the working capacity of the solution. Here the working capacity is defined as the difference between  $\text{CO}_2$  loadings behind the absorber and behind the desorber. The solution rate can be influenced by the pump upstream the absorber. The lean loading depends on the reboiler heat duty and thus is directly affected by the steam mass flow which is condensed in the reboiler. The liquid level of the absorber sump is controlled by a pump that conveys the solution to the desorber.

## 2.3 Oxyfuel Process

Conventional coal-fired power plants and power plants with PCC burn the coal with air. On the contrary, in the Oxyfuel process the coal is burnt in an atmosphere of oxygen from an air separation unit mixed with recirculated flue gas. As the nitrogen of the air is avoided in the combustion process, the flue gas contains mainly  $\text{CO}_2$  (70 vol.-%), water and small amounts of oxygen, nitrogen and argon. The flue gas fraction that is not recirculated is treated to remove the impurities in order to receive a  $\text{CO}_2$  stream with a purity higher than 96 %. The overall power plant net efficiency is decreased by approx. 8-10%-points when the Oxyfuel process is applied. This includes the cryogenic air separation unit and the compression of the captured  $\text{CO}_2$  to a pressure

of 110 bar. A detailed overview of the Oxyfuel process can be found in [9].

## 3 The ClaRaCCS Library

### 3.1 Library Structure

Creating a library covering a very broad range of physics that is at the same time well-arranged and user-friendly, demands an elaborate library structure. Figure 3 shows the top level content of the ClaRaCCS library. Beside the usual packages like *UsersGuide*, *Examples* and *Media* the library is structured into the main existing functional groups of the physical processes under consideration. *Components* is the package with the most basic models describing e.g. turbo machines, furnace, heat exchangers or thermal separation. In *SubSystems* these components are used to create more complex models e.g. a boiler or an air separation unit. The package *SubProcesses* then in turn contains models which are built from *SubSystems* models like whole  $\text{CO}_2$  capture cycles. *PowerPlants* consists of models representing whole power plants and is the package with the most complex models.

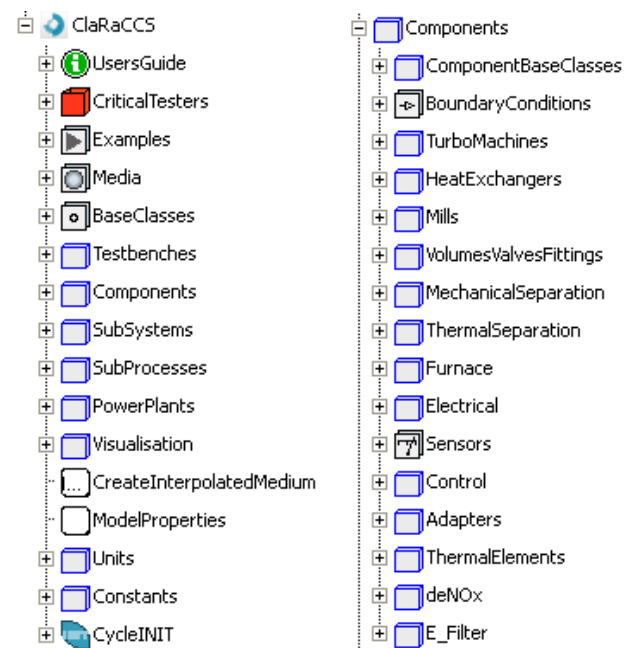


Figure 3: Top level content of the ClaRaCCS library and the central component package.

### 3.2 Model Design Principles

When setting up the model of a complex physical system such as a power plant, the first question to be answered is what physical fidelity is needed to cope with

the given simulation task. The answer to this question refers to the **level of detail** necessary for each component and sub-process. The next step is to define the general **physical effects to be considered** for solving the given task. Finally, the **level of physical insight** into the considered physical aspects must be chosen.

In what follows it will be explained how these three stages guide the model design of the ClaRaCCS library. For illustration the concept will be applied to the well-known example of a fluid flow in a pipe.

