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MECHANISM OF REDUCTION OF AIR POLLUTANTS ON CARBONS: SULFUR DIOXIDE AND OZONE

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Sulfur dioxide, ozone and nitrogen dioxide are air pollutants of the environment that cause acid rain and interfere with human health. The solid-gas kinetics were studied in a flow system with a tubular reactor under differential and steady state conditions. The reduction of XO_2 on carbons proceeds through a common primary mechanism with oxidized and reduced intermediates. The reactivity of the intermediates inserted on carbons (graphite, activated carbon, graphene oxide, carbon nanotubes) modified by SO_2 is selective. Theoretical study of the chemisorption of SO_2 on dehydrogenated pyrene as graphite active site model and computational quantum chemistry calculations, showed that at 900 °C the chemisorption occurs mainly on the diradical zigzag edge through cycloaddition formation of oxidized sulfur intermediates. Tetradehydrogenated-benzo[α]anthracene (TBA) was used as reactive site model of the reduction of SO_2 on graphite. The calculations of the pathways were consistent with the experimental results. Ozonation of graphite showed that the 1,2,3-trioxolane decomposes to an oxyrene, eliminating O_2. Both reactions, the SO_2 and O_3 with graphite, have the same experimental free energy of activation for the decarboxilation reaction. The SO_2 the desulfurization step has a much lower energetic demand than the decarboxylation route. Therefore, the reduction of SO_2 on carbons can occur without increasing the greenhouse effect due to the formation of CO_2.

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