NOx emission from a sulfur recovery unit thermal reactor with rounded corners or a vector wall

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Abstract. A sulfur recovery unit (SRU) thermal reactor is important equipment in a sulfur plant. Because its operating temperature is very high, the nitrogen oxides (NOx) produced by a SRU thermal reactor is one of the possible sources of air pollution. In this paper, NOx emission from a practical SRU thermal reactor is analyzed. Both the prototype thermal reactor and its modifications, including modifying the reactor geometry and using a vector wall are compared. Simulation results show that the SRU thermal reactor with a radius of curvature 1m at the zone 1 corner has the lowest NO emission. Compared with using a choke ring, the NO concentration at the reactor exit is higher using a vector wall.

1. Introduction
A SRU thermal reactor is the most important equipment in a sulfur plant. It converts the NH$_3$, H$_2$S and hydrocarbons in the reactants into sulfur. Most of the sulfur elements are recovered from the SRU thermal reactor. The first section of a SRU that uses the Claus process is composed of a burner, a thermal reactor and a waste heat exchanger. The configuration and dimensions of the first section of a SRU for a typical petroleum refinery are shown in Figure 1.

SRU thermal reactors are negatively affected by high temperature operations because high temperature can damage the refractory and the heat exchanger tubes. Our experience of operating a practical SRU thermal reactor in Taiwan shows that the refractories at the zone 1 corner and the choke ring are the parts of the thermal reactor that experience the greatest deterioration. The zone 1 corner has a suddenly expanded geometry and a recirculation zone forms behind it. The temperature at the zone 1 corner can exceed the maximum service temperature of the refractory and cause collapse or deformation. The choke ring is subjected to a bending moment from the rapid combustion gas stream and can collapse or deform.

NOx is a pollutant. It is one of the major sources of air pollution. NOx is a precursor for photochemical smog, contributes to acid rain, and causes ozone depletion. In addition, NOx has been recognized as one of the major causes of excessive peroxide concentration in the atmosphere. Thus, there is a common consensus that NOx control has become a worldwide problem. The formation of NOx can be attributed to four distinct chemical kinetic processes: thermal NOx, prompt NOx, fuel NOx, and intermediate N$_2$O. In general, the contribution from prompt NOx and intermediate N$_2$O is minor. Fuel NOx is produced by oxidation of nitrogen atoms contained in nitrogen-bearing fuels. Thermal NOx is formed by the oxidation of atmospheric nitrogen molecules present in the combustion air and strongly depends on the temperature. Considering the fuel composition for this study shown in Table 1, thermal NOx is the major source of NOx in this study. NOx emission consists of mostly nitric...
oxide (NO) (around 95%), and to a lesser degree nitrogen dioxide (NO₂) and nitrous oxide (N₂O) (around 5%). Therefore, the NO species is the major concern in this study.

![Figure 1](image)

**Figure 1.** The configuration and dimensions of the first section of the SRU for a typical petroleum refinery

The flow field in a SRU thermal reactor involves many complicated mechanisms, such as turbulent mixing, convection and radiation heat transfer modes, combustion, as well as NOx and SOx formations. These mechanisms are all highly complex and may interact with each other, which makes the analysis much more difficult. Hassan et al. [1] simulated the combustion process occurring in the combustion chamber of some domestic boilers. A two-dimensional CFD model is built to simulate the combustion chamber domain, and the partially premixed combustion model with a postprocessor for NOx calculations is used to simulate the combustion process inside the combustion chamber. Franco and Diaz [2] described the state of the art in the field of “clean coal technologies” showing the perspectives of improvement and the critical elements. They reviewed and analyzed the emission control of NOx and SOx, and particle matter as well as advanced coal conversion pathways such as ultra-supercritical (USC), pressurized fluidized bed combustion (PFBC), and integrated gasification combined cycle (IGCC). Normann et al. [3] reviewed available techniques for controlling both the emission of NOx to the atmosphere and the content of NOx in the captured carbon dioxide. Shin et al. [4] developed a comprehensive computer program to evaluate the efficiency of a selective non-catalytic reduction (SNCR) system for a boiler. The standard k-ε turbulence model and eddy breakup model were incorporated to analyze the Reynolds stresses and the turbulent reaction of major fuel species, respectively. Javed et al. [5] presented a review of NOx removal techniques with particular reference to SNCR technology. A review of various features related to selective non-catalytic gas phase injection of ammonia and ammonium salts (as reducing agent) was presented. CFD modeling was also applied to SNCR.
In this paper, NOx emissions from a practical SRU thermal reactor are analyzed. The purpose of this study is to compare the NOx emissions from the SRU thermal reactors (both prototype and its modifications). Practical operating conditions from a petrochemical corporation in Taiwan were used as the design conditions for the discussion.

