

**CHAPTER 4: OFF-GAS MODEL**

**4.1 INTRODUCTION**

An excellent approach to off-gas modelling would be to make use of CFD (Computational Fluid Dynamics). This approach is rigorous, and gives very accurate results. Unfortunately it also requires much expertise in the specific field, as well as much resources in terms of computation time. The derivation of a complete CFD model is outside the scope of this dissertation. Instead, an approximate transfer function model is derived using an alternate approach. The purpose with the off-gas model is to describe the dynamic behavior of the mass-flow of gas in the off-gas duct of the electric arc furnace. Off-gas duct design drawings for the furnace under study were used in the derivation of the off-gas model. An approximate illustration of the design drawings is given in Fig.4.1. Data from the design drawings relevant to the model derivation is given in Table 4.1.

The model accepts as input the electric power applied to the force draught fan motor in the off-gas system, and also the slip-gap width in the water-cooled duct. The model then calculates the mass-flow of gas resulting from the fan power. It also divides the mass-flow into two separate flows, namely, that which enters through the slip-gap and that which enters the duct from the EAF. Based on these flows, the temperature at the end of the cooling duct is calculated, and the composition of gas (% carbon monoxide) is calculated. The cross hair in Fig.4.1 indicates the location where the off-gas composition and temperature is under study.

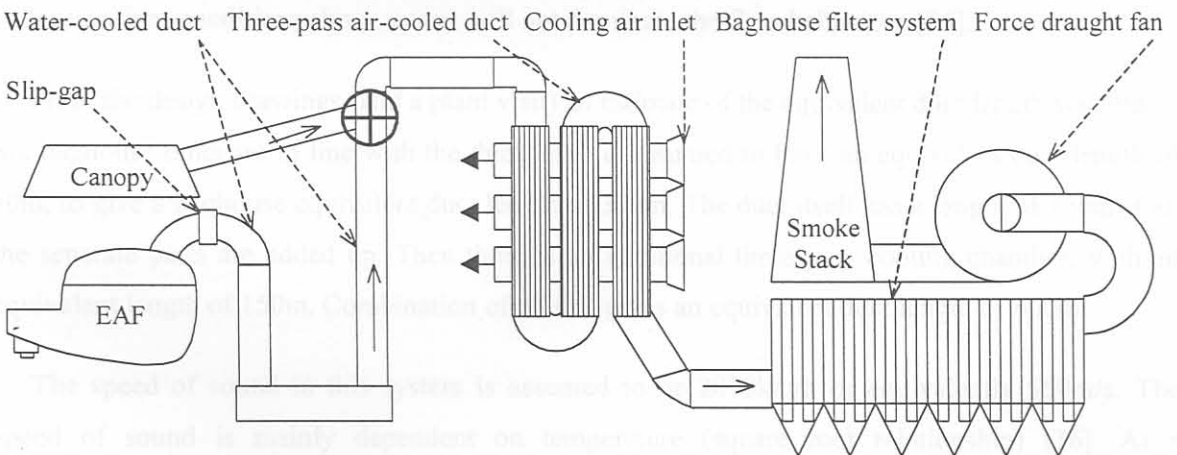


Figure 4.1 Off-gas system, with end of water-cooled duct marked

In Section 4.2 a transfer function model for the off-gas system is derived. First the necessary assumptions with respect to the steady state gain, time delay and time constants are given. Then the model approximation is discussed. In Section 4.3 the state space model is derived from the transfer function model. In Section 4.4 the mass-flow division at the slip-gap is discussed. Finally, in Section 4.5, the off-gas composition and temperature relations are derived.

## 4.2 TRANSFER FUNCTION MODEL

In the process industry, most SISO (single-input, single-output) processes can be represented by a first order transfer function (denominator is a first order polynomial) with time delay. The off-gas system is treated as two first order systems. Combination of the two systems yield a second order transfer function with time delay. One first order system relates the extraction fan power input and the relative pressure. The other first order system relates the relative pressure and the mass-flow. The time constants and the delay are related to the physical dimensions of the system.

### 4.2.1 Model Assumptions

#### 4.2.1.1 Steady-state Gain

A constant steady-state gain from fan power input to mass-flow is assumed. The gain would vary depending on the pressure difference between the fan entrance and atmosphere, or on the condition of the baghouse. For this dissertation the steady-state gain is assumed as  $11 \text{ (kg}\cdot\text{s}^{-1}\text{)}/\text{MW}$ .