### 3.2.1 Level of Detail

In [10] a classification of component models into different levels of detail was developed. It is mainly based on two criteria:

- Purpose of model. In which simulation context will the model be used? What questions and physical effects shall be analysed with the model?
- Applicability of model. What are the main assumptions the model is based on? Are there some structural limitations?

The model design of ClaRaCCS has been inspired by these ideas. Moreover it aims to provide a well balanced combination of readability<sup>1</sup>, modelling flexibility and avoidance of code duplication. Consequently, each component in the ClaRaCCS library is represented by a family of *freely exchangeable* models. Every component family is grouped into **four levels of detail**:

L1. Models are based on characteristic lines and / or transfer functions. This results in an idealised model, which shows physical behaviour. The model definition may be derived either from analytic solutions to the underlying physics or from phenomenological considerations. Applicability is limited to the validity of the simplification process. Non-physical behaviour may occur otherwise.

*Example:* transmission line model for fluid flow in a pipe.

L2. Models are based on balance equations. These equations are spatially averaged over the component. The models show a correct physical behaviour unless the assumptions for the averaging process are violated.

*Example:* single control volume for fluid flow in a pipe.

L3. Models are by construction subdivided into a fixed number of spatial zones. The spatial localisation of these zones is not necessarily fixed and can vary dynamically. For each zone a set of balance equations is used and the model properties (e.g. media data) are averaged zone-wise. The models show a correct physical behaviour unless the assumptions for the zonal subdivision and the averaging process over zones are violated.

*Example:* moving boundary approach for fluid flow in a pipe.

L4. Models can be subdivided into an arbitrary number of spatial zones (control volumes) by the user. They thus provide a true spatial resolution. For each zone a set of balance equations is used which is averaged over that zone. The model shows a correct physical behaviour unless the assumptions for the choice of grid and the averaging process over the control volumes are violated.

*Example:* finite volume approach with spatial discretisation in flow direction for fluid flow in a pipe.

### 3.2.2 Physical Effects to be Considered

Once the decision for a specific detail group of models is made, the set of required physical effects to be covered by a model may still differ according to the simulation goal. For instance, in a pipe model it might be necessary to resolve the spatial flow properties but unnecessary to analyse sound waves in detail. This is reflected in the complexity of the basic physical equations underlying the model.

Notice that, although the ClaRaCCS library is designed for dynamic simulations, it is still possible to include models, where parts of the basic physical equations correspond to the stationary behaviour of a component. Such models are often favourable with respect to computation time and stability. Their use is appropriate whenever certain aspects of the component dynamics can be neglected compared to the system dynamics under consideration. In the pipe example above this would be manifested by the fact that if only fluid flow properties (temperature profile, flow velocities, etc.) are of interest, sound wave propagation can be neglected, as long as the flow velocity is much less than the speed of sound. Consequently a stationary momentum balance for the fluid would be sufficient in this case.

<sup>1</sup>This results in a flat model hierarchy and restricts the use of inheritance.

In order to cope with these different needs, the ClaRaCCS library provides *component models at the same level of detail but covering different physical effects*. They are distinguished by different self-explaining names.

### 3.2.3 Level of Insight

By now, the fundamental equations of a model are defined by setting its level of detail and the physical effects of consideration. However, these equations declare *which* physical effects are considered, but not *how* they are considered. For instance, the pressure loss in a pipe may be modelled using constant nominal values or via correlations taking the flow regime and the fluid states into account. These physical effects are therefore modelled in *replaceable* models that complete the fundamental equations using predefined interfaces, e.g. the friction term in the momentum balance. By separating the governing model definition from the underlying sub-models, the flexibility of the model is enhanced without losing readability.

