



## SPECIALIZATION PROJECT 2011

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PROJECT TITLE:

Catalytic combustion control

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By

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# Abstract

Dynamic models for the different units of a catalytic waste gas incineration process were derived. The models were derived with a subsequent improvement of the existing control structure as the main objective. The processes were modelled using a lumped systems approach in order to avoid partial differential equations.

Process parameters, like heat transfer coefficients, were adjusted for each of the units in order to provide results as close as possible to the experimental plant data.

Functions computing the derivative of the given temperatures with respect to time were written in Matlab, and custom blocks solving these differential equations were implemented in Simulink using s-functions. Finally the different process units were connected in Simulink.

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# 1 Introduction

The Perstorp group is a world leader in several sectors of the speciality chemicals market, with sites located in different parts of the world. In this project, the site in Perstorp in Sweden is considered.

Catalytic incineration of waste gases is a common way of waste treatment which involves the catalytic combustion of organic substances, in this case volatile organic components that cannot simply be released to the atmosphere due to environmental restrictions. The catalytic incinerators at Perstorp treat gases from various parts of the plant, depending on the activity. As a result, the composition of the gas may vary rapidly, which makes the process control challenging.

A functional and stable control structure is important for many reasons – for optimal operation, for minimization of energy usage and for safety. Due to these variations in the inlet gas, the incinerators at Perstorp have had issues with absorption of organic compounds to the catalyst bed. This may lead to explosions due to rapid increase in temperature when they subsequently desorb and combust.

The main objective of this project was to get familiar with and derive a reasonable model for the catalytic waste gas incineration process at Perstorp. Identification of the most important aspects to include in the model and dynamic behaviour was the main focus. The model should be derived for the purpose of subsequent improvement of the process control structure. Familiarizing with implementation of custom blocks using s-functions in Simulink was also an important part of the project.

## 2 Background

### 2.1 Catalytic incineration<sup>1</sup>

Incineration is a waste treatment process which involves combustion of organic waste materials. Thus it is high-temperature, controlled combustion of unwanted compounds.

Incinerators are widely used in industry to avoid emissions of harmful organic compounds. Off-gases from chemical processes may contain organic compounds which cannot simply be released to the atmosphere in their current form. These can thus be lead through an incinerator where they are completely combusted to CO<sub>2</sub> and water.

Thermal incinerators are usually operated at high temperatures, approximately 800°C. This is to ensure complete combustion and stable operation. Firing auxiliary fuel is required to maintain and control this temperature as it most usual is not self-sustaining. However, at such a high temperature, harmful by-products like nitrogen oxides and carbon monoxide are also formed. Firing of auxiliary fuel also leads to increased emissions.

Today, catalytic incinerators are usually preferred over thermal incinerators. Catalysts can lower the temperature required for complete combustion to approximately 200°C-400°C. The advantages of this are many - mainly, reduced or zero fuel consumption and thus reduced CO<sub>2</sub> emissions, and negligible formation of secondary pollutants such as CO. In addition, less expensive construction materials can be used for the incinerator. Catalytic incinerators also have a high cleaning efficiency, usually of 99.8% or higher.

In this project, a catalytic incineration process is considered.

### 2.2 Process description

The process considered in this project is the catalytic incinerator at Perstorp, Sweden. The incinerator treats waste gases from various parts of the plant, like crystallizers, reactors, distillation columns and vacuum systems. The waste gases contain mainly MIBK (methyl isobutyl ketone), but also other volatile organic compounds like metachrolein, methanol, methylal and methyl formate.

The catalyst used is PPt-47, a common catalyst for volatile organic compounds oxidation purposes. It consists of 0.1 wt% platinum as an active component, on the support material alumina.

The concentrations of the different organic compounds in the waste gases vary significantly during operation. For example, FTIR analyses of the incoming waste gas to the process has shown the

concentration of MIBK to range from approximately 5000 to 10 000 mg/Nm<sup>3</sup> waste gas in 15 minutes (see appendix X).

An overview of the process is shown in figure 1.

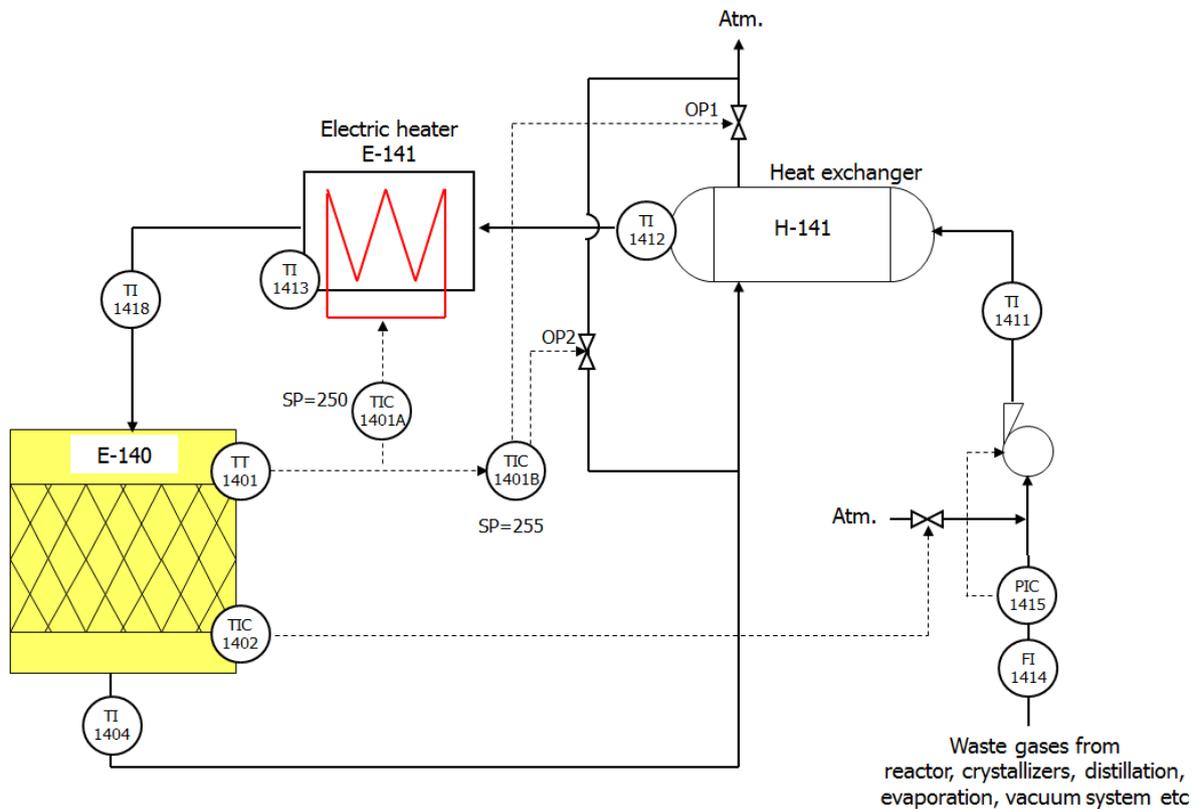


Figure 1 A simple overview of the catalytic incineration process at Perstorp and the current control structure.

The waste gases are preheated first in a heat exchanger, and further in an electric heater in order to reach minimum required temperature for the reactor inlet. In the reactor, the organic compounds are combusted to CO<sub>2</sub> and water under the influence of a catalyst. The hot outlet gases are then passed through the heat exchanger to preheat the incoming gases before being released to the atmosphere.

It is important to ensure that the temperature of the waste gases is above 250°C before entering the reactor. This is to avoid adsorption of organic compounds to the catalyst. The adsorbed compounds will subsequently desorb when the temperature in the reactor increases. This sudden increase in concentration of gaseous organic compounds in the reactor results in a large amount of heat being released from the combustion, which may in the worst case cause an explosion.

The temperature of the outlet gas from the reactor must be kept above 400°C in order to ensure complete combustion of the organic compounds. However, to minimize the risk of explosions, the temperature must be maintained below 500°C.

## 2.3 Current control structure and purpose

An overview of the current control structure of the catalytic incineration process can be obtained from figure 1.

As the figure shows, there are 3 controlled variables in this process:

- The gas temperature at the reactor inlet,  $T_{in}$
- The gas temperature at the reactor outlet,  $T_{out}$
- The pressure at the process inlet

### 2.3.1 Temperature controller TIC-1401

$T_{in}$  is controlled by the temperature controllers TIC-1401a and TIC-1401b. The purpose of these controllers is to provide a sufficiently high gas temperature before it enters the reactor, as explained in the previous section. TIC-1401a measures the temperature at the inlet of the reactor and controls it by manipulation of the effect to the electric heater E-141. It has a setpoint of 250°C. The latter has the same measurement, but manipulates the heat exchanger bypass, e.g. the two control valves TV1-1401 and TV2-1401 and has a setpoint of 255°C. This is a slightly higher setpoint than for the former controller to avoid unnecessary use of electricity.

### 2.3.2 Temperature controller TIC-1402

$T_{out}$  is controlled by the temperature controller TIC-1402. It measures the temperature at the outlet of the reactor, and controls it by manipulation of the control valve TV-1402. This valve adjusts the flow of air which is added to the waste gas stream. This controller has a setpoint of 450°C. If the reactor temperature exceeds the setpoint, the air flow is increased. This decreases the concentration of organic compounds in the waste stream, which results in a lower temperature increment due to the combustion.

### 2.3.3 Pressure controller PIC-1415

The pressure at the process inlet is controlled by the pressure controller PIC-1415. It measures the pressure upstream of the air inlet, and controls it by adjusting the power to the fan F-141. It has a setpoint of -20 mm Wg.

## 2.4 Modelling of chemical process systems<sup>2,3</sup>

There are many approaches when it comes to modelling of chemical process systems. Mainly, such mathematical models contain two aspects – an energy balance and a mass balance.

For control purposes, dynamic models, i.e. models containing the time derivatives of the states, are used. The more complex, local models for example for a reactor, may contain spatial derivatives in both axial and radial direction. For most applications, however, it is sufficient to use less complex area- or volume averaged models.

### 2.4.1 Basic energy balance

The total energy of a given chemical system can be described as the sum of the internal energy  $U$ , the potential energy  $P$  and the kinetic energy  $K$ :

$$E \hat{=} U + K + P$$

In chemical engineering, the control volumes generally have constant kinetic and potential energy, such that

$$\frac{d(K+P)}{dt} = \sum_{\forall m} \alpha_m (\hat{K}_m + \hat{P}_m) \approx 0$$

where  $m$  represents the mass flows,  $\alpha$  the direction of the flows with respect to a reference coordinate ( value  $\pm 1$  ) and  $\hat{K}_m$  and  $\hat{P}_m$  the changes in kinetic and potential energy due to mass flows. This assumption requires that the control volume is stagnant, and that the center of mass does not change in vertical direction. It also requires that there is no kinetic energy conserved in the mass flows in terms of turbulence or eddies.

Neglecting the change in potential and kinetic energy, the change in energy of the system can be described entirely by the change in its internal energy

$$\frac{dE}{dt} = \frac{dU}{dt}$$

The change in energy of a system is determined by energy flows. These can be divided into energy flows due to mass flows, heat flows, work flows and system volume work flow:

$$\frac{dE}{dt} = \frac{dU}{dt} = \sum_{\forall m} \alpha_m \hat{E}_m + \sum_{\forall m} \alpha_m p_m \hat{V}_m + \sum_{\forall q} \alpha_q \hat{q}_q + \sum_{\forall w} \alpha_w \hat{w}_w - p \frac{dV}{dt}$$

where the indices  $m$ ,  $q$  and  $w$  refer to mass, heat and work flows, respectively.