#### 4.2.1.2 Time Delay

The transfer function time delay is given by the quotient of the equivalent duct length and the speed of sound in air, as the force waves travel at the speed of sound. Shock waves are not considered, because the system under consideration will normally be at steady state, and even under transient conditions shock waves will not dominate the flow behaviour [36].

From the design drawings (and a plant visit) an estimate of the equivalent duct length was made. Six baghouse units are in line with the duct, each is assumed to have an equivalent duct length of 50m, to give a baghouse equivalent duct length of 300m. The duct itself has a length of 150m if all the separate parts are added up. Then there is an additional three-pass cooling chamber, with an equivalent length of 150m. Combination of all this gives an equivalent duct length of 600m.

The speed of sound in this system is assumed to be 2070km/h or equivalently 550m/s. The speed of sound is mainly dependent on temperature (square root relationship) [36]. At a temperature of 800K the speed of sound is 568.5m/s (2047km/h) while at 300K it is 348m/s (1253km/h). With the velocity of sound 550m/s and the equivalent duct length 600m the corresponding time delay is then equal to 1.09s.

### 4.2.1.3 Time Constants

For the time constant relating the extraction fan force to the duct relative pressure the same dimensions are considered as with the time delay. Due to the inertia and friction in the off-gas system, the gas in the off-gas duct flows with a velocity of eighteen times slower than the speed of sound. The motivation for this assumption stems from the worst case steady state analysis given in the design drawings. The applicable data is given in Table 4.1:

Table 4.1: Off-gas flow data

Location	Water-cooled duct entrance	Water-cooled duct exit
Mass Flow	143674 kg/h = 39.9 kg/s	143674 kg/h = 39.9 kg/s
Temperature	1425 K	879 K
Density	0.23 kg/m <sup>3</sup>	0.37 kg/m <sup>3</sup>
Volume Flow	173.48 m <sup>3</sup> /s	107.84 m <sup>3</sup> /s
Duct Area	4.3 m <sup>2</sup>	5.8 m <sup>2</sup>
Flow Velocity	40.3 m/s	18.6 m/s

The data given in Table 4.1 is regarded as a worst case scenario. As is apparent from the data, the average flow velocity is 29 m/s. This is about 18 times slower than the speed of sound in this environment. This justifies the assumption that under steady state conditions the flow velocity is eighteen times slower than the speed of sound. The corresponding time constant is then assumed to be eighteen to twenty times as large as the time delay. For a first order transfer function without time delay, the time constant is the time that the output response takes to reach 63% of its final value in reaction to a step input change. Using an average time delay of 1.09s the time constant is assumed to be 19.6s. Where the time delay was determined from the speed of sound, the time constant is determined from the speed of flow.

The time constant that relates the relative pressure to the mass-flow is much shorter since the cooling duct length is much shorter. As can be calculated from Fig.2.2 the length of the cooling duct is approximately 45m. The time constant corresponding to this length is 1.5s.

## 4.2.2 Model Approximation

The transfer function model has two factors in the denominator, a steady state gain and a time delay function as in equation (4-1):

$$\dot{m}(s) = \frac{K_M e^{-t_d s}}{(\tau_1 s + 1)(\tau_2 s + 1)} u_1(s) \quad (4-1)$$

A first order Padé approximation [21] is made to approximate the time delay. Since one of the time constants will always be at least ten times larger than the time delay, this is deemed to be an acceptable approximation. The first order Padé approximation for time delay is:

$$e^{-t_d s} = \frac{1 - 0.5t_d s}{1 + 0.5t_d s} \quad (4-2)$$

This approximation is substituted into equation (4-1) to obtain the approximated transfer function:

$$\dot{m}(s) = \frac{K_M (1 - 0.5t_d s)}{(1 + 0.5t_d s)(\tau_1 \tau_2 s^2 + (\tau_1 + \tau_2)s + 1)} u_1(s) \quad (4-3)$$

