MODEL STUDIES OF NO_X AND SO_X REACTIONS IN FLUE GAS TREATMENT BY ELECTRON BEAM

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Principalul obiectiv al acestei lucrări este acela de a realiza un model pentru procesul de îndepărtare a SO_2 şi NOx din gazele de ardere, prin iradiere cu electroni accelerați. Au fost studiate diferite compoziții: de la NO în N_2 până la NO într-un amestec complex de NO şi SO_2 dintr-un gaz care conține N_2, O_2, apă, CO_2 şi NH_3, având concentrații similare cu cele din gazele de ardere industriale. Pentru fiecare sistem de reacții s-a observat conversia NO în NO_2, N_2O, N_2O_5, NO_3, N_2, HNO_2, HNO_3, NH_4NO_2 şi NH_4NO_3. Rezultatele obținute din modelul matematic al procesului permit determinarea de efecte complexe.

The main objective of this paper is to realize a model for the SO_2 and NOx removal process from flue gases by electron beam irradiation. Different compositions were studied: from NO in N_2 to NO in a complex mixture of NO and SO_2 from a gas that contains N_2, O_2, water, CO_2 and NH_3, having similar concentrations with those of the industrial flue gases. For each reaction system was observed the NO conversion into NO_2, N_2O, N_2O_5, NO_3, N_2, HNO_2, HNO_3, NH_4NO_2 and NH_4NO_3. The obtained results from the mathematical model of the process allow determining complex effects.

Keywords: removal of NOx and SO_2, reaction mechanism, flue gas radiolysis, electron beam, G value

1. Introduction

During the combustion process of coal, the most important fossil fuel, a series of pollutants are generated: ash with heavy metals, SOx, NOx and volatile organic compounds (VOCs) [1]. Although, the use of alternative fuels [2] does not lead to increase in air emissions and the pollutants emissions remain within the limit values, their existence in the atmosphere in high concentration will affect not only the environment (acidic rain, photochemical smog), but also the public health. That is why they must be removed and several technologies are applied for air pollution control [3].

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The removal process of SO_2 and NOx from flue gases, by reaction with ammonia and by irradiation with electron beam, is one of the latest methods for the flue gases treatment and conversion of the pollutants into products with agricultural utilization (ammonia sulphate and nitrate) [1]. The process implies a great number of reactions, with a high complexity degree from the physico-chemical point of view. For a better understanding of this mechanism, a numerical simulation is necessary in order to solve the mathematical model associated to the process [3].

The main steps that take place during the electron beam irradiation process of a flue gases and ammonia mixture are: absorption of the electron beam energy with the formation of reactive species, chemical reactions in gaseous phase, aerosols formation and their growth and chemical reactions in liquid phase [4]. Researches regarding this domain were realized by a series of scientists [1, 3, 4, 5, 6, 8, 9], but full understanding of the mechanism is still not completely achieved.

2. Experimental

Until this moment, our main objective was to solve the mathematical model of the process constitute by reactions in gaseous phase. In a future paper, we will focus on the aspects regarding the liquid phase reactions with the formation of aerosols.

The steps that were followed for the model process of the SO_2 and NO removal accomplishment are presented in Figure 1:

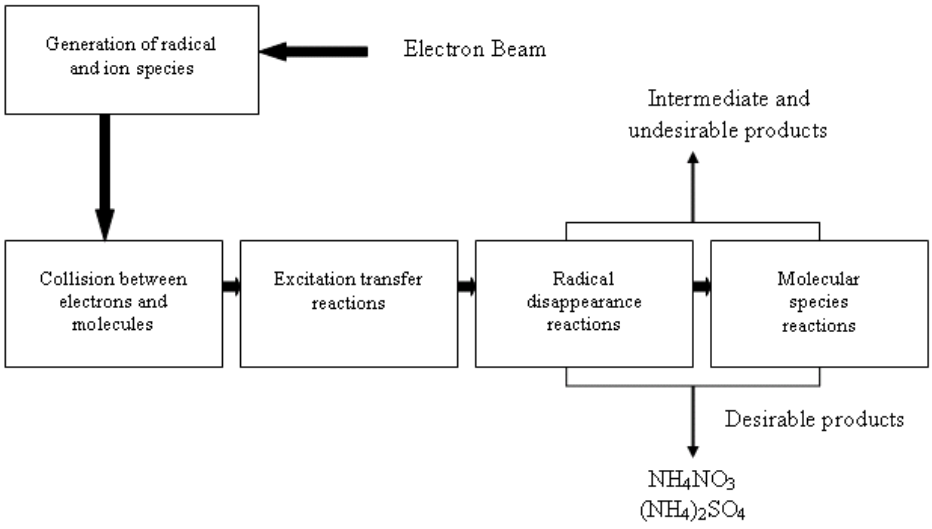

Fig. 1. The scheme of the NO and SO_2 removal mechanism [9]

For the removal mechanism reactions, the latest and the most complete information about kinetics were looked for in the literature. In Table 1 are presented the chemical reactions that describe the irradiation process of the acidic oxides. The rate constant k is expressed in cm^3 $molecules^{-1}$ s^{-1} for chemical reactions with two reactants and in cm^6 $molecules^{-2}$ s^{-1}, respectively for those with three reactants.

