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Modeling of the Steam Generation in a Sulfuric Acid Plant

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Abstract

An effort is made to model the steam generation at Kemira Kemi's sulfuric acid plant in Helsingborg, Sweden. The making of sulfuric acid starts with the oxidation of elementary sulfur in an exothermic reaction. The released energy is used in the waste heat boiler to produce high pressure steam. A model of this process consisting of burner, waste heat boiler and drum with controllers has been constructed. In the development of this model the theory of combustion and heat transfer is studied. The shrink-and-swell phenomenon, affecting the drum level dynamics, and the consequent control problem is given special attention. Modeling is done in Omola, an object-oriented modeling language, and simulation in OmSim. The developed plant model is simulated and the results are found in good resemblance with the actual plant. However, no real validation has been made.

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modeling, simulation, process control, steam generation, sulfuric acid plant

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Contents

1 Introduction

This masters thesis describes the modeling of the steam generation at the sulfuric acid plant at Kemira Kemi AB in Helsingborg. The effort to model the steam generation is a step in a process of developing a complete plant model. At Kemira Kemi AB there has been a continuous effort in increasing their employees competence. The model developed in this thesis, is part of this effort. Figure 1-1 shows the first steps in the making of sulfuric acid. The model describes the steam generation, the dotted square in Figure 1-1.

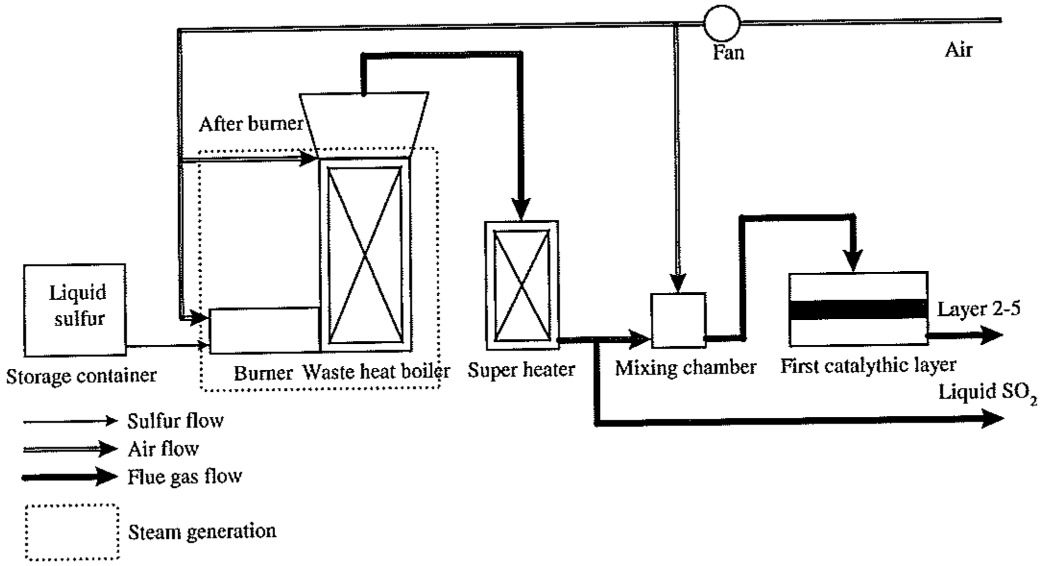


Figure 1-1 Principle sketch of the first steps of making sulfuric acid.

A model describing the steam generation could be of use in many different situations. Process supervisor support and training to increase the understanding of a large coupled system are some of the uses of the model.

The sulfuric acid plant is the heart of the Kemira Kemi AB facility in Helsingborg. The combustion of sulfur releases large amounts of energy. The energy released produces high pressure steam in a waste heat boiler. The steam is used for production of electricity in a turbine and also supplies process steam through a 6 bar pressure steam net to the other production facilities at the Kemira Kemi plant in Helsingborg.

This thesis has focused on modeling combustion and heat transfer. The components that are included in the model are burner and waste heat boiler complete with drum and controllers. Effort has been made to resemble the actual plan to every extent possible.

Modeling is done using Omola. Omola is an object-oriented modeling language for modeling of large systems. Omola is developed at the Department of Automatic Control at the Lund Institute of Technology.

1.1 Burner

Combustion of liquid sulfur takes place in a rotary burner. The sulfur is brought to the Kemira Kemi plant by sea transport and stored awaiting use. The sulfur is filtered and heated before use. Elementary sulfur is liquid between 100 and 150 °C and then becomes a liquid of high viscosity. A primary air flow atomizes the sulfur and is followed by a larger secondary air flow. The primary and secondary air flows are preheated and dried. The air is dried to prevent the reaction between the small amounts of formed sulfur trioxide and water, in air, forming sulfuric acid.

The combustion chamber is brick lined. There is some circulation of water in the foundation to ensure that the burner is kept in heat equilibrium with the flue gas pan but the combustion chamber is not part of the heat transfer process.

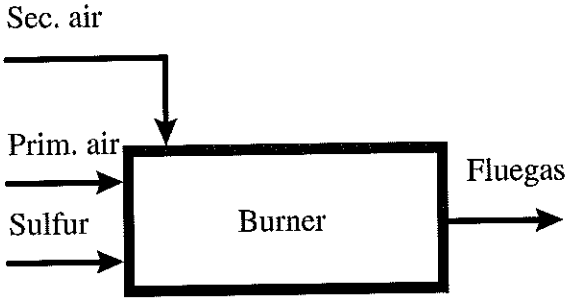


Figure 1-2: Description of burner flows.

1.2 Waste Heat Boiler

The waste heat boiler is eleven meters high and vertically mounted. Water is used as heat transfer medium and is circulated naturally. The burner is directly connected to the waste heat boiler at the base. The flame does not reach inside the waste heat boiler. On the inside heat transfer areas consist of vertically mounted tubes around the periphery of the boiler and a set of flag pipes at the top. The flag pipes at the top function as a lid on the waste heat boiler. This prevents radiation from being lost and thus increase heat transfer.

1.2.1 Circulation flow

The water flow in the waste heat boiler is upheld through natural circulation. Water leaves the drum through two down comers and is fed to the waste heat boiler and distributed to the risers, see Figure 1-3.

A mixture of water and steam enters the drum from the flue gas pan. The steam content in the risers is small, $x < 0.15$, where x is the steam mass ratio. This implies that the total flow of water, i.e. the circulation flow, is larger than the steam production and the feed water flow. To ensure that natural circulation is upheld the flow in the down comers and risers is ten to fifteen times the feed water flow. The size of the circulation flow is a design parameter and for different heat loads there are different circulation flows.

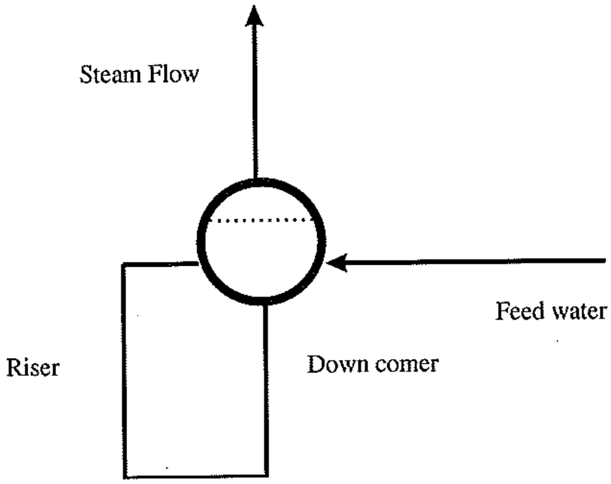


Figure 1-3 : The waste heat boiler.

1.3 Thesis outline

This masters thesis is focused on modeling the steam generation. Modeling of large systems, such as the steam generation, includes a variety of different engineering skills. In Chapter 2 the chemistry of combustion, the different forms of heat transfer and the shrink-and-swell phenomenon that affects the drum level are covered.

In the Chapter 3 concerns modeling and a introduction is first given to some of key points in object oriented modeling. An introduction to the used modeling language Omola with the central ideas of the class and inheritance are also included. At the end of the chapter there is a brief introduction to the simulator environment OmSim.

The description of the finished model of the steam generation is given in Chapter 4. There is a clear connection between the subjects covered in the theory- and modeling chapters and the model. A model hierarchy is developed and could be used in understanding the model. The different parts of the model are burner, waste heat boiler with drum and two controllers.

Finally, in Chapter 5, different simulations of the model are made to demonstrate some of the many aspects of the model. The shrink-and-swell phenomenon is captured as well as the effect of different sulfur loads on the total heat transfer.

2 Theory

Modeling a complex system as the steam generation at Kemira Kemi in Helsingborg involves theory from many different areas of engineering. Below, the theory concerning combustion of sulfur and the derivation of the combustion temperature is studied. A thorough look is also taken on heat transfer, with the three contributors radiation, convection and conduction. Finally, the shrink-and-swell phenomenon concerning drum level dynamics is studied.

2.1 Combustion

The first step in making sulfuric acid is the oxidation of elementary sulfur to sulfur dioxide. The oxidation of sulfur is done in a burner where sulfur reacts with the oxygen in air. At the Kemira Kemi plant, the combustion is run with a oxygen deficit to keep the formation of nitrous oxides low. The molar ratio of sulfur and oxygen fed to the burner is denoted λ and a λ value of 0.95 indicates a five percent deficit, on a molar basis, of oxygen.

Combustion of sulfur to sulfur dioxide is an exothermic reaction:

1. $S\,(l) + O_2\,(g) \rightarrow SO_2\,(g) \quad \Delta H_1 = -297$ kJ/mol.

With oxygen deficit the remaining sulfur reacts according to:

2. $S\,(l) \rightarrow \frac{1}{2} S_2\,(g) \quad \Delta H_2 = 55$ kJ/mol.

Further oxidation of sulfur dioxide to sulfur trioxide also occurs together with the formation of small amounts of nitrous oxides. A λ value of 0.95 is practice and thus 95 percent of the sulfur fed to the burner reacts according to reaction (1). Reaction (1) is exothermic and reaction (2) is endothermic and because the largest part of the sulfur reacts according to (1), there is a net release of energy increasing the flue gas temperature. The temperature of the combustion gases can be derived in many ways. Here it is assumed that no energy is lost to the environment. The process is said to be adiabatic. This is a fair assumption although to some extent energy is lost to the environment. The adiabatic combustion temperature, see [Reklaitis,1983], derived takes only into account reactions (1) and (2).

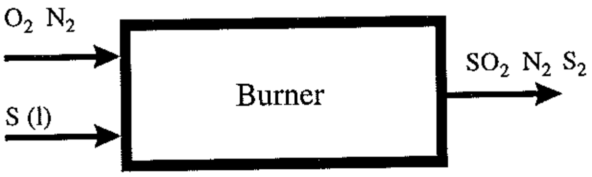


Figure 2-1 Description of the burner.

A simple mass balance states that:

IN + PRODUCED = OUT + ACCUMULATED

The IN term consists of the sulfur flow to the burner plus the amount of air that is supplied. The PRODUCED term is zero. The ACCUMULATED term is zero because mass is not accumulated in the burner. The OUT term is equal to the IN term. The mass balance can be translated into a mole balance.

A similar energy balance is made:

IN + PRODUCED = OUT + ACCUMULATED

The IN term is the energy of the reactants, oxygen and sulfur, plus the energy of nitrogen. The energy of the products is the OUT term. After start up there is no accumulation of energy in the burner which renders the ACCUMULATED term zero.

The size of the PRODUCED term depends on how much sulfur and oxygen that is fed to the burner and the ratio between them. The λ value determines how much of the sulfur that reacts in the exothermic reaction producing energy and how much that reacts in the, energy consuming, endothermic reaction.

$$\text{PRODUCED} = -\lambda \cdot n_{\text{sulfur,in}} \cdot \Delta H_1 - (1 - \lambda) \cdot n_{\text{sulfur,in}} \cdot \Delta H_2$$

The energy that is generated increases the temperature of the flue gas. An equation for the adiabatic combustion temperature can be derived:

$$\Sigma n_{i,\text{prod}} \cdot Cp_{i,\text{prod}} \cdot T_{i,\text{prod}} = \text{PRODUCED} + \Sigma\, n_{i,\text{reac}} \cdot Cp_{i,\text{reac}} \cdot T_{i,\text{reac.}}$$

The Cp values are temperature dependent and their value increase with temperature. The adiabatic combustion temperature is the same as $T_{i,\text{prod}}$.

2.2 Heat transfer

Heat transfer occurs in the waste heat boiler directly adjacent to the burner. As the flue gas passes through the boiler, heat is transferred to the water side. Heat exchange from gas to metal is due to both radiation and convection. There is conduction through the metal and convection from metal to water, see Figure 2-2.

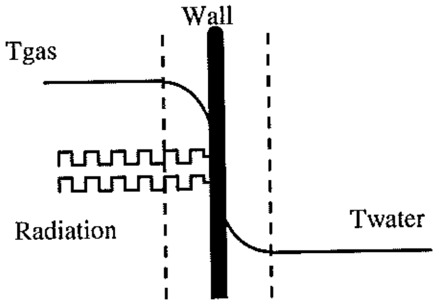


Figure 2-2 : Heat transfer.