2. Numerical methods and physical models
In this study, the FLUENT commercial code is used to simulate the reacting and fluid flow in a SRU thermal reactor. The SIMPLE algorithm by Patankar[6] is used to solve the governing equations. The discretizations of convection terms and diffusion terms are respectively performed using the power-law scheme and the central difference scheme. In terms of physical models, considering the accuracy and stability of the models and the evaluations of other researchers, the standard $k$-$\varepsilon$ Model [7], the P-1 radiation model [8] and the non-premixed combustion model with $\beta$–type probability density function [9] are respectively used for the turbulence, radiation and combustion simulations. The standard wall functions [10] are used to resolve the flow quantities (velocity, the temperature, and the turbulence quantities) at the near-wall regions. The detailed governing equations and convergence criterion were described in previous studies by the author [11, 12].

In this study, the numerical model of a SRU thermal reactor is constructed using an unstructured grid. Figure 2 shows the numerical model of the prototype SRU thermal reactor. In Figure 2, the heat exchanger section consists of 19 cooling tubes, which have a diameter of 0.5m, as shown schematically in Figure 3. The heat absorption rate for each heat exchanger tube is 40,000 W/m² and the other walls are adiabatic. No slip condition is applied on any of the solid walls. The exit of the heat exchanger section is connected to other equipment at 300 K and 1 atm by a pipe that is 1.372m in diameter and 11.5m in length.

![Figure 2. Numerical model for the SRU thermal reactor investigated](image)

![Figure 3. Illustration of the arrangement of heat exchanger tubes](image)

In this study, two types of oxygen supplies are investigated: an oxygen-normal supply and an oxygen-rich supply. An oxygen-rich supply increases sulfur recovery. The design conditions (including the species compositions, the temperature, the pressure and the velocity) at the acid gas inlet holes of zone 1 and zone 2 and at the air inlet hole are listed in Table 1. These conditions are practical operating conditions that are used by a petrochemical corporation in Taiwan. The turbulence
kinetic energy is 10% of the inlet mean flow kinetic energy and the turbulence dissipation rate is computed using Eq. (1).

\[ \varepsilon = C_\mu \frac{k^{3/2}}{l} \]  

where \( t = 0.07L \) and \( L \) is the hydraulic diameter.

