Modeling of the Gasification Island with Modelica

Julia Fahlke[1] Stephan Püschel[1] Frank Hannemann[2] Bernd Meyer[1]
[1]TU Bergakademie Freiberg, Institut für Energieverfahrenstechnik und Chemieingenieurwesen
Fuchsmühlenweg 9, Haus 1, 09596 Freiberg
[2]Siemens Fuel Gasification Technology GmbH
Halsbrücker Straße 34, 09599 Freiberg

Julia.Fahlke@iec.tu-freiberg.de

Abstract

For the modeling and simulation of the Gasification Island a new Modelica library *GasificationIsland* was developed. Therefore new components had to be generated, like the gasifier or the components of the pneumatic feeding system. The developed models are based on the Modelica_Fluid and the Modelica.Media libraries. In this paper the structure of the most important component models and the main modeling assumptions are illustrated.

Keywords: Gasification Island modeling; SFG

1 Introduction

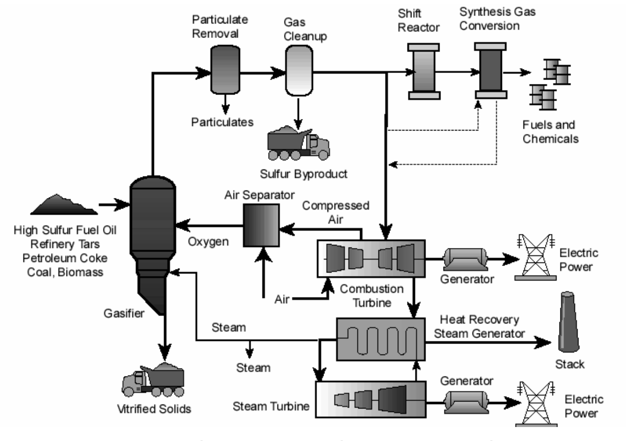

Figure 1: usage of the syngas from the gasification [1]

The gasification process is of great importance for the electrical and basic chemical industry as it converts any carbon-containing material into a synthesis gas (syngas) composed primarily of carbon monoxide and hydrogen. This syngas can be used as a fuel in a combined cycle to generate electricity (**I**ntegrated **G**asification **C**ombined **C**ycle). But it can also be used as a basic chemical for a large number of syntheses in the petrochemical and refining industry, like Methanol or Fischer Tropsch Synthesis (Figure 1). The modeling of the gasification process is till this day a great challenge.

1.1 The gasification process

Gasification means the thermo-chemical conversion of fuels with a reactant to a combustible gas, which is rich of the components CO, H_2 and CH_4. The most proceeded reactions are partial oxidation procedures, which take place with oxygen in free (elemental) or bounded form (H_2O, CO_2). These partial oxidations are interfered in dependence of the process and the process parameters with pyrolysis or devolatilization and hydrogenation processes [2].

The gasification process can be divided into different types according to the gasification agent/heat supply (autothermic, allothermic or hydrogenating gasification), the gas-solid-contacting (fixed/moving bed, fluidized bed or entrained flow gasification) or concerning the process temperature (above or below ash melting point).

This paper deals with the SFG gasification process, which is an autothermic, entrained flow gasifier with temperatures in the gasifier above the ash melting point.

In the gasification process a large number of reactions take place. Principle chemical reactions are those involving carbon, carbon monoxide, carbon dioxide, hydrogen, water (or steam) and methane [3]:

combustion reactions

$C + 0.5O_2 \rightarrow CO$ -111 MJ/kmol

$CO + 0.5O_2 \rightarrow CO_2$ -283 MJ/kmol

$H_2 + 0.5O_2 \rightarrow H_2O$ -242 MJ/kmol

Boudouard reaction

$C + CO_2 \leftrightarrow 2CO$ +172 MJ/kmol

water gas reaction

$C + H_2O \leftrightarrow CO + H_2$ +131 MJ/kmol

methanation reaction

$C + 2H_2 \leftrightarrow CH_4$ -75 MJ/kmol

CO shift reaction

$CO + H_2O \leftrightarrow CO_2 + H_2$ -41 MJ/kmol

steam methane reforming reaction

$CH_4 + H_2O \leftrightarrow CO + 3H_2$ +206 MJ/kmol

Most fuels contain additional components beside carbon, hydrogen and oxygen, e.g. sulfur, nitrogen or minerals. Sulfur in the fuel is converted into H_2S and COS and the nitrogen into elemental nitrogen, NH_3 or HCN.