Enthalpy is defined as:

$$H \triangleq U + pV$$

Differentiation yields

$$\frac{dH}{dt} = \frac{dU}{dt} + \frac{dp}{dt}V + p \frac{dV}{dt}$$

Assuming constant pressure and inserting the remaining terms into the total energy balance, this yields

$$\frac{dU}{dt} + p \frac{dV}{dt} = \frac{dH}{dt} = \sum_{\forall m} \alpha_m \hat{H}_m + \sum_{\forall m} \alpha_m p_m \hat{V}_m + \sum_{\forall q} \alpha_q \hat{q}_q + \sum_{\forall w} \alpha_w \hat{w}_w$$

Enthalpy is a function of pressure, temperature and composition:

$$H \triangleq H(p, T, m_1, m_2, \dots, m_n)$$

Thus, its total derivative can be written as:

$$\frac{dH}{dt} = \frac{\partial H}{\partial p} \frac{dp}{dt} + \frac{\partial H}{\partial T} \frac{dT}{dt} + \sum_{\forall i} \frac{\partial H}{\partial n_i} \frac{dn_i}{dt}$$

As constant pressure is assumed, the first term on the right hand side can be neglected. Further, the partial derivative of enthalpy with respect to temperature is defined as

$$\frac{\partial H}{\partial T} \triangleq \rho V c_p$$

where  $\rho$  is the density of the fluid,  $V$  is the volume of the given system and  $c_p$  is the specific heat capacity at constant pressure.

Further, the partial derivative of enthalpy with respect to the component masses is defined as the partial molar enthalpy

$$\frac{\partial H}{\partial n_i} \triangleq h_i$$

Introducing these terms into the total energy balance gives the expression

$$\rho V c_p \frac{dT}{dt} = \sum_{\forall m} \alpha_m \sum_{\forall i} h_{i,m} n_{i,m} - \sum_{\forall i} h_i \frac{dn_i}{dt} + \sum_{\forall m} \alpha_m p_m \hat{V}_m + \sum_{\forall q} \alpha_q \hat{q}_q + \sum_{\forall w} \alpha_w \hat{w}_w$$

With the time derivative of the masses of the components  $i$  being the component mass balance assuming no significant chemical reaction

$$\frac{dn_i}{dt} = \sum_{\forall m} \alpha_m \hat{n}_{i,m}$$

the total energy balance can be written as

$$\rho V c_p \frac{dT}{dt} = \sum_{\forall m} \alpha_m \sum_{\forall i} (h_{i,m} - h_i) \hat{n}_{i,m} + \sum_{\forall m} \alpha_m p_m \hat{V}_m + \sum_{\forall q} \alpha_q \hat{q}_q + \sum_{\forall w} \alpha_w \hat{w}_w \quad (1)$$

where the second last term is normally describes using simple heat transfer laws.

## 2.5 Methods for simulation and solving of ODE systems<sup>5</sup>

In Matlab, ordinary differential equations can be solved using built-in solvers. These solvers, for example ode15s in Matlab or s-functions in Simulink, are mainly based on numerical integration methods like Runge-Kutta.

Differential equations can be built directly in Simulink using predefined blocks connected accordingly. However, this does not provide a very flexible model. For example for models consisting of a series of lumped systems, increasing or decreasing the number of lumped elements is an inconvenient task as the number of differential equations increases or decreases. On the other hand, if one defines the system of ODEs in a Matlab function, for example using if-loops, these can be implemented in custom Simulink blocks using s-functions. An s-function, or system-function, is a computer language description of a Simulink block written in Matlab, C, C++ or Fortran.

Matlab s-functions have the following form:

$$[sys,x0]=f(t,x,u,flag)$$

where t (current time), x (state vector), u (input vector) and flag (integer value indicating task to be performed by s-function) are arguments that the Simulink engine passes to the s-function.

In this project, only the flags 0, 1 and 3 are used. Flag = 0 defines initialization, which means that initial conditions and the size of the system, like number of inputs, states and outputs, is defined. Flag = 1 defines calculation of the derivatives of the continuous state variables, and flag=3 calculates the outputs of the s-function.

## 3 Modelling and implementation

### 3.1 Objective

The main objective of this project is the derivation of a mathematical model of the catalytic incineration process at Perstorp. The accuracy and thus level of complicity of such a model has to be determined on a case-by-case basis.

In this project, the main objectives for the model were as follows:

- **Provide realistic simulations.** The model should provide simulation results and responses corresponding to the provided experimental plant data from the actual process at Perstorp.
- **Not make an unnecessarily complicated model.** The model should be derived with its actual purpose in mind, which is improvement of the control structure. This implies that the main focus should be on providing the correct *dynamic* behaviour of the process, and not on achieving the *exact* same temperatures and conditions as provided from plant data.
- **Control implementation convenience.** The model should be constructed with the subsequent control, and thus implementation in Simulink, in mind.

### 3.2 Modelling and assumptions

The model derived for the process will be explained for the 3 main parts separately, which are the heat exchanger, the electric heater and the catalytic incinerator. However, some basic assumptions that were made apply to the derivation of all of these models.

Firstly, in order to avoid the more complicated partial differential equations, the heat exchanger and the reactor were decided to be modelled as a series of lumped systems. This means that instead of introducing a spatial or axial derivative, the process is divided into a series of  $N$  connected “lumps”, which are assumed to be perfectly mixed and thus have no gradients. The temperature and conditions of the stream exiting the lump are thus the same as inside of the lump. Using this approach, each lump represents a spatial position throughout the process.

Further, due to lack of knowledge about the pressures throughout the process, the pressure drop is neglected. In addition, the mass based flow rate of the gas is assumed not to change throughout the process.

The density of the gas in each lumped element is computed using the ideal gas law:

$$\rho_g = \frac{PM}{RT} \quad (2)$$

where P is the given pressure in atm, M is the molecular mass in kg/mol, R is the universal gas constant in m<sup>3</sup>\*atm/K\*mol

### 3.2.1 Heat exchanger <sup>4</sup>

The countercurrent heat exchanger with a hot side bypass is modelled using the lumped systems approach. This means that the cold gas side, the hot gas side and the heat transfer wall are divided into a number of N lumped elements as shown in figure 2.

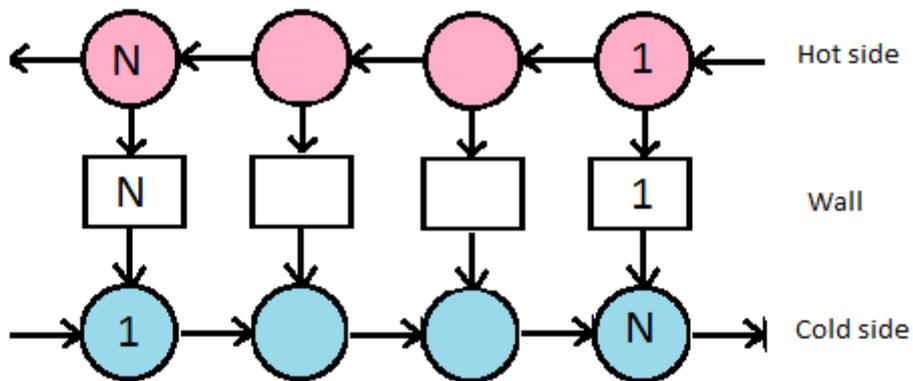


Figure 2 – Flow configuration and numbering of the elements for modelling the countercurrent heat exchanger

The following assumptions were made during the modelling of the heat exchanger:

- No conductive heat transfer between the different heat exchanger wall elements.
- The gas on both the hot and cold side is assumed to have a residence time of approx.1 second.
- Negligible pressure drop
- Constant heat capacities of the gas and wall
- Constant heat transfer coefficients
- Negligible heat loss to the environment

- The cold and hot side heat exchanger volumes are split up into an equal number of lumped elements with equal volumes, thus the heat transfer areas are equal on both sides
- The heat transfer coefficients from the gas to the wall are equal on hot and cold side

From equation 1 and using the configuration as shown in figure 2, application of these assumptions yields

for the cold side fluid:

$$\frac{\rho_g V_c c_{p,g}}{N} \frac{dT_c(i)}{dt} = \dot{m}_g c_{p,g} (T_c(i-1) - T_c(i)) - \frac{h_w A_w}{N} (T_c(i) - T_w(N+i-1)) \quad (3)$$

for the hot side fluid:

$$\frac{\rho_g V_h c_{p,g}}{N} \frac{dT_h(i)}{dt} = (1-\alpha) \dot{m}_g c_{p,g} (T_c(i-1) - T_c(i)) - \frac{h_w A_w}{N} (T_c(i) - T_w(i)) \quad (4)$$

and for the wall elements

$$\frac{m_w c_{p,w}}{N} \frac{dT_w(i)}{dt} = \frac{h_w A_w}{N} [(T_c(N+i-1) - T_w(i)) + (T_h(i) - T_w(i))] \quad (5)$$

where N is the number of elements,  $\dot{m}_g$  is the mass flow of gas,  $\rho_g$  is the gas density computed from ideal gas law,  $c_{p,w}$  and  $c_{p,g}$  are the specific heat capacities for the heat transfer wall and gas,  $T_c(i)$ ,  $T_w(i)$  and  $T_h(i)$  are the cold side, wall and hot side temperatures in element number I according to figure 2,  $A_w$  is the heat transfer area,  $h_w$  the heat transfer coefficient,  $V_h$  and  $V_c$  the hot and cold side volume and  $\alpha$  is the hot side bypass fraction.

### 3.2.2 Electric heater

The electric heater is modelled very simply as a single lumped system, without gradients. Energy is supplied directly to the gas phase, not taking into account heat transfer coefficients. Heat loss to the environment is also neglected.

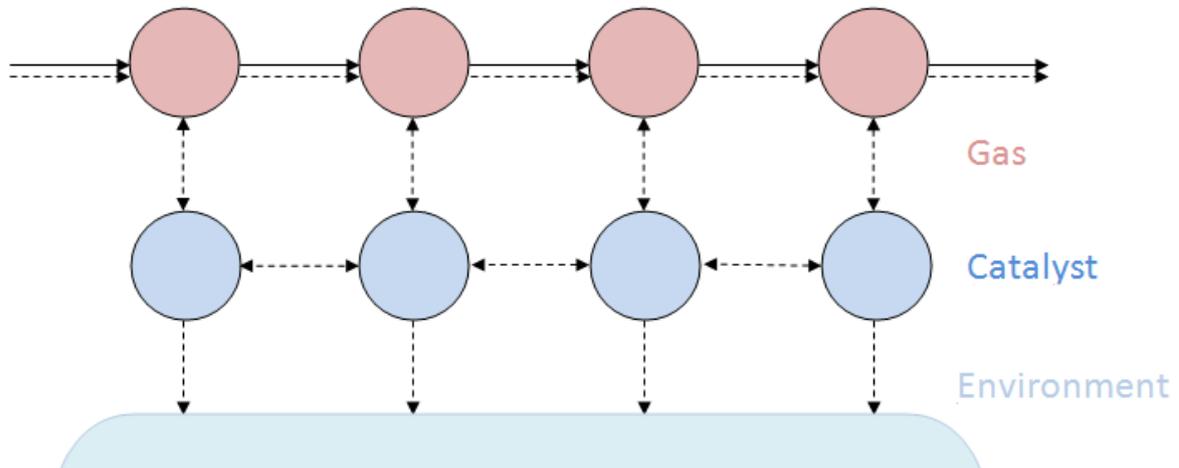
From equation 1, this yields:

$$\rho_g V c_{p,g} \frac{dT_{out}}{dt} = \dot{m}_g c_{p,g} (T_{in} - T_{out}) + \dot{W} \quad (6)$$

where V is the volume of the heater and  $\dot{W}$  is the added effect.

### 3.2.3 Catalytic incinerator

The catalytic incinerator is also modelled using the lumped systems approach. The gas volume and the catalyst phase inside the reactor are divided into a number  $N$  of lumped elements as shown in figure 3.



**Figure 3 – Schematic of the mechanisms included in the incinerator model**

The features included in the model can also be seen from the figure. These are convective mass transfer in the gas phase, convective heat transfer in the gas phase, heat of reaction in the gas phase, heat transfer between the gas- and catalyst phase, conductive heat transfer in the catalyst phase and heat loss through the reactor wall.

