# Effect of Reagent Injection Amount and Hole Size on NOx Reduction by SNCR in a CO Boiler

Chun-Lang Yeh

Abstract—This study investigates numerically the NOx reduction by SNCR in a CO boiler. The combustion and fluid flow in the FPC CO boiler is examined with emphasis on the effects of injection amount and hole size of reducing agent on NOx reduction. Simulation results indicate that NOx is formed mainly in the high temperature region near the boiler inlet where the mixing caused by swirler is strong. When reducing agent is injected from the boiler inlet, NOx reduction efficiency increases with the amount of reducing agent but gradually levels off. When the amount of reducing agent is increased to 2.5 times the default value, NOx reduction efficiency is 53%. On the other hand, when reducing agent is injected from 3.6m behind the boiler inlet, NOx concentration is not significantly influenced by the amount of reducing agent injected. Finally, when reducing agent is injected from the boiler inlet, the best NOx reduction efficiency is achieved when the size of reducing agent injection hole is the smallest. However, on the condition of fixed amount of reducing agent injected, NOx concentration is not significantly influenced by the injection hole size of reducing agent. On the other hand, when reducing agent is injected from 3.6m behind the boiler inlet, NOx concentration is not significantly influenced by the injection hole size of reducing agent.

Keywords—CO boiler; Combustion; Fluid Flow; SNCR; NOx Reduction

### 1. Introduction

Nitrogen oxide (NOx) is one of the major sources of air pollution affecting environment seriously. It is generated mainly from high temperature combustion processes and may result in acid rain and damage to the atmospheric ozone layer. In addition, NOx has been recognized as one of the major causes of excessive peroxide concentration in the atmosphere.

Several strategies have been developed to reduce NOx emission. Among them, selective non-catalytic reduction (SNCR) method is one of the most promising and cost-effective NOx reduction strategies for combustion systems. The gas-phase SNCR DeNOx process has been well studied and its deNOx efficiency is around 40% for utility boilers. Liang et al. [1] studied the influence of operating conditions (mixing, temperature, oxygen and residence time) on the SNCR process, in terms of the variations in the concentrations of NO, NH<sub>3</sub>, NO<sub>2</sub> and N<sub>2</sub>O. The results indicated that at lower temperatures, enriched O<sub>2</sub> enhanced NO reduction and N<sub>2</sub>O yield, with more NH<sub>3</sub> being consumed. At higher temperatures, increasing O<sub>2</sub> inhibited NO reduction and suppressed N<sub>2</sub>O formation, with the depletion of NH<sub>3</sub>. Gasnot

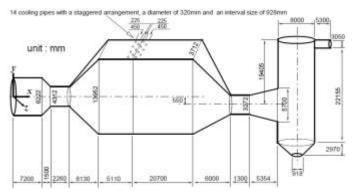
presented an experimental and kinetic study of the influence of additives on the SNCR process. The experimental results prove that the use of such additives allows the NO reduction process to be more efficient at lower temperatures. Ayoub et al. [3] performed an experimental study on the NOx reduction from gas stream by SNCR using urea as a reducing agent. Different types of additives were added during SNCR process to improve NOx reduction efficiency and enlarge temperature window. Anionic surfactants were found to give maximum efficiency for NOx reduction and provide maximum range for the temperature window. Nguyen et al. [4] studied the NOx controlling in a municipal solid waste incinerator by SNCR using urea-water solution by means of computational fluid dynamics (CFD) simulation, which is validated with on-site experiments. At normalized stoichiometric ratio (NSR) = 1.8, 70% NO reduction is obtained from on-site experiments, while 66% NO reduction is from the CFD simulation.

Carbon monoxide (CO) boilers play an important role in the petroleum-refining process. They can retrieve the thermal energy of CO from the regenerator. A CO boiler utilizes the burning gas (CO) from the regenerator as fuel, and CO then reacts to form CO<sub>2</sub> and release large amount of heat. The hightemperature flue gas flows through the superheating section and exchanges heat with water in the cooling tubes to produce superheated steam that can be used by other equipment. The performance of a CO boiler can have a detrimental influence on operation and production in petrochemical industries, steel & iron industries and other relevant industries. This study adopts a CO boiler from the Formosa Petrochemical Corporation (FPC) in Taiwan as the model for numerical investigation [5,6]. Configuration and dimensions of the CO boiler investigated are shown in Fig. 1. In the author's previous studies, the combustion and fluid flow [5] and the application of reburning technology to the NOx reduction in the FPC CO boiler [6] were investigated. In this study, the discussion is focused on the application of SNCR method to the NOx reduction in the FPC CO boiler. Reducing agent for the SNCR method is ammonia (NH<sub>3</sub>). The influences of injection amount and hole size of the reducing agent on SNCR method are inspected.

