A SIMULATION FOR PREDICTION THE NITROGEN OXIDE EMISSIONS IN LEAN PREMIXED COMBUSTOR

Nguyen Thanh Hao(1), Nguyen Thanh Nam(2), Jungkyu Park(3)

(1) HoChiMinh City University of Industry

(2)DCSELAB, University of Technology, VNU-HCM

(3) Department of Mechanical Engineering, Konkuk University, Korea

(Manuscript Received on October 21th, 2010, Manuscript Revised January 21st, 2011)

ABSTRACT: *The development of chemical reactor models to predict NOx emission is very important for the modern combustion system design. In this study, chemical reactor networks (CRN) models are constructed base on the computational fluid dynamics (CFD). The boundary and operating conditions used for these CRN model reflect the typical operating conditions of the lean premixed gas turbine combustor. The global mechanism has been developed by GRI 3.0 in the UW chemical reactor code [2]. For reliability of the predictive model, the model was analyzed and compared to the experimental test combustor.*

Keywords*: Chemical Reactor Networks (CRN), Computational Fluid Dynamics (CFD), Perfectly Stirred Reactor (PSR), Plug Flow Reactor (PFR), Lean Premixed Combustor, NOx, Emission*

1. INTRODUCTION

Controlling pollutant emission remain is one of the most important design goal in developing combustion system. Detailed knowledge of NOx formation in the flame is required for the the ultra-low NOx lean premixed combustors. Relatively small changes in the system boundary conditions can lead to a large emission increase. Therefore, modeling of the combustion process becomes an integral part of the gas turbine engine design process.

Different methods have been presented in the mechanical literature for modeling the turbulent combustion process. However, there are no computer models available that incorporate the full set of chemical kinetic reactions coupled with turbulent flow modeling. In order to model complex combustions, various simplified global kinetic mechanisms developed. Even the use of simplified chemistry in conjunction with CFD for an industrial combustor can take long time for a combustor designer. An intelligently designed CRN can provide answers regarding the quantitative NOx and CO behavior of the combustor.

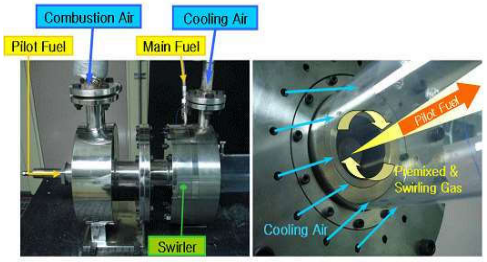
The concept of modeling combustor using chemical reactor such as PSR and PFR was introduced by S. L. Bragg [1]. Zonal combustion modeling was proposed by Swithenbank as an improvement for combustor design via correlation parameters, and followed experimental testing [13]. In the zonal modeling,

the combustor volume is divided into zones represented by idealized reactor elements, such as PSR, PFR, and MIX. Rubins & Pratt applied the zonal model to study emission control in gas turbine combustion [9].

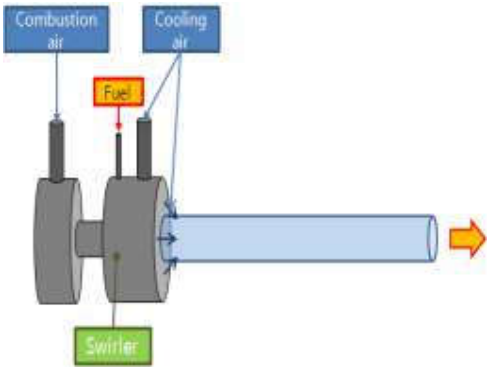
Chemical reactor modeling of combustion systems is not necessarily limited to the use of extensive chemical reactor networks. Recently, Rutar et al. [10], Rutar and Malte [11], Park, J. K. [7], and Lee et al. [3] shown the methodology for modeling the pollutant emissions of the experimental jet stirred reactor with a simple idealized reactor scheme.

