

MODELING STUDY OF NO_x REMOVAL IN FLUE GAS IN THE PRESENCE OF C₂H₆ UNDER ELECTRON BEAM IRRADIATION

Electron Beam Flue Gas Treatment (EBFGT) technology has demonstrated its efficiency in purification flue gases from SO_x and NO_x for coal and oil fired boilers [1]. High removal efficiency of SO₂ (> 95%) and NO_x(>70%) has been demonstrated and industrial plant applying this process has been built in Poland [2]. However SO₂ removal from off-gases by using EB is relatively easy, but NO_x removal needs higher energy consumption. It demands a new method to remove NO_x with lower energy consumption. Our previous work showed that NO_x removal efficiency was improved with the presence of alcohol [3]. In this work we theoretically studied NO_x removal with presence of C₂H₆ with the aid of computer simulation.

The computer simulation of NO_x removal in flue gas under EB-irradiation was carried out by using self-developed computer code "ELO", GEAR method was used. 883 reactions involving 94 species were considered for NO_x+ (air +CO₂ + H₂O) + C₂H₆ (0 – 400 ppm) system, and 998 reactions involving 137 species were considered for NO_x + (air +CO₂ + H₂O) + 400 ppm C₂H₆ + 700 ppm SO₂. Five main groups of reactions were included, the rate constants of reactions were mostly taken from the literatures [4, 5, 6]. The units of rate constant are /s, m³/mole s and m⁶/mole² s for first-, second and third- order reactions, respectively.

When fast electrons from electron beams are absorbed in the carrier gas, they cause ionization and excitation process of the nitrogen, oxygen, CO₂ and H₂O molecules in the carrier gas. Primary species and secondary electrons are formed.

The generation of active species under the electron beam is described by [6]:

$$\frac{dn_i}{dt} = G_{n_i} \dot{D} x_i \rho, \quad (1)$$

where n_i - concentration of i-th component, mole/m³; G_{n_i} - radiation yield of the i-th component of the gas, mole/J; x_i - mole fraction of i-th component; \dot{D} - dose rate, J/(kg·s); ρ - gas density, kg/m³.

Kinetics of chemical reactions of species formed during the gas irradiation with molecules of the gas medium and with one another is described by differential equations:

$$\frac{dn_i}{dt} = n_i \sum_n k_i^{(n)} \prod_{k=1}^n n_k \quad (2)$$

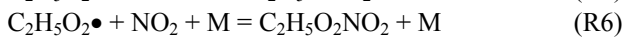
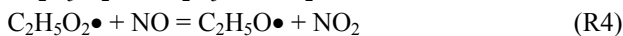
For given initial concentrations:

$$n_i(0) = n_{i0} \quad (3)$$

where, n_i - concentration of i-th component, mole/m³; $k_i^{(n)}$ - the rate constant for n-order chemical reaction between the i-th and the k-components of gas; n_k - concentration of k-th component, n_{i0} - the initial concentration of the i-th component. Calculations were made in the following conditions:

- NO = 494 ppm, NO₂ = 38 ppm, CO₂ = 7 %, H₂O = 10-11 % (v/v), O₂ = 10 %, N₂ as balance, T = 70 °C (no any additives);
- NO = 494 ppm, NO₂ = 38 ppm, CO₂ = 7 %, H₂O = 10-11 % (v/v), O₂ = 10 %, N₂ as balance, T = 70 °C (with presence of 100 ppm and 400 ppm C₂H₆, respectively);
- NO = 494 ppm, NO₂ = 38 ppm, CO₂ = 7 %, H₂O = 10-11 % (v/v), O₂ = 10 %, N₂ as balance, T = 70 °C (with presence of 700 ppm SO₂ and 400 ppm C₂H₆).

Fig.1 presents calculation and experimental results of NO_x removal in flue gas vs. dose under EB-irradiation. Calculation results agree with the experimental results [3] to some extent. NO_x removal under influence of additives is presented in Fig.2. It is seen that NO_x removal efficiency is slightly improved with the presence of C₂H₆. The key reactions are listed below:



The oxidation–reduction cycle between NO₂ and NO is toward the oxidation path and an increase in NO_x removal efficiency is favored.

From calculation results, following conclusions are drawn:

1. Removal efficiency of NO_x is increased by 3 % at a dose of 10.9 kGy with the presence of C₂H₆ when concentration of C₂H₆ is in the range of 100 ppm to 400 ppm.
2. Removal efficiency of NO_x is decreased by 23.84 % at a dose of 10.9 kGy with the presence of

400 ppm C₂H₆ and 700 ppm SO₂. SO₂ presence decreases removal efficiency of NO_x when ammonia is not added.

References

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List title of figures

Fig.1 Experimental and calculation results of NO_x removal from flue gas vs. dose under EB irradiation

Fig.2 Experimental and calculation results of NO_x removal from flue gas vs. dose under EB irradiation with/without the presence of additives