The following assumptions were made during the modelling of the catalytic incinerator:

- The reaction happens instantaneously in the lump in which the gas temperature exceeds the ignition temperature, which is 270°C.
- The reaction reaches 100% conversion, i.e. it is not limited by equilibrium.
- Heat loss through to the environment primarily happens from the catalyst phase through the reactor wall

Applying these assumptions to the general energy balance given in equation 1, this yields for the gas phase

$$\frac{\rho_g V_g c_{p,g}}{N} \frac{dT_g(i)}{dt} = \dot{m}_g c_{p,g} (T_g(i-1) - T_g(i)) - \frac{(UA)_{cat}}{N} (T_g(i) - T_{cat}(i)) + \dot{m}_g \omega_{VOC} \Delta_r H \quad (7)$$

and for the catalyst phase

$$m_{cat} c_{p,cat} \frac{dT_{cat}(i)}{dt} = \frac{(UA)_{cat}}{N} (T_g(i) - T_{cat}(i)) + (kA)_{cat} N [T_{cat}(i-1) + T_{cat}(i+1) - 2T_{cat}(i)] - \frac{(UA)_{wall}}{N} (T_{cat}(i) - T_{amb}) \quad (8)$$

where  $m_{cat}$  is the mass of catalyst,  $(UA)_{cat}$  and  $(UA)_{wall}$  are the heat transfer coefficients times heat transfer area between the gas and the catalyst and the catalyst and the environment,  $(kA)_{cat}$  is the thermal conductivity coefficient times the heat conduction area internally in the catalyst phase,  $(UA)_{wall} \omega_{VOC}$  is the mass fraction of volatile organic components and  $T_{amb}$  is the ambient temperature.

### 3.3 Implementation in Matlab/Simulink

The models for the heat exchanger, electric heater and catalytic incinerator were all simulated with the help of Matlab and Simulink. For each of the units, one function that calculates the time derivatives of the temperature was made in Matlab, and a corresponding custom Simulink block for solving the model was implemented using the s-function interface.

The implementation structure in terms of states, inputs and outputs for each unit will be described in the following subsections. Their respective Matlab codes are provided in appendices I-IX.

The choice and number of inputs and outputs is easily changed through the s-function and m-file if needed.

#### 3.3.1 Heat exchanger

The function computing the time derivatives of the temperatures of the cold gas side, hot gas side and wall elements, is given in the file HEX.m in appendix I. This function calculates the derivatives as given by equations 3-5. The s-function file HEXs.m in appendix II connects the function to Simulink which solves the differential equations numerically.

The states are:

- The cold side gas temperatures in each of the  $N$  elements, given as  $T_c$
- The hot side gas temperatures in each of the  $N$  elements, given as  $T_h$
- The wall temperatures in each of the  $N$  elements, given as  $T_w$

Thus, the system has  $3*N$  states.

The inputs to the function are:

- The mass flow rate of gas, given as  $m$
- The inlet cold side gas temperature to the process, given as  $T_{c0}$
- The bypass fraction, given as  $a$
- The inlet hot side gas temperature, which is the gas output temperature from the incinerator

The output returned by the Simulink block is:

- The cold side gas outlet temperature

### 3.3.2 Electric heater

The function computing the time derivative of the outlet temperature from the electric heater is given by the file `elheater.m` in appendix IV in accordance to equation 6. The corresponding s-function for simulation in Simulink is given in appendix V.

The state is:

- The outlet gas temperature , given as  $T$

The inputs to the block are:

- The inlet gas temperature  $T_c$ , i.e. the output from the heat exchanger block
- The mass flow  $m$ , given as input to the HEX block and defined globally for the process
- The effect  $W$

The output returned by the block is:

- The outlet gas temperature

### 3.3.3 Catalytic incinerator

The function computing the time derivatives of the temperatures of the gas phase and catalyst phase elements is given in the file `incin.m` in appendix VII. This function calculates the derivatives as given by equations 7-8. The s-function file `incins.m` in appendix VIII connects the function to Simulink which solves the differential equations numerically.

As shown in the Matlab code, the heat released in the gas phase due to the combustion reaction is implemented as an if-statement, and the mass fraction of reactive components is set to zero after the occurrence. This statement implies that the reaction occurs instantaneously and in only the first lumped element in which the temperature exceeds the ignition temperature of 270°C.

The states are:

- The gas phase temperatures in each of the  $N$  elements, given  $T(1:N)$
- The catalyst phase temperatures in each of the  $N$  elements, given as  $T(N+1:2*N)$

The inputs to the block are:

- The inlet gas temperature, which is the output temperature  $T$  from the electric heater
- The mass flow  $m$ , given as input to the HEX block and defined globally for the process
- The mass fraction of combustible volatile organic components, given as  $w$

The outputs returned by the block are:

- The gas temperature at the inlet of the reactor
- The gas temperature at the outlet of the reactor

## 4 Parameter fitting and simulation results

During the modelling of the given process, some parameters were known, some had to be assumed to have a given value and some had to be estimated and adjusted in order to provide results corresponding reasonably to the provided experimental data. This chapter will explain the parameters that are used in the Matlab files, and show the resulting simulation graphs.

### 4.1 General process parameters and conditions

The following are parameters that are used in all the modelled units, and that have been assumed based on given plant data and reason.

**Table 1 - Assumed properties of process system**

Parameter	Value
Fluid pressure [atm]	1
Molecular mass of gas (air) [g/mol]	29
Heat capacity of gas (air, at 200°C) [J/°C*kg]	1030
Approx. average flowrate of gas (1300 Nm <sup>3</sup> /h) [kg/s]	0.23

### 4.2 Heat exchanger

The data provided by Perstorp and literature regarding the heat exchanger are given in table 2. Appendix X shows the datasheet of the actual heat exchanger.

**Table 2 – Countercurrent heat exchanger H-141 data**

Shell (hot side) volume [m <sup>3</sup> ]	2.3
Tube (cold side) volume [m <sup>3</sup> ]	1.8
Heat transfer area [m <sup>2</sup> ]	115
Mass [kg]	2400
Wall heat capacity (steel) [J/kg°C]	500

For estimation of the heat transfer coefficient between the gas and heat exchanger wall, data from Perstorp where the bypass was not active were used. The data are shown in figure 4.

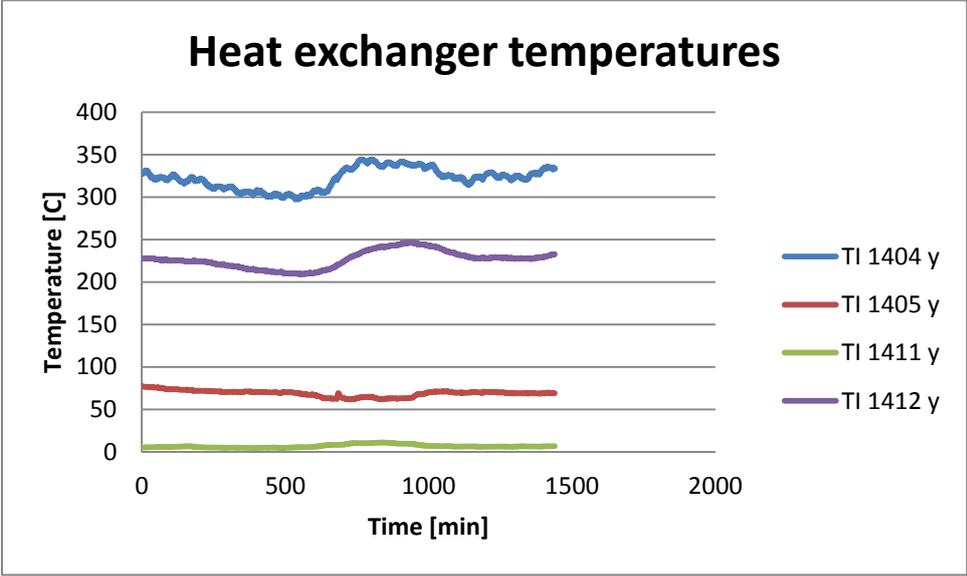


Figure 4 – Experimental temperature indicator data from the catalytic incineration process

Adjusting the heat transfer coefficient between the gas and heat exchanger wall using data given in table 2 and the given inlet temperatures from figure 4, i.e. 5°C for the inlet cold side temperature and 330° for the inlet hot side temperature, gave the results in figure 5. The value found for the heat transfer coefficient was 14 W/m<sup>2</sup>K.

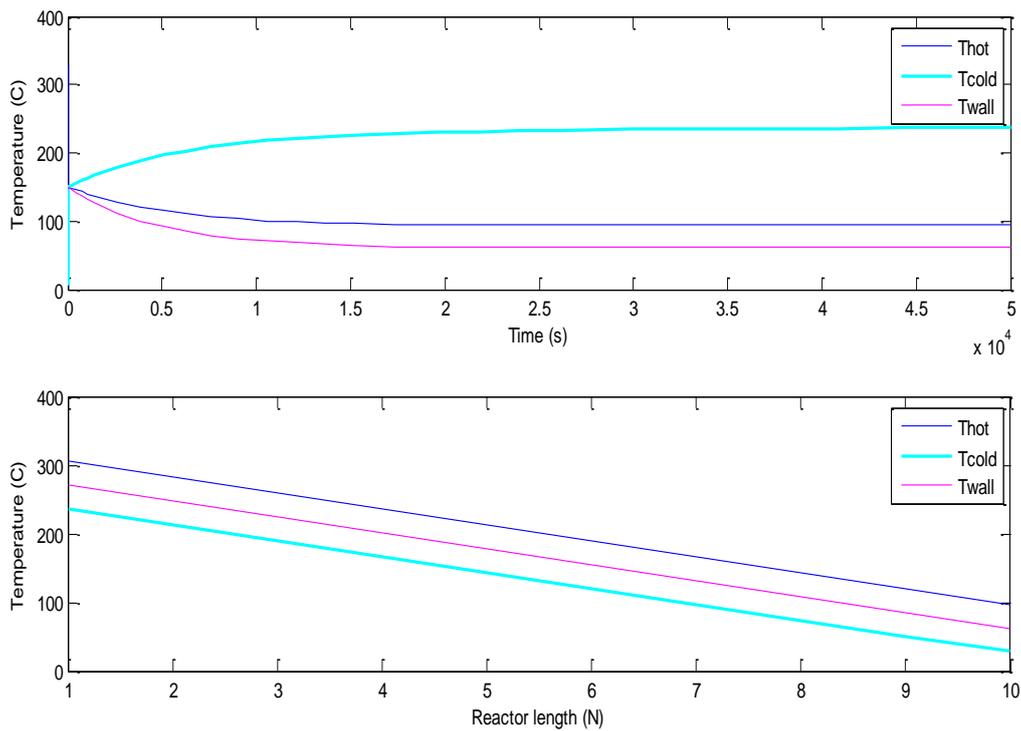


Figure 5 – Hot gas side, cold gas side and wall temperatures of the countercurrent heat exchanger simulated in Matlab

### 4.3 Electric heater

The information provided by Perstorp regarding the electric heater is given in the technical drawing in appendix X. The used information is given in table 3.