When the factors in the numerator and denominator are multiplied out, the result is:

$$\dot{m}(s) = \frac{K_M - 0.5K_M t_d s}{((0.5t_d \tau_1 \tau_2) s^3 + (0.5t_d (\tau_1 + \tau_2) + \tau_1 \tau_2) s^2 + (\tau_1 + \tau_2 + 0.5t_d) s + 1)} u_1(s) \quad (4-4)$$

When the coefficient of the  $s^3$ -term in the denominator is divided out, the result is:

$$\dot{m}(s) = \frac{(2K_M/t_d \tau_1 \tau_2) - (K_M/\tau_1 \tau_2) s}{(s^3 + (1/\tau_1 + 1/\tau_2 + 2/t_d) s^2 + ((2\tau_1 + 2\tau_2 + t_d)/(t_d \tau_1 \tau_2)) s + 2/(t_d \tau_1 \tau_2))} u_1(s) \quad (4-5)$$

### 4.3 STATE SPACE MODEL

Since the main model in the previous chapter is derived as a state-space model it is logical to convert this transfer function model to an equivalent state-space model. The desired state space model is given in equation (4-6):

$$\begin{aligned} \frac{d(\delta x(t))}{dt} &= \mathbf{A} \cdot \delta x(t) + \mathbf{B} \cdot \delta u(t) \\ \mathbf{y}(t) &= \mathbf{C} \cdot \delta x(t) + \mathbf{D} \cdot \delta u(t) \end{aligned} \quad (4-6)$$

The matrices are in the companion (Luenberger's second controllable canonical-) form [37]:

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -a_1 & -a_2 & -a_3 \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \quad \mathbf{C} = [c_1 \ c_2 \ c_3] \quad \mathbf{D} = 0 \quad (4-7)$$

The plant SISO transfer function can be obtained from the state space model in companion form. The output  $y$  is the mass flow  $\dot{m}$  in equation (4-1). Then the SISO equation is:

$$y = G_p(s) u_1 \quad (4-8)$$

which is the same as equation (4-1). The transfer function  $G_p(s)$  is obtained from the state space companion form as in equation (4-9):

$$G_p(s) = C[sI - A]^{-1}B + D \tag{4-9}$$

After matrix inversion and matrix multiplication the result is:

$$G_p = \frac{c_1 + c_2s + c_3s^2}{s^3 + a_3s^2 + a_2s + a_1} \tag{4-10}$$

Now equation (4-10) and equation (4-5) are equated and the various coefficients are determined:

$$\begin{aligned}
 c_1 &= 2K_M/(t_d\tau_1\tau_2); & c_2 &= -K_M/(\tau_1\tau_2); & c_3 &= 0; \\
 a_1 &= 2/(t_d\tau_1\tau_2); & a_2 &= (2\tau_1 + 2\tau_2 + t_d)/(t_d\tau_1\tau_2); & a_3 &= (1/\tau_1 + 1/\tau_2 + 2/t_d).
 \end{aligned}$$

A similar derivation is given in [38]. In order to incorporate this into the model, three states,  $x_{15}$  to  $x_{17}$ , are added to the state space. The output of these three state equations is the mass flow given by  $y = c_1x_{15} + c_2x_{16}$ . The equations for  $x_{15}$  to  $x_{17}$  are:

$$\dot{x}_{15} = x_{16} \tag{4-11}$$

$$\dot{x}_{16} = x_{17} \tag{4-12}$$

$$\dot{x}_{17} = -2/(t_d\tau_1\tau_2)x_{15} - (2\tau_1 + 2\tau_2 + t_d)/(t_d\tau_1\tau_2)x_{16} - (1/\tau_1 + 1/\tau_2 + 2/t_d)x_{17} + u_1 \tag{4-13}$$

The equivalent mass flow in the cooling duct is then given by equation (4-14):

$$\dot{m} = (2K_M/(t_d\tau_1\tau_2))x_{15} - (K_M/(\tau_1\tau_2))x_{16} \tag{4-14}$$

#### 4.4 MASS-FLOW DIVISION

At the slip-gap air is entrained from the atmosphere to combust the CO remaining in the extracted EAF gas, and to cool the off-gas. The duct area at the slip gap has a characteristic dimension  $h_d$ . The slip gap width ( $u_2$ ) is the other manipulated variable and is the characteristic dimension of the slip-gap area. Fig.4.2 gives a close look at the slip-gap structure:

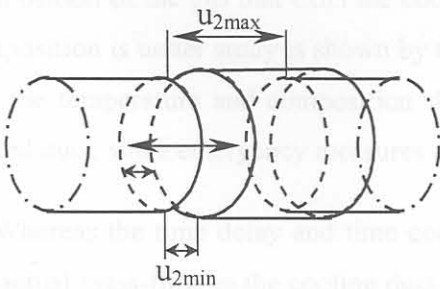


Fig.4.2 Slip-gap Structure

The flow rate through each area is proportional to the ratio of the respective characteristic dimension to the sum of the characteristic dimensions. Expressed as a fraction of  $\dot{m}$ , the rate of gas extraction from the EAF is:

$$\frac{\dot{m}}{\dot{m}_{\text{EAF}}} = \frac{h_d}{k_U u_2 + h_d} \quad (4-15)$$

To improve the approximation a dimensionless constant  $k_U$  is used to adjust the influence of  $u_2$ . The mass-flow through the EAF gas exit is then given by equation (4-16), while the mass-flow through the slip-gap is given by equation (4-17).

$$\dot{m}_{\text{EAF}} = \frac{h_d ((2K_M/t_d \tau_1 \tau_2) X_{15} - (K_M/\tau_1 \tau_2) X_{16})}{k_U u_2 + h_d} \quad (4-16)$$

$$\dot{m}_{\text{air}} = \frac{k_U u_2 ((2K_M/t_d \tau_1 \tau_2) X_{15} - (K_M/\tau_1 \tau_2) X_{16})}{k_U u_2 + h_d} \quad (4-17)$$

#### 4.5 OFF-GAS TEMPERATURE AND COMPOSITION

In the duct the off-gas from the furnace mixes with the air from the atmosphere that enters at the slip-gap. The carbon monoxide combusts with oxygen that enters with the air. The fraction of carbon monoxide that combusts is determined by the temperature, pressure and concentrations of oxygen and carbon monoxide in the mixed gas in the cooling duct [39].

The temperature of the gas at the end of the cooling duct is determined by the amount of air that is mixed with the EAF gas. It is also determined by the initial EAF gas temperature, the combustion of carbon monoxide in the duct and the amount of cooling done by the cooling water in the walls of the duct. Since the cooling duct has a length of approximately 45m there is a time delay between when gas enters and exits the cooling duct. This time delay is not determined by the velocity of sound, but by the velocity of the gas flow in the cooling duct.

Note that the cooling duct temperature and gas composition refer to the temperature and composition of the gas that exits the cooling duct. The location where the off-gas temperature and composition is under study is shown by the cross hair in Fig.4.1. The motivation for this location is that the temperature and composition should be monitored and controlled in advance of the air-cooled duct, since emergency measures are available to operators to prevent baghouse explosions.

Whereas the time delay and time constants derived in Section 4.2 were necessary to calculate the actual mass-flow in the cooling duct, the time delay in this case is dependent on the magnitude of mass-flow in the cooling duct. Previously approximations to determine the mechanism that

causes mass-flow had to be relied on. In this case the time delay can be calculated precisely from the knowledge of the actual mass-flow, the geometry of the cooling duct and the state (pressure and temperature) of the gas in the cooling duct. In the following three sub-sections algebraic equations will be developed to give the time delay resulting from the actual mass-flow, and then the composition and temperature of the gas that exits the cooling duct.

#### 4.5.1 Composition and Temperature Time Delay

To calculate the off-gas temperature at the entrance of the water-cooled duct, an average between the air temperature and the EAF temperature is taken, based on the ratio of mass-flows:

$$T_{\text{mixed}} = \frac{T_{\text{air}}k_U u_2 + x_{12}h_d}{k_U u_2 + h_d} \quad (4-18)$$