1.2 The SFG Gasification Island

The SFG Gasification Island consists of the SFG gasifier itself, the pneumatic feeding system and the gas treatment system (Figure 2).

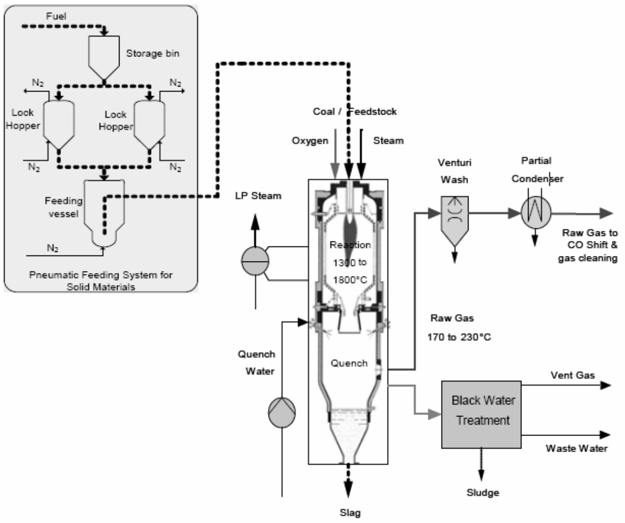

Figure 2: SFG Gasification Island [4]

The solid fuel (e.g. coal) is fed into the SFG-Reactor through a pneumatic feeding system. In the reactor the carbon rich fuel will be partially oxidized under high pressure and under the addition of oxygen as gasifying agent and steam as temperature moderator into a raw gas. Minerals in the fuel are separated and leave the bottom of the gasifier as an inert glass-like slag. The raw gas is cooled down and saturated in the quench. Afterwards it flows in the venturi wash and in the partial condenser, where the raw gas is cooled down and the solid particles are separated from the raw gas.

2 *GasificationIsland* Library Overview

The *GasificationIsland* library is an in-house Modelica library for the transient simulation of the Gasification Island process. The library is designed in a joint project with Siemens Fuel Gasification Technology GmbH Freiberg. The intention of the project is to apply these models to analyze the behavior of the different sub-processes as well as the whole Gasification Island at load changes or disturbances and to test new control strategies (see chapter 4). Furthermore the library shall be utilized in the plant shop tests prior real commissioning on site.

The developed models are based on the Modelica_Fluid and the Modelica.Media libraries.

The library is divided into functional sub-packages. In Figure 3 a screen shot of the first hierarchical level of the library is shown.

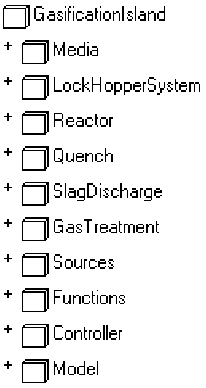
GasificationIsland
+ Media
+ LockHopperSystem
+ Reactor
+ Quench
+ SlagDischarge
+ GasTreatment
+ Sources
+ Functions
+ Controller
+ Model

Figure 3: screen shot of the GasificationIsland library in the package browser

The **Media** package contains all the used media models like raw gas, slag or coal. The solids are simulated as media with constant properties, like the *ConstantPropertyLiquidWater* in the Modelica.Media library.

The package **LockHopperSystem** includes all component models of the pneumatic feeding system, e.g. lock hopper, storage bin or feeding vessel.

The packages **Reactor/Quench** comprise the models of the gasification reactor and the quench.

The **SlagDischarge** package includes the models of the slag hopper and the flushing tank.

The **GasTreatment** package contains models of the venturi scrubber, partial condenser and drums.

The **Controller** package includes the sequence control of the batch processes for the pneumatic feeding system and the slag discharge system. The controllers were modeled by the Modelica.StateGraph library.

The package **Model** comprises the different simulated sub processes of the gasification island and a model of the complete process.

In the following section the structure and the main modeling assumptions for some selected components will be illustrated.