### Table 1. The design conditions at the acid gas inlet holes and the air inlet hole

| Location | Oxygen-Normal Supply | Oxygen-Rich Supply |
|----------|----------------------|--------------------|
|          | Acid Gas to Zone 1   | Acid Gas to Zone 2 | Air Inlet | Acid Gas to Zone 1 | Acid Gas to Zone 2 | Air Inlet |
| Species  | x (%)                | x (%)              |
|----------|----------------------|--------------------|
| \( \text{O}_2 \) | 0                    | 0                  | 19.87     | 0                    | 0                  | 23.85     |
| \( \text{N}_2 \) | 0                    | 0                  | 74.98     | 0                    | 0                  | 71.26     |
| \( \text{H}_2\text{O} \) | 7.83                 | 4.12               | 5.15      | 4.12                 | 27.97             | 4.89      |
| \( \text{CO}_2 \) | 1.27                 | 1.5                | 0         | 1.48                 | 0                  | 0         |
| \( \text{H}_2\text{S} \) | 82.06                | 89.88              | 0         | 89.9                 | 39.61             | 0         |
| \( \text{CH}_4 \) | 2.28                 | 2.7                | 0         | 2.7                  | 0                  | 0         |
| \( \text{C}_2\text{H}_6 \) | 1.52                 | 1.8                | 0         | 1.8                  | 0                  | 0         |
| \( \text{NH}_3 \) | 5.04                 | 0                  | 0         | 0                    | 32.42             | 0         |
| \( T \) (K) | 319.92               | 316.15             | 403.15    | 313.15               | 316.15             | 397.15    |
| \( P \) (N/m\(^2\)) | 76,920               | 75,068             | 74,382    | 75,068               | 75,068             | 89,572    |
| \( V \) (m/s) | 11.62                | 2.08               | 12.4 (Radial) | 11.46               | 1.88              | 10.8 (Radial) |
| title | 34.1 (Tangential)   |                    | 29.8 (Tangential) |

The grid independence test and validation of the numerical methods have been performed in the author’s previous studies [11, 12].

### 3. Results and discussion

#### 3.1. Effect of reactor geometry

Table 2 shows the exit NO concentrations for SRU thermal reactors with different radii of curvature at the zone 1 corner. Five different radii of curvature at the zone 1 corner, including 0m (i.e. without streamlining), 0.5m, 1m, 1.5m and 2m, are calculated to investigate the geometric effects of the zone 1 corner. Figure 4 shows the numerical models of a SRU thermal reactor with different radii of curvature at the zone 1 corner. From the author’s previous study [13], it was found that the lowest peak temperature is obtained with a radius of curvature 1m at the zone 1 corner. Figure 5 shows the temperature profiles for the SRU thermal reactors using a radius of curvature 1m at the zone 1 corner [13]. With a streamlined zone 1 corner, the average temperature is increased due to the compression effect caused by the decreased volume in zone 1. However, the corner recirculation zone in zone 1 becomes smaller due to the streamlining effect, which yields a reduction in temperature. These two effects (compression effect and a smaller corner recirculation zone) lead to an optimal radius of curvature at zone 1 corner. With larger radii of curvature at zone 1 corner, the compression effect overwhelms the effect of a smaller corner recirculation zone and therefore the peak temperature is higher.

From Table 2, it is observed that the SRU thermal reactor with a radius of curvature 1m at the zone 1 corner has the lowest NO emission because of its lowest peak temperature.
Table 2. Simulation results for SRU thermal reactors with different radii of curvature at the zone 1 corner

(a) oxygen-normal supply

| radius of curvature (m) | peak temperature (K) | average temperature (K) | Exit sulfur concentration (mole fraction) | Exit NO concentration (ppm) |
|------------------------|----------------------|-------------------------|----------------------------------------|----------------------------|
| 0                      | 1902                 | 1500                    | 0.0791                                 | 1.18                       |
| 0.5                    | 1895                 | 1502                    | 0.0792                                 | 0.99                       |
| 1.0                    | 1890                 | 1505                    | 0.0793                                 | 0.93                       |
| 1.5                    | 1913                 | 1508                    | 0.0795                                 | 2.45                       |
| 2.0                    | 1942                 | 1515                    | 0.0798                                 | 3.16                       |

(b) oxygen-rich supply

| radius of curvature (m) | peak temperature (K) | average temperature (K) | Exit sulfur concentration (mole fraction) | Exit NO concentration (ppm) |
|------------------------|----------------------|-------------------------|----------------------------------------|----------------------------|
| 0                      | 2103                 | 1595                    | 0.0902                                 | 14.7                       |
| 0.5                    | 2092                 | 1601                    | 0.0911                                 | 13.7                       |
| 1.0                    | 2071                 | 1609                    | 0.0915                                 | 13.5                       |
| 1.5                    | 2097                 | 1610                    | 0.0915                                 | 14.9                       |
| 2.0                    | 2111                 | 1611                    | 0.0915                                 | 16.1                       |