The cross sectional area of the cooling duct is  $5.2\text{m}^2$  on average. The density ( $\rho$ ) of the gas [ $\text{kg}/\text{m}^3$ ] is calculated using equation (4-19), where  $M_{\text{Gas}}$  is an average molar mass of the gas in the duct and  $T_{\text{mixed}}$  is the average temperature of the mixed gas before combustion.  $P$  is the absolute pressure, and  $R$  is the universal gas constant:

$$\rho = \frac{M_{\text{Gas}} P}{RT_{\text{mixed}}} \quad (4-19)$$

The velocity of flow ( $v$ ) can be calculated from the density, mass-flow and cross sectional area. This is shown in equation (4-20):

$$v = \frac{\dot{m}}{\rho A} \quad (4-20)$$

Substitute equations (4-19) and (4-14) into equation (4-20) to get the equation for the actual velocity of flow:

$$v = (RT_{\text{mixed}} ((2K_M/t_d \tau_1 \tau_2)x_{15} - (K_M/\tau_1 \tau_2)x_{16}))/AM_{\text{Gas}}P \quad (4-21)$$

The time delay is equal to the length of the cooling duct divided by the velocity of flow:

$$t_{\text{tcd}} = L/v \quad (4-22)$$

Substitute equation (4-21) into (4-22) to obtain the final equation for the time delay:

$$t_{\text{tcd}} = ALM_{\text{Gas}}P/(RT_{\text{mixed}} ((2K_M/t_d \tau_1 \tau_2)x_{15} - (K_M/\tau_1 \tau_2)x_{16})) \quad (4-23)$$

### 4.5.2 Cooling Duct Exit Composition

The composition of the off-gas at the cooling duct exit is determined by the amount of CO that combusted since the off-gas was mixed with air. The rate of reaction is dependent on the temperature, mol-fraction CO and mol-fraction O<sub>2</sub>. The time delay limits the time the reaction has to take place. The assumption here is that no combustion can occur after the gas exits the cooling-duct. Once again, this is a worst case approximation.

The mol-fractions of CO and O<sub>2</sub> are given by equations (4-24) and (4-25):

$$X_{CO} = \frac{x_9 h_d / M_{CO}}{(x_9 / M_{CO} + x_{10} / M_{CO_2} + x_{11} / M_{N_2})(k_U u_2 + h_d)} \quad (4-24)$$

$$X_{O_2} = \frac{0.2 k_U u_2}{(k_U u_2 + h_d)} \quad (4-25)$$

The fraction of CO (QC<sub>CO</sub>) that will then combust in the cooling duct is given by equation (4-26) where  $\gamma$  is given by equation (4-27). The natural exponential decay relationship is typical for this type of chemical reaction process.

$$QC_{CO} = 1 - e^{-\gamma} \quad (4-26)$$

$$\gamma = k_{\text{combust}} X_{CO} X_{O_2} T_{\text{mixed}} t_{\text{tcd}} \quad (4-27)$$

To determine the rate constant  $k_{\text{combust}}$  the values of the four variables were given their limiting values, and QC<sub>CO</sub> was set equal to 0.95, which is the highest value it should reach.

The limiting values (according to a steady state calculation) for the four variables were:

- $T_{\text{mixed}} = 1250 \text{ K}$
- $t_{\text{tcd}} = 6 \text{ s}$
- $X_{CO} = 0.28$
- $X_{O_2} = 0.14$

This resulted in a value of  $k_{\text{combust}} = 0.01 \text{ K}^{-1} \text{ s}^{-1}$ . The final CO fraction can be derived from equations (4-23) to (4-27). Note that the temperature in equation (4-23) is the same as  $T_{\text{mixed}}$ , and therefore cancels out. The final exit CO fraction is then:

$$FX_{CO} = \frac{x_9 h_d e^{-\gamma}}{(x_9 + x_{10} + x_{11})(k_U u_2 + h_d)} \quad (4-28)$$

Where  $\gamma$  is given by:



$$\frac{0.2k_{\text{combust}}k_U u_2 x_9 h_d M_{\text{Gas}} L_{\text{CD}} A_{\text{CS}} P_{\text{ABS}}}{R \left( \left( \frac{2K_M}{t_d \tau_1 \tau_2} \right) x_{15} - \left( \frac{K_M}{\tau_1 \tau_2} \right) x_{16} \right) \left( \frac{x_9}{M_{\text{CO}}} + \frac{x_{10}}{M_{\text{CO}_2}} + \frac{x_{11}}{M_{\text{N}_2}} \right) M_{\text{CO}} (k_U u_2 + h_d)^2} \quad (4-29)$$