2.2.1 Radiation

Many gases are transparent to thermal radiation, i.e. they do not absorb nor emit radiation. Inert gases, e.g. argon and symmetric diatomic molecules e.g. oxygen and nitrogen, are non radiant transparent gases. This means radiation to the environment can be neglected. Certain gases with asymmetrical molecule structures, however, emit and absorb radiation to and from surrounding surfaces. This is due to vibrational and rotational motions within the molecule. Sulfur dioxide is a radiant gas with both a vibrational spectrum and a rotational spectrum.

In [Holman,1992] a method is described for calculating gas emittance for engineering purposes. This method can be used to calculate the radiant exchange between a gas and its surrounding. Gas emittance is temperature dependent. To distinguish between different geometrical cases a characteristic dimension is defined called L_e, *the mean beam length.* L_e is tabulated for a wide range of different geometries. The waste heat pan at Kemira Kemi, with its cylindrical geometry gives:

$$L_e = 0.6 \cdot D$$

D = Interior diameter of the waste heat boiler.

Stefan Boltzman´s law

$$E_b = \sigma \cdot T^4$$

$$\sigma = 5.669 \cdot 10^{-8}\ (W/m^2\ K^4)$$

states that the total energy emitted, E_b, is proportional to the temperature of the fourth order where σ is Stefan Boltzman's constant.

Heat transfer from a gas to a cooler surface is:

q/A = Heat emitted by gas - Heat emitted from enclosure absorbed by gas.

$$q/A = \varepsilon_g(p,T_g,L_e \cdot pSO_2) \cdot \sigma \cdot T_g^4 - \alpha_g(p,T_g,T_w,L_e \cdot pSO_2) \cdot \sigma \cdot T_w^4 \quad (kW/m^2)$$

q	=	net heat transfer	kW/m^2
p	=	total pressure	bar
pSO_2	=	partial pressure of sulfur dioxide	bar
ε_g	=	emittance	
α_g	=	absorbance	
T_g	=	gas temperature	K
T_w	=	water/wall temperature	K
σ	=	Stefan Boltzman´s constant	(W/m^2K^4)
L_e	=	mean equivalent length	m

The emittance, ε_g, and the absorbance, α_g, are temperature dependent, see Figure 2-3 and [Vortmeyer,1984]. At a certain temperature the emittance equals the absorbance and the gas is no longer radiant. This occurs at temperatures below

800 K, which means that in the case studied at Kemira Kemi, the gas is radiant all through the waste heat pan. Note that α_g is dependent of the wall temperature as well as the gas temperature .

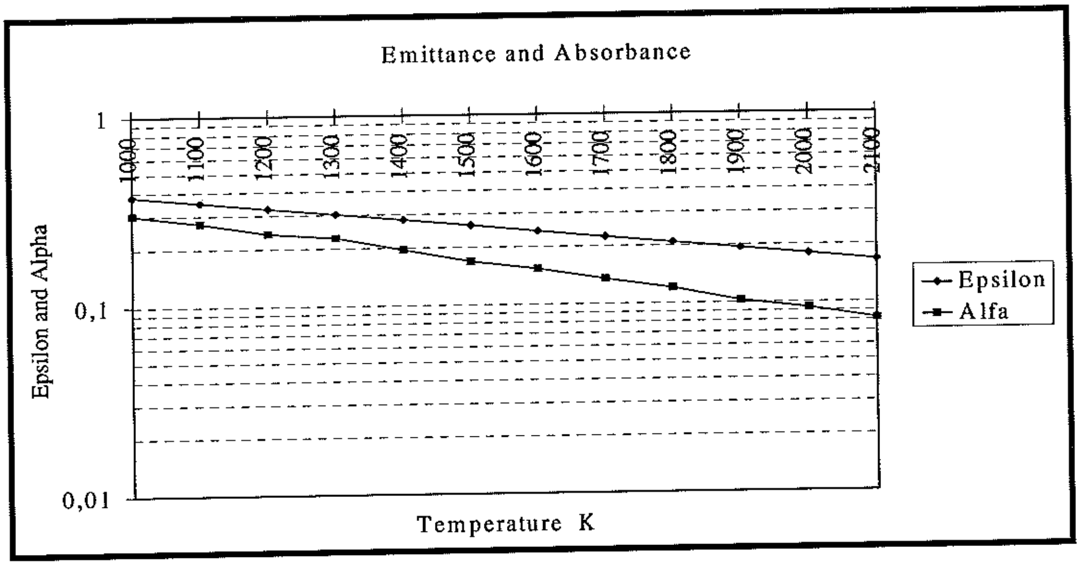


Figure 2-3 : Emittance and absorbance. Wall temperature is 260 °C.

The energy transfer, per square meter of surface exposed to radiation, will be higher at the bottom of the waste heat boiler than at the top. A series of calculations at different flue gas temperatures results in a net heat transfer chart, see Figure 2-4. The chart shows how heat transfer varies with different flue gas temperatures. The wall temperature is equal to the water temperature, see Section 2.2.3.

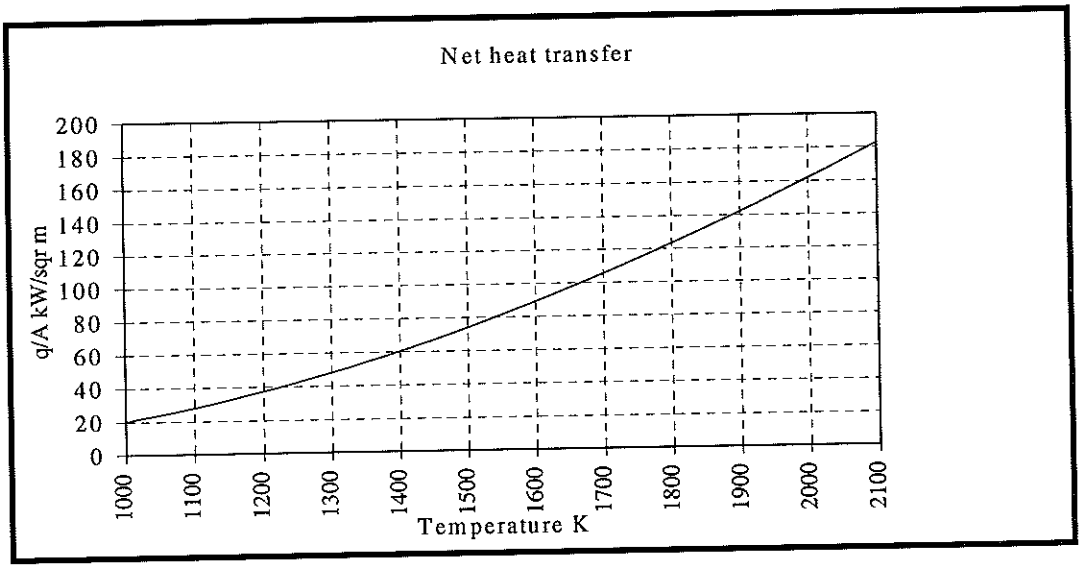


Figure 2-4 : Net heat transfer due to radiation.

A very high energy transfer is achieved due to radiation from the gas. This has influenced the design of the flue gas pan with almost no enlargement of heat transfer areas. The heat transfer at 1000 K is still high compared to the heat transfer achieved through convection from gas to metal wall, see Section 2.2.2.

2.2.2 Convection

Convection in the waste heat boiler is from flue gas to metal wall and from metal wall to water. It is a fair assumption that the convection from gas to metal wall is rate determining. A calculation of the heat transfer due to convection gives values in the 1-10 kW/m^2 range. This is almost negligible compared with the larger heat transfer due to radiation.

To calculate the heat transfer due to convection, dimension less numbers are used:

$$\mathrm{Re} = \frac{v \cdot \rho \cdot d}{\eta}$$

$$\mathrm{Pr} = \frac{c_p \cdot \eta}{\lambda}$$

$$\mathrm{Nu} = 0.33 \cdot \mathrm{Re}^{0.6} \cdot \mathrm{Pr}^{0.33}$$

$$\mathrm{Nu} = \frac{\alpha \cdot d}{\lambda}$$

$$\frac{1}{k} = \frac{1}{\alpha_{gas}} + \frac{d_{wall}}{\lambda} + \frac{1}{\alpha_{Water}}$$

$$q = k \cdot A \cdot \Delta T$$

EXAMPLE:

To determine the effect of heat transfer due to convection compared to the total heat transfer, a simple problem will be solved. Data have been taken from ASPENPlus and [Mörtstedt and Hellsten,1987]. Gas and water flows are from the simulation of the complete plant model. The flue gas temperature of 1300 °C implies that the example is from the middle of the waste heat boiler.

Gas:
T_{gas} = 1300 °C
v = 6.2 m/s
d = 3.8 m
ρ = 0.35 kg/m^3
η = 55$\cdot$ 10^{-6} Pa $\cdot$ s
c_p = 1130 J/kg
λ = 0.08 W/m$\cdot$ °C

$\Rightarrow$ Re = 1.5 10^5
Pr = 0.78
Nu = 390

α_{gas}= 8

Wall:
λ = 50 W/m$\cdot$ °C
d = 0.001

k = 8

Water:
T_{water} = 260 °C
v = 0.18 m/s
d = 0.063 m
ρ = 1000 kg/m^3
η = 114 $\cdot$ 10^{-6} Pa $\cdot$ s
c_p = 5000 J/kg
λ = 0.60 W/m$\cdot$ °C

$\Rightarrow$ Re =1 $\cdot$ 10^5
Pr = 0.95
Nu = 320

α_{water}= 3000

The derived k-value is equal to α_{gas}. From this it is concluded that the heat resistance of the metal and on the water side can be neglected.

$$q_{convection}/A = 8 \text{ kW/m}^2$$

The heat transfer due to convection is small compared to the heat transfer due to radiation. The heat transfer due to convection is not included in the model because of its little impact on the total heat transfer.

The difference between α_{water} and α_{gas} leads to different characteristics of the boundary layers on the gas and water sides. The major part of the temperature difference will be on the gas side.

2.2.3 Conduction

Metal is a very good heat conductor. The heat transfer tubes are in equilibrium with the water. The temperature of the wall is very close to the temperature of the water.

2.3 Shrink-and-swell

The shrink-and-swell phenomenon is encountered in the boiler drum and affects the drum water level. The shrink-and-swell occurs when the pressure of the drum is altered.

In the drum water-steam equilibrium steam bubbles rise through the water and leave the water surface. Of the total volume of steam in the drum a fraction is always submerged in the water. This is this volume of steam that accounts for the shrink-and-swell phenomenon. If there is an increase of energy flow to the flue gas pan a new larger equilibrium circulation flow is produced. But before this happens a larger amount of steam bubbles, in the risers and submerged steam bubbles in the drum, are generated which alters the drum pressure. Shrink-and-swell is causing large problems during start-up. If there is no steam production there can be no circulation flow, because it is the steam bubbles in the risers that pushes water up into the steam drum.

A possible solution to the problems during start-up is to install a pump to uphold a circulation flow. At start-up the heat load is low and the steam content in the risers is small. When the heat load is increased steam, of lower density, begins to form in the risers, and water needs to be supplied. If there is no circulation flow the water level in the drum will drop drastically and the pressure in the drum will rise. If instead a pump upholds the circulation flow water will be supplied to the risers continually and reduce the problem. Today there is no pump.

Shrink-and-swell is also responsible for the non-minimum-phase character of the drum. When there is a disturbance in the heat load additional steam is produced. This calls for the feed water valve to open which leads to that water of lower enthalpy enters the drum. This in turn lowers the total enthalpy in the drum and the volume of submerged steam bubbles decrease.

2.3.1 Drum level dynamics

Modeling of the drum level dynamics has been of interest for a long time. In [Bell and Åström, 1996] a fourth order model is derived describing drum boiler dynamics. The drum level is defined:

$$\text{level} = \frac{V_w + V_{sd}}{A}.$$

The level is composed of two variables, V_w which is the volume of water in the drum and V_{sd} which is the volume of steam that is submerged under water in the drum. If there is a change in the heat load there will be a transient change in V_{sd}. The transient will last until a new steady state in circulation flow is achieved. The drum controller will also try to lower the effects of an increase in V_{sd} and drum level, but the response is fast and difficult to control.

The quantity of V_{sd} depends on the drum pressure. If the drum pressure is increased the volume of the submerged bubbles will decrease and the opposite, a lowering of drum pressure, will increase the amount of V_{sd}.

Using mass and energy balances an equation for V_{sd} is derived:

$$\frac{dV_{sd}}{dt} = -\frac{V_{sd}}{T} + \frac{h_{fw} - h_w}{h_c \rho_s} q_{fw} - \left(\frac{V_{sd}}{h_c} \frac{\partial h_s}{\partial p} + \frac{\rho_w V_w}{\rho_s h_c} \frac{\partial h_w}{\partial p} + \frac{V_{sd}}{\rho_s} \frac{\partial \rho_s}{\partial p} \right) \frac{dp}{dt} + \frac{V_{0sd}}{T}$$

V_{0sd} = the submerged volume of steam in the drum at steady state.
V_{sd} = the submerged volume of steam in the drum during a transient change in pressure.
h_{fw}, h_w, h_s = enthalpies of feed water, water in the drum and steam.
h_c = h_s-h_w; enthalpy of condensation.
ρ_s = density of steam.
q_{fw} = feed water flow.
T = time constant, approximately equal to the residence time of the steam bubbles under the water surface in the drum.