The radiolysis process generates a series of reactive species which have a concentration that was computed by the following formula:

$$\frac{d\,|C_i|}{dt} = G_i \times \dot{D} \times \rho \times X_i \tag{1}$$

where: $|C_i|$ is the reactive species concentration that comes from the *i* species and has a X_i molar fraction in the flue gases; G_i is the corresponding radiochemical yield and it is expressed in molecules/100 eV; $\dot{D} \times \rho$ is the irradiation dose flow times the medium density and it is expressed in 100 eV/cm^3s [3]. The G values proposed by Matzing were used [5].

Table 1

Ion and radical reactions for the irradiation mixture of NO-N_2-O_2-H_2O-CO_2-SO_2-NH_3

Reaction No.	Chemical Reaction	Rate Constant [$cm^3 \times molecules^{-1} \times s^{-1}$]	Reference
Generation of radical and ion species			
$4.43N_2 \rightarrow 0.29N_2^* + 0.885N(^2D) + 0.295N(^2P) + 1.87N(^4S) + 2.27N_2^+ + 0.69N^+ + 2.96e$ $5.377O_2 \rightarrow 0.077O_2^* + 2.25O(^1D) + 2.8O + 0.18O^* + 2.07O_2^+ + 1.23O^+ + 3.3e$ $7.33H_2O \rightarrow 0.51H_2 + 4.25OH + 4.15H + 0.46O + 1.99H_2O^+ + 0.01H_2^+ + 0.57OH^+ + 0.67H^+ + 0.06O^+ + 3.3e$ $7.54CO_2 \rightarrow 4.72CO + 5.61O + 2.24CO_2^+ + 0.51CO^+ + 0.21O^+ + 0.07C^+ + 3.03e$			[5]
Collision between electrons and molecules			
1	$N_2^+ + e \rightarrow N(^4S) + N(^2D)$	1×10^{-7}	[6]
2	$e + NO^+ \rightarrow N(^2D) + O$	4×10^{-7}	[6]
3	$e + NO^+ \rightarrow NO + h\nu$	1×10^{-12}	[6]
4	$e + NO_2 + N_2 \rightarrow NO_2^- + N_2$	$1.5 \times 10^{-30} \times [N_2]$	[6]
5	$e + O_2 + N_2 \rightarrow O_2^- + N_2$	$4.8 \times 10^{-31} \times [N_2]$	[6]
6	$CO_2^+ + e \rightarrow CO + O$	$4 \times 10^{-7} \times (300/T)^{0.5}$	[3]
7	$CO_2^+ + e + N_2 \rightarrow CO_2 + N_2$	$6 \times 10^{-27} \times (300/T)^{0.5} \times [N_2]$	[3]
8	$CO^+ + e + N_2 \rightarrow CO + N_2$	$6 \times 10^{-27} \times (300/T)^{2.5} \times [N_2]$	[3]
Excitation transfer reactions			
9	$N_2^+ + NO \rightarrow NO^+ + N_2$	5×10^{-10}	[6]
10	$N_2^+ + O_2 \rightarrow O_2^+ + N_2$	5×10^{-10}	[6]
11	$N_2^+ + CO_2 \rightarrow N_2 + CO_2^+$	8.3×10^{-10}	[3]
12	$O_2^+ + NO \rightarrow NO^+ + O_2$	6.3×10^{-10}	[6]
13	$O_2^+ + NO_2^- \rightarrow O_2 + NO_2$	1×10^{-7}	[6]
14	$O_2^+ + O_2^- \rightarrow 2O_2$	4.2×10^{-7}	[6]

