Modeling of natural gas reburning process with pressure pulsations

L.Szecówka

Technical University of Czestochowa, Armii Krajowej 19, 42–200 Częstochowa, Poland e-mail: szecowka@mim.pcz.czest.pl R.Jarnicki, A.Teodorczyk^{*} Warsaw University of Technology, ITC, Nowowiejska 25, 00-665 Warszawa, Poland, ^{*}e-mail: ateod@itc.pw.edu.pl

Introduction

Computational fluid dynamics (CFD) has become an established tool for the design and understanding of practical combustion systems. Multidimensional models has proven their value in reducing the need for physical experimentation, the benefit of which has been a reduction in product development time and cost.

Combustion is still the most important process of energy generation in the world and at the same time it is the main source of pollution. Combustion generates about 75-85% of NO_x emission, 55-75% of CO, 55-80% of particulates and 100% of CO₂. Therefore, combustion processes should be optimized both according to power and environment criteria. The NO_x emission is one of the most hazardous pollutants and great effort is made to reduce this emission by the primary and secondary methods. Reburning is one of the most effective primary methods used to reduce NO_x emission. The idea of this process is fuel staging in order to reduce fuel NO_x. This process is currently extensively developed in many countries that have large deposits of fossil fuel, i.e. USA. UK. Ukraine, Poland and other. The reason for large interest in reburning lays in the large effectiveness of this process (50–70%), in comparison to relatively low investment and exploitation costs.

The process of NO reduction by reburning depends on many parameters, i.e.:

- type of reburning fuel,
- primary zone stoichiometry,
- reburning zone stoichiometry,
- residence time of reactants in the reburning zone,
- temperature in the reburning zone,
- intensity of mixing of reburning fuel with primary combustion products
- other.

The air excess ratio in the reburning zone λ_{RB} is very important because it directly influences chemistry of the process, and most of all concentration of radicals CH_i, O, H, i OH. In particular CH_i radicals have fundamental importance in the process of NO reduction. Some quantity of O and H radicals is also necessary in the reburning zone in order to form CH_i radicals and to convert HCN to NCO.

Intensity of mixing of reburning fuel with primary combustion products is another important parameter. The intensity of mixing can not be measured in most laboratory tests and therefore it is difficult to determine the characteristic mixing time of reactants. Generally this parameter is determined from mathematical models [1]. Not sufficient mixing may result in the formation of zones too rich or too lean in reburning fuel which in result lowers the efficiency of the process. In particular this is important in large installations. Getting similar effects of reburning process in industrial installations as in the laboratory stand depends on the establishment of similar mixing conditions. Different technical approaches are used to reach this goal, based on experimentation and mathematical modeling with continuous control of the process.

Models of reburning process

Modeling of NO reduction processes is closely connected with the processes of their formation. First models contained mainly chemistry of the process and concerned the kinetcs of chemical reactions. Introduction of hydrocarbon radicals to primary combustion products at particular stoichiometry results in NO reduction to molecular nitrogen. It was first described by Fenimore [2] who studied NO reduction in hydrogen flame with addition of HCN and NH₃. Second model of this process was given by Thorne [3] who studied NO reduction in enriched in fuel C₂H₂ flame. Other models [4] were based on reactions with CH_i radicals. Finally Bose and Wendt [1] have presented a model describing reburning process based on the assumption of partial equillibrium of NH_i radicals. Several other models were based on NO_x reduction by coal fuel [1]. Other models were also developed which included temperature action in the reburning zone [3]. Due to the large importance of mixing intensity in the reburning zone many attempts to include circulation in the process were undertaken by many researchers [1]. This resulted in the development of more sophisticated model by Weber and Wisser [1]. The flow from the burner with fuel staging was modeled by description of the shape of flame resulting from the combustion of coal dust and by introduction of the rate of mixing between primary combustion products and reburning fuel stream. Flow aerodynamics was described by fundamental conservation equations and turbulence model. Several fundamental reactions of NO reduction were also included. Original method of coal particles trajectory tracking was used. Heat transfer process included convection, radiation and heat from coal particles combustion. The model was tested and verified on experimental test stand and gave many important data.

Mathematical model and computations

Reburning is a very complex process, containing heat and flow phenomena connected with chemical kinetics. Having in mind that many researchers underlined the role of mixing we decided to intensify mixing by introduction of pressure pulsations. Our experiments [5 - 8] have confirmed the influence of generated pressure pulsations on mixing of reactants and their combustion. Further studies have revealed the influence of pulsations on emissions of NO_x and CO), and other on spatial location of CH and C₂ radicals in disturbed flame. These observations were used in further experiments consisted in cold and hot model tests.

In the next stage the simulation model was developed of the process of reburning with pulsations. The primary combustion products of fixed chemical composition from the main burner are flowing into the reburning zone, where mixing with additional reburning fuel (natural gas) occurs. Mixing process proceeds in natural way or it can be assisted by pressure pulsations.



