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Dynamic modeling of a thermally coupled waste heat boiler in an industrial catalytic reactor

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ABSTRACT

In this paper, dynamic modeling of an internal waste heat boiler is investigated which is used to capture reaction heat of an industrial reactor for water vapor production. Waste heat boiler system consists of evaporator and superheater tubes sections and a make-up steam drum. A mathematical lumped model has been used to describe the dynamics of this system in case of drainage. The effect of mass flow rate of drainage on gas side and superheated steam side temperature were presented. The model results showed the same trend in comparison to plant data. It is estimated that there should be an appropriate drainage to inhibit the temperature of superheated steam not to exceed from design value and safe operation of plant.

KEYWORDS

Dynamic modeling;
Waste Heat Boiler;
Drainage;
Lumped model.

INTRODUCTION

Ammonia oxidation over a platinum catalyst is a part of nitric acid production plant. Nitric acid production is one of the large-scale processes in chemical industry. The process involves the catalytic oxidation of ammonia by air (oxygen) in a catalytic reactor which is also referred to as ammonia burner yielding nitrogen oxide then oxidized into nitrogen dioxide and absorbed in water. Nitric acid is then widely used to synthesize explosive and fertilizer production such as ammonium nitrate. The oxidation of ammonia on platinum gauzes produces mainly molecular nitrogen and NO under industrial operating temperature (800-950°C). These products are formed on the catalyst surface by reactions (1) and (2) which are highly exothermic[1]:

$$NH_3 + 5/4\ O_2 \rightarrow NO + 3/2\ H_2O \quad (\Delta H = -226\ kj/mol NH_3) \qquad (1)$$

$$NH_3 + 3/4\ O_2 \rightarrow 1/2\ N_2 + 3/2\ H_2O \quad (\Delta H = -318\ kj/mol\ NH_3) \qquad (2)$$

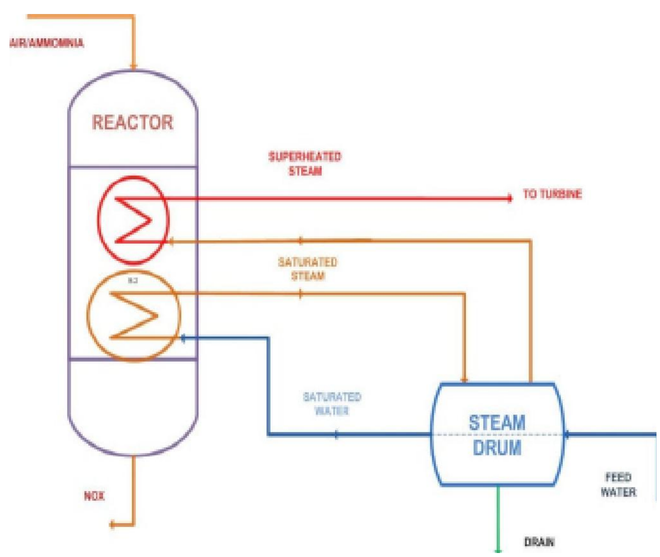

Figure 1 : Schematic diagram of WHB internally coupled in ammonia oxidation reactor

According to the operating conditions of the catalyst, other secondary reactions, which they can reduce the output nitrogen oxide, were not considered.

In this plant, oxidation is obtained by a downward flow of ammonia and air mixture on platinum gauzes. Reaction heat produced in the burner is recovered in the heat recovery unit of ammonia oxidation reactor which is often called waste heat boiler (WHB) by generating 40 bar steam for turbine power generation section. The WHB works as a heat exchanger for cooling the reaction mixture and steam production. Waste heat boiler consists of a water-tube evaporative unit connected in forced circulation flow with the steam drum and a steam superheater which is schematically shown in Figure 1. Superheaterstubes expose to the highest failure probability as reported by French[2] and have finite life contributing to prolonged exposure to high temperature, stress and aggressive environment which was assessed by Ray[3].