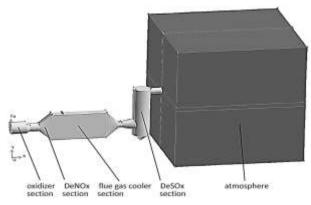
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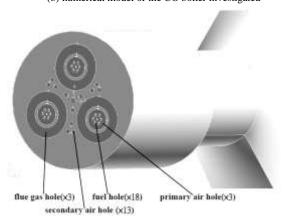




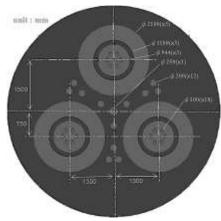
(a) dimensions of the CO boiler investigated



(b) numerical model of the CO boiler investigated



(c) enlarged view of the CO boiler inlet



(d) dimensions of the CO boiler inlet

Figure 1. Configuration and dimension of the CO boiler

### п. Numerical Methods

In this study, the ANSYS FLUENT 12.1 commercial code is employed to simulate the reaction and fluid flow in the FPC CO boiler, and the SIMPLE algorithm by Patankar is used to solve the governing equations. Discretizations of convection terms and diffusion terms are carried out by the power-law scheme and the central difference scheme, respectively. For physical models, by considering the accuracy and stability of the models and by referring to the evaluation of other researchers, the standard k- $\varepsilon$  Model, P-1 radiation model, eddy-dissipation-concept model [7], and the Ostberg and Dam-Johansen's two-step scheme [8] are adopted for turbulence, radiation, combustion and SNCR simulations, respectively. The standard wall functions are used to resolve the flow quantities (velocity, temperature and turbulence quantities) at the near-wall regions. Species compositions at the flue gas inlet holes and the fuel inlet holes, which are provided by Formosa Petrochemical Corporation, are listed in Tables 1 and 2, respectively.

Table 1. Species composition at flue gas inlet ( mole % )

carbon dioxide (CO <sub>2</sub> )	0.131
carbon monoxide (CO)	0.0271
nitrogen (N <sub>2</sub> )	0.7092
water (H <sub>2</sub> O)	0.1327

Table 2. Species composition at fuel inlet ( mole % )

methane (CH <sub>4</sub> )	0.482
ethane $(C_2H_6)$	8.04×10 <sup>-2</sup>
propane (C <sub>3</sub> H <sub>8</sub> )	4.05×10 <sup>-2</sup>
butane (C <sub>4</sub> H <sub>10</sub> )	2.88×10 <sup>-2</sup>
carbon monoxide (CO)	1.69×10 <sup>-2</sup>
oxygen (O <sub>2</sub> )	4.3×10 <sup>-3</sup>
nitrogen (N <sub>2</sub> )	5.48×10 <sup>-2</sup>
hydrogen (H <sub>2</sub> )	0.2919
sulphur (S)	4×10 <sup>-4</sup>

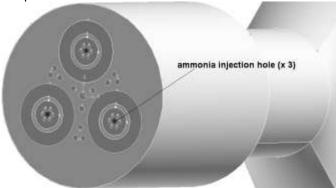
### ш. Results and Discussion

In this study, a numerical model of the CO boiler is constructed by an unstructured grid. A mesh of 351,742 cells is adopted after grid independence test for the original CO boiler in subsequent discussion.

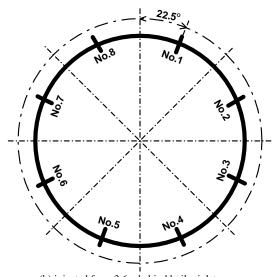
In this study, we investigated two reducing agent injection positions: boiler inlet and 3.6m (at the middle of the oxidizer section) behind the boiler inlet. When reducing agent is injected from the boiler inlet, the three injection holes are located at the centers of the primary air holes, as shown in Fig. 2(a). When reducing agent is injected from 3.6m behind the boiler inlet, the eight injection holes are located at the circumferential wall with 45° intervals, as shown in Fig. 2(b). Default injection hole diameter ( $D_{NH3}$ ) of the reducing agent is 3mm. Default injection velocity of the reducing agent is 194.5m/sec for reducing agent injected from the boiler inlet, and 72.9m/sec for other injection positions. The injection temperature and pressure of the reducing agent are 38°C and 1atm, respectively. In addition to the default injection hole