Fig. 1 Schematic of reburning unit with modeling area

The region of computations contained the central element of the setup (Fig. 1). The reburning fuel was supplied to the reaction zone. The burnout air was added downstream of the analyzed region.

Numerical computations were performed for undisturbed and disturbed flow. The reburning gas pulsating disturbance was assumed to be of sinusoidal character with average flow velocity of 3.65 m/s and the period of 0.1s. Simulations were carried out for two values of gas velocity amplitude: 1 m/s and 3 m/s.

Numerical simulations were performed with the use of KIVA3V code [9] with detailed chemistry model for natural gas combustion. The model was prepared with the use of CHEMKIN program and consists of 34 chemical species and 170 reactions [10, 11]. The calculations were performed on SGI Octane computer with one R10000 processor. One simulation was running for about 15 days. Several changes in the program were done, to allow reburning simulation application (oscillations of reburning fuel) and to achieve the best comparison to reality.

Results of simulations for undisturbed flow and for two pulsating cases are presented in Fig. 2. Colour graphs show distribution of NO in axial section of the reburning tube and in three cross sections at the distance of 50, 75 and 100 cm from the inlet.

It is evident that the largest reduction of NO occurs in the lower part of the tube in the zone of intense action of reburning fuel. The size of the region of lowered NO concentration depends on the mixing conditions of primary combustion products with reburning gas. When the gas is not subjected to disturbances (Fig. 2a), then the range of reaction does not exceed tube axis. On the other hand the impulsive addition of reburning gas clearly intensifies the mixing process due to wider gas distribution inside the tube. In result the region of lowered NO concentration is increased (Fig. 2b and 2c). The larger amplitude of disturbance (higher energy), the higher effectiveness of reburning process. The calculations show that introduction of pulsations reduces NO concentration in combustion products exiting the tube by 40 to 60%.

Summary

The results of this study confirmed the lowering of NO concentration in combustion products after introduction of pressure pulsations to the reburning zone. The increase of

amplitude of disturbance intensifies the process of mixing of reburning fuel with primary combustion products, which results in higher reduction of NO concentration.

Pressure pulsations influence also the spatial distribution of CH radical. The larger propagation of CH into the upper part of reburning tube occurs together with better equalization of concentration in cross section.

Computations confirmed also the increase of CO concentration in the reburning zone downstream of the point of gas inflow, which was observed in the experiments. After-burning of CO occurs in the third zone after introduction of additional air to the tube.

Quantitative computational results differ from experimental but still they can serve as qualitative guidance in running experimental program, in modernization of installation and in choosing the parameters of the study. For example the graph of NO spatial distribution in axial section (decaying wave) suggests the possibility of mixing intensification by decrease of pulsation period (increase of frequency).

References

- 1 Knill K.J.: Fuel staging and its implementation in a novel internally staged burner, The International Flame Research Foundation, IJmuiden, 1990
- 2 Fenimore C. P.: Studies of fuel nitrogen species in rich flame gases, Combustion and Flame, 26, 1979, s. 249
- 3 Thorne L.R., Branch M.C., Chandler D.W., Kee R.J., Miller I.A.: Hydrocarbon / nitric oxide interactions in low pressure flames, Twenty first Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, 1986, s. 965
- 4 Wendt J. O. L., Pershing D. W., Lee J. W., Glass J. W.: Pulverized coal combustion: NO_x formation mechanisms under fuel – rich and staged combustion conditions, Seventeenth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, 1979, s. 77
- 5 Szecówka L., Radomiak H.: Effect of external disturbances on mixing distance of gaseous substrates and jet configuration. 12-th International Symposium on Combustion Processes, Bielsko-Biała 1991, s. 121
- 6 Szecówka L.: Effect of pulsatory disturbances of substrates on turbulent intensity and combustion conditions. XIII-th International Symposium on Combustion Processes, Cracow 1993, s. 143
- 7 Szecówka L.: Influence of generated large scale pulsation on emission of toxic combustion products, Work Shop on Combustion Safety in Industrial Processes, Cracow 1994
- 8 Szecówka L.: Velocity measuring in flame and isothermal flow subjected to a large scale pulsation, XIV International Symposium on Combustion Processes, Częstochowa 1995
- 9 Amsden, A.A., KIVA-3V: A Block-structured KIVA Program for Engines with Vertical or Canted Valves, LA-13313-MS, (July 1997)
- 10 Golovitchev, V.I., Nordin, N., Jarnicki, R., Chomiak, J., 3-D Diesel Spray Simulations Using a New Detailed Chemistry Turbulent Combustion Model, SAE 00FL-447 (2000)
- 11 Golovitchev, V.I., http://www.tfd.chalmers.se/~valeri/MECH (1998)



Fig. 2. Spatial distribution of NO concentration in modeled tube section

a – without pulsations, b – with pulsations (amplitude of velocity pulsation - 1m/s), c – with pulsations (amplitude of velocity pulsation - 3m/s)