3 Developed Models

3.1 Lock Hopper System

3.1.1 Storage bin

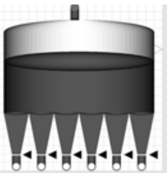

Figure 4: screen shot of the storage bin icon

The storage bin should ensure the uninterrupted service of the gasification reactor with coal. The storage bin works at ambient pressure.

In practice the pneumatic feeding system consists of more then one lock hopper, so the storage bin needs as many outlets as lock hoppers exist. For solid flow the outlet form is conical (Figure 4). To simulate the filling level of this geometrical form the storage bin was divided into segments. The single segments are connected through valves. These valves have a huge *Kv* flow coefficient and ensure the mass flow between the segments. So it can be guaranteed that the filling level in each storage bin segment is the same. There is only one exception: if the filling level is lower than the high of the cone no more mass transfer between the segments occurs. This is realized by setting the outlet pressure of the segment connections to a defined minimum value. Furthermore the inlet flow is split to the segments. Figure 5 shows the implementation of a storage bin with six outlets in the Dymola Diagram Layer.

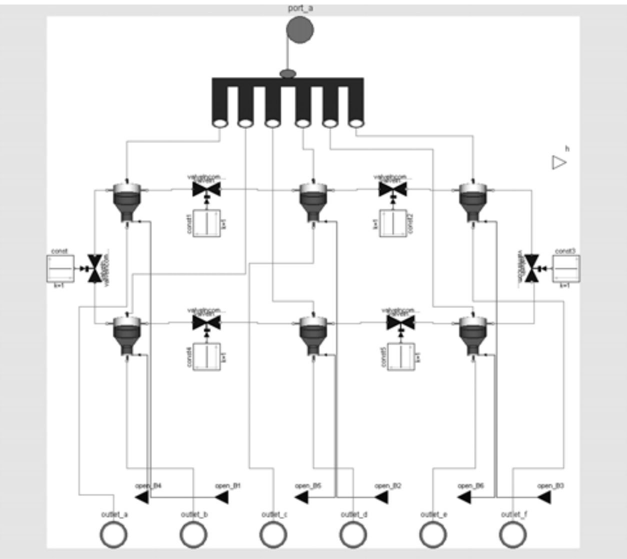

Figure 5: screen shot of the Implementation of a storage bin with 6 outlets in the Dymola Diagram Layer

For the outlet ports the coal mass flow is defined. The following function is used [5]:

$$\dot{m}_{c,out} = 0.3 \cdot \left(1 - e^{-0.1 \cdot \frac{d_A}{d_P}}\right) \cdot \frac{\rho_P \cdot g^{0.5} \cdot d_A^{\,2.5}}{\tan(\gamma) \cdot \beta^{0.36}} \cdot h^{0.5} \cdot \mu$$

There d_A is the diameter of the lock hopper outflow, d_P is the mean diameter of the coal particle, ρ_P is the particle density, γ is the repose angle, β is the cone angle and h is the fill level of the coal.

3.1.2 Lock Hopper

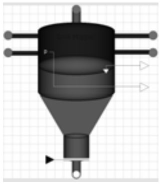

Figure 6: screen shot of the lock hopper icon

For dosing of the pulverized coal into the reactor it is necessary to bring it into a pressure system that operates at a pressure level higher than the reactor pressure. This is fulfilled by the lock hoppers. Therefore 4 sequences appear:

- filling of the lock hopper with coal until the maximum level is reached
- pressurizing of the coal. Therefore a pressurized inert gas is fed into the lock hopper
- discharging of the lock hopper into the feeding vessel
- depressurizing of the gas

In the lock hopper are two different media: the gas and the coal medium. For each a mass balance is considered but only one energy balance is implemented. Furthermore the wall material is regarded as a heat storage system and convective heat transfer between the gas and the wall is implemented.