15	$O_2^+ + O_2^- \rightarrow 2O + O_2$	2×10^{-6}	[6]
16	$N(^4S) + NO \rightarrow N_2 + O$	2.2×10^{-11}	[6]
17	$N(^4S) + NO_2 \rightarrow 2NO$	5.9×10^{-12}	[6]
18	$N(^4S) + NO_2 \rightarrow N_2O + O$	7.7×10^{-12}	[6]
19	$N(^4S) + NO_2 \rightarrow N_2 + O_2$	1.8×10^{-12}	[6]
20	$N(^4S) + NO_2 \rightarrow N_2 + 2O$	2.3×10^{-12}	[6]
21	$N(^4S) + O_2 \rightarrow NO + O$	1×10^{-16}	[6]
22	$N(^4S) + O_3 \rightarrow NO + O_2$	3.7×10^{-13}	[6]
23	$N(^4S) + N(^4S) + N_2 \rightarrow 2N_2$	$5 \times 10^{-33} \times [N_2]$	[6]
24	$N(^2D) + N_2O \rightarrow NO + N_2$	1.6×10^{-12}	[6]
25	$N(^2D) + NO \rightarrow N(^4S) + NO$	5.9×10^{-11}	[6]
26	$N(^2D) + O_2 \rightarrow NO + O$	5.2×10^{-12}	[6]
27	$N^+ + CO_2 \rightarrow N + CO_2^+$	1.3×10^{-9}	[3]
28	$N^+ + NO_2^- \rightarrow 2NO$	4.8×10^{-10}	[8]
29	$O + NO + N_2 \rightarrow NO_2 + N_2$	$1 \times 10^{-31} \times [N_2]$	[6]
30	$O + NO_2 \rightarrow NO + O_2$	1.0×10^{-11}	[7]
31	$O + NO_2 + N_2 \rightarrow NO_3 + N_2$	$1.3 \times 10^{-31} \times [N_2]$	[6]
32	$O + O_2 + N_2 \rightarrow O_3 + N_2$	$5.6 \times 10^{-34} \times [N_2]$	[6]
33	$O + O_3 \rightarrow 2O_2$	$1.5 \times 10^{-11} \times e^{(-2.240/T)}$	[6]
34	$O + O + N_2 \rightarrow O_2 + N_2$	$1.6 \times 10^{-33} \times [N_2]$	[6]
35	$O + HNO_2 \rightarrow NO_2 + OH$	1.7×10^{-11}	[6]
36	$O + HNO_3 \rightarrow NO_3 + OH$	1.7×10^{-11}	[6]
37	$O + NO_3 \rightarrow NO_2 + O_2$	1.7×10^{-11}	[7]
38	$SO_2 + O + N_2 \rightarrow SO_3 + N_2$	$1.4 \times 10^{-33} \times [N_2]$	[3]
39	$SO_3 + O + N_2 \rightarrow SO_2 + O_2 + N_2$	$8 \times 10^{-30} \times [N_2]$	[3]
40	$OH + NO + N_2 \rightarrow HNO_2 + N_2$	$7.4 \times 10^{-31} \times [N_2]$	[6]
41	$OH + NO_2 + N_2 \rightarrow HNO_3 + N_2$	$3.3 \times 10^{-30} \times [N_2]$	[6]
42	$OH + HNO_2 \rightarrow NO_2 + H_2O$	6×10^{-12}	[7]
43	$OH + HNO_3 \rightarrow NO_3 + H_2O$	1.5×10^{-13}	[7]
44	$OH + O_3 \rightarrow HO_2 + O_2$	$1.3 \times 10^{-12} \times e^{(-950/T)}$	[6]
45	$OH + NO_3 \rightarrow HO_2 + NO_2$	2×10^{-11}	[7]
46	$CO + OH \rightarrow CO_2 + H$	1.5×10^{-13}	[3]
47	$SO_2 + OH + N_2 \rightarrow HSO_3 + N_2$	$4.5 \times 10^{-31} \times [N_2]$	[3]
48	$HSO_3 + OH \rightarrow H_2SO_4$	9.8×10^{-12}	[3]
49	$HSO_3 + OH \rightarrow SO_3 + H_2O$	8.30×10^{-12}	[3]
50	$H + O_2 + N_2 \rightarrow HO_2 + N_2$	$5.4 \times 10^{-32} \times [N_2]$	[9]
51	$H + O_3 \rightarrow HO + O_2$	2.8×10^{-11}	[9]
52	$H + HO_2 \rightarrow 2OH$	7.2×10^{-11}	[7]
53	$H + HO_2 \rightarrow H_2O + O$	2.4×10^{-12}	[7]
54	$H_2O^+ + H_2O \rightarrow OH + H_3O^+$	9.8×10^{-14}	[4]
55	$H_3O^+ + NO_2^- \rightarrow H + NO_2 + H_2O$	4.8×10^{-12}	[4]
56	$CO_2^+ + O_2 \rightarrow O_2^+ + CO_2$	$6.5 \times 10^{-9} \times T^{-0.78}$	[3]
57	$CO_2^+ + H_2O \rightarrow H_2O^+ + CO_2$	1.7×10^{-9}	[3]
58	$CO_2^+ + O_2^- \rightarrow CO_2 + O_2$	$4 \times 10^{-7} \times (300/T)^{0.5}$	[3]
59	$CO^+ + O_2 \rightarrow O_2^+ + CO$	1×10^{-10}	[3]
60	$CO^+ + H_2O \rightarrow H_2O^+ + CO$	1.3×10^{-10}	[3]
61	$CO^+ + CO_2 \rightarrow CO_2^+ + CO$	8.5×10^{-10}	[3]