### 3.3 Media Data

The property data for all models will be provided by medium classes which then in turn call external C-functions. However, up to now only the models of the conventional part of the plant obtain their property data from external functions. The observed advantage of this procedure is the possible access to other commercial external fluid property libraries and a large increase in simulation speed of the models. The implementation of external property data for the multi-component media used in the PCC is still work in progress. The current state of this issue and the experiences with external, table-based media data for single-component media are very encouraging concerning simulation speed and simulation stability.

For the sake of initialisation and numerical stability the choice of different state variables may be of high importance. Depending on the selection of the respective state variables an index reduction can be necessary. Also phase and reaction equilibria can lead to high index systems which have to be reduced symbolically. In both cases it is likely that derivatives of property data are required to perform index reduction. Providing these derivatives still is a challenge to be overcome during this project.

## 3.4 Model Validation

Models in the ClaRaCCS library will be validated against established process modelling and power plant software (Aspen Plus and Epsilon [11, 12]) as well as dynamic measurement data.

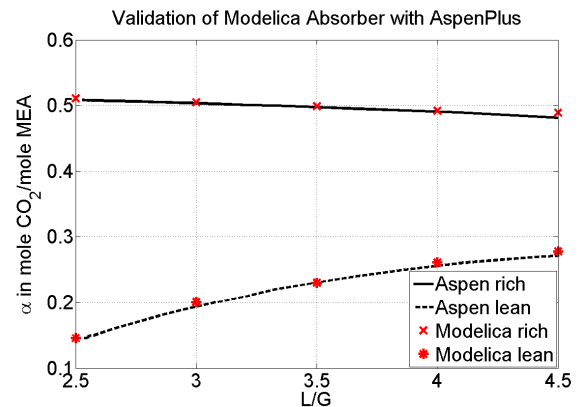


Figure 4: Validation example. Modelica absorber vs. [11]. Lean and rich solution. Here  $\alpha$  denotes the amount of substance  $\text{CO}_2$  per amount of substance solvent (MEA).  $L$  denotes the mass flow rate of the solvent and  $G$  is the flue gas mass flow rate.

For the water steam cycle this measurement data are provided by the coal fired power plant [13] at Rostock, Germany, with a net power output of 500 MW. For the PCC process the data are provided by a pilot plant [14] at Heilbronn, Germany, which has the capacity to clean approximately  $1150 \text{ Nm}^3/\text{h}$  of flue gas.

## 4 Modelling of Furnace

The purpose of this section is the illustration of the general modelling strategy as introduced in section 3. As an example the furnace model package that provides models for burner, flame rooms and hoppers with different levels of detail is considered. Here, predominantly the structure of the package is described without covering the physics inside in more detail.

### 4.1 Connectors

Although parts of ClaRaCCS and Modelica.Fluid cover similar fields of application own connectors for liquids, fluids and gas mixtures are necessary due to the usage of external media as motivated in 3.3. However, models of the Modelica standard library and ClaRaCCS may be connected using simple adapters included in the library. In addition, connectors for

aerosols (unburned coal dust, fly ash) are defined similar to the approach of Gall *et al.* [15]. These connectors instantiate the connectors for the flue gas, the coal and the slag. In contrast to Gall's approach, the fly ash is treated as substance of the flue gas so that there is no need for a fourth connector. The Modelica code of e.g. the CoalSlagFlueGas\_inlet connector reads

```
connector CoalSlagFlueGas_inlet
"Port describing Coal,Slag and FlueGas flow"
import ClaRaCCS;
// Media properties of coal and slag
parameter Media.Coal.PartialCoal coalType;
parameter Media.Coal.PartialSlag slagType;

BaseClasses.Interfaces.FlueGas_a flueGas;
BaseClasses.Interfaces.Coal_inlet
    coal(coalType = coalType);
BaseClasses.Interfaces.Slag_outlet
    slag(slagType = slagType);
end CoalSlagFlueGas_inlet;
```

Likewise, a connector for the coal dust and the primary air is available. In addition, components for splitting and joining are provided so that other components in the flue gas path having solely flue gas connectors (as e.g. a deNO<sub>x</sub> plant) can be connected to a combustion chamber model.

