A kinetic modeling study of propyne and allene pyrolysis: C1-C6 and PAH hydrocarbon products

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Abstract

Allene and propyne provide an early insight into the effects of structural differences on combustion performance and emissions while their consumption reactions are primary sources of the key propargyl and allyl radicals. In the present investigation, the pyrolysis of allene and propyne was studied by a combination of experimental and modeling work. Previously published experimental work on the atmospheric pressure pyrolysis of propyne is herein further enhanced with relevant data from allene pyrolysis in an isothermal laminar-flow reactor at temperatures between 970 – 1270 K and a residence time of 0.3 s [1-3]. Several products were observed and analyzed by GC/FID/MS and HPLC with diode-array ultraviolet-visible absorbance detection setup, leading to the identification of a wide range of H/C species with high accuracy. An existing detailed, in-house chemical kinetic mechanism [4, 5] was further developed and utilized for modeling key C1-C6 hydrocarbon products and major PAH species profiles, up to benzo[a]pyrene, obtained from the aforementioned novel pyrolysis data. Generally, excellent agreement between experimental and predicted species profiles is achieved, for major C1-C6 and typical PAH species such as, toluene, styrene and naphthalene. The results are critically assessed via rate-of-production and sensitivity analyses towards identification of the key controlling processes. The work demonstrates the connection between C3 and C5 chemistry, along with the role of these odd-carbon-number species in the formation and growth of higher aromatics. The importance of fuel destruction paths, and mainly propyne consumption channels, is shown to largely control the availability of CH_3 and C_3H_3 and to directly influence the formation of mono-substituted aromatics and two-PAH species.

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Figures

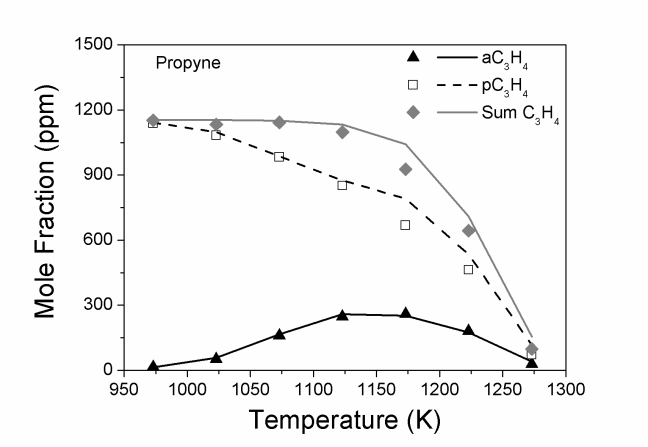

Figure 1. Comparison between computed (line, p.w.) and measured (symbols, [1], [2]) C_3H_4 profiles, p = 1 atm, τres = 0.3 s.

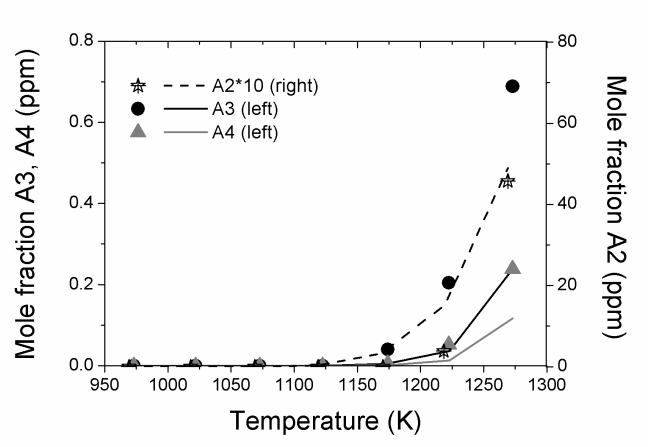

Figure 2. Comparison between computed (line, p.w.) and measured (symbols, [1], [2]) naphthalene, phenanthrene and pyrene profiles, p = 1 atm, τres = 0.3 s.

References

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