Table 3 - Data for electric heater E-141

Volume [m <sup>3</sup> ]	0.24
Max. effect [kW]	122.1

Figure 6 shows the response of the outlet temperature when inputting a step in effect from 0 to 1000 W for a mass flow rate of gas of 0.23 kg/s and an inlet temperature of 200°C

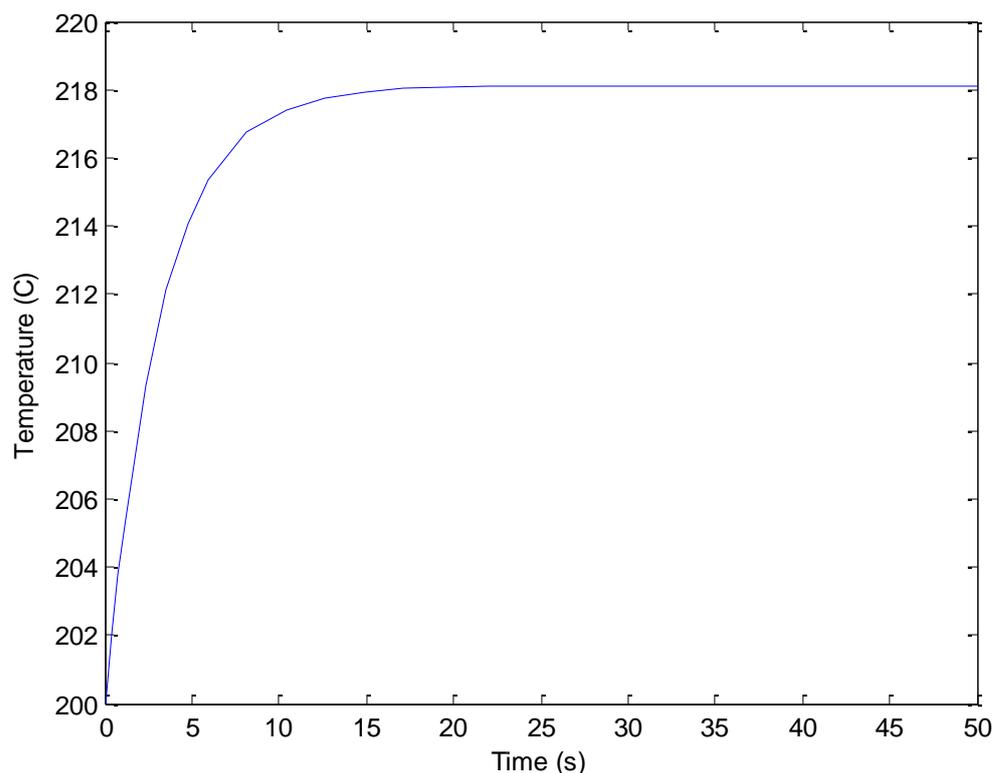


Figure 6 – Step response in outlet temperature from electric heater when inputting a step in added effect

## 4.4 Catalytic incinerator

The information provided by Perstorp regarding the catalytic incinerator is given in table 4.

Table 4 – Data for catalytic incinerator E-140

Mass of catalyst (kg)	280
Type of catalyst	Ppt-47

The catalyst consists of 99.9 wt% alumina. In various literature sources, alumina is stated to have a specific heat capacity of approx. 800 J/kg°C, so this value will be used in the simulations.

No information was provided regarding the void volume in the reactor, i.e. the volume which can be taken up by gas. Thus, it is assumed that a residence time of the gas in the order of magnitude of 1 second is reasonable. For the normal flowrate of about 0.23 kg/s and a gas density of about 0.5 kg/m<sup>3</sup> at 400°C, this yields a reactor volume of about 0.5 m<sup>3</sup>.

A mass fraction of 0.005 kg VOC/kg inert is used for the estimation of the heat transfer coefficients in the reactor. In addition, the heat of combustion of MIBK, which is 35 MJ/kg is used.

There are not given any corresponding data regarding mass fractions of combustibles and reactor temperatures, thus a random dataset for the temperatures was chosen. See appendix X for the placement of the temperature indicators.

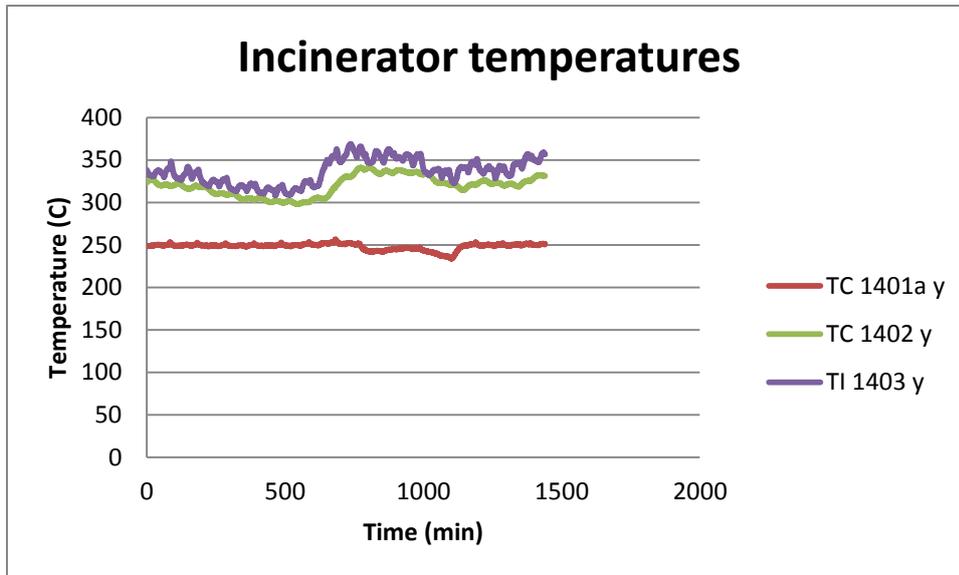


Figure 7 - Experimental temperature indicator data from the catalytic incineration process

Figure 7 shows that the temperature in the middle of the reactor is approximately 20°C higher than the temperature at the outlet of the reactor.

Simulation of the temperatures in the gas phase and catalyst phase as a function of reactor length and time, shows that for a value of the heat transfer coefficient times the heat transfer area for the catalyst,  $(UA)_{cat}$ , of 1000 W/K, and a heat loss coefficient  $(UA)_{wall}$  of 0.01 W/K, similar results are yielded. This is shown in figure 8, 9 and 10. In addition, a conductivity coefficient  $(kA)_{cat}$  of 100 Wm/K was used.

The simulations are done with an inlet temperature of 250°C for the gas phase, and initial condition 250°C in the gas phase for all elements and 350°C in catalyst phase for all elements.

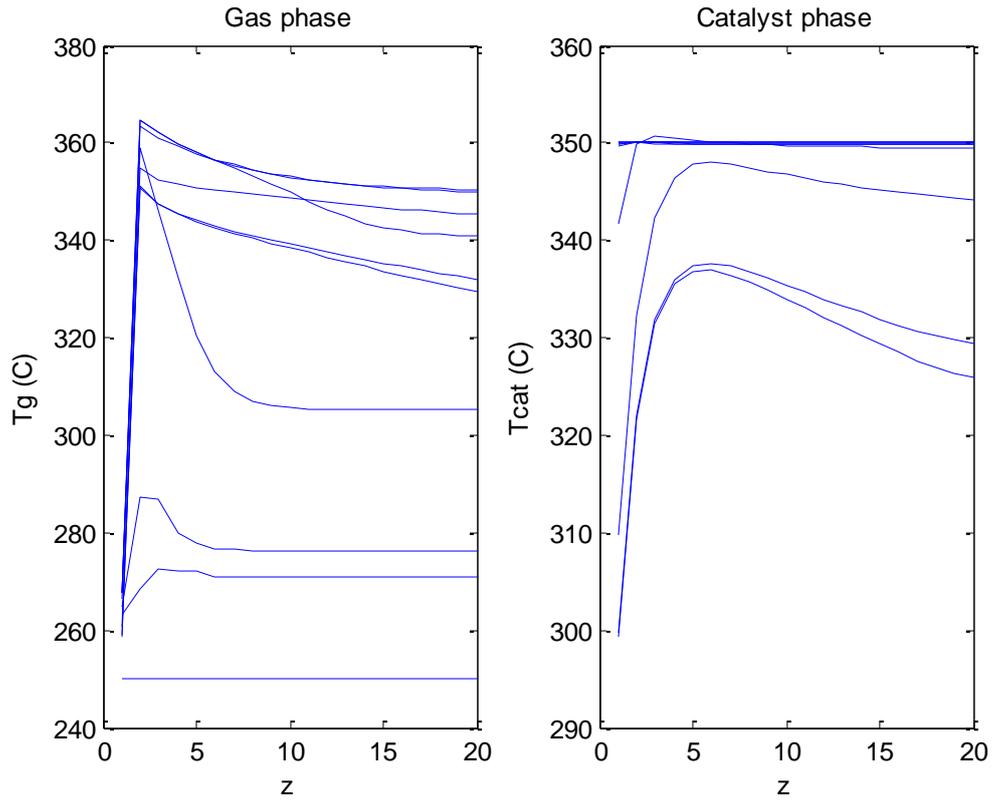


Figure 8 – The temperature profile throughout the reactor. The different lines represent different times.

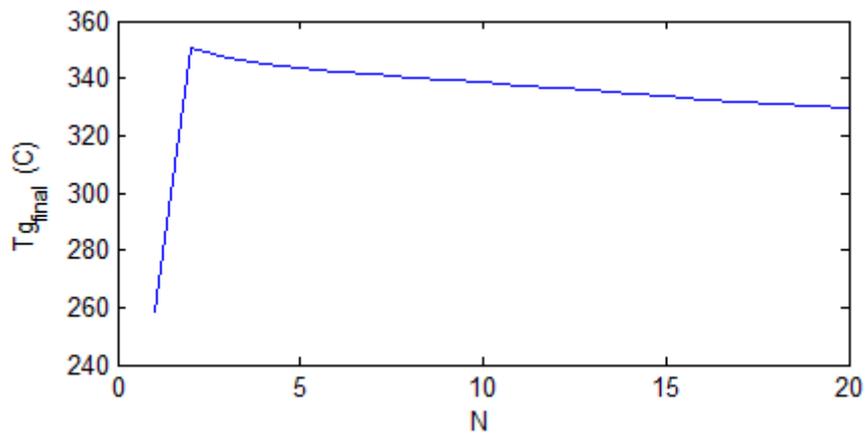


Figure 9 – The temperature profile throughout the reactor for the final integration time, i.e.  $t=10000$  s.

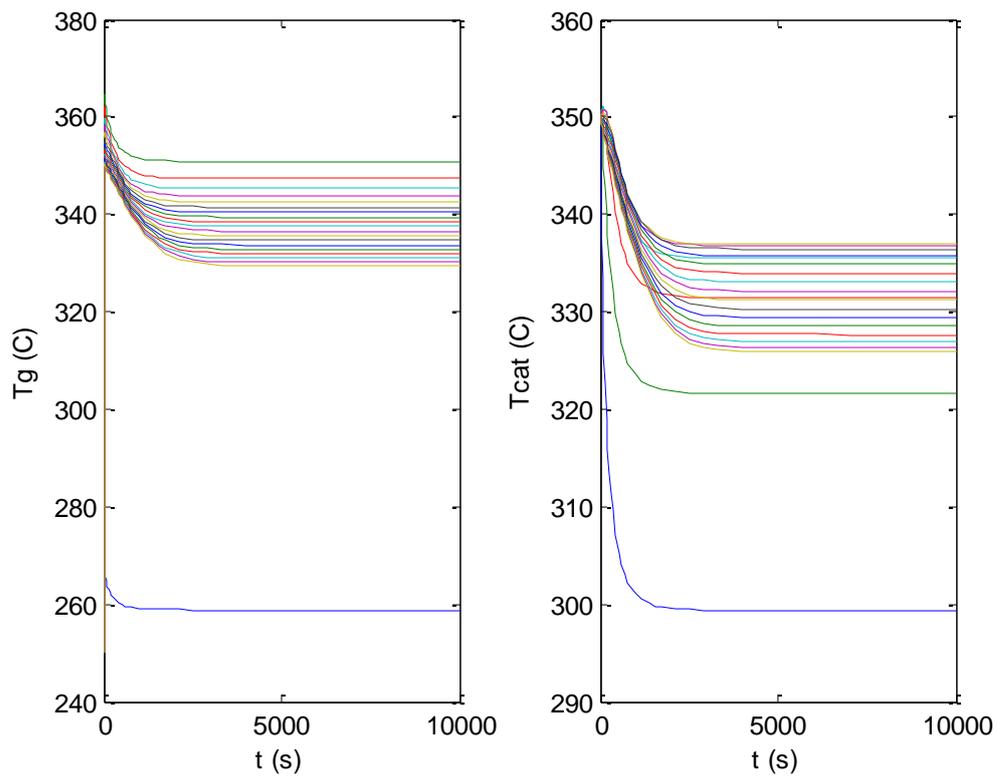


Figure 10 – The temperature evolution of the gas and catalyst phase over time. The different lines represent different elements.