## 4.2 Components in the Furnace Package

### 4.2.1 A Simplified Combustion Chamber Model

Figure 5 shows the tree of the furnace model package. At the top level it provides the model SimpleCombustionChamber which represents a simplified model of detail level 2 (refer to figure 6). It provides physical connectors for the coal dust and primary air, for the slag and flue gas outlet. Based on a stationary stoichiometric combustion calculation, the flue gas composition, the heat  $Q_{\text{combustion}}$  obtained from combustion and the stoichiometric air ratio  $\lambda = \dot{m}_{\text{air}}/\dot{m}_{\text{air,st}}$  are calculated. The model consists of stationary balance equations for the energy, the mass flow, the flue gas components and its composition (i.e. mass balance equations for each single substance considered in the used flue gas mixture). The user can

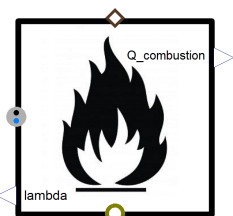


Figure 6: Diagram view of the simplified combustion chamber model.

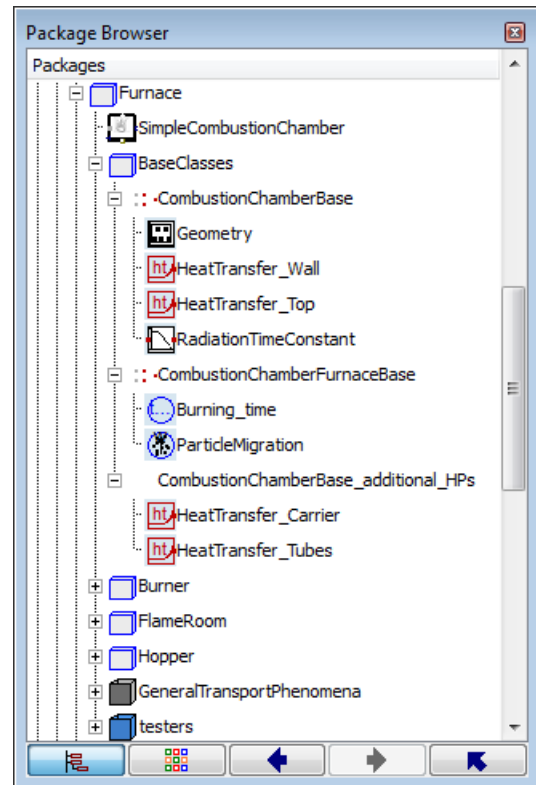


Figure 5: The tree of the furnace model package.

set values for the flue gas outlet temperature, the slag fraction, slag temperature, and the concentration of toxic substances (CO, NO<sub>x</sub> and SO<sub>x</sub>) in the flue gas. Whereas the flue gas and the slag are accessible via physical connectors,  $Q_{\text{combustion}}$  and  $\lambda$  are provided by *real outputs*. These important process variables can then be used as inputs to other models, such as a controller for the air ratio. The model has been compared to Epsilon [12] and has shown good consistency of the results.

### 4.2.2 Components for a Detailed Combustion Chamber Model

Besides the model SimpleCombustionChamber, the furnace package is intended to provide all required components from that a complete –more detailed– combustion chamber model can be built. These components are currently models of detail level 2, i.e. they represent single control volumes for the considered combustion process. Since a complete combustion chamber model will be built from several level of detail 2 models, it yields a spatial discretisation and will thus be a model of detail 3 or 4.

