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**Thermal behavior, reaction pathways and kinetic implications of using a Ni/SiO2 catalyst for waste tire pyrolysis**

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**Table S1.** Expressions for the most common reaction mechanisms in solid state reactions.



Additionally, the Random Scission model proposed by Sánchez-Jiménez et al.[1] was used. This model states that the conversion function is determined by the fraction of broken bonds (x) and the length of the polymeric unit (L). Then, it proposes the following law to describe the conversion:

(1)

This expression takes the form  for L = 2. However, for L ≠ 2 no symbolic solution can be obtained, and the equation should be solved numerically for specific *α*-values by applying the following equation:

(2)

The other alternative used was thetruncated Sestak–Berggren model (SB) represented in eq. 3:

(3)

**Table S2.** Identified compounds by Py–GC/MS during waste tire pyrolysis

|  |  |
| --- | --- |
| tR (min) | Compound |
|  | **Alkenes** |
| 2.1 | Isoprene |
| 3.2 | Cyclohexene |
| 4.4 | 3-methylcyclohexene |
| 4.8 | 1,4-cycloheptadiene |
| 5.1 | 2,6-dimethyl-1,4,6-heptatriene |
| 5.3 | 1-methyl-1,3-cyclohexadiene |
| 5.5 | 1,3,5-heptatriene |
| 7.6 | 4-ethenylcyclohexene |
| 11.7 | 2,6-dimethyl-1,3,6-heptatriene |
| 12.2 | 1,5,5,6-tetramethyl-1,3-cyclohexadiene |
| 14.0 | 4-ethenyl-1,4-dimethyl cyclohexene |
| 15.0 | 5-ethyl-1,5-dimethyl-1,3-cyclohexadiene |
| 15.2 | 3,7-dimethyl 2,4,6-octatriene |
| 15.4 | 2,6-dimethyl-1,6-octadiene |
| 15.6 | 3,7-dimethyl-2,6-octadiene |
| 15.8 | 3,7-dimethyl-1,3,6-octatriene |
| 16.5 | D,L-limonene |
| 16.7 | α-Terpinene |
| 16.9 | 2,4,6-trimethyl-1,3,6-heptatriene |
| 17.2 | p-cymene |
| 17.5 | γ-Terpinene |
| 18.2 | Terpinolene |
| 19.0 | 2,6-dimethyl-2,4,6-octatriene |
| 19.8 | 2,6-dimethyl-1,3,5,7-octatetraene |
|  | **Aromatic compounds** |
| 3.4 | Benzene |
| 5.9 | Toluene |
| 11.5 | Xylenes |
| 13.3 | Styrene |
| 17.0 | p-cymene |
| 17.4 | 1,2,3-trimethyl benzene |
| 18.0 | Isopropylbenzene |
| 18.5 | 4-Ethyltoluene |
| 18.8 | 4-Allyltoluene |
| 19.0 | p-cymenene |
|  | **Additives** |
| 6.4 | Methyl isobutyl ketone |
| 15.2 | Cyclohexanone |
| 18.7 | Aniline |
| 22.0 | 2-Methoxy-4-methylphenol |
| 23.1 | Benzothiazole |
| 23.9 | 4-Ethyl-2-methoxyphenol |
| 25.4 | 4-(2-Propenyl)-2-methoxyphenol |
| 26.1 | 2,6-Dimethoxyphenol |
| 26.7 | 2,4-Dimethylquinoline |
| 27.1 | 1,2-dihydro-2,2,4-trimethylquinoline |

**Table S3.** Main functional groups identified by FTIR during thermogravimetric analysis

|  |  |  |
| --- | --- | --- |
| **Wavenumber** | **Functional group/ Vibration** | **Pyrolysis product** |
| 1500 and 1600 cm-1 | C=C stretch | Aromatic ring |
| 740-690 cm-1 | C-H out-of-plane bend |
| 1600-1670 cm-1 | C=C stretch | Alkenes and Conjugated Dienes |
| 3000-2840 cm-1 | C-H stretch | Alkyls |
| 1330 -1500 cm-1 | C-H bend | Methyl and Methylene |
| 690 cm-1 | (ρCH2). | Methylene rocking vibrations |
| 1650 and 1750 cm-1 | C=O stretch | Carbonyl groups |
| 2320 and 2360 cm−1 | C=O stretch | CO2 |
| 3014 cm-1 | C-H stretch | CH4 |
| 1460 cm-1 | S=O stretch | Sulfur species |

Gráfico

Descripción generada automáticamente

**Fig. S1** FTIR of evolved gases of thermal decomposition of waste tire for (a) non-catalyzed and (b) catalyzed reaction.



**Fig. S2** Temperature effect on formation of aromatics and alkenes during waste tire decomposition for uncatalyzed and catalyzed reaction followed by absorbance.

Gráfico

Descripción generada automáticamente

**Fig. S3** Effect on product distribution of catalytic support (SiO2) during waste tire pyrolysis carried out at 400 °C.

**References**

1. Sánchez-Jiménez, P.E., Pérez-Maqueda, L.A., Perejón, A., Criado, J.M.: A new model for the kinetic analysis of thermal degradation of polymers driven by random scission. Polym. Degrad. Stab. 95, 733–739 (2010). https://doi.org/10.1016/j.polymdegradstab.2010.02.017