diameter of 3mm, four additional diameters are inspected to investigate the influence of injection hole size. They are 6mm, 12mm, 24mm and 48mm. Further, besides the default amount of reducing agent injected ( $Q_{\rm NH3}$ ), four additional amounts are also inspected to investigate the influence of injection amount. They are  $0.5Q_{\rm NH3}$ ,  $1.5Q_{\rm NH3}$ ,  $2Q_{\rm NH3}$  and  $2.5Q_{\rm NH3}$ . For the CO boiler with reducing agent injection holes, the numerical model is constructed by adding reducing agent injection holes to the above original CO boiler. By grid independence test, injection hole with a mesh size of 0.5mm is adopted in the subsequent discussion. The total number of meshes is around 390,000 and may differ slightly with the injection hole sizes and positions.



(a) injected from boiler inlet



(b) injected from 3.6m behind boiler inlet

Figure 2. Illustration of the arrangements and locations of the reducing agent injection holes

The inlet pressure is 1 atm. Primary air inlets are facilitated by swirlers at a  $60^{\circ}$  swirl angle. Axial and tangential velocity components are 6.31 and 10.93 m/sec, respectively. Temperature is  $450^{\circ}$ C. Turbulence kinetic energy is 10% of the inlet mean flow kinetic energy and turbulence dissipation rate is computed from Eq.(1) with a hydraulic diameter L=0.944m.

$$\varepsilon = C_{\mu}^{3/4} \frac{k^{3/2}}{l} \tag{1}$$

where l=0.07L and L is the hydraulic diameter. At the secondary air inlet, velocity is 40.154m/sec, temperature is

450°C, turbulence kinetic energy is 10% of the inlet mean flow kinetic energy, and turbulence dissipation rate is computed from Eq.(1) with a hydraulic diameter L of either 0.2m or 0.25m (Fig. 1(d)). At the fuel inlet, velocity is 0.015m/sec for the original boiler, temperature is 323K, turbulence kinetic energy is 10% of the inlet mean flow kinetic energy, and turbulence dissipation rate is computed from Eq.(1) with a hydraulic diameter L=0.1m. At the flue gas inlet, velocity is 13.35m/sec, temperature is 877K, turbulence kinetic energy is 10% of the inlet mean flow kinetic energy, and turbulence dissipation rate is computed from Eq.(1) with a hydraulic diameter L=0.912m. The heat absorption rate of the flue gas cooling tubes is  $13,286 \text{ W/m}^2$  and the other walls are adiabatic. No slip condition is applied on any of the solid walls. The atmosphere at the exit is taken as a cube with a side length of twenty times the exit diameter of the DeSOx section. The atmosphere is at 300K and 1 atm.

## 3.1 Effect of the amount of reducing agent

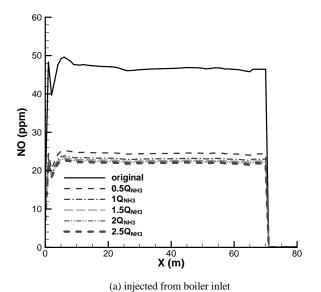
3 compares the cross-sectional averaged NO concentrations for different injection amounts of reducing agent with default injection hole size (D<sub>NH3</sub>=3mm). Fig. 4 shows the temperature distributions and streamtraces for different injection amounts of reducing agent with default injection hole size (D<sub>NH3</sub>=3mm). When reducing agents of 0.5 or 2.5 times the default amount are injected from the boiler inlet, Fig. 4(a) shows that reducing agent can pass through a region where temperature is suitable for the SNCR reaction and because of the good mixing and hence reaction of NOx and reducing agent caused by inlet swirling flow, NOx is reduced effectively. Fig. 3(a) shows that when reducing agent is injected from the boiler inlet, NOx reduction efficiency increases with the amount of reducing agent but gradually levels off. This result is consistent with other researchers' findings [4]. When the amount of reducing agent is increased to 2.5 times the default value, averaged NOx concentration inside the boiler is reduced from 46.2ppm to 21.7ppm, with an efficiency of 53%, which is better by 2% than that of default amount of reducing agent.