The level of the coal is determined by the fixed bulk density.

```
model LockHopper
   …
  // Total quantities
  m_coal = V_coal*coal.d;
  m_gas = (V-V_coal)*gas.d;
  U = coal.u*m_coal + gas.u*m_gas;
  U_wall = m_wall*cp_wall*T_wall;
  V_bulk = m_coal/rho_bulk;
  Q = alpha*A*(T_wall – gas.T);

  //Mass balances
  der(m_coal) =  in_c.m_flow + out_c.m_flow;
  der(m_gas) = sum(in_g.m_flow) + sum(out_g.m_flow);

  //Energy balances
  der(U) =   in_c.H_flow + out_c.H_flow + sum(in_g.H_flow)
  + sum(out_g.H_flow) + Q;
  der(U_wall) = -Q;
  …
end LockHopper;
```

3.1.3 Feeding Vessel

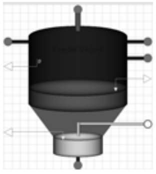

Figure 7: screen shot of the feeding vessel icon

The pulverized coal is fed from the feeding vessel into the gasification reactor. Therefore the feeding vessel remains a constant level of operating pressure above the reactor pressure. This is done through pressurizing and depressurizing of the feeding vessel with inert gas.

In the feeding vessel exist three layers: the fluidized bed, the bulk and the gas layer (Figure 8).

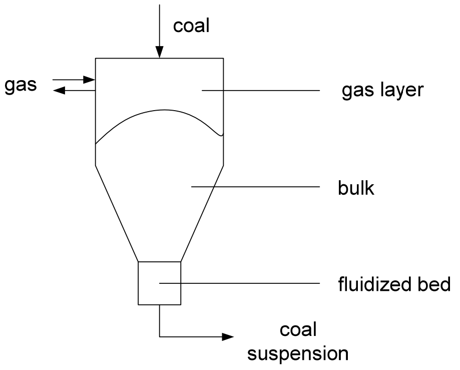

Figure 8: layers in the feeding vessel

From the fluidized bed the coal suspension is fed to the reactor. It is assumed that the height of the fluidized bed is fixed. Furthermore a functional correlation among the pressure drop between the feeding vessel and the reactor and the coal mass flow to the reactor exists. This functional correlation can be lodged.

In the feeding vessel only one energy balance is considered. The wall material as heat storage system is neglected because the appeared temperature fluctuations are only small.

3.2 Reactor

3.2.1 Gasification Reactor

In the gasification reactor the conversion of the coal into a combustible raw gas occurs.

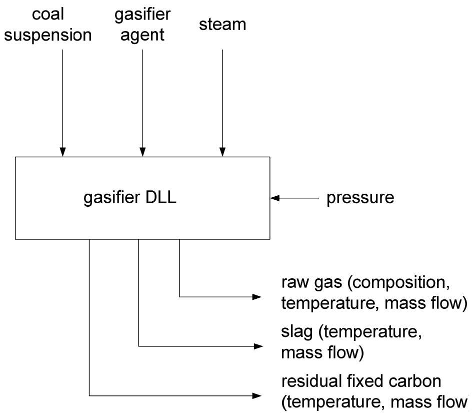

Figure 9: calculation of the gasifier DLL

The gasifier is implemented in a Dynamic Link Library (DLL), which was developed by the Siemens Fuel Gasification Technology GmbH Freiberg. In the DLL the thermodynamic equilibrium is calculated. Therefore the equilibriums for the reversible reactions mentioned in chapter 1.1 are calculated.

Figure 9 shows the in- and outputs of the gasifier DLL.

3.2.2 Quench

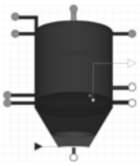

Figure 10: screen shot of the quench icon

In the quench the raw gas from the reactor is cooled down and saturated.

The quench consists of two zones the gas space and the sump. For each zone own mass and energy balances are considered. However convective heat transfer between the raw gas in the gas space and the water in the sump is assumed. In the gas space the raw gas from the reactor is saturated and therefore cooled down. This is done by the injection of fresh water at the top of the quench (Figure 11).

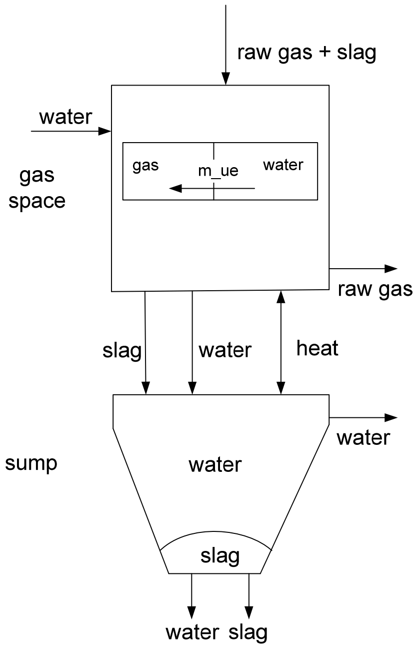

Figure 11: mass flows at the quench

In the gas space one energy balance for the media water, slag and gas is regarded.