Figure 7 shows the diagram of a burner model which extends the three base models– namely CombustionChamberBase,

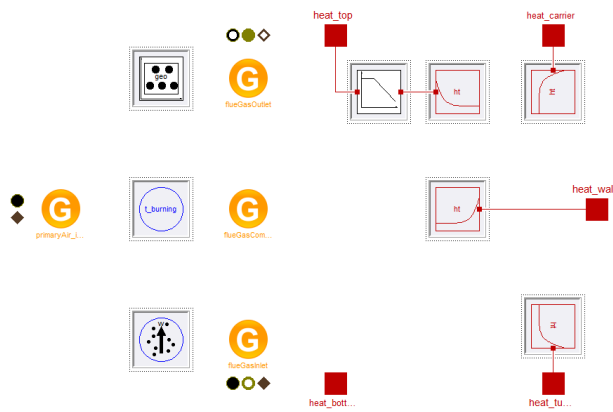


Figure 7: Diagram view of a burner model.

CombustionChamberFurnaceBase and CombustionChamberBase\_additional\_HPs that are provided by the BaseClasses package (see figure 5).

The partial model CombustionChamberBase provides the definition of the used Media, the instance of the corresponding medium objects and physical connectors. A *replaceable model* Geometry allows for an adaptation of the combustion chamber's dimensions to the user's needs. Also basic parameters that are common in all furnace components are defined in this base class whereby the duplication of code is avoided ensuring low maintenance effort.

Regarding the physical effects to be considered, besides the connectors for the gas and solid flow, this base model has three connectors for heat flows. They are required to model the heat transfer from the hot flue gas to the combustion chamber wall and the heat transfer between neighboured flame rooms/burners. The heat flows to the top and to the wall are calculated based on the *replaceable models* HeatTransfer\_Top and HeatTransfer\_Wall (refer to figure 5). Please note that the heat flow at the bottom connector is calculated from the heat transfer model HeatTransfer\_Top in the respective adjacent burner/flame room. In view of a numerical optimisation, the control volume temperature can be decoupled from that of neighboured ones by using differential states for the temperature at a heat port. Such a state with a certain time constant is provided with the *replaceable model* RadiationTimeConstant (see figure 5) and is placed in the burner model shown in figure 7 at the top heat connector. Whereas the CombustionChamberBase represents a basic control volume just describing the flow of the gas and solid phase and the heat transfer, the sec-

ond partial model CombustionChamberFurnaceBase accounts for the furnace process. It is extended by *replaceable models* for the burning time and the particle migration time. The third base model CombustionChamberBase\_additional\_HPs provides two additional heat ports. In this way also the heat flow from the flue gas to e.g. the carrier tubes and the tube bundles of the convective heat exchangers in a boiler model can be modelled. Again, for each heat port replaceable models for the heat transfer correlation are provided.

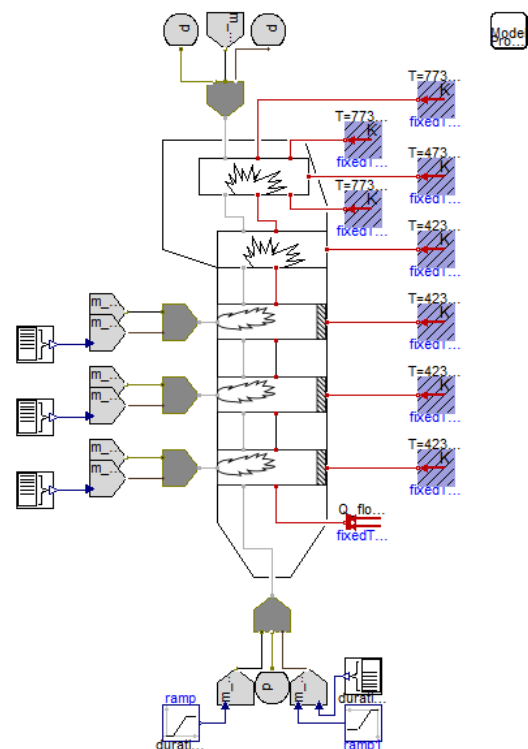


Figure 8: Diagram view of an exemplary combustion chamber model built by the furnace package components described above.

Figure 8 shows the diagram of an exemplary combustion chamber model. In a boiler model the fixed temperature boundaries on the right would be replaced by according water steam tube models.