62	$CO^+ + O_2^- \rightarrow CO_2 + O$	$4 \times 10^{-7} \times (300/T)^{2.5}$	[3]
63	$O^+ + CO_2 \rightarrow O_2^+ + CO$	1×10^{-9}	[3]
64	$NO_2^- + NO^+ \rightarrow NO_2 + NO$	3×10^{-7}	[6]
65	$O_2^- + NO^+ \rightarrow O_2 + NO$	4×10^{-7}	[6]
66	$O_2^- + NO_2 \rightarrow NO_2^- + O_2$	8×10^{-7}	[6]
	Radical disappearance reactions		
67	$N + CO_2 \rightarrow NO + CO$	4×10^{-13}	[3]
68	$HSO_3 + NO_2 \rightarrow HOSO_2ONO$	8.30×10^{-13}	[3]
69	$HSO_3 + O_2 \rightarrow HOSO_2O_2$	6.64×10^{-14}	[3]
70	$HSO_3 + O_2 \rightarrow SO_3 + HO_2$	4.3×10^{-13}	[7]
71	$HSO_3 + HO_2 \rightarrow H_2SO_5$	8.30×10^{-12}	[3]
72	$HSO_3 + HSO_3 \rightarrow H_2S_2O_6$	4.98×10^{-13}	[3]
73	$HOSO_2O_2 + HSO_3 \rightarrow 2HSO_4$	8.30×10^{-14}	[3]
74	$HOSO_2O_2 + NO \rightarrow HSO_4 + NO_2$	8.30×10^{-12}	[3]
75	$HOSO_2O_2 + NO \rightarrow HOSO_2ONO_2$	8.30×10^{-12}	[3]
76	$HOSO_2O_2 + SO_2 \rightarrow HSO_4 + SO_3$	1.66×10^{-12}	[3]
77	$HOSO_2O_2 + N \rightarrow HSO_4 + NO$	5.81×10^{-12}	[3]
78	$HSO_4 + NO \rightarrow HOSO_2ONO$	1.66×10^{-12}	[3]
79	$HO_2 + NO \rightarrow NO_2 + OH$	8.8×10^{-12}	[7]
80	$HO_2 + NO_2 \rightarrow HNO_2 + O_2$	3.7×10^{-14}	[6]
81	$HO_2 + NO_3 \rightarrow HNO_3 + O_2$	2.1×10^{-12}	[6]
82	$HO_2 + O_3 \rightarrow OH + 2O_2$	3×10^{-15}	[6]
83	$HO_2 + OH \rightarrow H_2O + O_2$	2×10^{-10}	[6]
84	$SO_2 + HO_2 \rightarrow SO_3 + OH$	1.49×10^{-15}	[3]
85	$NH_3 + OH \rightarrow H_2O + NH_2$	1.6×10^{-13}	[7]
86	$NO + NH \rightarrow N_2 + HO$	4.75×10^{-11}	[8]
87	$NH_2 + NO \rightarrow N_2 + H_2O$	1.6×10^{-11}	[7]
88	$NH_2 + NO_2 \rightarrow N_2O + H_2O$	2×10^{-11}	[7]
	Molecular species reactions		
89	$NO + O_3 \rightarrow NO_2 + O_2$	1.8×10^{-14}	[7]
90	$NO + NO_3 \rightarrow 2NO_2$	2.6×10^{-11}	[7]
91	$NO_2 + NO_3 \rightarrow NO + NO_2 + O_2$	4×10^{-16}	[6]
92	$NO_2 + NO_3 + N_2 \rightarrow N_2O_5 + N_2$	$3.6 \times 10^{-30} \times [N_2]$	[6]
93	$NO_2 + O_3 \rightarrow NO_3 + O_2$	3.5×10^{-17}	[7]
94	$2NO_2 + H_2O \rightarrow HNO_2 + HNO_3$	1.49×10^{-37}	[7]
95	$N_2O_5 + N_2 \rightarrow NO_2 + NO_3 + N_2$	$1.2 \times 10^{-19} \times [N_2]$	[6]
96	$NO + HNO_3 \rightarrow HNO_2 + NO_2$	1.7×10^{-22}	[6]
97	$HNO_2 + HNO_3 \rightarrow 2NO_2 + H_2O$	1.1×10^{-17}	[6]
98	$2HNO_2 \rightarrow NO + NO_2 + H_2O$	$1.4 \times 10^{-11} \times (T/300)^{-0.4} \times e^{(-8.843/T)}$	[6]
99	$N_2O_5 + H_2O \rightarrow 2HNO_3$	2.5×10^{-22}	[7]
100	$NO_3 + CO \rightarrow NO_2 + CO_2$	$1.6 \times 10^{-11} \times \exp(-3250/T)$	[3]
101	$SO_3 + H_2O \rightarrow H_2SO_4$	6×10^{-15}	[3]
102	$NH_3 + HNO_2 \rightarrow NH_4NO_2$ (s)	1.05×10^{-7}	[8]
103	$NH_3 + HNO_3 \rightarrow NH_4NO_3$ (s)	1.05×10^{-7}	[8]
104	$2NH_3 + H_2SO_4 \rightarrow (NH_4)_2SO_4$ (s)	1×10^{-7}	[8]