A hybrid CFD-CRN model for gas turbine combustors was proposed by Sturgess & Shouse [12]. The post-processing of the CFD simulations was employed for the development of CRN model. Roby et al. modeled the experimental results of Mellor using a CRN with the main combustion zone split into two streams to account for imperfect fuel-air premixing [4, 8]. Novesselov also employed a CRN for NOx and CO emissions prediction of the lean premixed gas turbine combustor of Mellor [4, 5, 6]. The CRN development was based on the CFD solution of the combustor using eight-step global chemistry. Chemical reactor modeling is found to be valuable tool in the evaluation of pollutant formation and blow-out performance of combustion systems. The methodologies of the development vary between authors.

In this work, the CRN approach is applied to predict NOx for lean premixed combustor. The prediction of NOx by the CRN approach is compared to experimental data for the verification of the model. The effects of equivalence ratio, swirler vane angle, pilot fuel ratio are investigated.



(a) Experiment



(b) Schematic diagram

Figure 1. Experimental combustor model

2. DESCRIPTION OF MODELS

2.1 Model Test Combustor

Figure 1 shows the experiment and the schematic diagram of the combustor which is used in experiment. The model system is composed with the combustor liner and the injector which has premixer and pilot. Cooling air is supplied through hole to impact the combustor liner. For measurement of emission density, Testo 360 Gas analyzer was used. This equipment extracts the emission gas sample. Also, the R-type thermocouple probe, which is possible to use from room temperature to 1700K,

was used for measuring the combustor exit temperature. The measurement location was from R/2 points of radius direction. The preheated air temperature was fixed at 650K and the pressure condition is 1 atm. The overall fuel-air equivalence ratio was changed from 0.5 to 0.8. Three different swirler vane angles 30°, 45°, and 60° were used. Pilot fuel-air mixture ratio was varied from 0 to 10% of the injector flow rate, the rich pilot corresponds to the lower than normal premixer equivalence ratio.

2.2. CFD Analysis

CFD modeling provides basic insight of the flow, temperature and species fields/profiles in the combustor. These fields/profiles aid the visualization, interpretation of the combustor flow and reaction space. They are also necessary for constructing an accurate CRN. In this study, the model combustor is modeled using STAR-CD version 4.06 which is a commercial CFD code. For a turbulent model, the k-ε model which has a good convergence, was used. Combustion reactions were analyzed with the Eddy Break-Up combustion model.

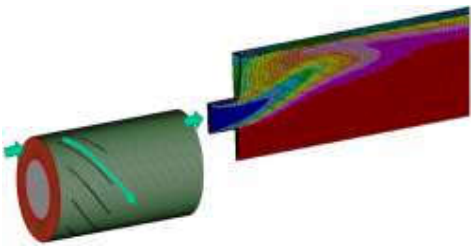


Figure 2. The geometry of swirler vane angle and chamber

The model combustor shown in Figure 2 is a 3D partial model of the swirler and the combustor, which was designed by simplifying the experimental combustor for rapid calculation. The model combustor is composed of the combustion chamber, the main swirl piece and the injector which has pilot fuel nozzle piece. The combustor used in the actual experiment is more complex, but it is simplified for modeling. A five million cell, sector geometry (one complete injector and sector of the annular combustor) with periodic boundary condition is used. The fuel used in the CFD modeling is assumed as methane for the actual natural gas used in engine rig testing.

A representative temperature field in the combustor is shown in Figure 3. This figure shows the zone with a 20% CO concentration, compared with its maximum, which assumes the main flame, the zone where the axial velocity is zero, and the temperature field in the combustor at the equivalent ratio 0.6 for three different swirl ratios without pilot fuel injection. The flame zone was identified with the criteria of 20% of CO concentration (as dotted line in Figure 3), and the other parts as post flame zones. The recirculation zone on the wall surface of the liner is the dome recirculation zone where the temperature distribution is lowest due to forced cooling in the entire combustion zone. The main recirculation zone is the recirculation zone at the center of the combustor and is highly affected by the swirl at the entrance. Figure 3 also shows that the swirl has an effect on the size of the flame zone, recirculation zone.