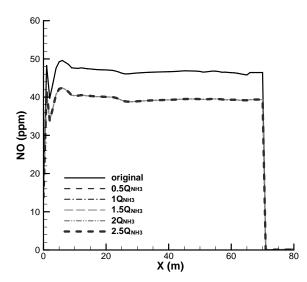
On the other hand, when reducing agent is injected from 3.6m behind the boiler inlet, the reducing agent is injected perpendicular to the main stream. A larger injection amount results in a larger penetration depth of reducing agent. Further, temperature distribution and streamtraces in Fig. 4(b) show that the highest temperature is around 960K which is not within the suitable temperature range for SNCR reaction. However, Fig. 4(c) shows that the recirculating flow in the lower portion of the oxidizer section can recirculate part of the reducing agent upstream into the high temperature region near the boiler inlet suitable for SNCR reaction. This is the dominant factor contributing to NOx reduction and injection amount or penetration depth of reducing agent are instead of minor importance. Therefore, Fig. 3(b) shows that when reducing agent is injected from 3.6m behind the boiler inlet, NOx concentration is not significantly influenced by the injection amount of reducing agent.



3.2 Effect of the injection hole size of reducing agent

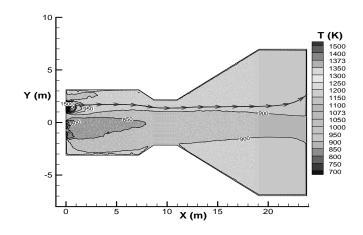
Fig. 5 compares the cross-sectional averaged NO concentrations for different injection hole sizes of reducing agent with default injection amount (Q<sub>NH3</sub>) of reducing agent. Because the injection amount of reducing agent is kept at the default value, the larger the injection hole size is, the smaller the injection velocity would be. It can be observed from Fig. 5(a) that when reducing agent is injected from the boiler inlet, the best NOx reduction efficiency is achieved when the injection hole size of reducing agent is the smallest (D<sub>NH3</sub>=3mm), but the influence of injection hole size on NO concentration is not significant. This result can be interpretated from Fig. 6(a) which shows the temperature distributions and streamtraces for injection hole size D<sub>NH3</sub>=48mm and default injection amount (Q<sub>NH3</sub>) of reducing agent. The temperature distribution and streamtraces in Fig. 6(a) shows that when reducing agent is injected from the boiler inlet, reducing agent can pass through a region where temperature is suitable for the SNCR reaction and hence NOx can be effectively reduced. Therefore, on the condition of fixed amount of reducing agent injected, NOx concentration is not significantly influenced by the injection hole size of reducing agent.





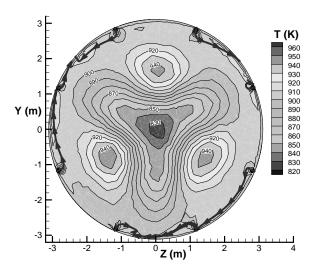
(b) injected from 3.6m behind boiler inlet

Figure 3. Comparison of cross-sectional averaged NO concentrations for different injection amounts of reducing agent ( $D_{NHB}$ =3mm)

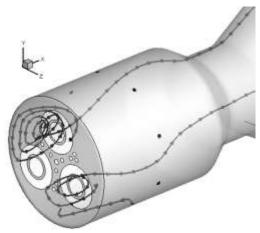


(a) injected from boiler inlet with 2.5  $Q_{\text{NH}3}$ 





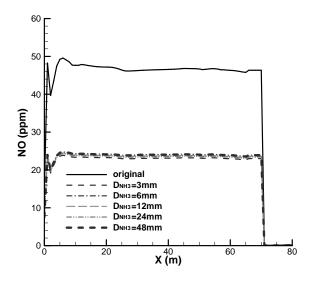
(b) injected from 3.6m behind boiler inlet with 2.5  $Q_{NH3}$ 



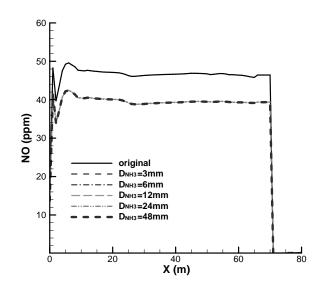
(c) injected from 3.6m behind boiler inlet with  $2.5~Q_{NH3}$ 

Figure 4. Temperature distributions and streamtraces for different injection amounts of reducing agent (D<sub>NH3</sub>=3mm)

On the other hand, when reducing agent is injected from 3.6m behind the boiler inlet, because the reducing agent is injected perpendicular to the main stream, a larger injection hole size leads to smaller injection velocity and penetration depth of reducing agent. Further, temperature distribution and streamtraces in Fig. 6(b) show that the highest temperature is around 960K which is not within the suitable temperature range for SNCR reaction. However, Fig. 6(c) shows that the recirculating flow in the lower portion of the oxidizer section can recirculate part of the reducing agent upstream into the high temperature region near the boiler inlet suitable for SNCR reaction. This is the dominant factor contributing to NOx reduction. Injection hole size or penetration depth of reducing agent are instead of minor importance. Therefore, Fig. 5(b) shows that when reducing agent is injected from 3.6m behind the boiler inlet, NOx concentration is not significantly influenced by the injection hole size of reducing agent.