### 4.5.3 Cooling Duct Exit Temperature

The cooling entrance temperature is given by equation (4-18). After the gas enters the cooling duct, it mixes and the carbon monoxide combusts with the oxygen which leads to an increase in the enthalpy. At the same time the forced circulation of cooling water through the duct walls extracts some of the heat. Both of these process rates are proportional to the temperature difference between the off-gas and the atmosphere (cooling water) and inversely proportional to the mass-flow. Since their mechanics are approximately the same, they can be treated in a single relationship. To justify this approximation, recall that in addition to the water-cooled duct, there is also a three-pass air-cooled duct before the off-gas enters the baghouse filter. Thus the water-cooled duct is not the last cooling stage, and the exit temperature is not critical, and an approximation suffices.

The temperature change of gas that flows from the cooling duct entrance to the exit is related to the heat rate of change (DH) in the cooling duct as in equation (4-30). (Units: [K])

$$DT = \frac{DH M_{\text{gas}}}{\dot{m} C_p (\text{gas})} \quad (4-30)$$

The heat change is a combination of the cooling and combustion heats. The cooling heat (DH<sub>1</sub>) and combustion heat rates (DH<sub>2</sub>) are approximated as follows (Units: kJ/s):

$$DH_1 = k_{\Delta C1} \Delta T \quad (4-31)$$

$$DH_2 = k_{\Delta C2} \Delta T \quad (4-32)$$

These rate constants are determined for a specific example, and the two equations are then combined to give the effect of the cooling-duct conditions (cooling as well as combustion) on the off-gas temperature. For this purpose the data in Table 4.1 is used again.

Additional information is obtained from the design drawings. The heat removed between the duct entrance and exit was DH<sub>1</sub> = 39.8 MW = 39800 kJ/s. This value is given in the design drawing. The mass-flow rate is given in Table 4.1 (39.9 kg/s). The atmosphere (and also cooling water) is assumed to be at a temperature of 33°C. The off-gas temperature at the cooling duct entrance is identical with T<sub>mixed</sub> and is 1425 K = 1152°C. The temperature difference is then 1119 K. Substitute the necessary variables into equation (4-31), and the rate constant is k<sub>ΔC1</sub> = -35.57 (kJ)/(sK). If only the cooling heat extraction is considered, the temperature change is:

$$DT = \frac{(39800 \text{ kJ/s})}{(39.9 \text{ kg/s})(0.034 \text{ kJ/molK})} (0.032 \text{ kg/mol}) = 939 \text{ K} \quad (4-33)$$

Here the  $C_p$  and  $M$  values of oxygen were used, since the gas is heavier after some combustion, and the average is comparable to oxygen. At the cooling entrance, the mixed gas has a temperature of  $1152^\circ\text{C} = 1425 \text{ K}$ . If the combustion heat is ignored, then the temperature at the exit is supposed to be  $T_{\text{exit}} = 1425 \text{ K} - 939 \text{ K} = 486 \text{ K} = 213^\circ\text{C}$ . However, this is not the case. The exit temperature (according to the limiting case in the design drawings) is  $606^\circ\text{C}$ , indicating that the combustion heat may not be ignored. The temperature change due to the combustion heat is then calculated as  $606^\circ\text{C} - 213^\circ\text{C} = 393 \text{ K}$ . The corresponding heat change is:

$$DH_2 = \frac{(393 \text{ K})(39.9 \text{ kg/s})(0.034 \text{ kJ/molK})}{(0.032 \text{ kg/mol})} = 16661 \text{ kJ/s} \quad (4-34)$$

From this the second rate constant can be obtained as  $k_{\Delta C2} = 14.89 \text{ (kJ)/(sK)}$ . The combined rate constant is then  $k_{\Delta C} = 14.89 - 35.57 = -20.68 \text{ (kJ)/(sK)}$ . The final equation for the temperature change is then given here in (4-35):

$$DT = \frac{k_{\Delta C} \Delta T M_{\text{gas}}}{m C_p (\text{gas})} \quad (4-35)$$

## 4.6 CONCLUSION

In this chapter the transfer function model for the off-gas system was derived. The necessary assumptions with respect to the steady state gain, time delay and time constants were given and then the model approximation was discussed. The state space model was derived from the transfer function model and the mass-flow division at the slip-gap was discussed. Finally, the off-gas composition and temperature relations were derived.