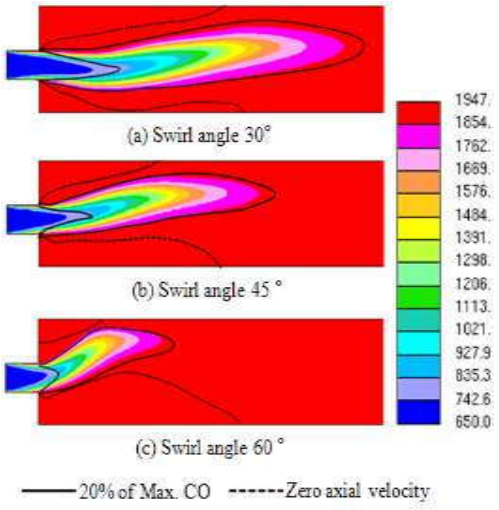


Figure 3. The results of temperature, CO and zero axial velocity at Φ=0.6 for non-pilot injection case

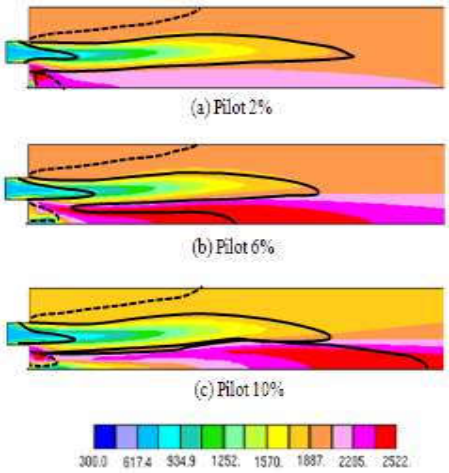
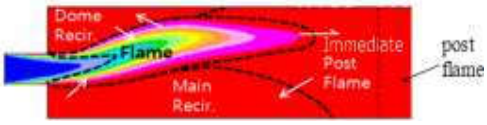


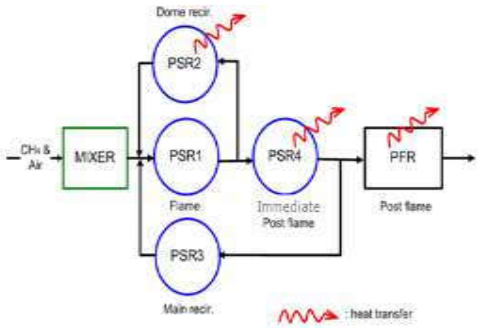
Figure 4. The results of temperature, CO and zero axial velocity at Φ=0.6 for pilot fuel injection case

The CFD analysis was also carried out for the combustor with the pilot fuel injection. In this pilot fuel injection case the swirl number is zero in the main fuel entrance, because the swirler is not attached. The calculation was performed for pilot ratio 2%, 6%, and 10%. Figure 4 shows the results of the temperature and 20% CO concentration compared with its maximum in the case of equivalence ratio 0.6 for three different pilot ratio. The main flame shape is straight and long because the swirler is not used. The temperature in the pilot flame increases as the pilot fuel ratio increases. Although the entire temperature distribution has a similar pattern in all cases, the size of the pilot flame and the main recirculation zone is varied. The length of pilot flame increases abruptly with the increase of pilot fuel ratio.