For the calculation of the saturated steam fraction the following equation is used:

$$\varphi_{Steam} = \frac{p_{S,S}(T_G) \cdot M_s}{p_G \cdot M_G}$$

φ_{Steam} is the mass fraction of steam, $p_{S,S}(T_G)$ is the saturation vapor pressure at the temperature T_G, p_G is the gas pressure and $M_{S,}\ M_G$ are the molar masses of steam and the gas.

The vaporization flow has to be regarded in the mass balances of the water and the gas in the gas space. Furthermore the heat of vaporization has to be taken into account in the energy balance of the gas space.

```
model quench
  …
  //mass balances gas space
  der(m_gas) = in_g.m_flow + out_g.m_flow + m_ue;
  der(mXi[s]) = in_g.mXi_flow[s] + out_g.mXi_flow[s] +
  m_ue;
   0 = in_w.m_flow + out_w.m_flow – m_ue;
  …
  //energy balance gas space
  der(U) = … - delta_hv*m_ue;
  …
  //calculation of the saturated steam fraction
  gas.Xi[s] = p_steam*M_s/gas.p*gas.MM;
  p_steam = saturationPressure(gas.T);
  …
end quench;
```

3.3 Gas Treatment

3.3.1 Venturi Scrubber System

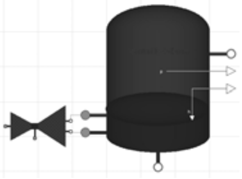

Figure 12: screen shot of the venture scrubber icon

The venturi scrubber system is located between the quench and the partial condenser. It consists of a venturi jet and a drum. The venturi jet is a pressure drop component. There are two different types of venturi's: controlled and uncontrolled.

The raw gas, which leaves the venturi scrubber system, is saturated. For the calculation of the saturated gas properties the same equations as in the quench are used.

3.3.2 Partial Condenser

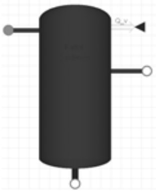

Figure 13: screen shot of the partial condenser icon

The partial condenser is located between the venturi scrubber system and the synthesis gas system. There the raw gas is cooled down and the condensate is separated. The raw gas leaving the partial condenser is saturated.

For the calculation of the gas properties the same equation as in the quench were used. Furthermore the energy balance equation is enlarged by the heat loss flux $\dot{Q}$. This heat flux is a real input value. It should be so adjusted that the temperature difference between the inlet and the outlet of the partial condenser reaches a given value.

3.4 Slag Discharge System

3.4.1 Slag Hopper

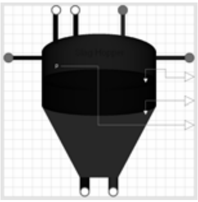

Figure 14: screen shot of the slag hopper

The function of the slag hopper is to discharge the slag from the pressurized system of the quench into the atmospheric pressure environment. Therefore 5 steps appear:

- filling of the slag hopper with water
- pressurizing until the pressure of the quench is reached
- filling of the slag hopper with slag (thus lead to a displacement of water from the slag hopper into the quench)
- depressurizing of the slag hopper
- drawdown of the slag hopper

As in the below explained components only one energy balance is considered.

3.5 Initialization

For every component the temperature and the filling levels can be defined. For the components which cover to the saturation of gas the dry gas composition and for all other components the gas composition have to be deposited.

Furthermore the user can decide for each component if the pressure should be initialized or not.

4 Simulation Results

As mentioned in the introduction the developed models shall be used to enhance process control. Therefore existing control methods can be verified and in addition tests of advanced process control conceptions like kinds of MPC (**M**odel **P**redictive **C**ontrol) and virtual sensors are allowed.