The reaction rates were computed taking into consideration the differential equations that correspond to chemical and radiochemical reactions, as follows [3]:

$$\frac{d\,|C_i|}{dt} = G_i \times \dot{D} \times \rho \times X_i + \textit{rate of formation} - \textit{rate of disappearance} \qquad (2)$$

In order to determine the irradiation dose flow, the following values were used: 1×10^{-3} μA the current of the electrons that were absorbed by 1 cm^3 of gas; 1×10^6 eV/cm^3 the kinetic energy and 0.1 seconds the time step. The G values (molecules/100 eV) for the reactive species formed by the radiolysis of the N_2, O_2, CO_2 and H_2O molecules were those presented in Table 1.

3. Results and Discussions

Seven distinct cases were solved. In the beginning, a simple gas formed by NO and N_2 was used, then O_2, CO_2, H_2O, SO_2 and NH_3 were successively added. In all cases, the same initial concentration of NO (250 ppm) was maintained and the most complex composition was similar to the flue gases obtained at the combustion of some fuels with a high degree of sulphur content.

From the mathematical model results, the variation of the molecular species based on nitrogen concentration was obtained. The most interesting thing was the monitoring of the NO concentration profile with the irradiation dose increasing. Figures 2, 3, 4, 5, 6, 7, 8 present the concentration variation [ppm] function of the irradiation dose [MRad] for each of the seven gas mixtures.

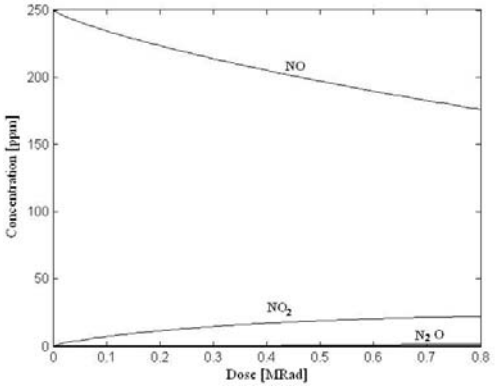

Fig. 2. Concentrations profile function of the irradiation dose for gas mixture 1 – NO (250 ppm) and N_2 (99.975%)

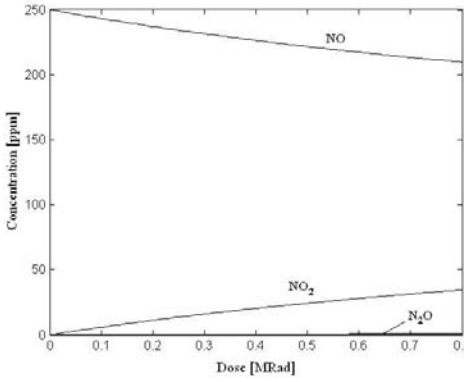

Fig. 3. Concentrations profile function of the irradiation dose for gas mixture 2 – NO (250 ppm), N_2 (91.975%) and O_2 (8%)

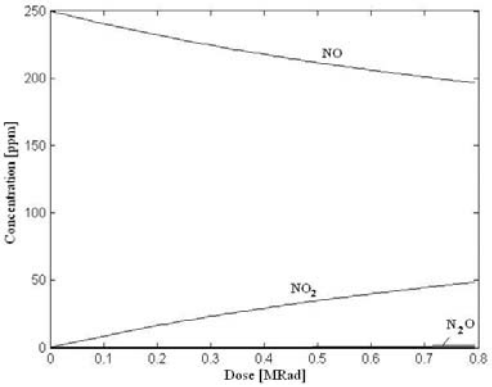

Fig. 4. Concentrations profile function of the irradiation dose for gas mixture 3 – NO (250 ppm), N_2 (81.975%), O_2 (8%) and CO_2 (10%)