2.3. Chemical Reactor Network (CRN) Modeling



(a) Zone mapping based on CFD result @ swirl 45°, Φ=0.6



(b) Schematic of the six-element CRN model

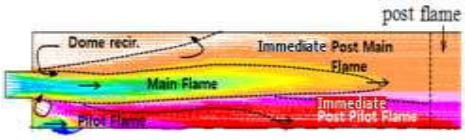
Figure 5. CRN modeling for non-pilot injection case

CRN for the lean premixed test combustor without pilot fuel injection is developed here. The chemical reactor code, CHEMKIN with the detailed chemical kinetic mechanism GRI 3.0 is used for the modeling. The fuel used in the modeling is methane. The combustor can be

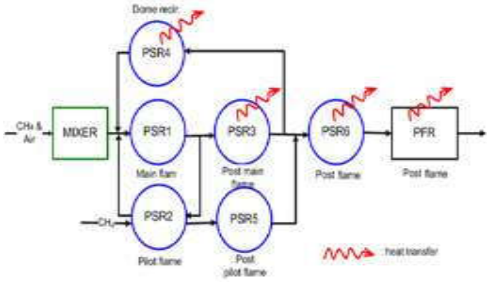
divided into the zones based on the flow temperature, velocity, and chemical species concentrations from CFD analysis. Figure 5(a) shows the flame shape and location, the entrainment of gas from dome and main recirculation zone into the flame, the gas flow from the flame into dome and post flame zone, and gas flow from the post flame zone into main recirculation zone.

Figure 5(b) shows the layout of six-element CRN is constructed based on the CFD-predicted results. The network consists of one MIX, four PSRs and one PFR elements. PSR is generally defined as a reactor where mixing to the molecular is assumed to happen instantaneously compared to chemical reaction. The combustion occurs homogeneously in the reactor. A Plug Flow Reactor (PFR) is the reactor where the flow is assumed to move as a plug and the chemical reaction proceeds one-dimensionally, longitudinal mixing in the reactor is assumed to be zero. MIX stands for an element in which the entering streams are uniformly mixed without chemical reaction. The first element in the CRN arrangement is the MIX, which represent the cone shape zone of inlet mixture where the mixture is not ignited yet. The flame zone, the dome and the main recirculation zone, and the immediate post flame zone are modeled by using PSR., while the post flame zones is modeled by using PFR.

The main flame volume in the CFD simulation can be estimated by calculating the volume confined by iso-CO surface (the value is 20% of the maximum CO concentration). The volume of the dome and main recirculation zone can be determined from the flow pattern and temperature field. The volume of post flame where the flow is assumed to be plug flow is determined by the flow result. Then, the volume of the immediate post flame is finally determined. Flow splits between the elements in the six-element CRN are chosen based on the CFD results for the combustor as shown in Figure 5(a). The mass flow rates toward each reactor were calculated at the boundary of each reactor by taking a surface integral of mass flux over the surface. The cooling of the combustion liner is achieved by convection heat transfer. The averaged heat transfer coefficient is used in this study even though the heat flux varies along the liner. The heat loss in PSR which contact the combustor liner, is calculated using the averaged heat transfer coefficient.



(a) Zone mapping based on CFD result @ pilot fuel ratio 6%, Φ=0.6



(b) Schematic of the eight-element CRN model

Figure 6. CRN modeling for pilot fuel injection case

The CRN modeling was also conducted for the combustor with the pilot fuel injection. Figure

6(a) shows the main and pilot flame shape and location, the entrainment of gas from dome recirculation zone and pilot flame zone into the flame, the gas flow from the flame into immediate post main flame zone and pilot flame zone, and gas flow from the post main flame zone into dome recirculation zone and post flame, gas flow from pilot flame to immediate post pilot flame zone, and gas flow from immediate post main flame zone and immediate post pilot flame into post flame zone.

Figure 6(b) shows the layout of eight-element CRN developed for the combustor with pilot fuel injection. The flame, recirculation and immediate post flame zone are modeled by using PSR. The immediate post flame zone is divided into immediate post main flame zone and immediate post pilot flame zone because of the big temperature difference. Flow splits between the elements in the eight-element CRN are chosen based on the CFD results for the combustor as shown in Figure 6(a).