In the drum model h_w is equal to h_{fw}. The feed water is at saturation temperature. This means that the second term disappears. The partial derivative $\partial h_s/\partial p$ is negative and $\partial h_w/\partial p$ and $\partial \rho_s/\partial p$ is positive when the pressure is increased. The reverse is true if there is a drop in drum pressure. This has been verified from steam tables.

2.3.2 Drum control

The control of the drum level is complicated. This is a result of that the drum level reacts opposite to an expected way. If the feed water valve is opened water of lower enthalpy enters the drum and in the equilibrium with steam lowers the drum level at first. If the steam valve is opened the drum pressure is lowered and the steam volume increases and the drum level increases. This is called a non-minimum phase system and constitutes a complicated control problem.

In the control of the drum level, feed forward control is used. A three-point controller, see [Hägglund,1990], is used where not only the drum level is measured but also feed water flow and steam flow. The difference in flow of feed water and steam is used as a feed forward to the level controller.

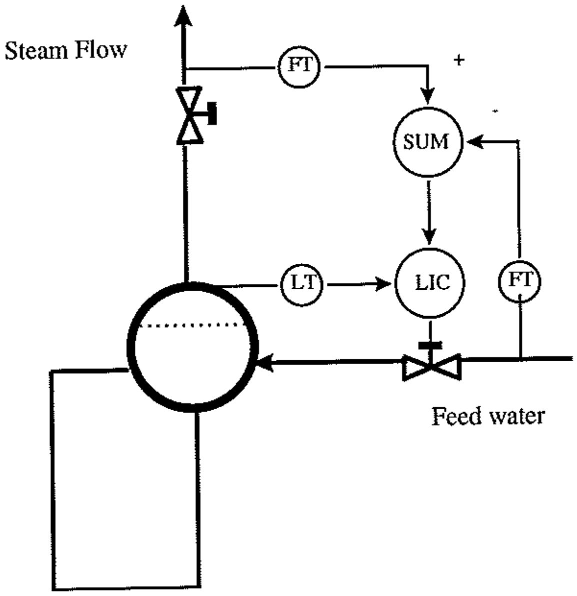


Figure 2-5 : Drum with a three-point controller.

3 Modeling

There are many different approaches to computer modeling in process engineering, see [Nilsson,1993]. The field span from flow sheeting packages, that furnish steady state solutions, to an equation-oriented dynamic approach. Here is a dynamic model desired and an object-oriented approach is used.

Two important aspects of computer modeling is decomposition and composition. Decomposition is a useful tool to fully understand and successfully model a complex chemical environment. The idea is to end up with small well defined areas that are easy to model. When each component is successfully modeled and its interaction with other components is fully described, composition leads to a complete model. The composition of smaller parts into a complex system is easier if the building block models are made in such a way that they can be used in many different instances. For example a model computing the Reynolds number in a heat transfer model could also be used in a pressure drop calculation and so forth. This is called modularisation and facilitates reuse.

The finished model can be used for many different purposes. It can be used for feasibility studies, process supervision, education and as a support when making difficult decisions in everyday situations. It is important that the model is validated for the specific situation in which it is to be used. A model in a feasibility study has a lower demand on accuracy compared to a model used as a support to a process supervisor at a chemical plant.

3.1 Modeling concepts

The use of decomposition-composition and encapsulation, in modeling, can in many ways simplify both the modeling effort and the understanding of the finished model. These are key ideas and important.

3.1.1 Decomposition - Composition

A central idea of model making is decomposition and composition. A part of a plant is extracted and decomposed in to smaller parts. If a heat exchanger is used as an example it can be pictured as two compartments with an intertwining wall, see Figure 3-1. A compartment can be further decomposed and furnished with a Medium model, Heat exchange model and a Pressure drop model. This decomposition can be taken even further until the system can be described with simple building blocks. Another aspect of decomposition is the way the different building blocks communicate with each other, which must be fully stated. The opposite of decomposition is composition. A system of great complexity can be built with small primitive building blocks.

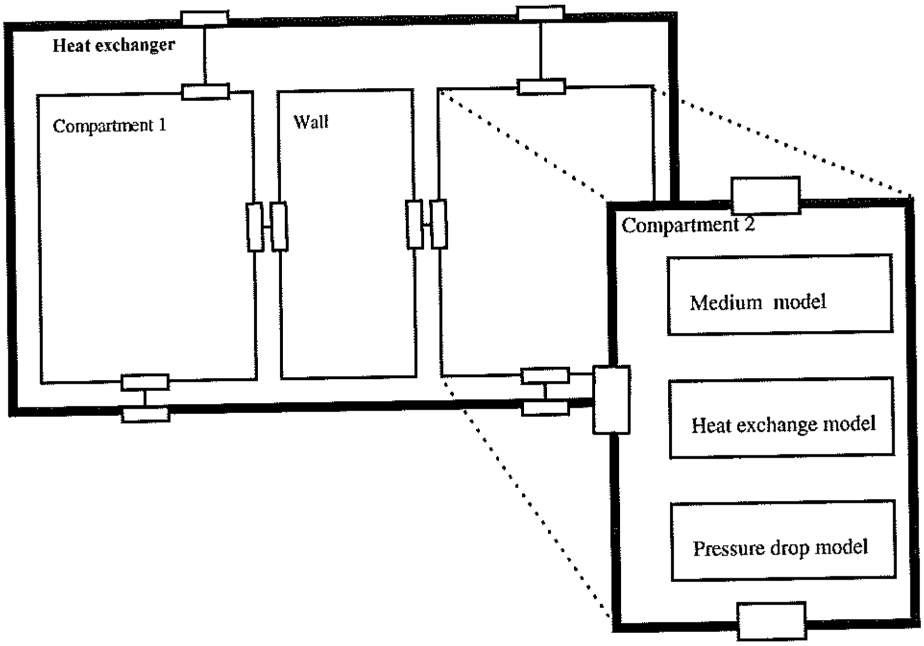


Figure 3-1 : Compartment 2 of the Heat exchanger decomposed.

3.1.2 Encapsulation

The idea of encapsulation is to separate the interior of a model from its interaction with other models. By applying a simple interface one should be able to make use of the model without knowledge of the interior. With the same example of an heat exchanger, the interior of the model is abstracted with an image explaining the function of the model and its points of interaction with other models, see Figure 3-2. The encapsulation icons are made in a bitmap editor and can then be associated with a model.

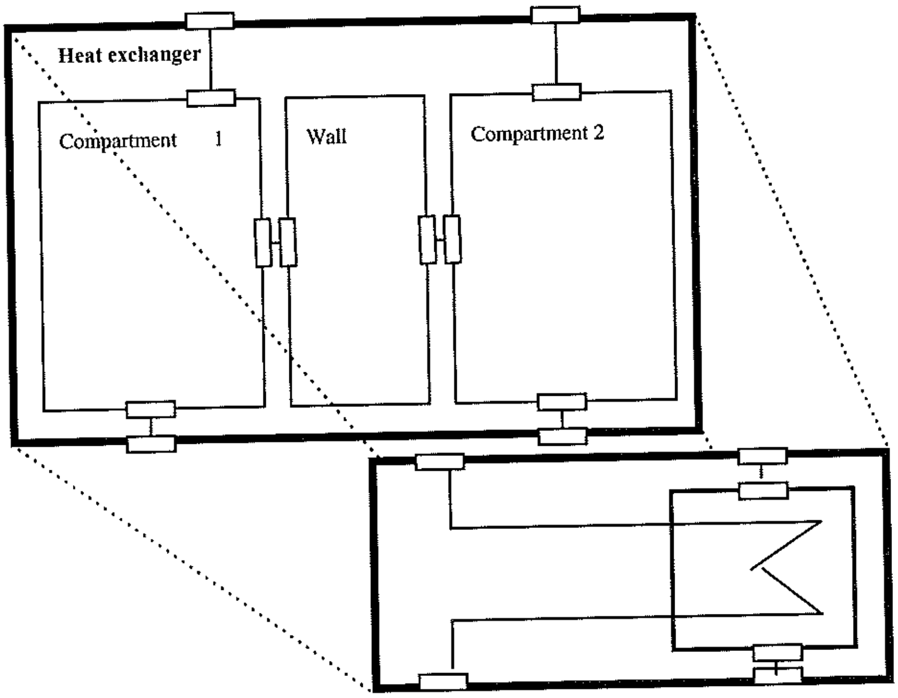


Figure 3-2 : Abstraction of Heat exchanger.

3.2 Omola

Omola, see [Mattsson *et al*,1993], is an equation based object-oriented modeling language and is developed at the department of Automatic Control at Lund Institute of Technology. Omola is the third generation of modeling software developed at the department. Omola supports ideas from object-oriented programming such as classes and inheritance. Omola is written in C++ and implemented in a UNIX environment. A LINUX version for PC is also available.

3.2.1 Class and inheritance

The concept of class is central in object-oriented modeling. Inheritance is another where an object class inherits properties from its super class. The idea is to group common properties together forming an object. This object class can be a subclass of another class and inherit attributes from this class. The attributes of a class can be a collection of data, equations and other class definitions.

Inheritance of properties from a class to a subclass simplifies modeling and results in a hierarchy between classes. This hierarchy supports the ideas of reuse, specialization and polymorphism. A class can reuse definitions of its superclass where the superclass is the nearest class above in the hierarchy.

If additional attributes are added to a class it alters or specializes the class. In the case of the heat exchanger the default media might be water/water. If instead there is heat transfer from water to air a new medium model is needed. The heat exchanger is then specialized by exchanging the medium model of the original heat exchanger with a new medium model describing the properties of air.

Polymorphism is when a new model can be used in an old model structure without any alterations of model structure. Polymorphism results in a standard way of modeling where the interaction of the model with its surroundings must be well defined. The new model with a different interior communicates with the surroundings in the same way as the replaced model.

3.2.2 Basic Omola

A simple class definition:

```
{name} ISA {name of super class} WITH
    {class body}
END;
```

The class is the basic entity in Omola. It is composed of an arbitrary name, the name of its superclass and a class body. The name can be chosen arbitrarily and the connection with the super class defines its position in the model hierarchy.

A set of class definitions already exists in Omola. These predefined classes have certain characteristics which define the attributes they can have. The root class is called Class and has four subclasses; Model, Terminal, Parameter and Variable, see Figure 3-3.

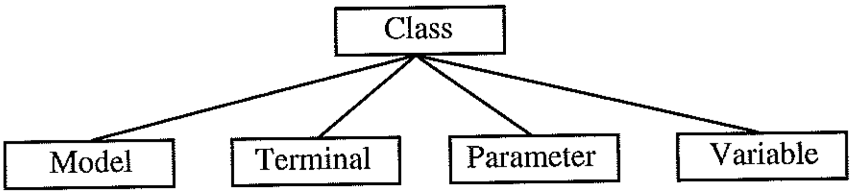


Figure 3-3 : Class definitions.

- The `Model` class is the root class for all defined models. A model can be simulated in a simulator.
- The `Terminal` class describes interactions between models i.e. it connects models. It has several subclasses. A connection is only valid if two terminals with the same internal structure are connected.
- The `Parameter` is a variable that the user can alter.
- The `Variable` is variable definition

3.2.3 Terminals

The idea of interaction between different models is the key in object-oriented modeling. It is important to assure that proper communication between models is achieved. This is done through the use of well defined terminals. The Terminal class has several predefined subclasses, see Figure 3-4.

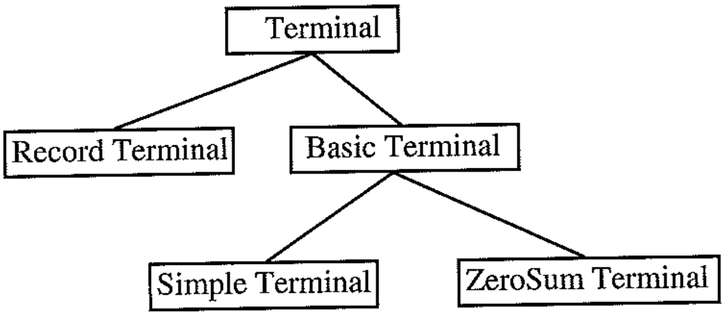


Figure 3-4 : Class tree of terminals.

- The `Record Terminal` is a structured terminal and describes a set of connections. All individual connections between terminals must be of the same sort for the connection to be valid.
- The `Simple Terminal` constitutes of a single value of interaction and a connection results in a equality e.g. the pressure of a class through the terminal is equal to the flow into the adjacent, connected terminal.
- The `ZeroSum Terminal` introduces the direction of an interaction e.g. the direction of a flow. A connection results in an equation where the values are summed to zero.