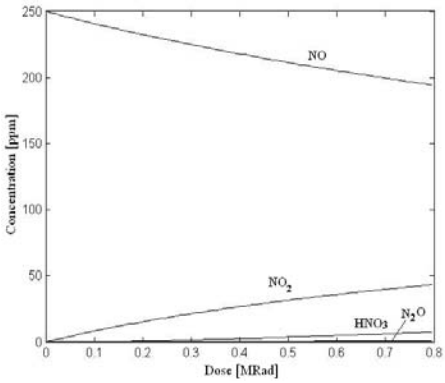

Fig. 5. Concentrations profile function of the irradiation dose for gas mixture 4 – NO (250 ppm), N_2 (81.975%), O_2 (8%) and H_2O (10%)

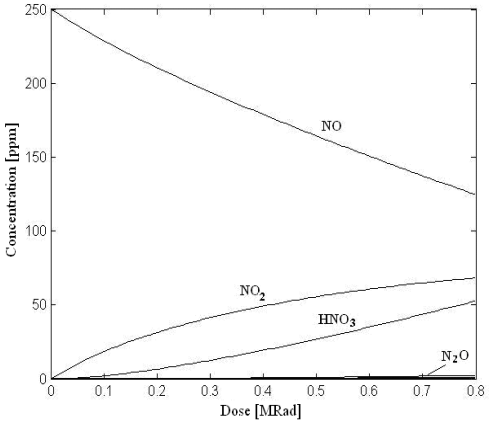

Fig. 6. Concentrations profile function of the irradiation dose for gas mixture 5 – NO (250 ppm), N_2 (71.975%), O_2 (8%), CO_2 (10%) and H_2O (10%)

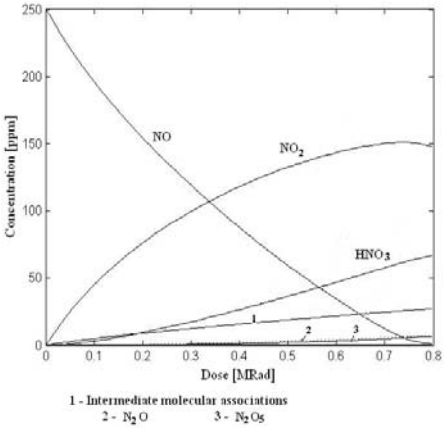

Fig. 7. Concentrations profile function of the irradiation dose for gas mixture 6 – NO (250 ppm), N_2 (71.775%), O_2 (8%), CO_2 (10%), H_2O (10%), SO_2 (2000 ppm)

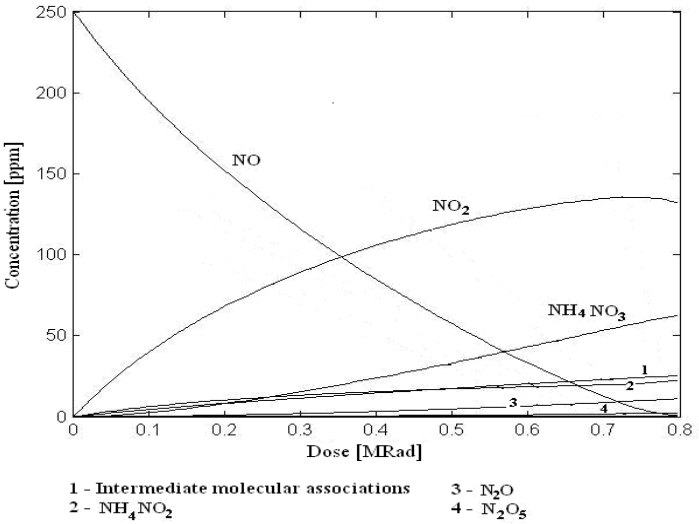

Fig. 8. Concentrations profile function of the irradiation dose for gas mixture 7 – NO (250 ppm), N_2 (71.325%), O_2 (8%), CO_2 (10%), H_2O (10%), SO_2 (2000 ppm) and NH_3 (0.45%)

Table 2 lists the initial used compositions, the NO concentrations from the exit and the quantities of the new formed NO during the process. The initial concentration of NO was 6.722×10^{15} molecules/cm^3. According to Figure 9, the radiolysis of the nitrogen will lead to the formation of active species such as N(^{2}D) and N(^{4}S) that can generate NO (see 17, 21, 22, 26 reactions). In the same time, new amounts of NO can be formed in the above mentioned 28, 67 and 77 reactions.