3. RESULTS AND DISCUSSIONS

3.1. CRN Prediction for Non-Pilot Fuel Injection

Figure 7 shows the NOx predictions with variable equivalence ratio for three different swirler vane angle, 30°, 45°, and 60° without pilot fuel injection for the methane as fuel by using six-element CRN as shown in Figure 5, and the comparison of the predicted results to the experimental data for natural gas as fuel. The lines denote the predicted results and the dots denote the experimental data. The CRN predicted NOx emissions results show the reasonably good agreement with the experimental data. Both the CRN predicted results and the experimental data show that the NOx increase as the equivalent ratio increases. The CRN model underpredicts compared to experimental data when equivalence ratio is low ($\Phi<0.6$), and overpredicts compared to the experimental data when equivalence ratio is high ($\Phi>0.6$). The effects of swirler vane angle on NOx emission is not strong as can be seen in the Figure 7, but both the CRN predicted results and the experimental data show that the lowest NOx emission is found at swirler vane angle 45°, while the higher NOx emissions are found at larger swirler vane angle 60°, and smaller swirler vane angle 30°.

Figure 8 shows the NOx concentration at each reactor zone for three different equivalence ratio, 0.5, 0.6, and 0.7 at swirl vane angle 45° without pilot fuel injection. The NOx concentration in each reactor zone (flame, main recirculation, dome recirculation, immediate post flame zone) increases as the equivalence ratio increases because the temperature in each reactor zone increases with the increase of equivalence ratio as can be seen in Figure 9. The temperature in the dome recirculation zone is lowest among the reactor zones due to heat transfer in the wall. The increase of NOx concentration from equivalence ratio from 0.6 to 0.7 is much larger than the increase of NOx concentration from 0.5 to 0.6 because the NOx formation increases exponentially as the temperature increases.

Figure 10 shows the NOx concentration at each reactor zone for three different swirler vane angle, 30°, 45°, and 60° at equivalence ratio 0.6

without pilot fuel injection. The smallest mole fraction of NOx emission is found at swirler vane angle 45°, while the larger mole fraction of NOx emission is found at swirler vane angle 30°, 60°, because the temperatures in all the reactor zones increase to higher temperatures at swirler vane angle, 30°, 60° as can be seen in Figure 11.

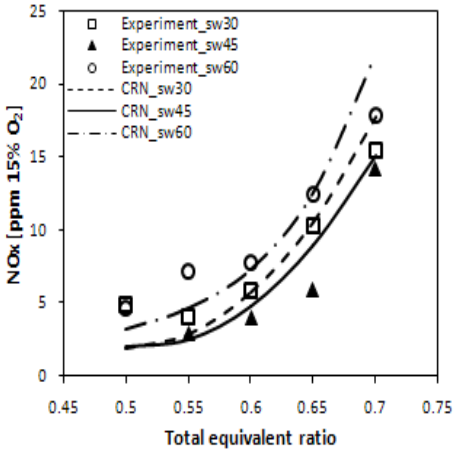


Figure 7. The mole fraction of NOx emission vs. equivalence ratio for non-pilot injection case

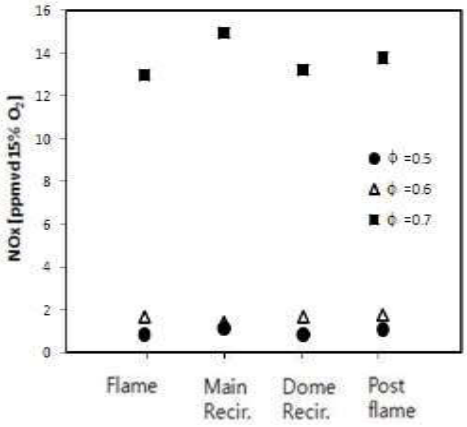


Figure 8. The mole fraction of NOx in each reaction zone for non-pilot injection case