## 5 Discussion

The simulations for the different units separated seem to provide reasonable results, corresponding to the trends shown in the provided experimental data from Perstorp. The units were also assembled. This was done according to the description of output/input-coupling as described in section 3.3.1-3.3.3. However, due to insufficient time, not enough simulations were performed to include it in the report. Thus, some further response testing and simulations for the whole process assembled is necessary in order to investigate its validity.

For the heat exchanger, the most important aspect was to match the outlet cold side temperature, as this is used as the input further throughout the process.

For the incinerator, the desired temperature distribution with a somewhat higher temperature in the middle of the reactor than at the outlet was achieved.

The heat transfer coefficients inside the heat exchanger were estimated to be  $14 \text{ W/m}^2\text{K}$ . This is a reasonable order of magnitude for a gas/metal system.

The actual data for the weights of the heat exchanger and the catalyst bed were provided by Perstorp. This is an advantage for the model, as such high masses and thus capacities may influence the dynamics of the process to a significant extent.

For the whole process, pressure drop was neglected and thus the pressure was assumed constant. Due to lack of information about the process pressures, the validity of the assumption is hard to judge. However, judging by the operating pressures of for example the heat exchanger, there seems to be no large pressure variations.

## 6 Conclusions and further work

Models describing the behaviour of the different process units were derived. Functions computing the derivative of the state temperatures with respect to time were written in Matlab, and custom blocks solving these differential equations were implemented in Simulink using s-functions. Finally the different process units were connected in Simulink.

Process parameters, like heat transfer coefficients, were adjusted for each of the units in order to provide results as close as possible to the experimental plant data.

Simulations and step responses of the whole assembles process need to be performed in order to investigate the model validity. This will be part of the following Master thesis. When the model has been validated, the current control structure will be implemented, and further the control structure will be attempted improved.

## 7 References

1. Edward C. Moretti, Baker Environmental Inc, June 2002: "Reduce VOC and HAP emissions"
2. Heinz A. Preisig, 2010: Lecture notes TKP4140 Process Control
3. Tore Haug Warberg, 2006: "Den termodynamiske arbeidsboken"
4. Knut Wiig Mathisen, 1994: "Integrated design and control of heat exchanger networks"
5. [www.mathworks.se](http://www.mathworks.se) – "Developing s-functions"

## APPENDIX I – HEX.M

```
function Tprime=HEX(t,X,U)

N=10;

cph=1030;           % [J/kgC]
cpc=1030;           % [J/kgC]
cp_w=800;           % [J/kgC]

% Heat transfer areas given from Perstorp [m^2]

A  = 115;
Ac = A/N;
Ah = A/N;
A_i_w=A/N;

% Volumes given from Perstorp [m^3]
Vh_tot = 2.3;       % Hot side volume [m3] for HE2 and HE3
Vc_tot = 1.8;       % Cold side volume [m3] for HE2 and HE3

Vh      = Vh_tot/N;
Vc      = Vc_tot/N;

hc      = 14;       % [W/m2K]
hh      = hc;       % [W/m2K]

mhex=2400;          % [kg]
mw      =mhex/N;

P=1;                % [atm]
M=0.029;            % [kg/mol]
R=8.2057*10^-5;    % [M3atm/Kmol]
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Splitting the states
Th=X(1:N);
Tc=X(N+1:2*N);
Tw=X(2*N+1:3*N);

% Inputs and disturbances
Tc0      = U(1);      % Inlet temp. cold side
Th0      = U(2);      % Inlet temp. hot side
m        = U(3);      % Mass flow
a        = U(4);      % Hot side bypass

dTdhdt=zeros(N,1);
dTcdt=zeros(N,1);
dTwdt=zeros(N,1);
```

```
rho_h=1;
rho_c=1;
```

```
% Initial
```

```
dTcdt(1) = (Tc0-Tc(1))*(m*R*(Tc(1)+273.15)/(P*M*Vc) ...
- (Tc(1)-Tw(N))*(hc*Ac*R*(Tc(1)+273.15)/(cpc*P*M*Vc));
```

```
dThdt(1) = (Th0-Th(1))*(m*R*(Th(1)+273.15)/(P*M*Vh) ...
- (Th(1)-Tw(1))*(hh*Ah*R*(Th(1)+273.15)/(cph*P*M*Vh));
```

```
dTwdt(1) = ((Th(1)-Tw(1))*hh + (Tc(N)-Tw(1))*hc)*(A_i_w/(mw*cp_w));
```

```
% Interior
```

```
for i=2:N
```

```
dTcdt(i) = (Tc(i-1)-Tc(i))*(m*R*(Tc(i)+273.15)/(P*M*Vc) ...
- (Tc(i)-Tw(N+1-i))*(hc*Ac*R*(Tc(i)+273.15)/(cpc*P*M*Vc));
```

```
dThdt(i) = (Th(i-1)-Th(i))*(m*R*(Th(i)+273.15)/(P*M*Vh) ...
- (Th(i)-Tw(i))*(hh*Ah*R*(Th(i)+273.15)/(cph*P*M*Vh));
```

```
dTwdt(i) = ((Th(i)-Tw(i))*hh + (Tc(N+1-i)-
Tw(i))*hc)*(A_i_w/(mw*cp_w));
```

```
end
```

```
Tprime=[dThdt; dTcdt; dTwdt];
```

```
end
```

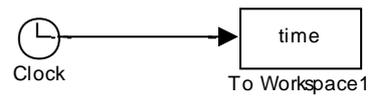
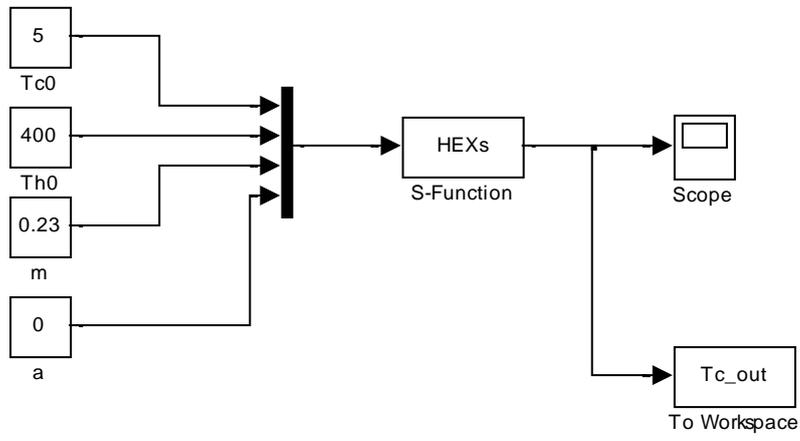
## APPENDIX II – HEXS.M

```
function [sys,x0] = incins(t,x,u,flag)

% Inputs:      t      - time in [s].
%              X      - States. A total of 3*N states.
%              Temperatures of cold side gas, hot side gas and heat
%              exchanger wall elements
%              U(1) - Inlet cold gas temperature, Tc0 [K]
%              U(2) - Inlet hot gas temperature, Th0 [K]
%              U(3) - Mass flow [kg/s], m
%              U(4) - Hot side bypass , a
% Outputs:     sys and x0 as described in the SIMULINK manual.
%              when flag is 0 sys contains sizes and x0 contains
%              initial condition.
%              when flag is 1, sys contains the derivatives,
%              and when flag is 3 sys contains outputs;

N=10;
Xinit=[ones(N,1)*400; ones(N,1)*5; ones(N,1)*250];
if abs(flag) == 1
    % Return state derivatives.
    sys = HEX(t,x,u);
elseif abs(flag) == 3
    % Return system outputs.
    sys(1,1) = x(2*N);           % Outlet temp. cold side
elseif flag == 0
    % Initialize the system
    x0 = Xinit;
    sys = [3*N, 0, 1, 4, 0, 0];
else
    sys = [];
end
```

APPENDIX III – HEXSIM.MDL



## APPENDIX IV – ELHEATER.M

```
function dTdt=elheater(t,X,U)

% Inputs and disturbances
T0      = U(1);           % Inlet temp. [C]
W       = U(2);           %Effect elheater [W]
m       = U(3);

cpg=1013;
Vg=0.24;

P=1;
M=0.029;
R=8.2057*10^-5;

T=X;

dTdt    = (T0-T)*(m*R*(T+273.15)/(P*M)) + W*(R*(T+273.15)/(P*M*cpg*Vg));

end
```

## APPENDIX V - ELHEATERS.M

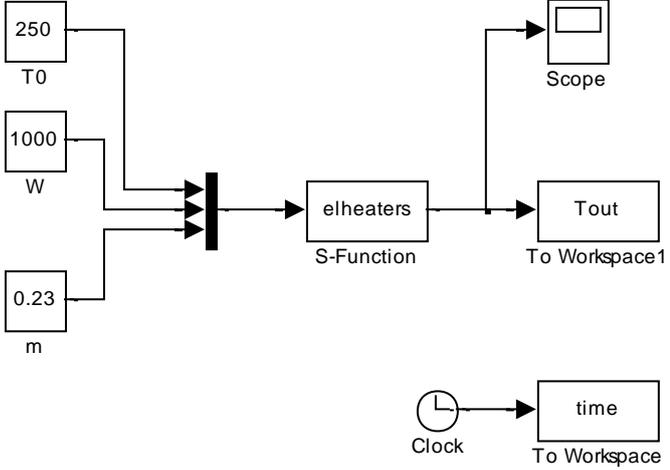
```
function [sys,x0] = elheaters(t,x,u,flag)

Xinit=250;

if abs(flag) == 1
    % Return state derivatives.
    sys = elheater(t,x,u);
elseif abs(flag) == 3
    % Return system outputs.
    sys(1) = x(1);

elseif flag == 0
    % Initialize the system
    x0 = Xinit;
    sys = [1, 0, 1, 3, 0, 0];
else
    sys = [];
end
```

APPENDIX VI – ELHEATERSIM.MDL



## APPENDIX VII – INCIN.M

```
function dTdt=incin(t,X,U)
```

```
% Inputs:      t      - time in [s].
%              X      - States. A total of 2*N states.
%                  Temperatures of gas (1-N) and catalyst (N+1 -
%                  2*N) in each mixing tank
%              U(1)   - Inlet gas temperature, T0 [K]
%              U(2)   - Mass flow gas [kg/s]
%              U(3)   - massfrac of VOC
```

```
% Outputs:    sys and x0 as described in the SIMULINK manual.
%              when flag is 0 sys contains sizes and x0 contains
%              initial condition.
%              when flag is 1, sys contains the derivatives,
%              and when flag is 3 sys contains outputs;
%              y(1:N)   - Gas temperature in element N [K]
%              y(N+1:2*N)- Catalyst temperature in element N [K]
```

```
N=10;
```

```
Cpcat   = 800;
UAcat   = 1000;
UAwall  = 0.01;
Tamb    = 15;
mcat    = 280;
kAcat   = 100;
```

```
deltaHc = 35000000; %[J/kg]
Vg       = 0.5;
Cpg      = 1013;
P=1;
M=0.029;
R=8.2057*10^-5;
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```
T=X(1:2*N)';
```

```
% Inputs and disturbances
```

```
T0      = U(1);           % Inlet temp.
m        = U(2);           % Mass flow of gas
w        = U(3);           % Mass fraction of VOC
```

```
% T(1:N) is the gas temperature
% T(N+1:2*N) is the catalyst temperature
```

```

%%% ~~~~~ Model ~~~~~

% Initial elements
dTdt(1) = ((N*m*R*(T(1)+273.15)/(P*M*Vg))* (T0-T(1))) ...
          - ((UAcat*R*(T(1)+273.15)/(P*M*Vg*Cpg))* (T(1)-(T(N+1))));

dTdt(N+1) = (UAcat/(mcat*Cpcat))* (T(1)-T(N+1)) ...
            + ((kAcat*N/(mcat*Cpcat))* (T(N+2)-T(N+1))) -
            (UAwall/(mcat*Cpcat))* (T(N+1)-(Tamb));

% Interior elements
for i=2:(N-1)
    if T(i)>=270 % ignition temperature exceeded
        dTdt(i) = ((N*m*R*(T(i)+273.15)/(P*M*Vg))* (T(i-1)-T(i))) ...
                  - ((UAcat*R*(T(i)+273.15)/(P*M*Vg*Cpg))* (T(i)-(T(N+i)))) ...
                  + (m*w*deltaHc*N*R*(T(i)+273.15)/(P*M*Vg*Cpg));
        w=0;
    else %below ignition temperature
        dTdt(i) = ((N*m*R*(T(i)+273.15)/(P*M*Vg))* (T(i-1)-T(i))) ...
                  - ((UAcat*R*(T(i)+273.15)/(P*M*Vg*Cpg))* (T(i)-(T(N+i))));
    end
    dTdt(N+i) = (UAcat/(mcat*Cpcat))* (T(i)-T(N+i)) +
                (kAcat*N/(mcat*Cpcat))* (T(N+i-1)+T(i+N+1)-2*T(N+i)) ...
                - (UAwall/(mcat*Cpcat))* (T(N+i)-(Tamb));
end

% Final elements
dTdt(N) = ((N*m*R*(T(N)+273.15)/(P*M*Vg))* (T(N-1)-T(N))) ...
          - ((UAcat*R*(T(N)+273.15)/(P*M*Vg*Cpg))* (T(N)-T(2*N)));
dTdt(2*N) = (UAcat/(mcat*Cpcat))* (T(N)-T(2*N))
+ ((kAcat*N/(mcat*Cpcat))* (T((2*N)-1)-T(2*N))) ...
  - (UAwall/(mcat*Cpcat))* (T(2*N)-(Tamb));