3.3 OmSim

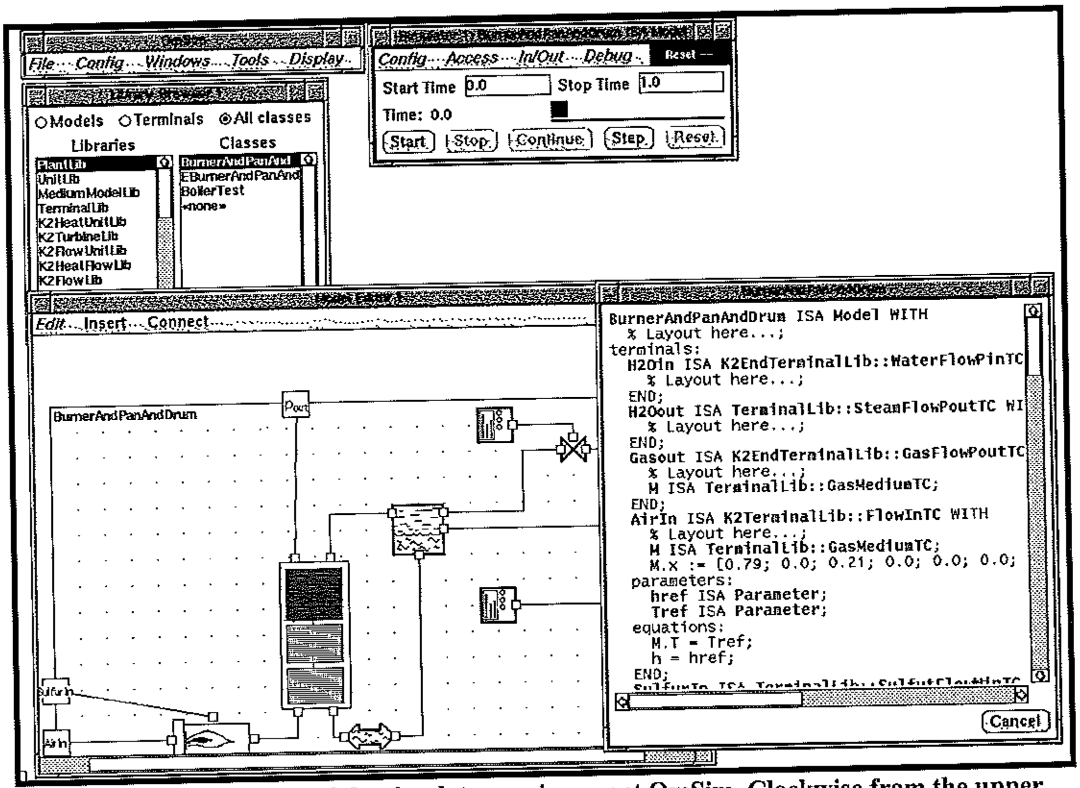
OmSim is the Omola Simulation environment i.e. the simulator. It is the place were the textual description of an Omola model is compiled into an equation system that can be simulated. OmSim also offers a model building environment where different building blocks can be accessed. The model composition takes place in the graphical model editor, MED. The abstracted building blocks can be connected to each other with graphical connections. The model built in MED is transformed to and saved as textual Omola.

The model building blocks are stored on file. These files are grouped together in libraries. These libraries can be accessed in a browser. The contents of a library can be full models or parts there of.

3.3.1 Simulation

When a model is complete, simulation can take place. The process, within OmSim, of transforming the Omola model into simulation code is complex. The model compilation for simulation includes syntactical and semantical checks as well as a mathematical analysis. Connection consistency is also verified which ensures that the model parts are connected correctly.

When a model is compiled successfully, simulation can take place. Interaction during simulation is supported without need for a new compilation. Any variable of a simulation can be connected to a plotter and followed during the simulation. Figure 3-5 shows a description of the OmSim environment.



```
BurnerAndPanAndDrum ISA Model WITH
  % Layout here...;
terminals:
  H2Oin ISA K2EndTerminalLib::WaterFlowPinTC
    % Layout here...;
  END;
  H2Oout ISA TerminalLib::SteamFlowPoutTC WI
    % Layout here...;
  END;
  GasOut ISA K2EndTerminalLib::GasFlowPoutTC
    % Layout here...;
    M ISA TerminalLib::GasMediumTC;
  END;
  AirIn ISA K2TerminalLib::FlowInTC WITH
    % Layout here...;
    M ISA TerminalLib::GasMediumTC;
    M.X := [0.79; 0.0; 0.21; 0.0; 0.0; 0.0;
  parameters:
    href ISA Parameter;
    Tref ISA Parameter;
  equations:
    M.T = Tref;
    h = href;
  END;
```

Figure 3-5 : Screen dump of the simulator environment OmSim. Clockwise from the upper left corner it features the OmSim control bar, a Simulator for the BurnerAndPanAndDrum model, the textual description of the model, the MED and a library browser.

3.3.2 Model initialization and OCL

In the simulator Omola code is compiled for simulation. Usually, the state variables need to be set to allow for the system to be solvable. These state variables can be accessed under the simulator bar. For a large system the number of state variables increase and the work can be elaborate. The Omola Command Language script, the OCL, is used as a kind of description of the simulator environment. In an editor outside OmSim the parameters of a simulation are set. Variables and plotters can be accessed.

4 Plant Model

The plant model describes the steam generation at Kemira Kemi in Helsingborg. It is a model including burner, waste heat boiler and steam drum. It also includes two controllers, one controlling drum level and the other steam pressure, see Figure 4-1.

The plant model is dynamic and an alteration of a parameter results in a transition from one steady state into another. All time dependent changes during the transition can be followed. This allows for an appreciation of the different time horizons in chemical and physical changes, e.g. a change in gas pressure is fast but a change in circulation flow is slow.

The model is constituted of different submodels. Some models are reused directly from the K2 project, see (Nilsson and Eborn, 1995), and some are reused with alterations. The K2 project is a Sydkraft AB sponsored research project at the Department of Automatic Control. K2 is an effort to model a bio gas power plant in Värnamo, Sweden. When modeling the steam generation, effort has been made to reuse and/or specialize as much of the work already done in the K2 project as possible.

Each model is symbolized with a bitmap picture. The bitmap picture is made in a separate editor and is associated to the respective model. If a bitmap picture is missing the model is represented by a square and the model name. The interaction between models is symbolized with connections. The connections can represent flows of different media or in the case of controllers, control signals. The connections between submodels, are made between terminals.

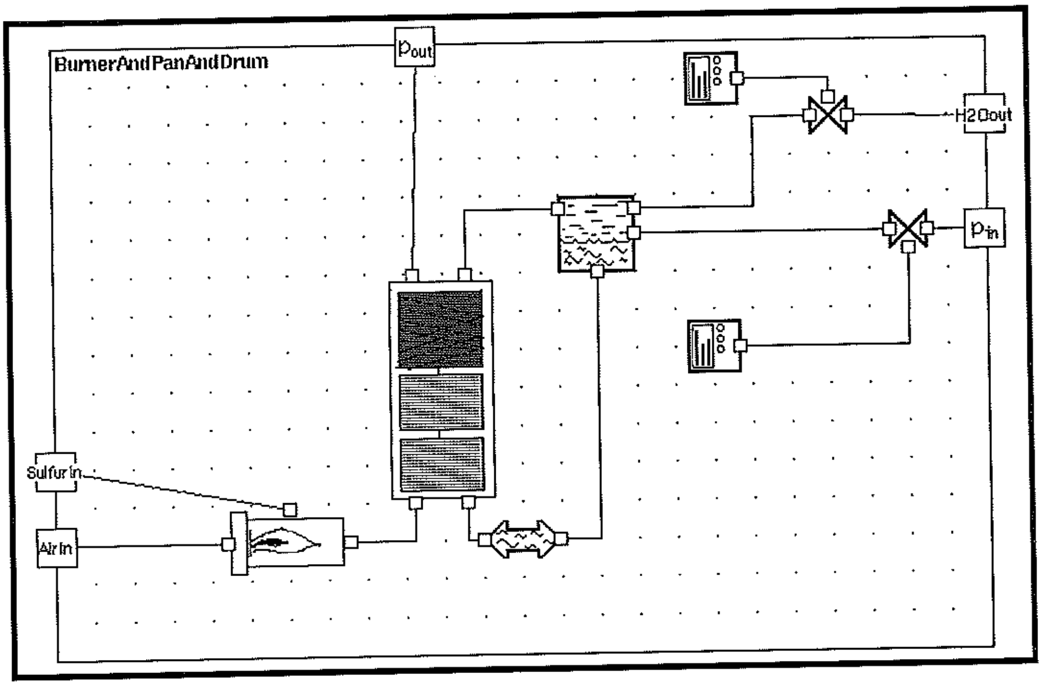


Figure 4-1 : MED picture of BurnerAndPanAndDrum.

4.1 Model Hierarchy

The Omola modeling language results in a model hierarchy. If the hierarchy is studied, the interaction between different submodels becomes clearer, see Figure 4-2. The top model's name is BurnerAndPanAndDrum. The top model consists of different sub models which in turn consists of yet different sub models.

The idea of reuse is clearly demonstrated in the sub model NewPan. NewPan has five submodels: SteamComp, FlashFlowResistor and PanSection1-3. The three different pan sections have the same submodels and are in a larger sense the same. In the PanSection1-3 heat transfer areas are specialized and customized to fit the description of the interior by an alteration of parameter values.

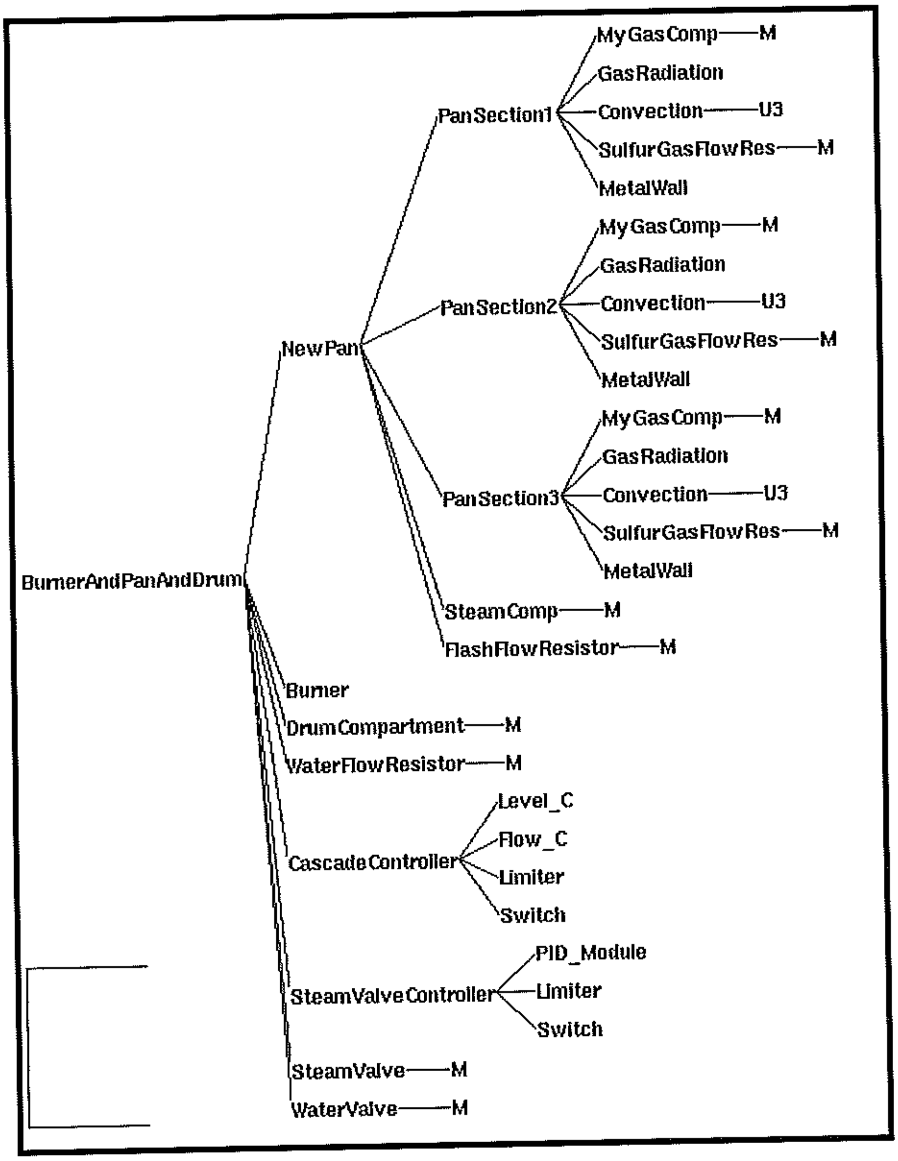


Figure 4-2 : Plant model hierarchy

4.2 Terminals

The key to understanding the interaction between models is to fully grasp the idea of the use of terminals. Many terminals are used in the model with different names but share common characteristics. Most terminals are flow terminals from the K2 library. The terminals passes information from one model to another. Depending on which type the terminal is it can result in forwarding a value or result in an equation.

A closer look will be taken at the category of flow terminals. These are responsible for nearly all connections in the BurnerAndPanAndDrum model. The terminals are defined in the K2 library TerminalLib and serve well. TC stands for TerminalClass.