## 5 Example of Use

The current capabilities of the ClRaCCS library can be illustrated by a model of an anthracite-fired steam power plant with a coupled post combustion capture unit. For the sake of simplicity and due to current library limitations the complex topology of current Rankine cycles is reduced to the main features.

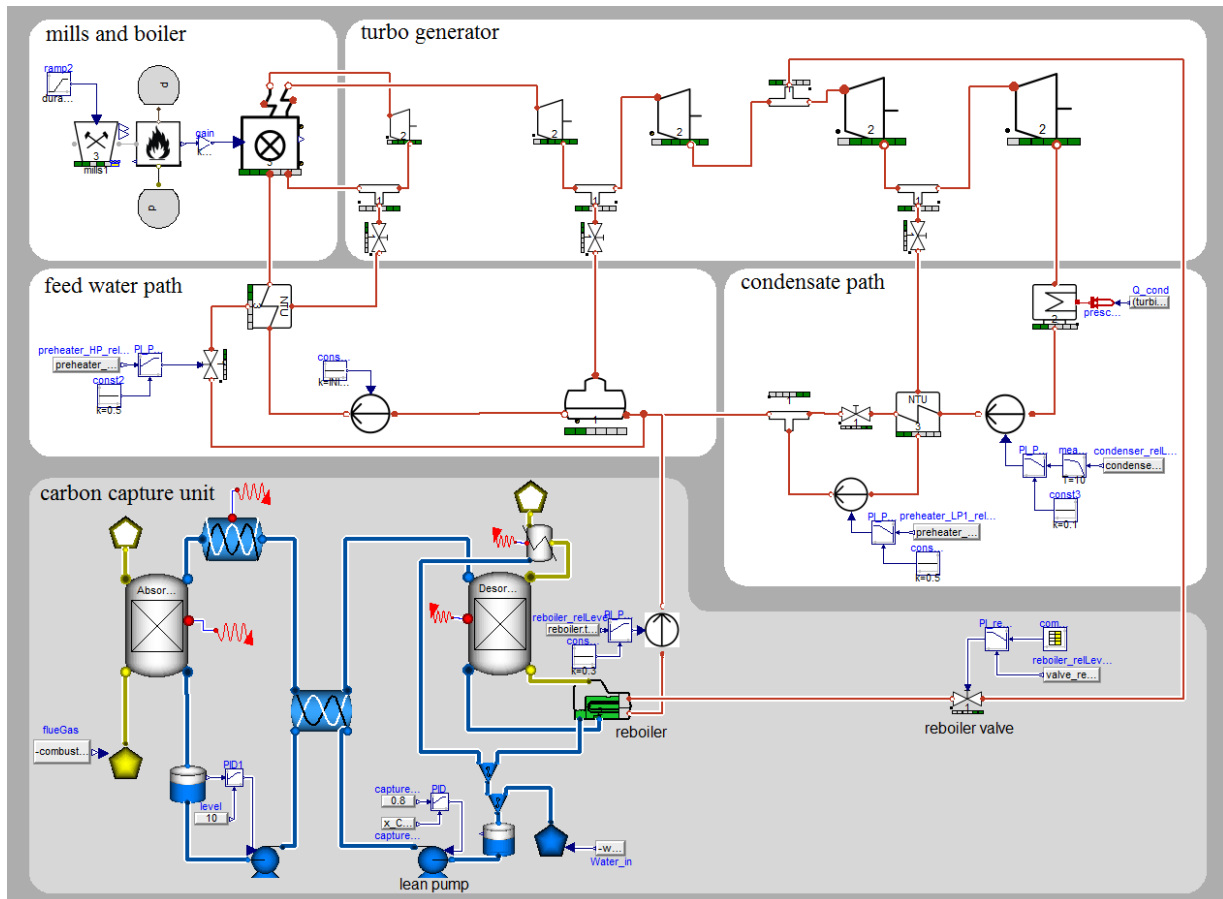


Figure 9: Diagram view of coupled steam plant with carbon capture unit.