Figure 4. Numerical models of a SRU thermal reactor with different radii of curvature at the zone 1 corner

Figure 5. Temperature profiles for the SRU thermal reactors using a radius of curvature 1m at the zone 1 corner

3.2. Effect of a vector wall
The specific arrangement of the holes of a vector wall results in spiral motion behind the vector wall and thereby increases the residence time. In addition, a vector wall enhances mixing and temperature uniformity.

![Diagram of vector wall](image)

**Figure 6.** Numerical models of a SRU thermal reactor with a choke ring or a 36-hole vector wall

![Graph and curve plots](image)

**Figure 7.** Comparison of cross-sectional average temperature for the SRU thermal reactor with a choke ring or a vector wall

(a) oxygen-normal supply  
(b) oxygen-rich supply
Figure 8. Temperature profiles for the SRU thermal reactors using a vector wall

(a) using a choke ring (oxygen-normal supply)
(b) using a vector wall (oxygen-normal supply)
(c) using a choke ring (oxygen-rich supply)
(d) using a vector wall (oxygen-rich supply)

Figure 9. Stream traces for the SRU thermal reactors using a choke ring or a vector wall

Figure 6 shows the numerical models of a SRU thermal reactor with a choke ring or a 36-hole vector wall. The choke ring or vector wall is located at 6m away from the zone 1 corner. From the author’s previous study [13] (Figure 7), it was found that with a vector wall, the average temperature in zone 2 is increased due to better mixing. However, the larger surface area of a vector wall results in
a larger blockage effect and hence the average temperature in zone 1 is also increased. Figure 8 shows the temperature profiles for the SRU thermal reactors using a vector wall [13]. It is observed that the average temperature across a vector wall becomes more uniform due to better mixing. Figure 9 shows the stream traces for the SRU thermal reactors using a choke ring or a vector wall [13]. The spiral motion behind the vector wall is clearly observed.

Table 3 shows the sulfur and the NO concentration at exit. In a practical SRU thermal reactor, the refractory may be ruptured due to high temperature, for example, near the zone 1 corner. It can be seen from Table 3 that the sulfur and NO concentration at exit are higher using a vector wall. The exit sulfur concentrations are increased by 0.6% and 2.5% for the oxygen-normal operation and the oxygen-rich operation, respectively, while the exit NO concentrations are increased by 14.4% and 16.3% for the oxygen-normal operation and the oxygen-rich operation, respectively.

**Table 3. Sulfur and NO concentration at the exit for SRU thermal reactors with a choke ring or a vector wall**

|                      | (a) oxygen-normal supply | (b) oxygen-rich supply |
|----------------------|--------------------------|------------------------|
|                      | Exit sulfur concentration (mole fraction) | Exit NO concentration (ppm) | Exit sulfur concentration (mole fraction) | Exit NO concentration (ppm) |
| choke ring           | 0.0791                   | 1.18                   | 0.0902                     | 14.7                     |
| vector wall          | 0.0796                   | 1.35                   | 0.0925                     | 17.1                     |

4. Conclusion
In this paper, NOx emissions from the SRU thermal reactors are analyzed. Both the prototype thermal reactor and its modifications, including modifying reactor geometry and using a vector wall, are compared. Practical operating conditions from a petrochemical corporation in Taiwan were used as the design conditions for the discussion. From the simulation results, it is found that the SRU thermal reactor with a radius of curvature 1m at the zone 1 corner has the lowest NO emission. The NO concentration at exit is higher using a vector wall in comparison with using a choke ring. The result of this study is helpful to the design of a low-nox SRU thermal reactor.

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