Dynamic modeling and simulation are becoming increasingly important in engineering since there is a growing need to analyze the unsteady operation of complex systems. Control of heat integrated systems has been studied by several workers. Heat integration of chemical reactors was studied by Worthey and Georgakis[4]. Tyreus and Luyben[5] studied the dynamics of one type of heat integrated distillation column system. Chaiang[6] explored several other types. Many papers have appeared in the literatures that discuss the dynamics and control of reactors. Stephens[7] investigated a methanol plant consisting of four adiabatic catalyst beds with cold-shot cooling and showed that the exit temperature control failed but the inlet temperature control was successful. Luyben[8] discussed the effect of design and kinetic parameters on the control of cooled tubular reactor systems.

This paper investigates a dynamic modeling of a WHB which can provide significant understandings of a drainage effect on superheated steam temperature, which is supported by information available in the nitric acid plant in Shiraz Petrochemical Complex.

PROCESS DESCRIPTION

The air/ammonia mixture at about 214°C is introduced into the reactor or ammonia oxidizer where it crosses a perforated sheet-plate which distributes it uniformly over the platinum catalysis gauzes. The complete technical design data of the catalyst and input data of heat recovery unit are summarized in TABLES 1 and 2.

Heat released by the ammonia oxidation reaction, added to the air/ammonia mixture's sensible heat, brings the temperature of the catalysis gauzes and gases to about 880°C. The nitrous gas is subjected to cooling in the WHB, which consists of a water-tube evaporative unit connected in forced circulation flow with the steam drum and a steam superheater Figure 2. Treated feed water which is fed to the steam drum is used as the coolantfor cooling reaction mixture. The water is supplied by forced circulation via circulating pump to the evaporative heating surface and returned as a saturated steam to the drum. The produced saturated steam in the steam drum at a pressure of 44 bar g maximum feeds the steam superheater tubes which in turn is led to the steam turbine and for heating the unit's apparatus after it is desuperheated.

TABLE 1 : Gas analyses at inlet of waste heat recovery unit.

Parameters	Value	Unit
Gas flow	kg/h	116000
NO	vol.%	9.81
O_2	vol.%	5.35
N_2	vol.%	67.90
H_2O	vol.%	16.94
Gas density (0°C; 1.013 bar)	kg/m^3	1.1932
Gas pressure (design)	barg	5.54
Gas temperature inlet	°C	880
Gas temperature outlet	°C	475

TABLE 2 : Physical characteristics of catalyst.

Parameters	Unit	Value
Outside diameter	mm	3710
Bordered edge	mm	22
Meshes	per cm^2	1024
Thread diameter	mm	0.076
Weight of Pt-Rhodium	g/m^2	630
Total weight of installed gauzes	kg	55
Life timedays		120

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Figure 2 : Uninstalled connecting tubes of WHB.

DRAINAGE DESCRIPTION

Even with the best pretreatment programs, boiler feed water often contains some degree of impurities, such as suspended and dissolved solids. The impurities can remain and accumulate inside the boiler as the boiler operation continues. The increasing concentration of dissolved solids may lead to carryover of boiler water into the steam (by foaming), causing damage to piping, steam traps and even process equipment. The increasing concentration of suspended solids can form sludge, which impairs boiler efficiency and heat transfer capability. To avoid such problems in boiler, water must be periodically discharged or "blown down" from the boiler to control the concentrations of suspended and total dissolved solids in the boiler. Surface water drainage is often done continuously to reduce the level of dissolved solids, and bottom drainage is performed periodically to remove sludge from the bottom of the boiler.

TABLE 3 : Feed water Quality(< 68 bar g operating pressure; > 250 KW/m²).

Parameters	Unit	Value
General appearance	clear	colorless
Hardness		not detectable
Carbone dioxide as CO_2		not detectable
Total iron as Fe	mg/l	< 0.02
Total copper as Cu	mg/l	< 0.003
Silica as SiO_2	mg/l	< 0.02
Sodium as Na	mg/l	< 0.01
Oxygen (O_2)	mg/l	< 0.1
Conductivity at 25°C	μS/cm	< 0.20
pH at 25	°C	> 9

The analytical requirements are used for safe running of system are shown in TABLES 3 and 4. The problem appears when measured values exceed these limits.

TABLE 4 : Boiler Water Quality(< 68 bar g operating pressure; > 250 KW/m²)

Parameters	Unit	Value
Total iron as Fe	mg/l	< 1.0
Total copper as Cu	mg/l	< 0.12
Hardness		not detectable
Silica as SiO_2	mg/l	< 0.8
Caustic alkalinity	mmol/l	0.02 -0.1
Oxygen (O_2)	mg/l	< 0.1

MATHEMATICAL MODEL

In terms of modeling the dynamics of WHB, a series of mathematical formulations were used.