4.2.1 FlowInTC

FlowInTC is a structured terminal used when connecting components in BurnerAndPanAndDrum. FlowInTc is a RecordTerminal. A RecordTerminal consists of two or more terminals. FlowInTC consists of four. The idea behind using the FlowInTC terminal is that it should be able to handle the majority of all connections in the model with smaller alterations.

```
FlowInTC ISA RecordTerminal WITH
  w ISA MassFlowInTC;
  p ISA PressureTC;
  h ISA EnthalpyTC;
  M ISA WaterMediumTC;
END;
```

MassFlowInTC terminal describes the mass flow into the class. It is defined as a MassFlowTC which is a ZeroSumTerminal. The ZeroSumTerminal has three defined attributes. The quantity attribute is defined as a mass flow rate which has the specified SI unit kg/s. The ZeroSumTerminal has also a default setting of the direction of flow. The default direction is In.

```
MassFlowInTC ISA MassFlowTC;

MassFlowTC ISA ZeroSumTerminal WITH
  quantity := "mass.flow.rate";
  unit := "kg/s";
END;
```

MassFlowOutTC is also a MassFlowTC with a different direction of flow. MassFlowOutTC can be said to be a specialization of the MassFlowTC.

```
MassFlowOutTC ISA MassFlowTC WITH
  direction := 'out;
END;
```

FlowOutTC is the same as the FlowInTC except for a different direction on the mass flow.

```
FlowOutTC ISA FlowInTC WITH
  w ISA MassFlowOutTC;
END;
```

PressureTC and EnthalpyTC are straight forward terminal definitions.

```
PressureTC ISA SimpleTerminal WITH
  quantity := "pressure";
  unit := "Pa";
END;

EnthalpyTC ISA SimpleTerminal WITH
  quantity := "specific.enthalpy";
  unit := "kJ/kg";
END;
```

WaterMediumTC is a RecordTerminal with two sub terminals, PhaseTC and HeightTC.

```
WaterMediumTC ISA RecordTerminal WITH
      q ISA PhaseTC;
      z ISA HeightTC;
    END;

HeightTC ISA SimpleTerminal WITH
  quantity := "height";
  unit := "m";
END;

PhaseTC ISA SimpleTerminal WITH
  value TYPE (Water, Steam, Flash, Gas,
  Sulfur);
  % default TYPE :='Water;
END;
```

The definition of the WaterMediumTC in the FlowInTC serves well for water and steam flows. However, flue gas flow demands for a new definition. GasMediumTC is a RecordTerminal with three sub terminals. The q terminal alters the default set phase from Water to Gas. The GasCompositionTC allows for control of all the different components of the gas.

```
GasMediumTC ISA RecordTerminal WITH
  q ISA PhaseTC WITH value:='Gas; END;
  T ISA TemperatureTC;
  x ISA GasCompositionTC;
END;

TemperatureTC ISA SimpleTerminal WITH
  quantity := "thermodynamic.temperature";
  unit := "K";
END;

GasCompositionTC ISA Std::VectorTerm WITH
% Composition description = [ N2, CO2, O2, S2,
  SO2, NO, H2O]
  n := 7;
END;
```

4.3 Burner

The model of the burner describes the combustion of sulfur and the consequent oxidation of sulfur to sulfur dioxide. Because of the fact that burner modeling is time consuming the derived burner model can be considered a primitive model. The model does not capture most phenomena that occur in the burner e.g. the formation of NOx gases. The burner model uses Cp-data and reaction enthalpies to calculate the combustion temperature. The model is guided by the amount of sulfur fed to it. The amount of sulfur together with the lambda value determines the airflow. On a molar basis we get:

$$\text{Oxygen flow} = \lambda \cdot \text{Sulfur flow}$$

$$\text{Nitrogen flow} = \text{Oxygen flow} \cdot 0.79/0.21$$

The different Cp-values are temperature dependent. The variation of the Cp-values with temperature are approximated with a polynomial $Cp(T_{gas})$ of the fourth degree. MATLAB was used to calculate the coefficients of the polynomial. This results in an implicit equation to determine the adiabatic combustion temperature T_{gas}, where NN2out, NSO2, NO2in, NN2in and NS are the molar flow rates.

$$\left(NN_{2out} \cdot CpN_{2out} + NSO_2 \cdot CpSO_2\right) \cdot T_{gas} = \left(NO2_{in} \cdot CpO_{2in} + NN_{2in} \cdot CpN_{2in} \right) \cdot T_{air} + NS \cdot Cps \cdot T_s - NO_{2in} \cdot \Delta H_1 - (NS - NO_{2in}) \cdot \Delta H_2$$

4.4 Waste Heat Boiler

The purpose of the waste heat boiler is to cool the combustion gas and produce high pressure steam. The model of waste heat boiler is decomposed into three sections. The reason for this is that the geometry of the waste heat boiler is different at the bottom of the pan compared to the top i.e. the gas inlet makes the heat transfer area smaller at the bottom of the boiler.

On the gas side of the waste heat boiler the gas is viewed as flowing unhindered through a pipe with a large diameter. The flag pipes at the top of the waste heat boiler are not modeled, see Section 2.2.2. The water that enters the waste heat boiler is distributed, and is viewed as flowing in tubes with a small diameter. The tubes form a cylinder along the periphery of the waste heat boiler.

4.4.1 Lay out

The interior of the waste heat boiler model can be seen in Figure 4-3. Three gas compartments transfer energy to a single steam compartment. The steam compartment is a compartment which allows for two phase flow. The flow resistor has a height description with the inlet at the bottom of the waste heat boiler.

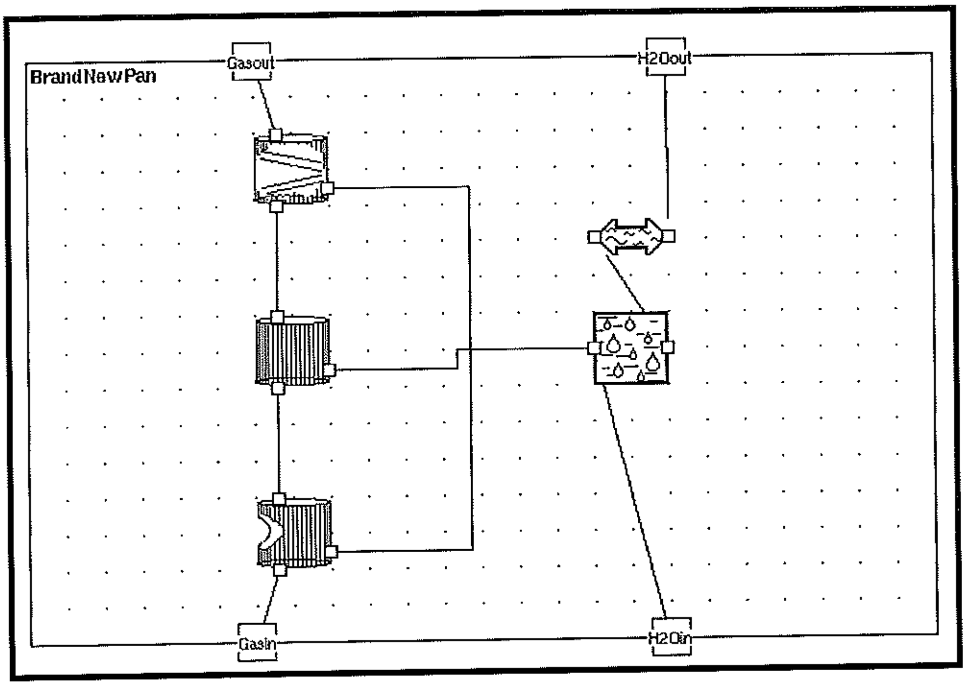


Figure 4-3 : The interior layout of the waste heat boiler.

4.4.2 Heat transfer

Heat transfer is modeled using the theory described in Section 2.2. The heat transfer model was refined several times. Early models consisted of separate models for radiation and convection on the gas side. The gas-convection contribution to the overall heat transfer is small and therefore omitted from the final model. This leads to a model with well abstracted parts which is easy to understand, see Figure 4-4. The gas flows through the PanSection and heat is transferred to the water side. The heat flows through a wall. The wall has a mass and a heat capacity. This has been done to resemble the behavior of a mass of metal with an environment of changing temperatures. If the heat load is changed a new equilibrium wall temperature is reached with a time delay which in turn affects the heat transfer. The calculation of the metal masses involves some uncertainty. The model uses values derived from waste heat boiler drawings supplied by Kemira Kemi.

The amount of energy that is transferred through the heat terminal, q, is guided by the heat resistor Convection. Convection is a K2 library heat resistor. From flow data and dimension less numbers a heat resistance is calculated. The heat resistance divided with the logarithmic mean temperature difference decides the size of q. This is an analogy of the $I = U/R$ for electrical circuits.

$$q = \frac{\Delta T_m}{\text{Heat Resistance}}$$

The heat transfer model does not allow for heat conduction from one wall segment to another in the vertical direction. The complete model has three different wall segments. The temperature difference between the segments are so small that the conduction would not affect the total heat transfer.

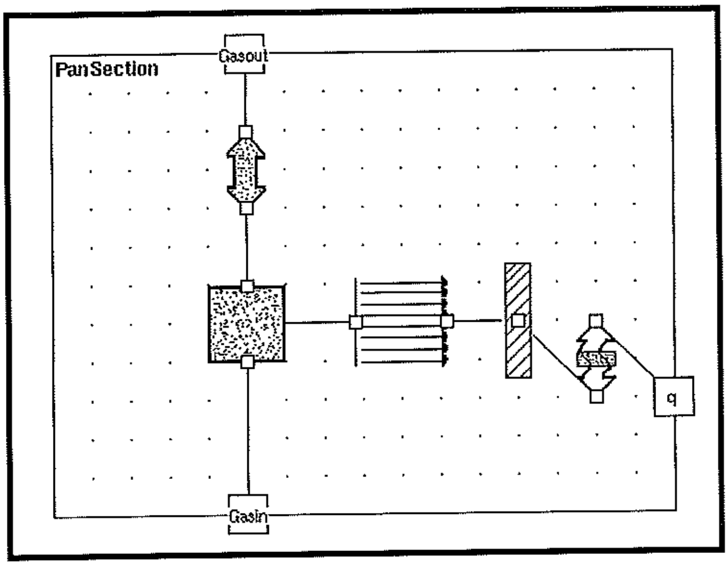


Figure 4-4 : Interior layout of the PanSection.

4.5 Drum

The drum model is taken from the K2 library. It is basically a compartment containing water and steam in equilibrium with four terminals. Feed water flows down through two down comers and the risers supply a mixture of water and steam to the drum. Water is supplied at the same rate as the production of steam. The water and steam flows are controlled by two controllers.

The K2 library DrumCompartment and its subclass SaturatedWaterSteamMM make use of the Omola built in steam tables. The steam tables are functions that can be accessed to calculate thermodynamic properties. The partial derivatives are approximated with difference approximations. The drum compartment has a height description. As a result of this the down comer flow leaves the drum at a level lower than the drum water surface, which leads to the formation of a circulation flow.

In the model of the drum at the Kemira Kemi plant additional equations are added to describe the shrink-and-swell phenomenon, see Section 2.3.1.

4.6 Controllers

Two controllers are used in the BurnerAndPanAndDrum model. The SteamValveController is controlling the steam valve, ensuring that steam of the right pressure is fed to the high pressure steam net. The CascadeController is a three point controller controlling the level of the drum. Both controllers feature manual over-rides.

The SteamValveController is a controller taken directly from the K2 library. The CascadeController is a three-point level controller, see Figure 4-5. The three points are: drum level, water flow and steam flow. It is composed of two PID-controllers. The difference between steam- and water flow is fed forward to the first controller. The first controller's control signal acts as a set point for the second controller that controls the feed water valve setting. The CascadeContoller also features an actuator saturation model.

Both controllers in the BurnerAndPanAndDrum model use the same parameters as in the actual plant.

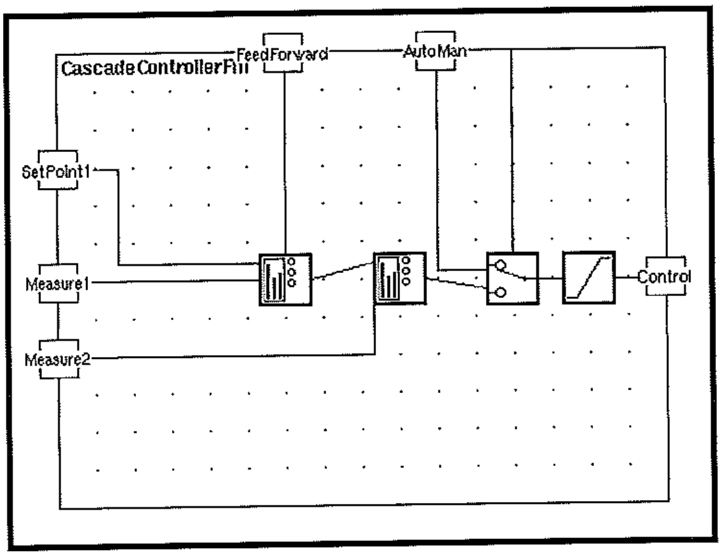


Figure 4-5 : Interior layout of CascadeController.