```

## APPENDIX VIII – INCINS.M

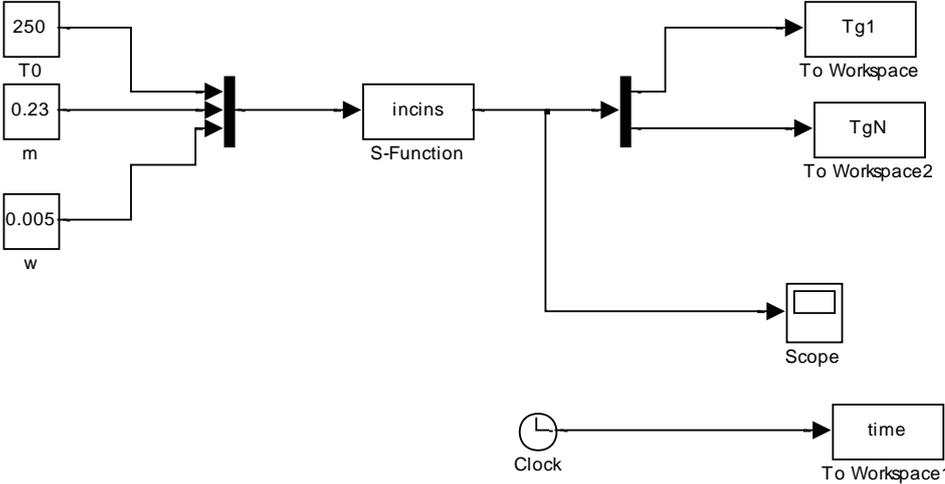
```
function [sys,x0] = incins(t,x,u,flag)

% Inputs:      t      - time in [s].
%              X      - States. A total of 2*N states.
%                  Temperatures of gas (1-N) and catalyst (N+1 -
%                  2*N) in each mixing tank
%              U(1)   - Inlet gas temperature, T0 [K]
%              U(2)   - Massflow of gas [kg/s]
%              U(3)   - Massfrac of VOC

% Outputs:     sys and x0 as described in the SIMULINK manual.
%              when flag is 0 sys contains sizes and x0 contains
%              initial condition.
%              when flag is 1, sys contains the derivatives,
%              and when flag is 3 sys contains outputs;
%              y(1:N)   - Gas temperature in element N [K]
%              y(N+1:2*N)- Catalyst temperature in element N [K]

N=10;
Xinit=[ones(N,1)*250; ones(N,1)*350];
if abs(flag) == 1
    % Return state derivatives.
    sys = incin(t,x,u);
elseif abs(flag) == 3
    % Return system outputs.
    sys(1,1) = x(1);      % Gas temperature in element 1.
    sys(2,1) = x(N);     % Gas temperature in element N.
elseif flag == 0
    % Initialize the system
    x0 = Xinit;
    sys = [2*N, 0, 2, 3, 0, 0];
else
    sys = [];
end
```

APPENDIX IX – INCINSIM.MDL



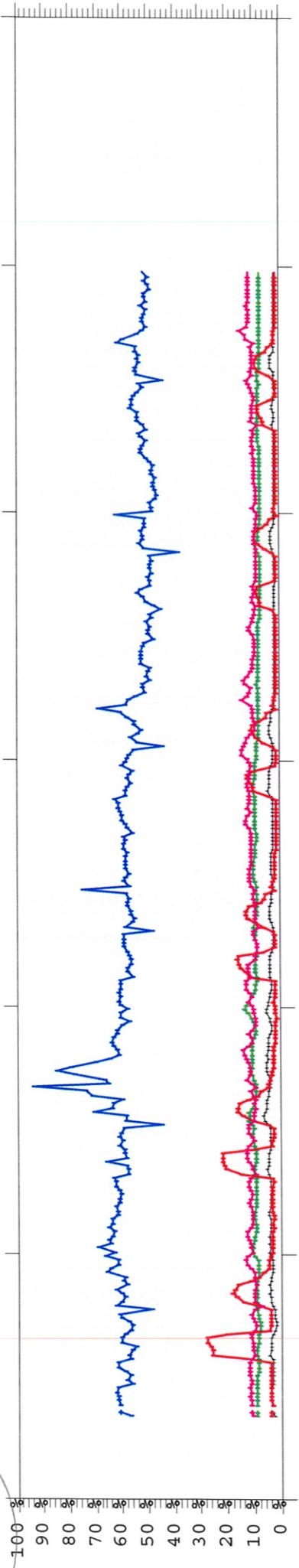
Halter i ingående gas till kal. förbr.

D:\Mätningar 2011\Penta\20110810\PEL20\_00681.SPE  
 2011-08-10 23:55:54 PEL20\_110811.LIB

Ch	Component	Concentration	Unit	Output	Compensation	Range	Resid
1	Water vapor H2O	1.82	vol-%		wet	25	0.0017
2	Carbon dioxide CO2	0.38	vol-%		wet	20	0.0044
3	Carbon monoxide CO Low	254	mg/nm3tg		dry	2000	0.0027
13	Formaldehyde CHOH Low	19.05	mg/nm3tg		dry	500	0.0010
15	Dimethyl ether	39.83	mg/nm3tg		dry	515	0.0086
17	Metanol hög	239	mg/nm3tg		dry	1500	0.0048
18	Myrsyra	16.34	mg/nm3tg		dry	1000	0.0217
23	Metakrolein	459	mg/nm3tg		dry	1000	0.0091
27	Acetaldehyd	21.95	mg/nm3tg		dry	515	0.0070
28	MIBK	5142	mg/nm3tg		dry	10000	0.0173
36	Metylal	15.33	mg/nm3tg		dry	2000	0.0170
40	Metylformiat	343	mg/nm3tg		dry	3000	0.0079
219	Pressure	998	mbar		wet	2000	
231	Sample cell temperature	180	C		wet	200	
232	Interferometer temp	40.00	C		wet	100	
233	Detector temperature	36.00	-C		wet	40	
234	IFG peak height	2.00			wet	6	
235	IFG center position	2334			wet	5000	

*Desse halter avser  
(Endast sista analysen)*

% of range

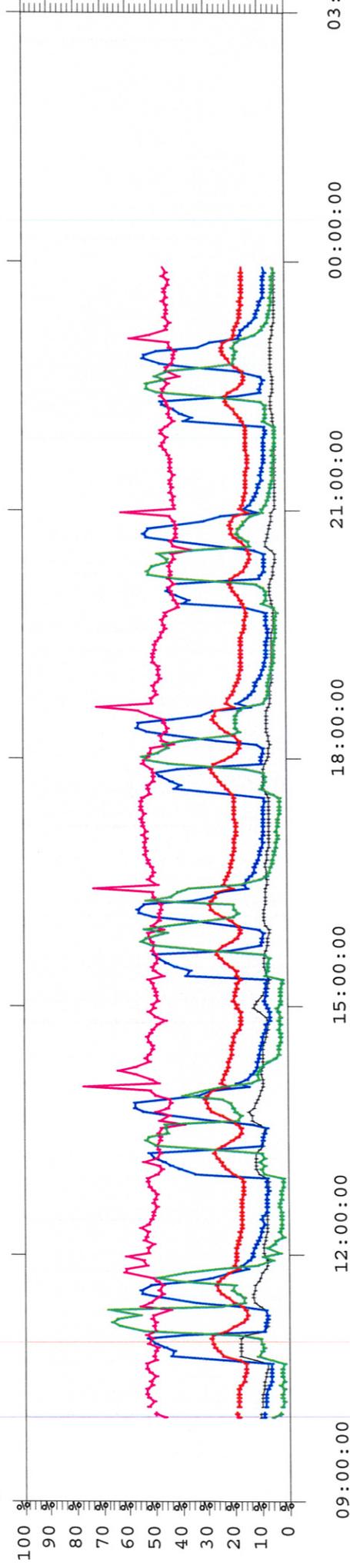


09:00:00 12:00:00 15:00:00 18:00:00 21:00:00 00:00:00 03:00:00

HIF  
tel. 38443

Ch	Component	Concentration	Unit	Output	Compensation	Range	Resid
1	Water vapor H2O	1.82	vol-%		wet	25	0.0017
2	Carbon dioxide CO2	0.38	vol-%		wet	20	0.0044
3	Carbon monoxide CO Low	254	mg/nm3tg		dry	2000	0.0027
13	Formaldehyde CHOH Low	19.05	mg/nm3tg		dry	500	0.0010
15	Dimethyl ether	39.83	mg/nm3tg		dry	515	0.0086
17	Metanol hög	239	mg/nm3tg		dry	1500	0.0048
18	Myrsyra	16.34	mg/nm3tg		dry	1000	0.0217
23	Metakrolein	459	mg/nm3tg		dry	1000	0.0091
27	Acetaldehyd	21.95	mg/nm3tg		dry	515	0.0070
28	MIBK	5142	mg/nm3tg		dry	10000	0.0173
36	Metylal	15.33	mg/nm3tg		dry	2000	0.0170
40	Metylformiat	343	mg/nm3tg		dry	3000	0.0079
219	Pressure	998	mbar		wet	2000	
231	Sample cell temperature	180	C		wet	200	
232	Interferometer temp	40.00	C		wet	100	
233	Detector temperature	36.00	-C		wet	40	
234	IFG peak height	2.00			wet	6	
235	IFG center position	2334			wet	5000	