Model assumption

a. Lumped formulation was employed.
b. All of the boiler water content vaporizes passing through the evaporator tubes.
c. Conduction heat transfer in tubes wall is negligible compared to convection termdue to high thermal conductivity of tube metal.
d. Ideal gases are assumed.
e. The temperature of saturated vapor was assumed to be constant.
f. The heat transfer coefficient was also assumed to be constant.

The energy equation for the evaporator can be written as follow:

$$c_{pv} T_{s.v} \frac{dm_v}{dt} = h_{gs.v} A_e (T_g - T_{s.v}) + Q_{G.R} - \frac{dm_v}{dt} h_{fg} \qquad (3)$$

Where, $T_{S.V}$ and m_V are the temperature and mass flow rate of saturated vapor, respectively and h_{fg} is the latent heat of water. $Q_{G.R}$ is defined as the amount of heat transferred by gas radiation inside reactor which relevant calculations and equations were given as follow:

$$\frac{Q_{G.R}}{A_e} = \varepsilon_g(T_g)\sigma T_g^{\ 4} - \alpha_g(T_{s.v})\sigma T_{s.v}^{\ 4} \qquad (4)$$

Where $E_g(T_g)$ is the gas emittance at T_g and $\alpha_g(T_{s.v})$ is the gas absorptance for the radiation from the black enclosure at $T_{S.V}$ and is a function of both T_g and $T_{S.V}$. Regarding the data from TABLE 2, the highest value for volume fraction of mixture is due to water vapor which is the most important source of gas radiation. Though for a mixture including water vapor, empirical relations exist and they were used in these calculations[9].

The energy equation for the superheater also can be written as follow:

$$c_{ps}m_s\frac{dT_{s.h}}{dt} = h_{gs.h}A_s(T_g - T_{s.h}) + Q_{G.R} + f_s c_{ps}(T_{s.v} - T_{s.h}) \qquad (5)$$

Where, T_g and $T_{s.h}$ are the temperature of nitrous gas and superheated steam, respectively. The heat transfer coefficient can be calculated by[10]:

$$\frac{hd}{k_f} = C(Re)^n\, Pr_f^{\ 1/3} \qquad (6)$$

$$Re = \frac{\rho u_{max} d}{\mu} \qquad (7)$$

$$u_{max} = u_\infty \frac{S_n}{S_n - d} \qquad (8)$$

h, ρ, k_f, u, μ, Re, Pr are the properties of gas flowing downward on tubes (with diameter of *d*) and calculated at bulk temperature. Values of C and n in equation (6) exist in literature[10]. Equation (8) is determination of maximum flow velocity normal to in-line arrangement of tube banks where S_n is the tubes spacing (2 cm).

The energy equation inside reactor can be defined as:

TABLE 5 : Waste heat boiler Data.

Parameters	Unit	Value
Diameter of reactor	mm	3900
Average gas temperature	°C	650
Evaporator heating surface		m^{2}310
Superheater heating surface		m^{2}111
Saturated vapor temperature	°C	256

$$c_{pg}m_g\frac{dT_g}{dt} = h_{gs.v}A_e(T_g - T_{s.v}) + h_{gs.h}A_s(T_g - T_{s.h}) + Q_{G.R1} + Q_{G.R2} - \dot{m}_g\Delta H_r \qquad (9)$$

The relevant variables were tabulated in TABLE 5.

RESULTS AND DISCUSSION

Dynamic modeling results which it was validated with historical process data[11] for a conventional reactor under the design specifications are shown in Figure 3. Relevant input data were tabulated in TABLES 2 and 5. This Figure makes a comparison between the mass flow rate of drainage and temperature of superheated steam and gas flowing over tubes inside reactor. The model illustrates that decreasing the mass of water in steam drum by drainage and thus the mass of vapor results in simultaneous increasing the temperature of steam and gas as the heat source remains unchanged.