5 Simulation

This chapter deals with simulation of the plant model. First are, however, some of the results of the model presented. The remainder of this chapter deals with the simulation of the BurnerAndPanAndDrum model. In the first simulation different sulfur flows are fed to the burner and their impact on the total heat transfer is studied. Later the shrink-and-swell phenomenon in the drum is studied in two simulations. The figures are from OmSim. In all figures the x-axis unit is time in seconds.

5.1 Results

A simulation of the BurnerAndPanAndDrum model generates a vast amount of data. The model gives total access to all of the 1500 parameters and variables. In OmSim interesting variables can be high lighted by placing the variables in a special window. Another way to view the parameters and variables is to generate a Snapshot of all variables. This is also done in OmSim and the data is saved on a text file for easy access. Here follows an excerpt from a simulation where interesting variables are presented.

5.1.1 Simulation results

In all the simulations the initial sulfur flow to the burner is 15.5 ton/h. The sulfur flow determines the airflow which in turn determines the adiabatic combustion temperature and so forth. Most of the data in the model are given in SI-units. In some cases has transformation from SI-unit to a more conventional unit been done.

Burner:

Sulfur flow = 4.3 kg/s (15.5 ton/h)
Sulfur temperature = 180 °C (The sulfur temperature should be 135 °C)
Air flow = 17.6 kg/s
Air temperature = 220 °C
Flue gas flow = 21.9 kg/s ($\lambda = 0.95$)
Flue gas temperature = 1770 °C

Waste heat boiler:

Gas temperature IN = 1770 °C
Gas temperature OUT = 840 °C
Water flow down comer = 124 kg/s
Water temperature IN = 257 °C
Water temperature OUT = 257 °C
Steam mass ratio = 0.11
Total heat transfer = 23.7 MW

Steam drum:

Pressure = 45 bar
Level = 0.9 m (half full)
Submerged volume of steam = 0.5 m^3
Steam flow OUT = 14 kg/s
Water flow IN = 14 kg/s

5.2 Heat transfer

The heat transfer in the waste heat boiler is pretty clear cut. A decrease in sulfur flow rate to the burner decreases the heat transfer and an increase of the sulfur flow rate increases the heat transfer. But how does a change in sulfur flow rate affect the total amount of heat transferred?

5.2.1 Simulation

A decrease in sulfur flow rate is made which lowers the heat transfer. An increase in sulfur flow rate to the burner, increases the heat transfer. Noteworthy is that the changes in heat transfer are of a different order than the changes in sulfur flow rate. If you lower the sulfur flow rate with ten percent the change in total heat transfer is four percent, compare Figure 5-1 with Figure 5-3. This is accounted for by the different flue gas residence times in the waste heat boiler. A lower flow rate of flue gas increases the residence time and allows for additional heat transfer. A higher flow rate of flue gas lowers the residence time of the flue gas in the waste heat boiler. A look on the exit temperatures from the waste heat boiler confirm this reasoning, see Figure 5-2.

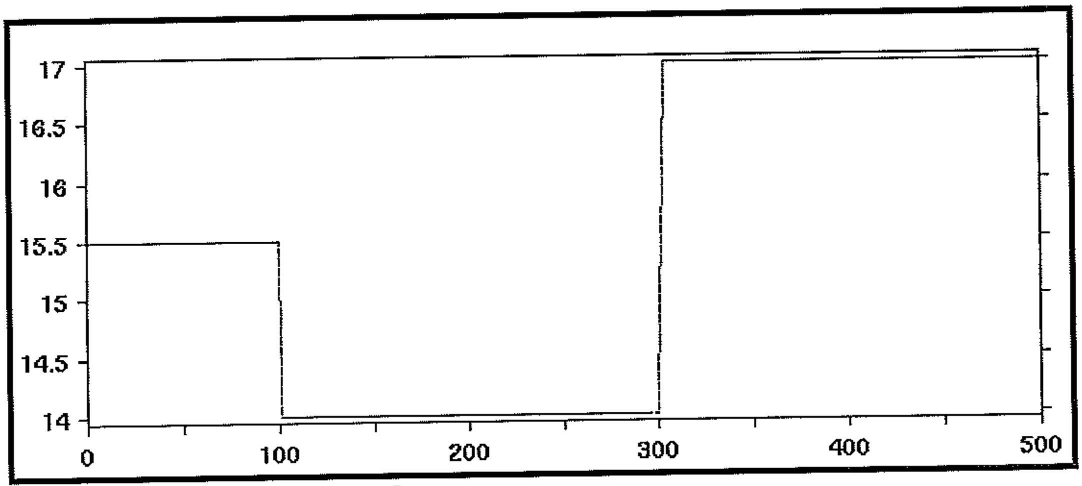


Figure 5-1: Sulfur flow Unit: ton/h.

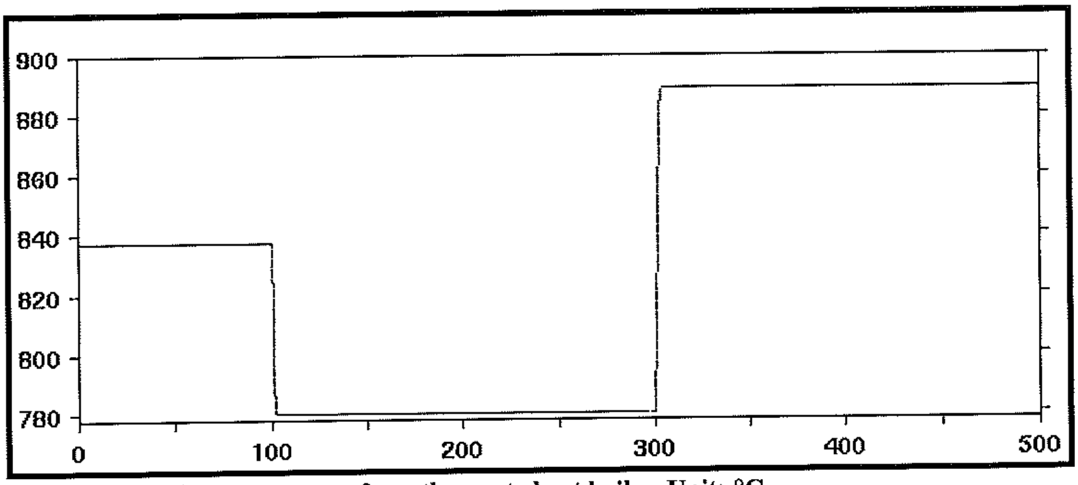


Figure 5-2: Exit temperatures from the waste heat boiler Unit: °C.

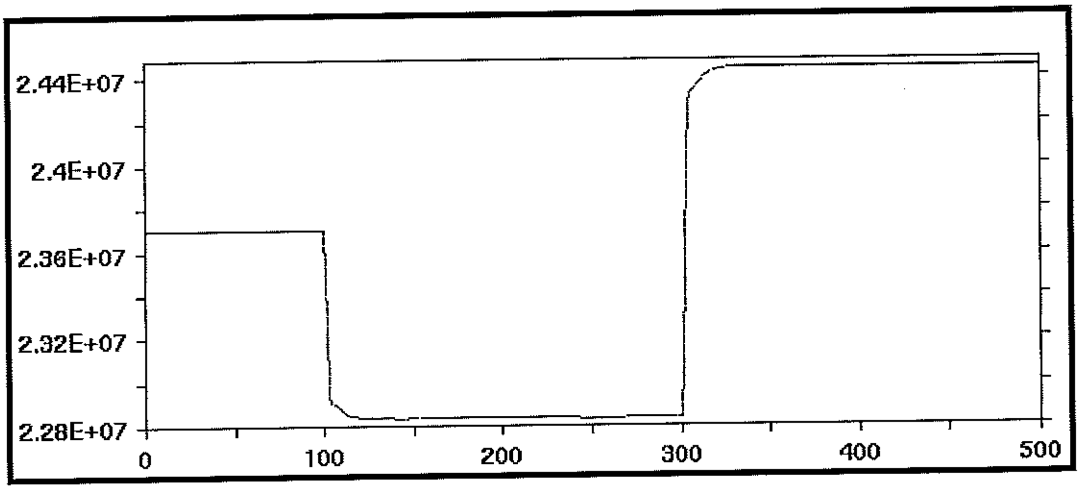


Figure 5-3: Total heat transfer Unit : W

5.3 Shrink-and-Swell

The shrink-and-swell phenomenon is difficult to understand. During the start up of the plant the problem is accentuated. The model captures this phenomenon. The equation in 2.3.1 concerning V_{sd} offers some kind of an explanation. The change in V_{sd} is proportional to the derivative of the pressure, dp/dt.

$$\frac{dV_{sd}}{dt} = -\frac{V_{sd}}{T} + \frac{h_{fw} - h_w}{h_c\rho_s} q_{fw} - \left(\frac{V_{sd}}{h_c}\frac{\partial h_s}{\partial p} + \frac{\rho_w V_w}{\rho_s h_c}\frac{\partial h_w}{\partial p} + \frac{V_{sd}}{\rho_s}\frac{\partial \rho_s}{\partial p} \right)\frac{dp}{dt} + \frac{V_{0sd}}{T}$$

In the simulations the enthalpies of the feed water and the water temperature of the drum is equal, $h_{fw} = h_w$. This leads to the expression for dV_{sd}/dt being zero at steady state when $V_{sd} = V_{sd0}$.

5.3.1 Simulation 1

The level of the drum is controlled by a level controller with a set point of 0.92 m. The pressure of the drum is controlled by a steam valve controller. Both these controllers have manual over rides. These manual over rides allows for a possibility to simulate sudden pressure drops by for instance increasing the control signal to the steam valve. In the simulation the system is disturbed at T = 100 s and again at T = 300 s. First the control signal to the steam valve is increased from 0.293 to 0.31, see Figure 5-4. If the steam valve opening is increased the pressure of the drum drops. At T = 300 s the steam valve controller is put back in action with the set point pressure of 45 bar. The effect of these changes in drum pressure can be seen in Figure 5-6, where the drum level is plotted. A pressure drop results in an increase of the volume of the steam bubbles submerged in the drum which affect the drum level. An increase in drum pressure leads to the opposite behavior.

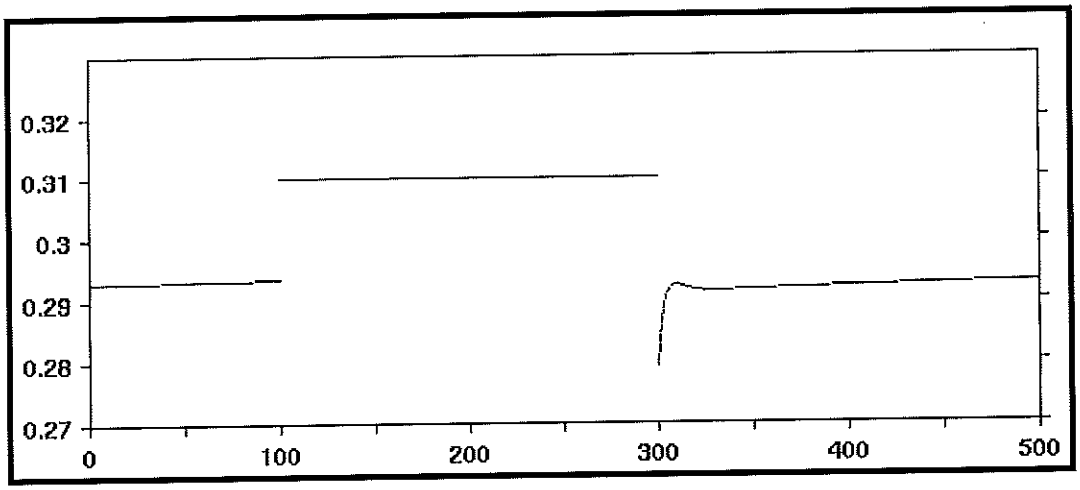


Figure 5-4: The control signal to the steam valve controller.

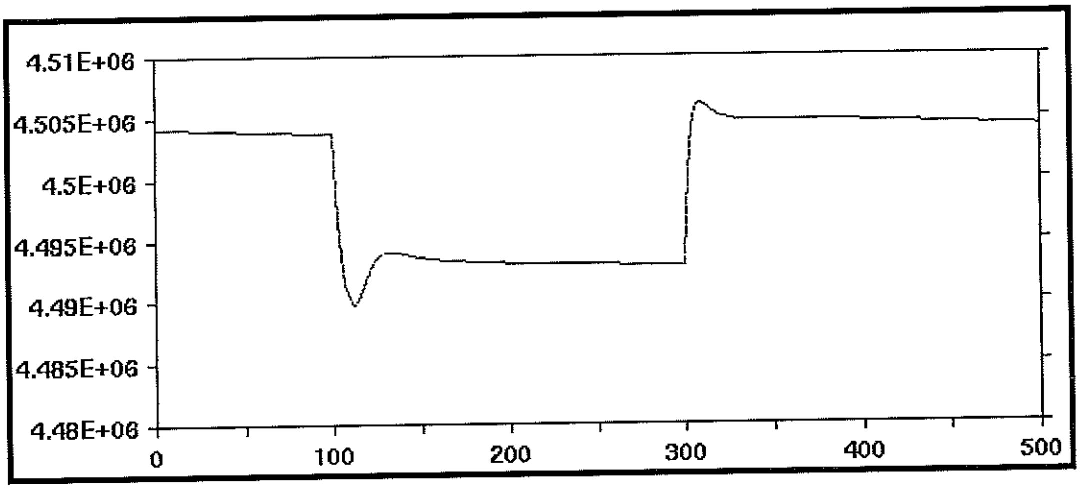


Figure 5-5: Drum pressure Unit: Pa.