% of range



09:00:00

12:00:00

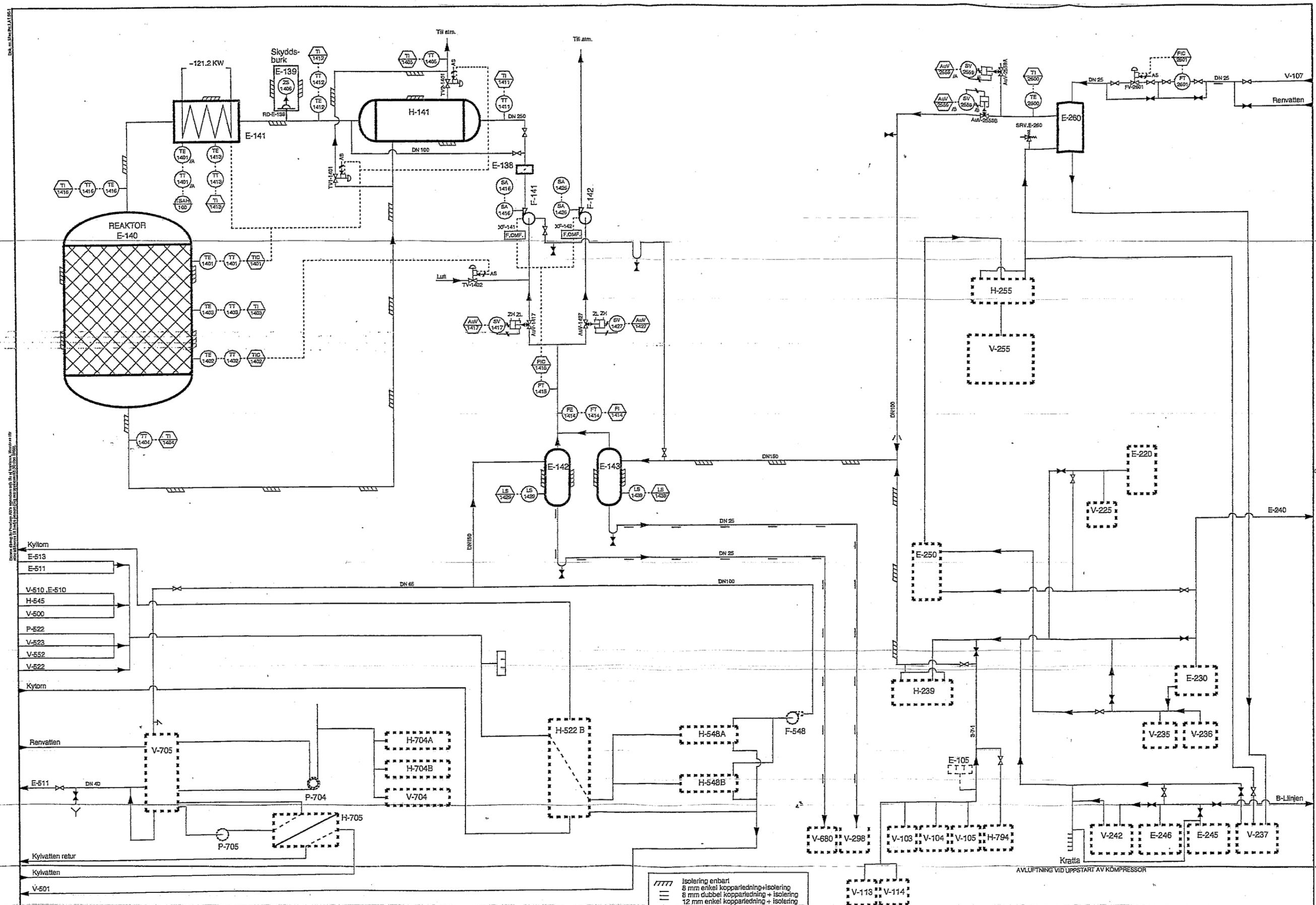
15:00:00

18:00:00

21:00:00

00:00:00

03:00:00



Dwg. nr. H-14217 H  
 10418 Skyddsburk för RD-E-139  
 10419 Isolerings- och rörledningsschema för H-794 och H-704  
 10420 Isolerings- och rörledningsschema för H-794 och H-704

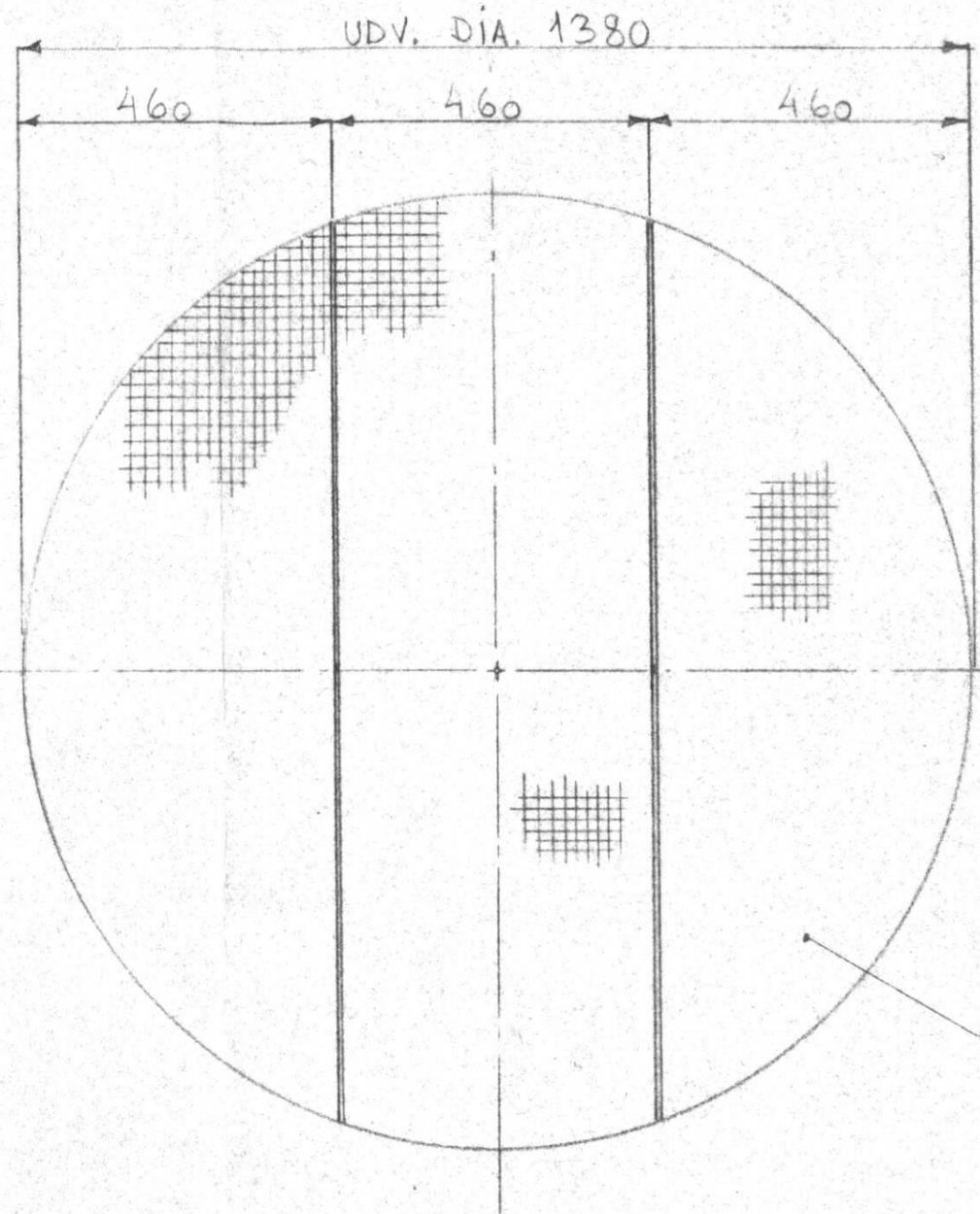
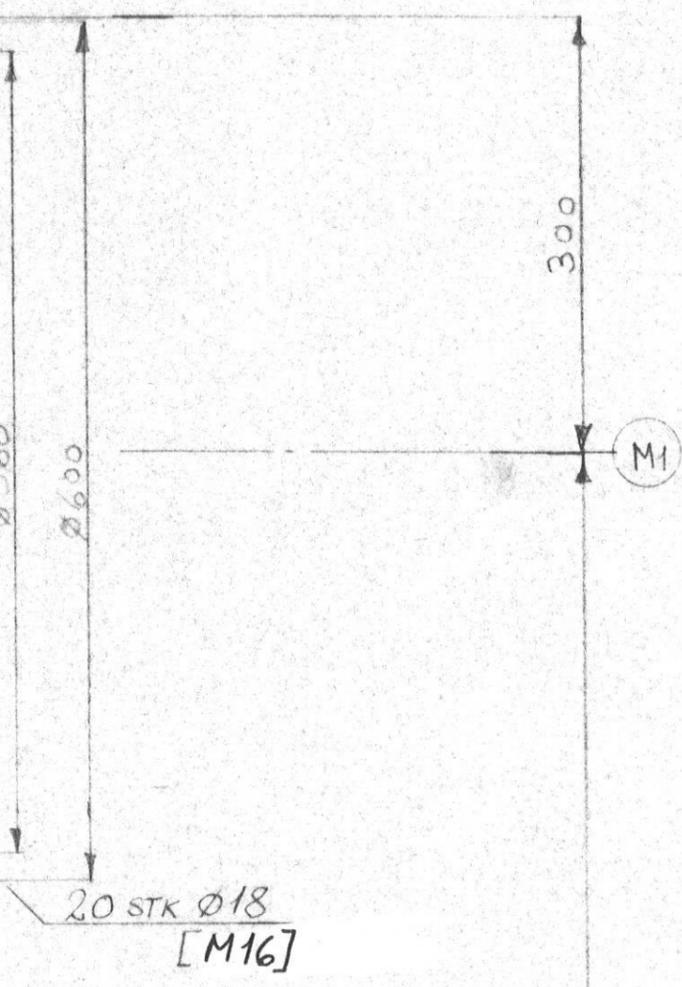
F	10125	Dw. ändringar Penta 401	031125	BL	BL
H	20200	Isolerings- och rörledningsschema för H-794 och H-704	070515	BL	BL
G	10418	Skyddsburk för RD-E-139	041015	BL	BL

- Isolering enbart
- 8 mm enkel kopparledning + isolering
- 8 mm dubbel kopparledning + isolering
- 12 mm enkel kopparledning + isolering
- 12 mm dubbel kopparledning + isolering
- 12 mm trippel kopparledning + isolering
- Elvärmeband + isolering

440 PENTA  
 Katalytisk förbränning  
 Del 18  
 Fjäderchema  
 211028  
 1-421747 H

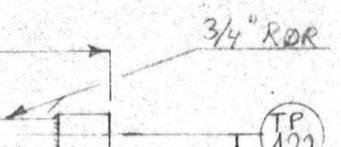
THIS DOCUMENT CONTAINS TRADE SECRET AND PROPRIETARY INFORMATION, THE PROPERTY OF HALDOR TOPSOE A.S. AND IS ISSUED ON CONDITION THAT IT IS RECEIVED AND HELD IN CONFIDENCE. NEITHER IT NOR THE INFORMATION HEREIN SHALL BE REPRODUCED, SOLD, LENT, DISCLOSED OR USED FOR ANY PURPOSE OTHER THAN THAT FOR WHICH IT HAS BEEN ISSUED WITHOUT WRITTEN AUTHORITY OF HALDOR TOPSOE A.S.