Some deviation is observed between model results and plant data which were shown in Figure 4. Such deviation roots in the controller influence on dynamic behavior of system which was not considered in our

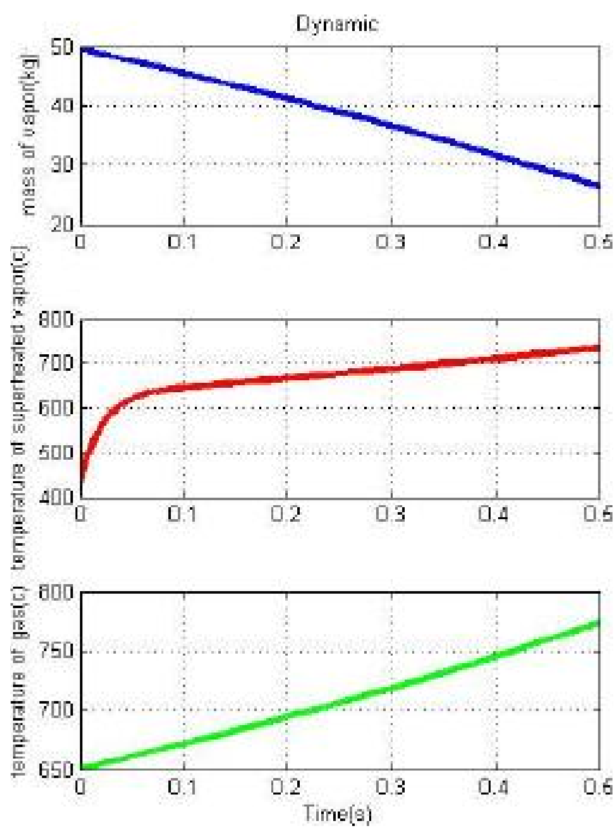

Figure 3 : Dynamic modeling

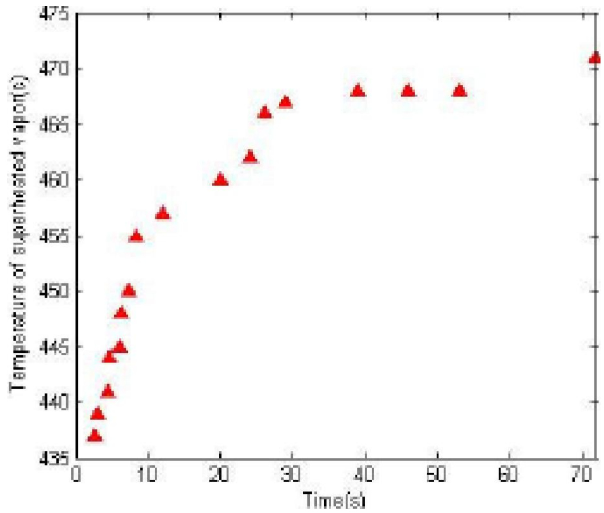

Figure 4 : Plant observed data

modeling. Plant dynamic data are available for a reactor-boiler system which also consists of a controller. However, the same trend is predicted by model.

Furthermore, it is absolutely necessary to observe some values and characteristics of feed and boiler water in order to ensure trouble free operation. One of the most common and serious problem which usually occurs is tube failure. Steam-carrying superheater tubes operating at high temperatures are subject to failure by creep-rupture. These tubes form an internal oxide layer that inhibits heat transfer through the wall and causes the tube metal temperature to increase over time. Creep is the process where metals exposed to high temperature and sustained stress over long periods of time will gradually deform and eventually fail.

The importance of boiler drainage is often overlooked. Inappropriate drainage can cause enhancement of feed water consumption, additional chemical treatment, and as the heat source (heat of reaction) can be assumed to be constant, increasing the temperature of produced steam is natural.

CONCLUSION

Dynamic modeling of a waste heat boiler thermally coupled in ammonia oxidation reactor has been investigated. The study concerns system behavior in case of change in the drainage flow rate in steam drum section. A dynamic mass and energy balance equations were written for the system due to very high heat of reaction and gas radiation which is also included in the model. Model results are compared to the available plant data. Some deviation is observed between model results and plant data due to effect of control system. The same trend is predicted by model while model values differ from plant data to some extent. Dynamic model exhibits poor flow and temperature transition prediction as drainage rate changes.

It is estimated that there should be an appropriate drainage to inhibit the temperature of superheated steam not to exceed from design value and safe operation of plant.

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