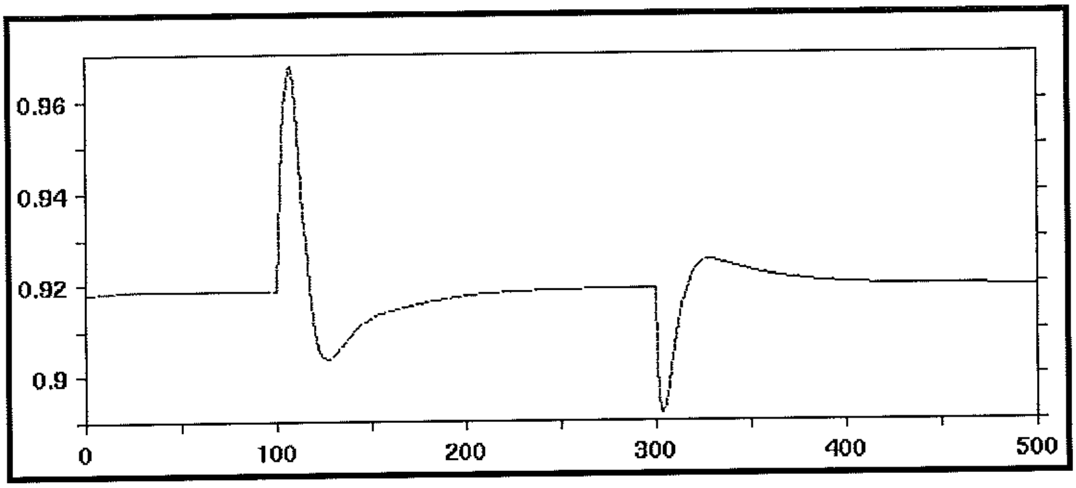


Figure 5-6: Drum level Unit: m.

5.3.2 Simulation 2

An increase of sulfur flow rate to the burner is made. This leads to an increase in the amount of flue gas that enters the waste heat boiler. At steady state there is an equilibrium circulation flow. A positive change in sulfur flow rate leads to a new greater equilibrium flow. In the time that elapses until this flow is established the steam content in the risers increases. This raises the pressure in the drum and thus lowering V_{sd} and the drum level.

Intuitively the drum level should increase when an increase in sulfur flow rate is made. A larger heat load would increase the steam content in the risers and thus increase the drum level. However this effect has not been accounted for in the model. Instead it is the opposite effect that the pressure has on V_{sd} that is visible, see Figure 5-9. The expression for V_{sd} states that the volume of the bubbles under the water surface in the drum is dependent on the derivative of the pressure. However an increase in riser flow can be detected with increased sulfur flow rate, due to an increase of the steam mass ratio in the risers. The steam bubbles pushes the water upwards. The increase in riser flow should give a higher water level but this effect is lost because of the magnitude of the effect related to V_{sd} and its pressure dependence. Without detailed validation it can not be determined which behavior is correct. A key issue is the steady state volume of submerged steam bubbles, V_{0sd}, which is a matter of uncertainty. The steam mass ratio in the risers is approximately ten percent. From this the volume of submerged steam in the boiler at steady state has been set to 0.5 m^3. This is ten percent of the water volume in the drum.

A decrease in sulfur flow rate to the burner gives the opposite behavior. A lower heat load lowers the pressure in the drum which in turn increases the volume of V_{sd}.

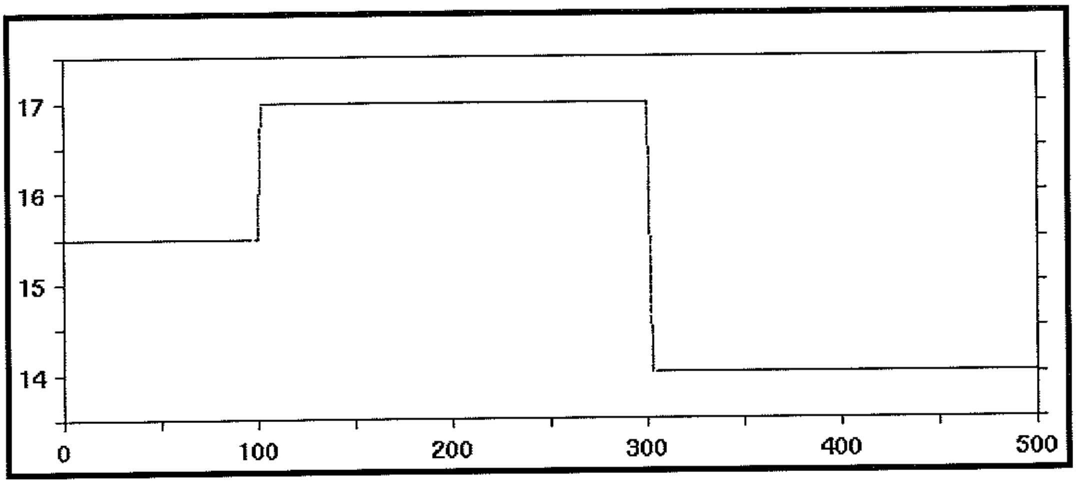


Figure 5-7: Sulfur flow changes. Unit : ton/h

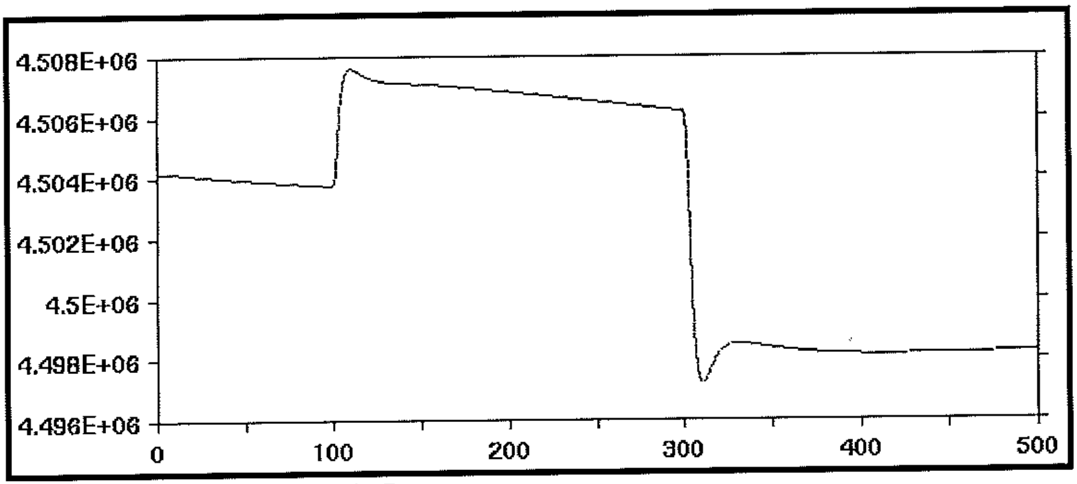


Figure 5-8: Drum Pressure Unit: Pa.

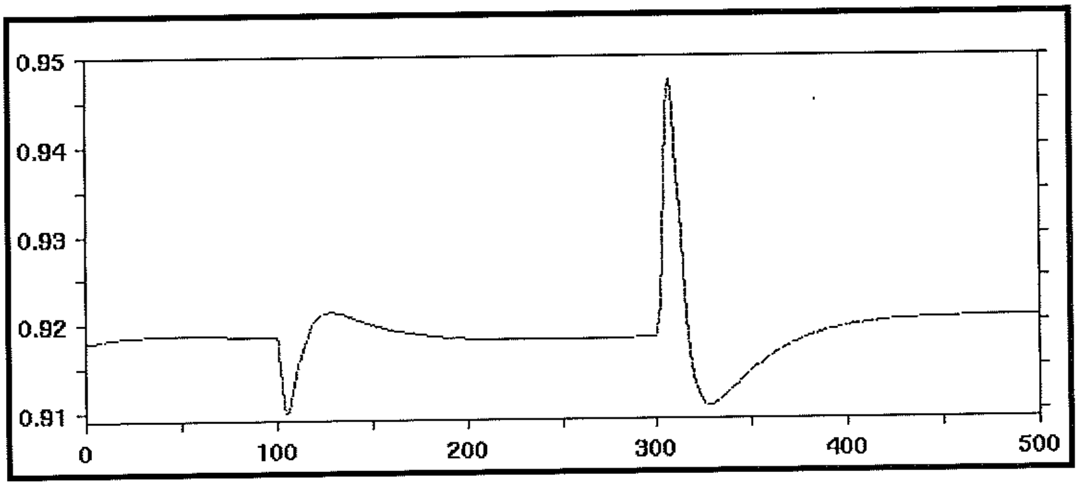


Figure 5-9: Drum level Unit: m.

6 Conclusions

Modeling is time consuming.

The developed plant model describes the steam generation at a sulfuric acid plant. The resemblance is good but no real validation against the actual plant has been done. Even if the model should over-emphasize certain phenomena, it offers plenty of opportunities of tailoring the plant model to increase the resemblance to the real facility at Kemira Kemi AB.

Modeling of large complex systems as the steam generation requires knowledge in a wide variety of areas. The plant model covers combustion chemistry, heat transfer through radiation, convection and conduction and process control. All of these different areas have been covered during my education and this thesis has been both a repetition and a possibility to develop new skills.

The model is developed using Omola, an object oriented modeling language. Omola is straight forward and quite easy to use and understand. But as in all other programming there is a large amount of time spent correcting code. However in Omola you have the opportunity to start with a small defined area and model that area and run a simulation to check for consistency. When several different areas have been covered these can be assembled to build a large system. I started to model the burner followed by the waste heat boiler, drum and controllers. A large part of the time was spent modeling the heat transfer in the waste heat boiler.

The OmSim simulation environment is under constant improvement but is already a nice tool. The OmSim environment features powerful tools for solving large equation systems.

Omola and OmSim are implemented in UNIX which takes a while to get used to if you are accustomed to the PC environment. It is important to concentrate effort to the understanding of Omola and try not to be hindered by the rough edges of UNIX and OmSim.

7 Acknowledgments

This report is a masters thesis in Chemical Engineering presented at the Department of Automatic Control, Lund Institute of Technology in collaboration with Kemira Kemi AB in Helsingborg, Sweden.

I would like to thank everybody who has helped me with this report; Leif Hansson, Lars Pålsson and Lars-Erik Lindell at Kemira Kemi AB; Sven-Erik Mattsson, Tomas Schönthal and Bernt Nilsson at the Department of Automatic Control. A special thank you to my supervisor Jonas Eborn for having patience with me and always being supportive.

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Appendix

Summary in the form of a scientific article, as required by the regulations for a masters thesis in Chemical Engineering at Lund Institute of Technology.

MODELING OF THE STEAM GENERATION IN A SULFURIC ACID PLANT.

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Abstract – This paper concerns an effort to model the steam generation at Kemira Kemi's sulfuric acid plant in Helsingborg, Sweden.

The making of sulfuric acid starts with the oxidation of elementary sulfur in an exothermic reaction. The released energy is used in the waste heat boiler to produce high pressure steam. A model of this process consisting of burner, waste heat boiler and drum with controllers has been constructed. In the development of this model the theory of combustion and heat transfer is studied. The shrink-and-swell phenomenon, affecting the drum level dynamics, and the consequent control problem is given special attention.

The developed plant model is simulated and the results are found in good resemblance with the actual plant. No real validation, however, has been made.

INTRODUCTION

This paper is a part of my Masters Thesis in Chemical Engineering at the Lund Institute of Technology. An effort is made to model the steam generation at a sulfuric acid plant. The plant modeled is Kemira Kemi's plant in Helsingborg, Sweden. At Kemira Kemi there has been a continuing effort to increase their employees competence and this model is a continuing of this effort.

The first step in the production of sulfuric acid is the oxidation of liquid sulfur to sulfur dioxide. This is an exothermic reaction and the release of energy raises the temperature of the gas to 1800 °C. The gas exchanges heat in a waste heat boiler to produce high pressure steam. The steam is used to produce electricity and furnish other facilities at the Helsingborg plant with high pressure steam.

The combustion- and heat transfer theory used in the model is covered in the theory chapter. Following this the developed model is described then an excerpt from simulations using the finished model is shown and finally conclusions.

Modeling is done using Omola, an object-oriented modeling language developed at the Department of Automatic Control.