The Gasification Island contains a multitude of control systems:

- level control systems
- temperature control systems
- pressure control systems
- mass flow rate control systems

In cooperation with the Siemens Fuel Gasification Technology GmbH Freiberg, analyses were carried out on how far advantages appear by applying the advanced process control strategies in comparison to the accepted PID controllers. As an example of use the coal mass flow control system from the feeding vessel to the reactor was chosen due to the occurred dead times. Furthermore this mass flow control system is of great importance to the gasification process, because of its impact to the quality (temperature, composition) of the formed raw gas.

The following two figures show the results of some simulations. Figure 15 shows the step response of the controlled coal mass flow for an accepted PI controller and a model based controller. To avoid overshooting both, controllers were designed for aperiodic transient behavior (this is an arbitrary chosen design case and doesn't reflect the behavior of the implemented control system in the gasification plant). The response of the system for a ramp like change of the coal mass set point is given in Figure 16.

Both figures show that the coal mass flow can be significantly enhanced for this control system design case by using advanced process control concepts.

The control tests were done in Matlab. Therefore, the developed Modelica/Dymola models were converted into a Simulink model.

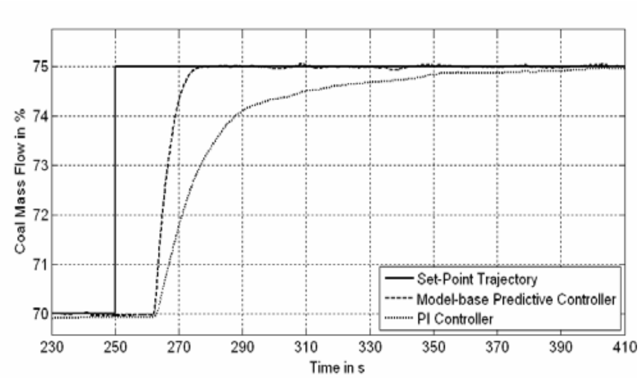

Figure 15: step response of the coal mass flow at sudden change of the coal mass flow set point value (arbitrary chosen design case: aperiodic transient behavior of the controllers)

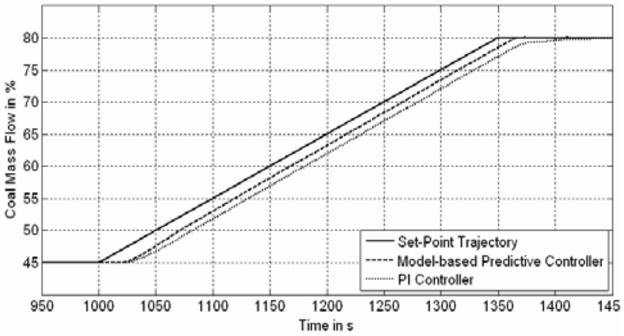

Figure 16: ramp like change of the coal mass flow set point (arbitrary chosen design case: aperiodic transient behavior of the controllers)

5 Conclusion and future work

The Gasification Island was developed in the Modelica language. Therefore new components were designed which are based on the Modelica_Fluid and Modelica.Media libraries. First analyses were done to enhance the process control of the coal mass flow from the feeding vessel to the reactor.

The further step is to enhance the gasifier model. Therefore the reaction kinetics of the reactions listed in 1.1 and the complex heat balance (heat radiation, convective heat transfer …) will be implemented.

Abbreviations

SFG	Siemens Fuel Gasifier

References

[1] http://www.gasification.org

[2] Klose, E.; Toufar, W.: Grundlagen der Vergasung, 1. Lehrbrief. Lehrbriefe für das Hochschulfernstudium, 1985

[3] Higman, C.; van der Burgt, M.: Gasification. Gulf Professional Publishing, Amsterdam, 2002

[4] Hannemann, F.: Siemens Fuel Gasification Technology at a Glance. Virtuhcon Workshop 2007, Freiberg, Germany

[5] Heyde, M.: Fluidisieren von Schüttungen.

[6] http://www.fossil.energy.gov

[7] Casella, F.; Otter, M.; Proells, K.; Richter, C.; Tummescheit, H.: The Modelica Fluid and Media Library for Modelling of Incompressible and Compressible Thermo-Fluid Pipe Networks. 5th International Modelica Conference Proceedings, 2006