## 5.1 Example Description

The model's definition is based on a PCC-retrofit of the existing power plant [13] of Rostock, Germany, see table 1 for its general operation parameters.

Table 1: General overview of power plant of Rostock, Germany

Net output	509 MW
Net efficiency	43.2 %
Live steam pressure	262 bar
Live steam temperature	545 °C
Live steam mass flow	417 kg/s
Re-heat temperature	562 °C
Re-heat pressure	54 bar

In particular, the model features a set of roller bowl mills, as reported in [16], a reduced combustion chamber and boiler, a turbo-generator with tapplings for one high pressure pre-heater, one low pressure pre-heater, the feedwater tank and the reboiler of the PCC. At the low pressure side a condenser, a condensate pump, the pre-heaters, the feedwater tank and the feedwater pump complete the cycle, see figure 9.

The coupling of furnace outlet and PCC inlet at the flue gas path is currently cut because of missing components for the flue gas cleaning.

The PCC features first-principle models for the absorber and desorber columns and simplified models for pumps and the inner heat exchanger, see [17] for a more detailed description on column modelling.

In order to get a pure feed-forward response of the model, only subordinate controllers are implemented in a simple way. Pumps are used to keep the filling levels of the storage devices within reasonable bounds. The generator power output is controlled by the reboiler valve, which sets the amount of steam that is used to supply heat for the reboiler. Additionally the carbon capture rate is controlled by the lean solvent pump downstream the desorber. Future investigations will have to consider an integrated unit control concept for both the steam cycle and the PCC unit, see [18] for a first approach.

Although the degree of simplification is too high to allow quantitative statements on the transient behaviour, the model is capable to capture the main dynamics in a qualitative manner and shows that the dif-



ferent aspects of the library work together as desired.

## 5.2 Simulation Results

The extensive steam tapping for the heating of the reboiler introduces the option to provide primary control power by throttling the reboiler valve. Doing so, the low pressure turbine mass flow rate is increased in short term resulting in a significant power step-up. However, a temporary drop of the carbon capture rate has to be accepted. In figure 10 the power output and the reboiler steam mass flow are displayed indicating that almost full throttling of the valve can lead to a power step of 5 %-pts within 30 s. After holding the primary control power for 5 min, the control band is set free within 10 min.

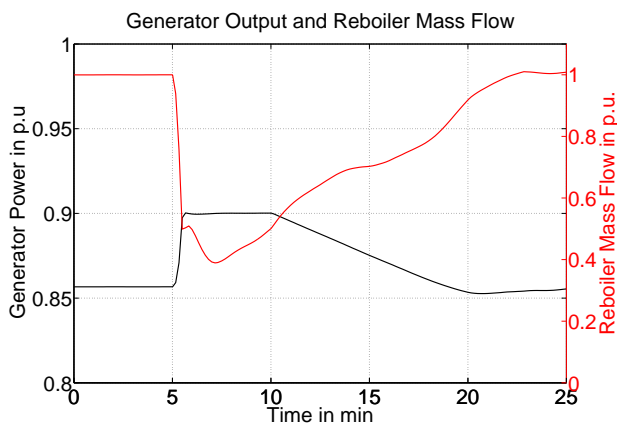


Figure 10: Power output applying reboiler feed reduction.

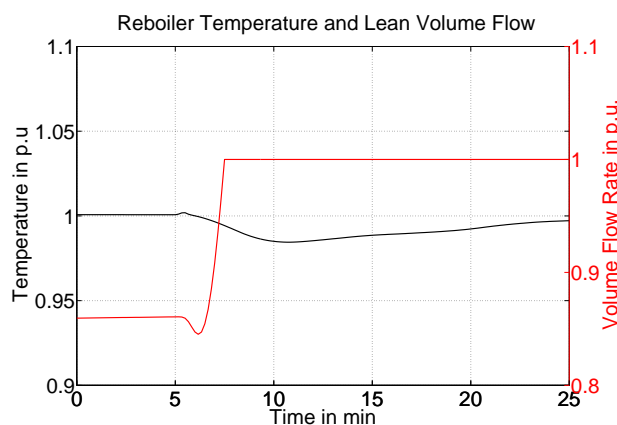


Figure 11: Amine gas treatment characteristic values.