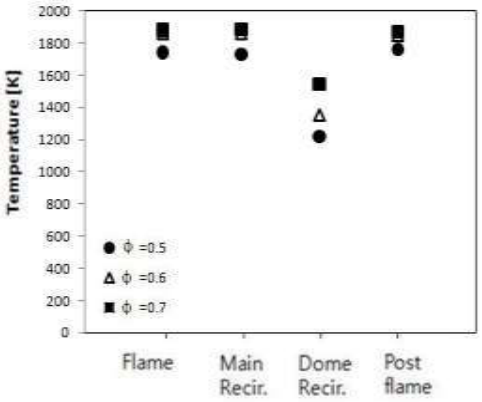


Figure 9. Temperature int each reaction zone for non-pilot injection case

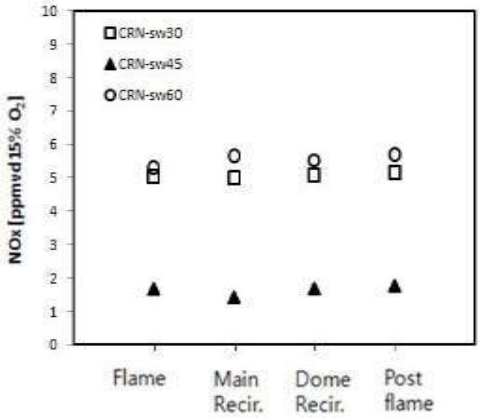


Figure 10. The mole fraction of NOx in each reaction zone for non-pilot injection case

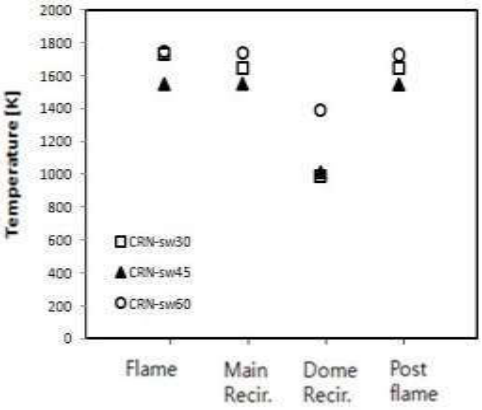


Figure 11. Temperature in each reaction zone for non-pilot injection case

3.2. CRN Prediction for Pilot Fuel Injection

Figure 12 shows the NOx predictions with the variable equivalence ratio for three different pilot fuel ratio, 2, 6, 10% without swirler vane by using the eight-element CRN as shown in Figure 6, and comparison of the predicted results to experimental data. The predicted results of NOx emission show the reasonably good agreement with the experimental data. Both the CRN predicted results and experimental data show that the NOx increase with increase of the overall equivalent ratio and the pilot fuel ratio.

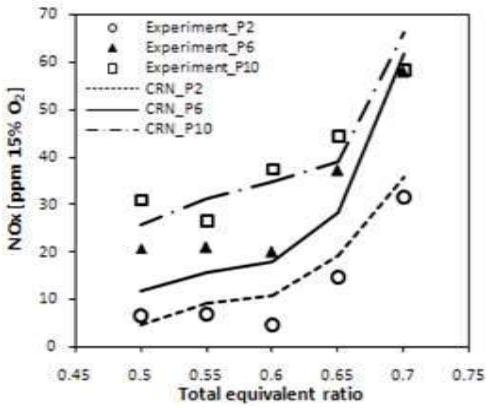


Figure 12. The mole fraction of NOx emission vs. equivalence ratio for pilot fuel injection case

Figure 13 shows the NOx concentration at each reactor zone (main flame, pilot flame, immediate post flame, dome recirculation, immediate pilot post flame zone) for three different pilot fuel ratio, 2, 6, and 10 % at equivalence ratio 0.6. When the pilot fuel ratio is little, the NOx concentration in each reactor is almost same except the pilot post. However, if the pilot fuel ratio increases, the NOx concentration in pilot flame and pilot post increase much more than other reactors because the temperature increases to very high temperature above 2000K as can be seen in Figure 14.

