

Cyclopentadiene conversion

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Despite the technological advances of recent decades, combustion processes remain as one of the main sources of pollution. One of the main pollutants emitted from combustion is particulate matter like soot. Conventional fossil fuels reserves are depleted, which would promote the use of alternative energy sources. Among those, a promising future alternative is the consideration of the fracking or hydraulic fracturing for the extraction of oil from unconventional reservoirs, and therefore the role of combustion process may still be on top.

Although the general characteristics of unconventional fuels (obtained from fracking) can be considered comparable to those of conventional fuels, the specific fuel composition can differ significantly, depending on their origin. In this context, it is of special relevance the fact that shale fuels may have a higher content of aromatics [1] and therefore, their conversion and soot formation trends would be expected not to be the same as for the conventional fuels. Cyclopentadiene (C_5H_6) is an important compound which may be present in such fuels, and also generated during the conversion of aromatics (e.g. benzene) [2]. Therefore, C_5H_6 may be present in the combustion process. Furthermore, it is known that cyclopentadiene may contribute significantly to the formation of polycyclic aromatic hydrocarbons (PAH) in the early stages of PAH and soot formation [3].

In this context, we performed a study of the conversion of cyclopentadiene under different operating conditions, and analyzed its tendency to form soot.

The C_5H_6 conversion experiments were performed at the Aragón Institute of Engineering Research of the University of Zaragoza in an experimental installation which has been used with success in a number of earlier works by our research group, addressing the formation of soot from different fuels (e.g. [4, 5]).

The experiments were focused on the pyrolysis of C_5H_6 in a quartz flow reactor, at atmospheric pressure. The operating conditions tested included the variation of the residence time, the initial fuel concentration and the reaction temperature. In each test, the soot formed were collected in a quartz fiber thimble allocated at the outlet of the reaction system and the product gases measured using a gas chromatograph equipped with a thermal conductivity detector (TCD) and HP Plot MoleSieve and HP Plot Q columns, and a flame ionization detector (FID) with an HP-PONA column. The gas chromatograph is calibrated to quantify CO , CO_2 , H_2 , CH_4 , C_2H_2 , C_2H_4 , C_2H_6 , C_3H_8 , C_3H_6 , 1,3-butadiene, i - C_4H_{10} , n - C_4H_{10} , C_5H_6 , C_6H_6 , C_7H_8 and C_8H_{10} .

The results obtained were used to analyze the product distribution from the C_5H_6 pyrolysis, and to evaluate the tendency of C_5H_6 to form soot. In addition, we performed a chemical-kinetic modeling study of the conversion of C_5H_6 in order to improve the knowledge of the main reaction pathways involved in the gas-phase processes.

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