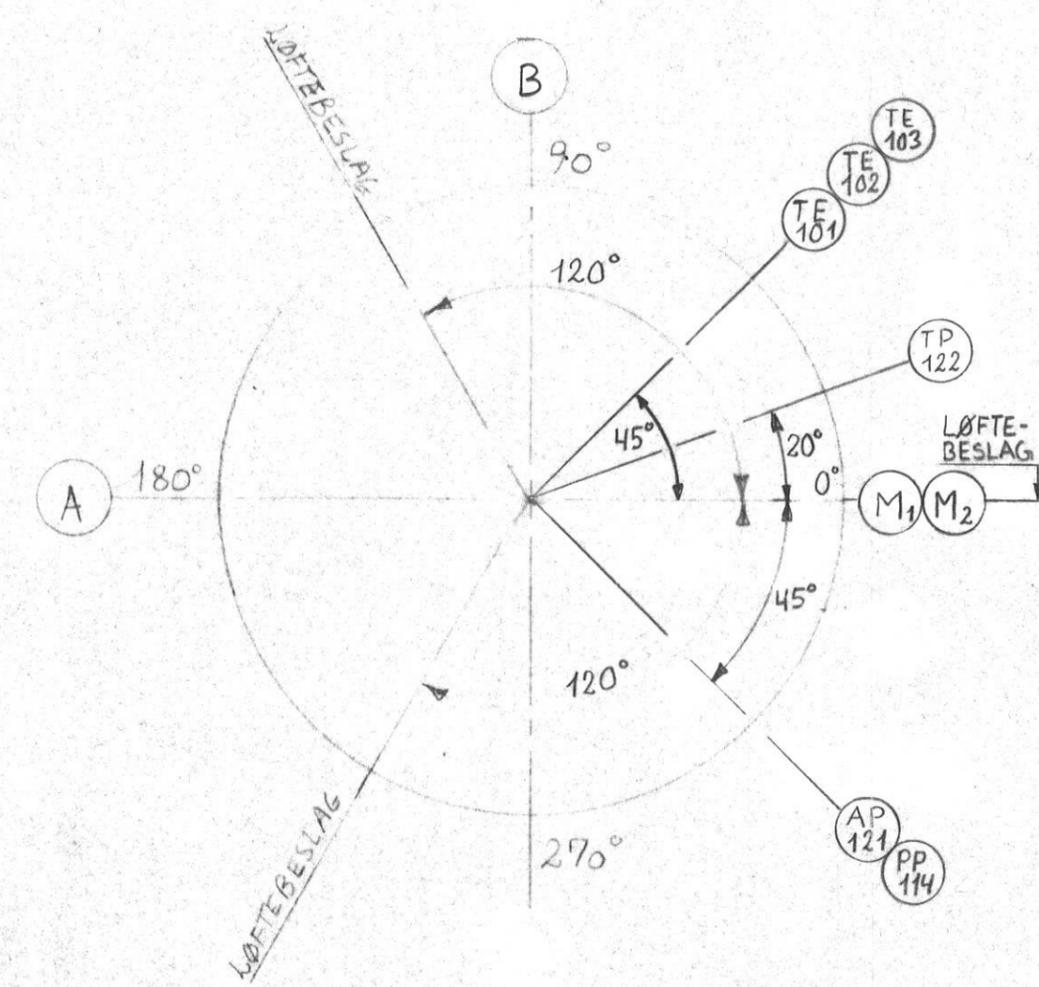
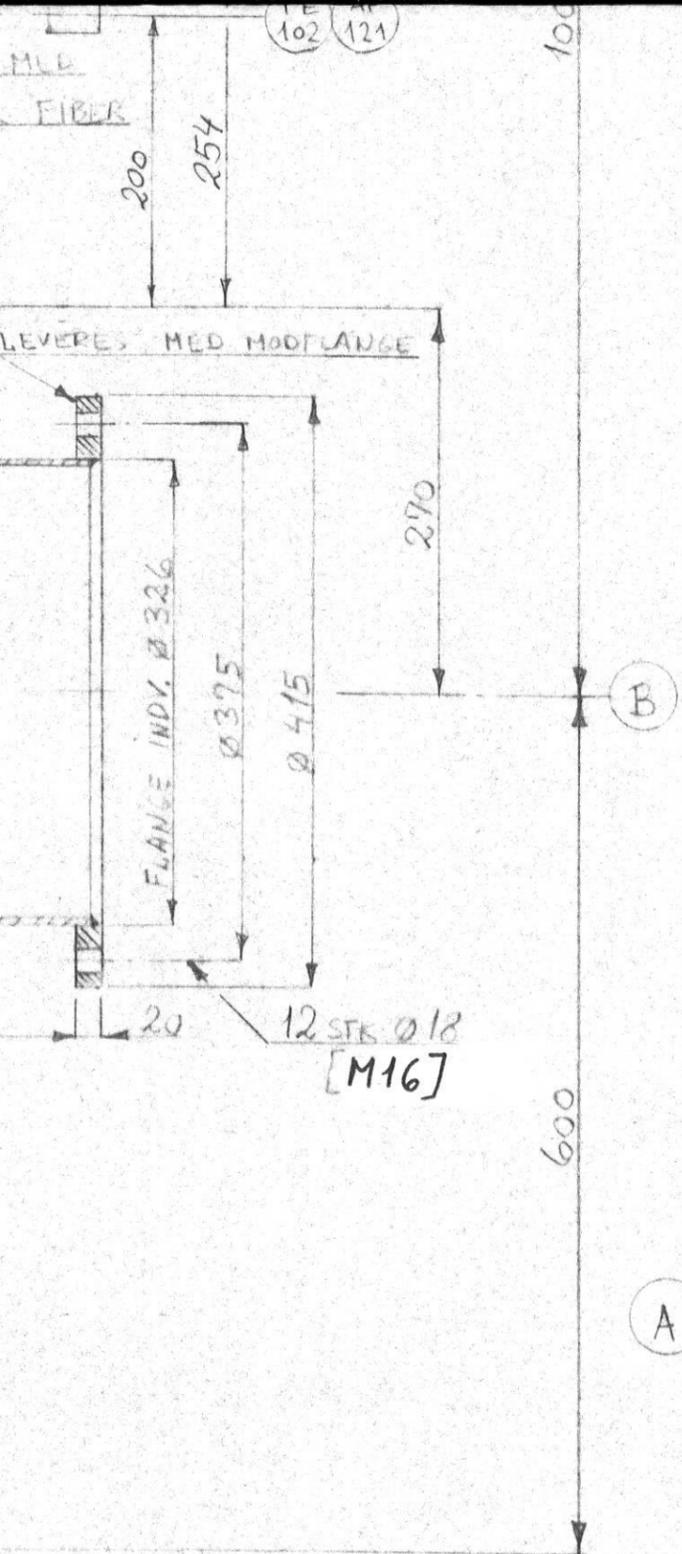
A



ELEFANTRISTE: MATR: AISI 316

DETALJE A  
SKALA: 1:10





STUDS ORIENTERING A-A

MATR.: AISI 304

ANMÆRKNINGER:

1) HVOR INTET ANDET ER NÆVNT ANVENDES  
MATERIALET: AISI 316

PAKNINGER					
STUDS	STØRRELSE ND	PAKNINGS MATR.	UDV. DIA.	INDV. DIA.	TYKKELSE
A	300	KLINGERSIL C4400	354	324	3
B	300	KLINGERSIL C4400	354	324	3
M1+2	500	KLINGERSIL C4400	538	508	3

REV	DESCRIPTION	DATE	DRAWN	CHECK	APPD.
5					
4					
3					
2	STUDSE ORIENTERING FASTLAGT	20.01.22	BH7	SDN	ESA
1	FOR UDBUD, OPDATERET	89.12.04	BH7	SDN	ESA

**HALDOR TOPSØE A/S**  
COPENHAGEN  
DENMARK

EQUIPMENT DIVISION

PERSTORP POLYOLS  
PERSTORP, SVERIGE  
1800 Nm<sup>3</sup>/h CATOX ANLÆG

REAKTOR R1

89.11.06 SDN EGH ESA

SCALE 1:5

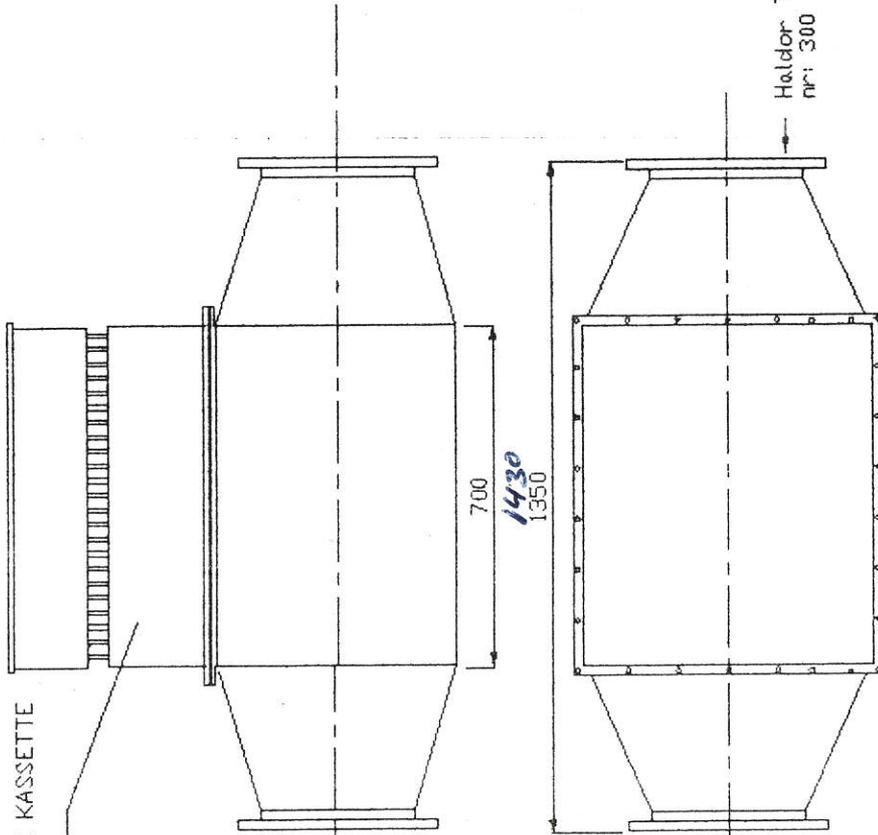
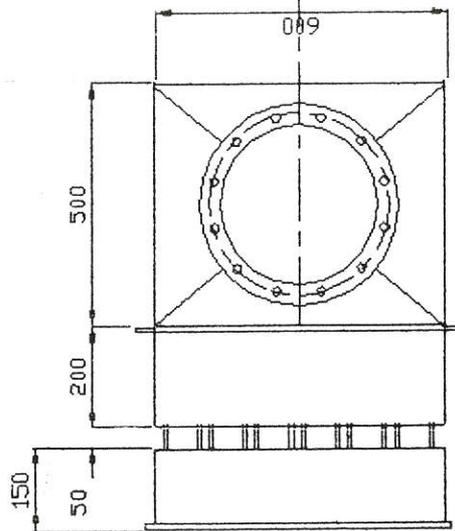
JOB NO. 55178

ITEM R1

DWG. NO. E 128800

REV. 2

INDSTIKS KASSETTE  
21705611

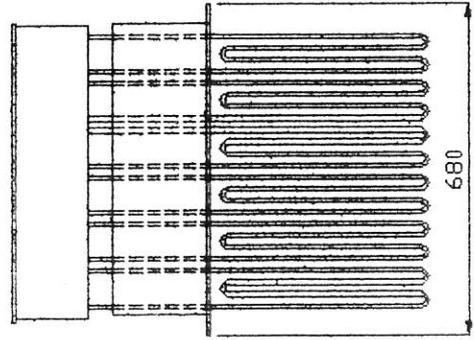
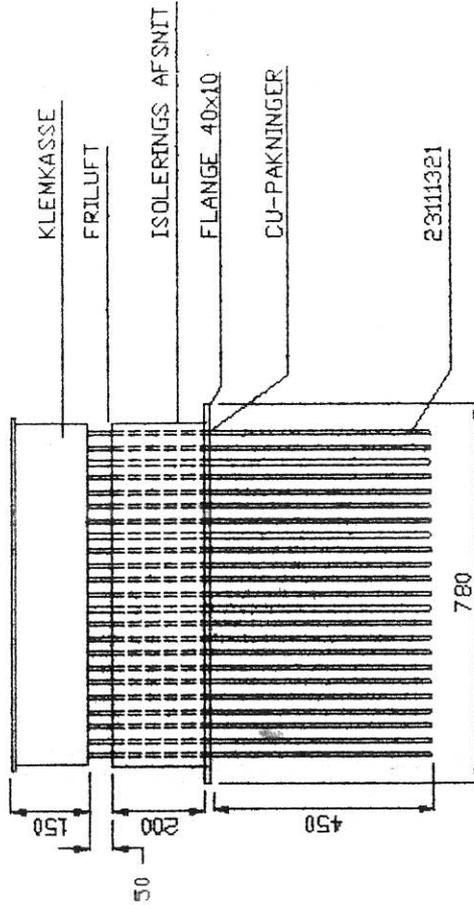


Tolerance DS 2075 grov

Kobles i åben trekant

Kabinet fremstilles i AISI316L  
Rørvl. 380V 1100watt i mat. AISI309

Kunder HALDOR TOPSØE		Målest. 110	Konst. N.
Emne: EL-HEATER 3X380V 122,1KV		Matr. AISI316L	Tegn. N.
			Dato, 2008
 <b>DEVI</b> IE-VI Industrial Heat		 <b>HI</b> <i>EL Heatfare</i>	Tegning nr. 21705553,



3X380V 122,1KW

Kunde: HALDOR TOPSØE		Målest.	Konst. N.
Emne: KASSETTE FOR VF 21705553		Matr. AISI316L	Tegn. N.
			Dato: 900116
			Tegning nr.
			21705611

