Publ. Astron. Obs. Belgrade No. 89 (2010), 163 *Topical Lecture*

EFFECT OF GAS MIXTURE COMPOSITION ON TAR REMOVAL PROCESS IN A PULSED CORONA DISCHARGE REACTOR

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Abstract. The simulation of naphthalene ($C_{10}H_8$) removal from several gas mixtures (pure nitrogen, mixtures containing N_2 with CO_2, CO, H_2, H_2O, and biogas - the product of biomass gasification), has been investigated. The modeling is based on the experimental data obtained in the reactor with a pulsed positive corona discharge. The problem of simulation of the cleaning process includes description of two stages. The first, fast stage is generation of primary active species during streamer propagation. The second, slow stage is the chain of chemical transformations triggered by these species. The input parameters for the modeling of the second stage are *G*-values for generation of primary active species, obtained under consideration of streamer dynamics. Simulation of the second stage of the removal process takes into account the processes of chemical kinetics and diffusion outside and inside of streamer traces during multi-pulsed treatment.

Besides neutral active species, streamer discharges produce electrons and ions. Primary positive ions (N_2^+, CO^+, CO_2^+, H_2^+, H_2O^+) in a chain of fast ion-molecule reactions transform into more stable positive ions. The ions recombine with electrons. Both ion-molecule reactions and electron-ion recombination process are additional (to dissociation of gas molecules by electron impact in the streamer head) sources of neutral active species. The relative contribution of these sources to the G-values for H, OH and O is rather large. In our modeling two approaches have been used. At the first approach the contribution of ion-molecule reactions is estimated approximately assuming that the dominating stable ion is N_4^+ (in pure N_2 and its mixtures with H_2) or CO_2^+ (in mixtures including CO_2). Other way is the calculations with kinetic scheme including the molecular ions, aquated ions such as $H_3O(H_2O)_m^+$, $NO_2(H_2O)^-$, $NO_2(H_2O)^+$ and other. The comparison of results of two approaches is presented. Only full kinetic scheme allowed describing the experimental results for 82.5%N_2+17.5%H_2O mixture on $C_{10}H_8$ removal.

Obtained dependencies of the remaining naphthalene fraction versus the specific energy input have been compared with the experimental data. The results agree rather well for considered mixtures. The best decomposition has been obtained in nitrogen with water vapor, a little better than that in pure nitrogen, both in experiments and in the simulation. It has been found that the reaction of naphthalene with excited nitrogen molecules $N_2(A^3\Sigma)$ plays a key role in the removal process. Addition to N_2 of such gases as CO, CO_2 and H_2 reduces the removal efficiency noticeably.