THEORY

Combustion

The first step in making sulfuric acid is the oxidation of elementary sulfur to sulfur dioxide

$$S\,(l) + O_2\,(g) \rightarrow SO_2\,(g)\ \Delta H_1 = -297\text{kJ/kmol}$$

The oxidation takes place in a rotary burner where sulfur is burnt. The oxygen is supplied in the form of dried and preheated air. The combustion chemistry is quite complex with many combustion products possible, for example SO_3. The air is dried to prevent the small amounts of formed SO_3 from reacting with water forming sulfuric acid. An oxygen deficit keeps the formation of NOx gases low. The λ value describes the ratio between sulfur and oxygen flow. A value of 0.95 means that for every mole sulfur fed to the burner there is 0.95 mole oxygen supplied. The remaining sulfur evaporates, in an endothermic reaction, according to:

$$S\,(l) \rightarrow \tfrac{1}{2} S_2\,(g)\quad \Delta H_2 = 55\text{ kJ/mol.}$$

The gas that enters the waste heat boiler is composed of N_2, SO_2 and S_2.

The resulting temperature of the combustion gases is a matter of some discussion. Here the adiabatic combustion temperature is derived, see (Reklaitis,1985). A simple energy balance:

IN + PRODUCED = OUT +
ACCUMULATED

leads to the formation of an implicit expression for the combustion temperature:

$$\Sigma n_{i,prod} \cdot Cp_{i,prod} \cdot T_{i,prod} = \text{PRODUCED} + \Sigma\, n_{i,reac} \cdot Cp_{i,reac} \cdot T_{i,reac.}$$

The Cp values are temperature dependent and their value increases with temperature. The PRODUCED term is the resulting heat release from the two reactions above:

$$\text{PRODUCED} = -\lambda \cdot n_{sulfur,in} \cdot \Delta H_1 - (1-\lambda) \cdot n_{sulfur,in} \cdot \Delta H_2$$

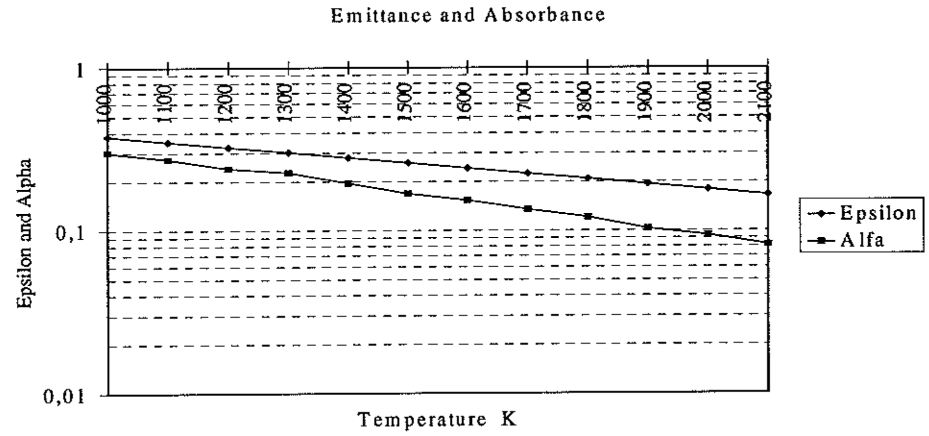


Fig 1 Emittance and Absorbance of the flue gas at different gas temperatures.

Heat transfer

Heat transfer occurs in the waste heat boiler directly adjacent to the burner. Heat is transferred from the gas to the water side. Heat transfer from the gas to the metal tube is due to both radiation and convection, conduction through the metal and convection on the water side, see Fig 2.

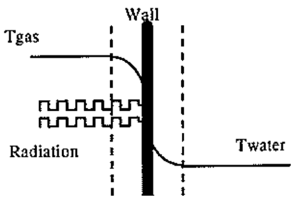


Fig 2 Heat transfer.

Many gases are transparent to thermal radiation, i.e. they do not absorb nor emit radiation. However due to the asymmetrical structure of SO_2 it is a radiating gas with both a vibrational spectrum and a rotational spectrum. In (Holman,1992) a method is described for calculating gas emittance for engineering purposes. The method involves Stefan Boltzman´s law:

$$E_b = \sigma \cdot T^4$$

which states that the total emitted energy is proportional to the temperature of the forth order. A geometry factor called the mean beam length, L_e, is added to take into account different possible geometries of the waste heat boiler. The resulting equation of the total heat transfer due to radiation is

$$q/A = \varepsilon_g(p, T_g, L_e \cdot pSO_2) \cdot \sigma \cdot T_g^4 - \alpha_g(p, T_g, T_w, L_e \cdot pSO_2) \cdot \sigma \cdot T_w^4$$

where ε_g is the gas emittance and α_g is the gas absorbance. ε_g is dependent on gas temperature and α_g is dependent on gas temperature and the temperature of the wall. Fig 1 shows the emittance and absorbance for different gas temperatures, the wall temperature is 260 °C. The total heat transfer due to radiation is very high, between 20 and 180 kW/m^2. As a result the heat transfer due to convection can be neglected.

Shrink-and-swell

The shrink-and-swell phenomenon occurs in the waste heat boiler drum and affects the drum level during pressure changes. Shrink-and-swell is also responsible for the non-minimum phase character of the drum, see (Hägglund, 1990). Modeling of the drum level dynamics has been of interest for a long time. In (Bell and Åström,1996) a fourth order model is derived. The drum level is defined:

$$\text{level} = \frac{V_w + V_{sd}}{A}$$

consisting of one volume of water Vw and one volume of steam, Vsd. Vsd is the volume of steam that is submerged under the water level in the drum. If a process alteration is made that influences the pressure of the drum, the volume of steam submerged in the drum changes according to the equation:

$$\frac{dV_{sd}}{dt} = -\frac{V_{sd}}{T} + \frac{h_{fw} - h_w}{h_c \rho_s} q_{fw} - \left(\frac{V_{sd}}{h_c} \frac{\partial h_s}{\partial p} + \frac{\rho_w V_w}{\rho_s h_c} \frac{\partial h_w}{\partial p} + \frac{V_{sd}}{\rho_s} \frac{\partial \rho_s}{\partial p} \right) \frac{dp}{dt} + \frac{V_{0sd}}{T}$$

V_{0sd} is the volume of steam under the water surface in steady state.

Drum control

The control of the drum level is complicated. At steady state there is a certain volume of steam submerged under the water surface. If the feed water valve opening is increased water enters the drum. This lowers the total enthalpy of the drum collapsing submerged steam bubbles and thus lowering the drum level. Control problems as these leads to the use of a three point controller, see (Hägglund,1990) and Fig 3, for drum level control.

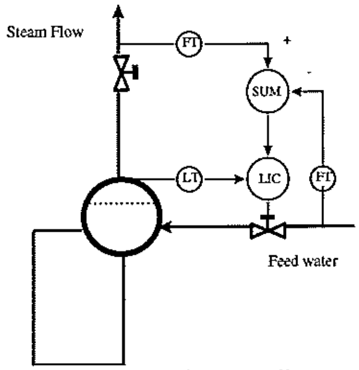


Fig 3 Three point controller

The three points refers to drum level, steam flow and feed water flow. The difference in feed water flow and steam flow is used as feed forward to the level controller.

MODELING

Modeling of complex systems can be done in many different ways. In this work a dynamic object-oriented approach has been used. Omola is an object-oriented modeling language developed at the Dept. of Automatic Control at Lund Institute of Technology. Omola is influenced by and captures many of the concepts of object-oriented programming such as inheritance and reuse. Omola supports dynamic simulation and is implemented in a UNIX environment. For an introduction to Omola see (Mattsson *et al*,1993). The developed plant model also makes use of work already done in the K2 project where an effort is made to model a Sydkraft biogas plant in Värnamo, Sweden.

The plant model describes the steam generation at Kemira Kemi in Helsingborg. The model includes burner, waste heat boiler and steam drum with controllers. The model is dynamic and a change of a parameter leads to a transition from one steady state to another. The model is composed of different submodels. Some are used from the K2 library unchanged, some with alterations and others are new.

A central idea in model making is decomposition and composition. In decomposition a part of a plant is extracted and decomposed into smaller parts. These can, if necessary, be further decomposed. The idea is to end up with small well defined areas that are easy to model. In Fig 4 the steam generation is decomposed into burner, waste heat boiler and drum with controllers.

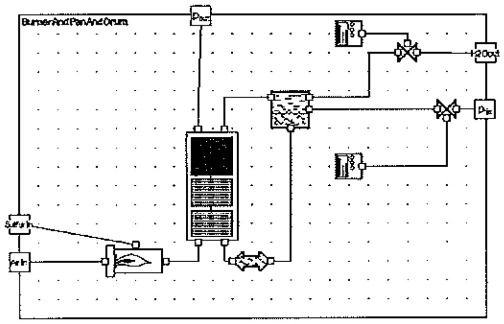


Fig 4 Steam generation - decomposed.

In Fig 5 the waste heat boiler is further decomposed, separating gas and water/steam flows indicating the heat transfer process. Three sections of the waste heat boiler deliver energy to a single water/steam compartment.

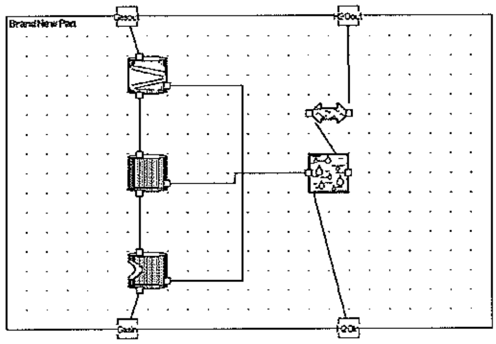


Fig 5 Waste heat boiler - decomposed.

SIMULATION

A simulation of the plant model generates a vast amount of data. A presentation of some interesting results is followed by a simulation of how a drum pressure change influence the drum level.

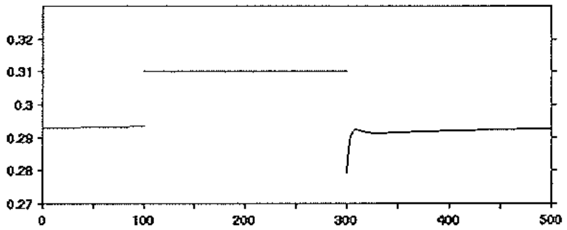
Simulation results

The sulfur flow to the burner determines the air flow, which in turn determines the adiabatic combustion temperature and so forth. The model uses SI units but in some cases more conventional units are used in parallel.

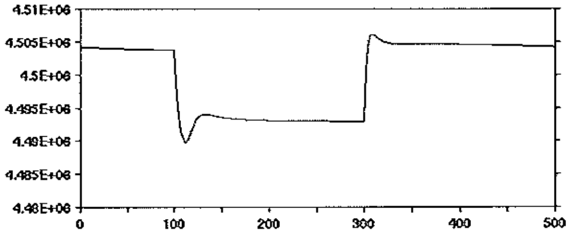
Burner:
Sulfur flow = 4.3 kg/s=15.5 ton/h
Sulfur temperature = 180 °C
Air flow = 17.6 kg/s, $\lambda = 0.95$
Air temperature = 220 °C
Flue gas flow = 21.9 kg/s
Flue gas temperature = 1770 °C
Waste heat boiler:
Gas temperature IN = 1770 °C
Gas temperature OUT = 840 °C
Water flow down comer = 124 kg/s
Water temperature IN = 257 °C
Water temperature OUT = 257 °C
Steam mass ratio = 0.11
Total heat transfer = 23.7 MW
Steam drum:
Pressure = 45 bar
Level = 0.9 m (half full)
Submerged steam = 0.5 m^3
Steam flow OUT = 14 kg/s
Water flow IN = 14 kg/s

Shrink-and-swell

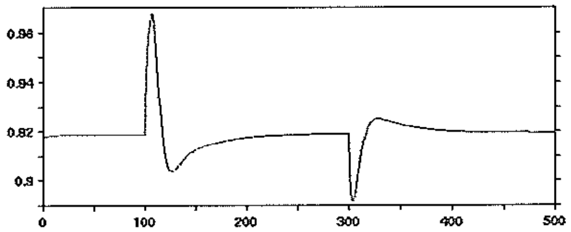
The shrink-and-swell phenomenon is difficult to understand. The problem is accentuated during start up. In this simulation the steam valve opening is increased manually at t=100s and the controller is put back in automatic again at t=300s. When the steam valve opening is increased this causes a drop in drum pressure. The pressure change influence the volume of submerged steam bubbles in the drum affecting drum level. In Fig 6 the change in drum level can be followed. The x-axis unit is time in seconds.



Valve setting [%]



Drum Pressure [Pa]



Drum level [m]

Fig 6 Simulation of steam valve changes.

CONCLUSIONS

Modeling of large systems as the steam generation requires knowledge in a wide variety of areas. The model covers combustion chemistry, heat transfer through radiation, convection and conduction and process control.

The developed plant model describes the steam generation at a sulfuric acid plant. The resemblance is good but no real validation against the actual plant has been done. Even if the model should over-emphasize certain phenomena, it offers plenty of opportunities of tailoring the model to increase the resemblance to the real facility at Kemira Kemi AB.

The model is developed using Omola, an object oriented modeling language. Omola is straight forward and quite easy to use. But as in all other programming there is a large amount of time spent correcting code. However, Omola gives you the opportunity to start with a small defined area and model that area. A simulation is run to check consistency. When several different areas have been covered these can be assembled to build a large system. In this work the burner was modeled first, followed by the waste heat boiler, drum and controllers. A large part of the time was spent modeling the heat transfer in the waste heat boiler.

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