Table 2

Mixtures composition at the entrance, NO concentration at the exit and the quantity of the new formed NO

Mixture	Entrance							Exit	
	NO	N_2	O_2	CO_2	H_2O	SO_2	NH_3	NO	NO new
	%	%	%	%	%	%	%	molec./cm^3/10^{15}	
NO,N_2	0.025	99.975						4.73	1.85
NO,N_2,O_2	0.025	91.975	8					5.64	0.93
NO,N_2,O_2,CO_2	0.025	81.975	8	10				5.3	0.54
NO,N_2,O_2,H_2O	0.025	81.975	8		10			5.23	0.78
NO,N_2,O_2,CO_2,H_2O	0.025	71.975	8	10	10			3.36	0.38
$NO,N_2,O_2,CO_2,H_2O,SO_2$	0.025	71.775	8	10	10	0.2		0.029	0.35
$NO,N_2,O_2,CO_2,H_2O,SO_2,NH_3$	0.025	71.325	8	10	10	0.2	0.45	0.024	0.35

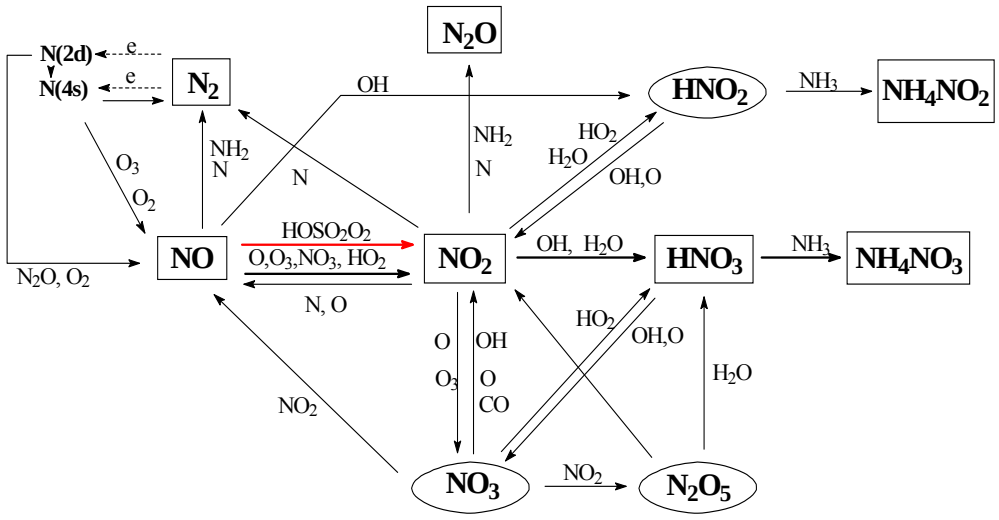

Fig. 9. The scheme of the chemical reactions involved in the conversion of nitrogen species during electron beam irradiation of flue gases mixture and ammonia

Taking into consideration the obtained results, two removal efficiencies of NO were determined and Table 3 presents the calculated efficiencies for each gas mixture.

$$Efficiency_{removal} = \frac{NO_{initial} - NO_{final}}{NO_{initial}} \times 100 \tag{3}$$

$$Efficiency_{total} = \frac{(NO_{initial} + NO_{formed}) - NO_{final}}{NO_{initial} + NO_{formed}} \times 100 \tag{4}$$

where: $NO_{initial}$ = NO initial concentration, ppmv;
NO_{final} = NO concentration after treatment, ppmv;
NO_{formed} = NO formed from nitrogen, ppmv.

From the above given Figures 2-8 and from the computations, it was observed that NO was consumed as much as the model became more and more complex. An important leap in the NO removal efficiencies rising was obtained when the gases contained water and CO_2, but the highest increase was calculated when the gases also contained SO_2 (the removal efficiencies for NO practically became double). Figure 10 presents the NO concentration profile function of the irradiation dose in all seven proposed gas mixtures.

Table 3

Removal efficiencies for NO

Mixture	Removal Efficiency	Total Efficiency
	%	%
NO, N_2	29.63	44.82
NO, N_2, O_2	16.10	26.29
NO, N_2, O_2, CO_2	21.15	27.02
NO, N_2, O_2, H_2O	22.20	30.29
NO, N_2, O_2, CO_2, H_2O	50.01	52.69
NO, N_2, O_2, CO_2, H_2O, SO_2	99.57	99.59
NO, N_2, O_2, CO_2, H_2O, SO_2, NH_3	99.64	99.66

During the electron beam irradiation process, a part of the total NO concentration that entered in the reaction gas mixture is consumed, but, in the same time, a certain amount of NO is formed, function of the chosen gas mixture.

The used computation program allowed us to separately calculate the total concentration of the new formed NO that was obtained from 17, 21, 22, 26, 28, 67 and 77 reactions.

The new formed NO concentrations functions of the irradiation dose are represented in Figure 11. It can be observed that the largest amounts were obtained when a mixture of nitrogen and NO was irradiated by electron beam. When a gas mixture with a concentration similar to flue gases was subjected to an electron beam irradiation, the new formed NO amounts decrease, being approximately 10 times lower than the initial NO concentration. It is observed that the presence of ammonia will lead to a certain increase of the new formed NO amount.

4. Conclusions

A complex kinetic model was obtained. It describes the gaseous phase reactions that take place during the radiolysis of a flue gases mixture and ammonia.