The reboiler temperature in figure 11 shows a moderate drop with a minimum at 10 min of simulation time. Due to the throttling of the valve and the subsequent temperature drop in the reboiler, the lean loading of the solution in the reboiler increases (because less

CO<sub>2</sub> is stripped from the solution). This means that a higher flow rate of solution is needed to maintain the targeted capture rate. Hence, the lean pump volume flow increases in order to compensate the higher loading, until the pump reaches its maximum capacity.

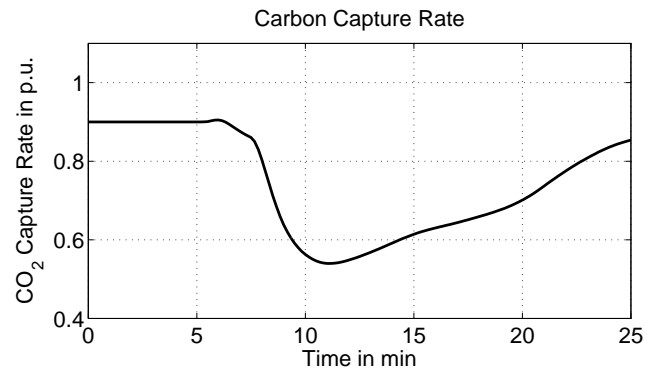


Figure 12: Carbon capture rate during reboiler hold-up.

As expected, the additional power output comes at the cost of a strongly reduced carbon capture rate showing its minimum of 55 % at approx. 11 min simulation time, see figure 12.

Although the simulation scenario might be strongly simplified and the applied control strategy technically not yet mature, it becomes obvious that the application of highly integrated sub-processes like the amine gas-treatment brings up new options for the plant's transient operation mode and economical shifting (trade-off between revenues from primary control power supply and costs due to CO<sub>2</sub> certificates) on the one hand. On the other hand new challenges for the power plant's control system must be tackled.

## 6 Summary and Outlook

In this paper the status of development of the C1aRaCCS library is presented, which is a central part of the DYNCAP project. In its final stage the library will allow detailed dynamic simulations of power plants coupled to a CO<sub>2</sub> capturing process.

It was demonstrated how the flexible library structure supports the user in order to build up complex power plant models individually tailored to specific simulation goals.

Although in an early state of development, the given simulation example proves that the library is already capable of simulating simplified dynamic operation scenarios for coal fired power plants coupled to a post-combustion CO<sub>2</sub> capture process.

Having almost completed the development of fundamental components for the water steam cycle and the post combustion process, the development will now proceed to the design of subsystems and complete power plant models including a CO<sub>2</sub> capturing unit. These models will be validated against measurement data from an existing hard coal power plant and a demonstration post combustion unit.

However, it should be noted that the design of ClaRaCCS allows the easy adaptation of component models in order to feature CCS-retrofits to existing power plants as well as to perform concept studies for planned ones. In this context the development of an integrated control concept is a major challenge. First steps into this direction have already been published in [18]. Moreover the automation of the initialisation process for complex simulations will be a major future direction of work.

Concerning the models for the CO<sub>2</sub> capture, the use of external media data shall be supported in the future. In this context it may be necessary to adapt the models in order to maintain performance.

## 7 Acknowledgements

On behalf of the authors we would like to thank all members of the ClaRaCCS team. This research project is supported by the Federal Ministry of Economics and Technology (project number 03ET2009). For valuable data input and discussions the staff of KNG, EnBW, Vattenfall and E.ON are gratefully acknowledged. We thank the anonymous reviewers for their valuable comments.



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