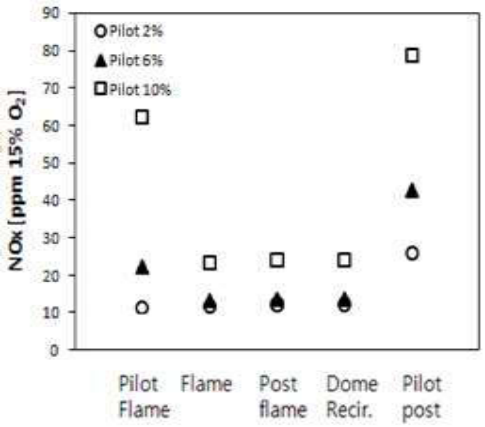


Figure 13. The mole fraction of NOx in each reaction zone for pilot fuel injection case

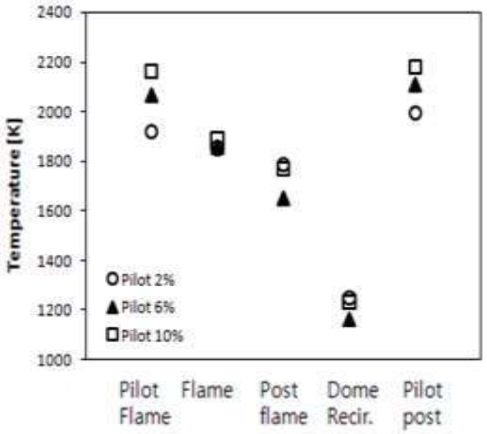


Figure 14. Temperature in each reaction zone for pilot injection case

4. CONCLUSIONS

This research has shown that the use of the combined CFD and CRN approach has the ability to accurately predict NOx emissions for lean-premixed combustion applications. The results are summarized as follows:

(a) The predicted NOx emission by CRN

model based on CFD agrees reasonably well with experimental data of test combustor.

(b) The effect of swirl on NOx emission is not large, but it was found that NOx emission is lowest at swirl vane angle 45°.

(c) The NOx emission increases as the pilot fuel ratio increases due to the increase of temperature at pilot flame and post pilot flame zone.

The CRN tool may be used as a means for parametric analyses and for design. It shows very good capability for prediction the NOx emission.

Nomenclature

CRN : Chemical Reactor Network
CFD : Computational Fluid Dynamic
EBU : Eddy Break Up
CO : Carbon monoxide
NOx : Nitrogen oxides
CH_4 : Methane
K : Kelvin temperature scale

NGHIÊN CỨU QUÁ TRÌNH HÌNH THÀNH KHÍ THẢI NOx TRONG BUỒNG ĐỐT CÔNG NGHIỆP BẰNG MÔ HÌNH MÔ PHỎNG KẾT HỢP CFD VÀ CRN 6 THÀNH PHẦN

Nguyễn Thanh Hào(1), Nguyễn Thanh Nam(2), Park Jung Kyu(3)

(1) Trường Đại học Công nghiệp TP.HCM

(2) DCSELAB, Trường Đại học Bách khoa, ĐHQG-HCM

(3) Konkuk University, Seoul, Korea

TÓM TẮT: *Bài báo trình bày kết quả nghiên cứu quá trình hình thành khí thải độc hại NOx trong buồng đốt công nghiệp bằng phương pháp kết hợp hai mô hình mô phỏng ứng dụng cơ học lưu chất tính toán (CFD) và mô hình mô phỏng ứng dụng mạng phản ứng hóa học 6 thành phần (CRN). Trong nghiên cứu này mô hình số CRN 6 thành phần dùng để xác định thành phần NOx trong buồng đốt được xây dựng dựa trên kết quả từ mô hình số CFD. Các điều kiện biên và điều kiện đầu vào của mô hình CRN 6 thành phần được lấy từ thực nghiệm. Kết quả nghiên cứu mô phỏng được kiểm chứng với thực nghiệm để khẳng định độ tin cậy và hướng phát triển trong việc dự đoán thành phần gây ô nhiễm môi trường đồng thời đảm bảo quá trình cháy sạch trong buồng đốt.*

Từ khóa**:** *mạng phản ứng hóa học 6 thành phần (CRN, cơ học lưu chất tính toán (CFD), Nox.*

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