Data about the conversion of nitrogen oxide into reactive species ($N(^4S)$, $N(^2D)$, N, NO_2^-, NO^+, N_2^+ and N^+), intermediate molecular associations ($HOSO_2ONO$ and $HOSO_2ONO_2$) and molecular species (NO_2, N_2O, N_2O_5, NO_3, N_2, HNO_2, HNO_3, NH_4NO_2 and NH_4NO_3) were obtained by solving the mathematical model.

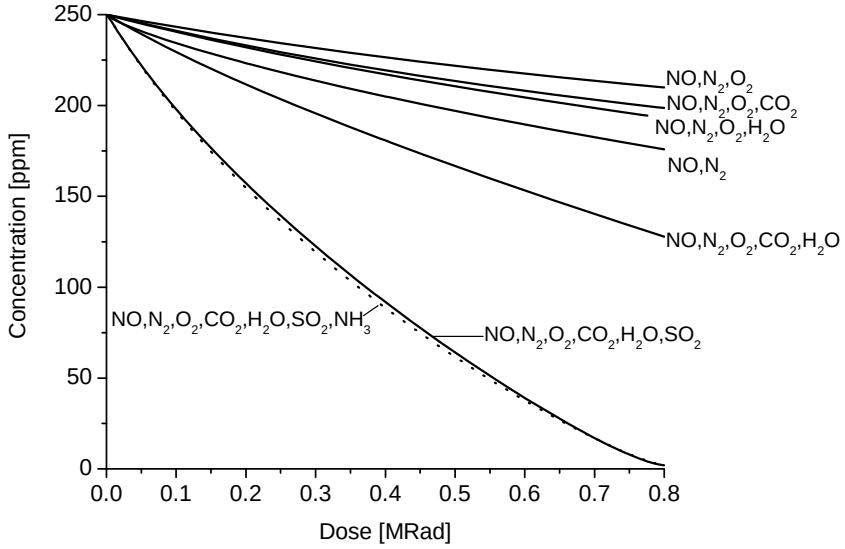

Fig. 10. The dependence of the consumed NO concentration upon the irradiation dose for different compositions of the gas mixture

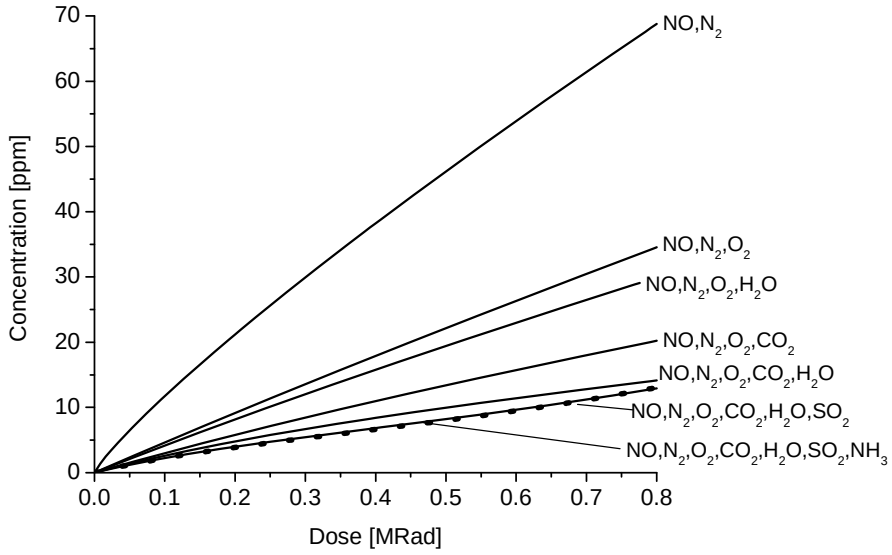

Fig. 11. The dependence of the new formed NO concentration upon the irradiation dose for different compositions of the gas mixture

The model was solved for seven different gas compositions. In the beginning, the gas mixture was a simple one, formed by NO and N_2, then O_2, CO_2, H_2O, SO_2 and NH_3 were successively added.

It was observed that the presence of some components in the gas that was subjected to radiolysis will favor the NO removal from the gas. The influence order of these components is:

$$CO_2 < H_2O < (CO_2+H_2O) << SO_2$$

The amount of the new NO, formed during the radiolysis process, was also put into evidence. When a gas mixture with a concentration similar to industrial flue gases was subjected to radiolysis, the amount of the new formed NO will not exceed 10 % from the initial NO concentration, existent in the gas mixture.

The formation of NO during this process is not a barrier as long as the final NO concentration is low. On the contrary, the NO formation will lead to a certain increase in the total amount of the formed ammonia nitrate, fact that is beneficial for the composition of the obtained product which is used as agricultural fertilizer.

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