(a) injected from boiler inlet



(b) injected from 3.6m behind boiler inlet

Figure 5. Comparison of cross-sectional averaged NO concentrations for different injection hole sizes of reducing agent ( with Q<sub>NH3</sub> )

### **IV.** Conclusions

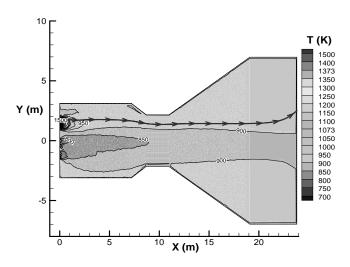
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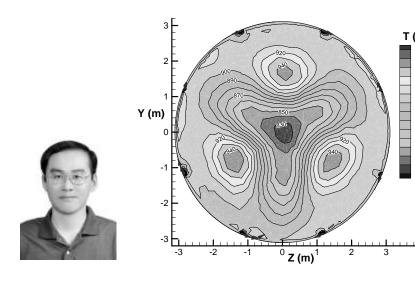
than that of default amount of reducing agent. On the other hand, when reducing agent is injected from 3.6m behind the boiler inlet, NOx concentration is not significantly influenced by the injection amount of reducing agent. Finally, when reducing agent is injected from the boiler inlet, the best NOx reduction efficiency is achieved when the size of reducing agent injection hole is the smallest. However, on the condition of fixed amount of reducing agent injected, NOx concentration inside the boiler is not significantly influenced by the injection hole size of reducing agent. On the other hand, when reducing agent is injected from 3.6m behind the boiler inlet, NOx concentration is not significantly influenced by the injection hole size of reducing agent.

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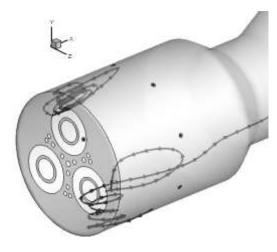
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(a) injected from boiler inlet



(b) injected from 3.6m behind boiler inlet



(c) injected from 3.6m behind boiler inlet

Figure 6. Temperature distributions and streamtraces for injection hole size  $D_{NH3}$ =48mm and default injection amount ( $Q_{NH3}$ ) of reducing agent

### References

- L. Liang, S. Hui, S. Pan, T. Shang, C. Liu, and D. Wang, "Influence of mixing, oxygen and residence time on the SNCR process," Fuel, Vol. 120, pp. 38-45, 2014.
- [2] L. Gasnot, D. Q. Dao, and J. F. Pauwels, "Experimental and kinetic study of the effect of additives on the ammonia based SNCR process in low temperature conditions," Energy & Fuels, Vol. 26, pp. 2837–2849, 2012.
- [3] M. Ayoub, M. F. Irfan, and K. S. Yoo, "Surfactants as additives for NOx reduction during SNCR process with urea solution as reducing agent," Energy Conversion and Management, Vol. 52, pp. 3083–3088, 2011.
- [4] T. D. B. Nguyen, T. H. Kang, Y. I. Lim, W. H. Eom, S. J. Kim, and K. S. Yoo, "Application of urea-based SNCR to a municipal incinerator: on-site test and CFD simulation," Chemical Engineering Journal, Vol. 152, pp. 36-43, 2009.
- [5] C. L. Yeh, "Numerical analysis of the combustion and fluid flow in a carbon monoxide boiler," Int. J. Heat Mass Transfer, Vol. 59, pp. 172-190, 2013.



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- [6] C. L. Yeh, "Numerical investigation of reburning flow in a carbon monoxide boiler," Num. Heat Transfer, Part A, Vol. 66, pp. 622-645, 2014.
- [7] B F. Magnussen, "On the structure of turbulence and a generalized eddy dissipation concept for chemical reaction in turbulent flow," 19th AIAA Aerospace Science Meeting, St. Louis, Missouri, Jan. 12-15, 1981.
  [8] M. Ostberg and K. Dam-Johansen, "Empirical modeling of the selective
- [8] M. Ostberg and K. Dam-Johansen, "Empirical modeling of the selective non-catalytic reduction of NO: comparison with large-scale experiments and detailed kinetic modeling," Chem. Engineering Science, Vol. 49, No. 12, pp. 1897-1904, 1994.

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