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PII: S1385-8947(17)32227-1
DOI: https://doi.org/10.1016/j.cej.2017.12.105
Reference: CEJ 18266

To appear in: *Chemical Engineering Journal*

Received Date: 27 October 2017
Revised Date: 15 December 2017
Accepted Date: 20 December 2017

Please cite this article as: Z. Cheng, B. Yang, Q. Chen, Z. Shen, T. Yuan, Quantitative relationships between molecular parameters and reaction rate of organic chemicals in Fenton process in temperature range of 15.8 °C - 60 °C, *Chemical Engineering Journal* (2017), doi: https://doi.org/10.1016/j.cej.2017.12.105

Quantitative relationships between molecular parameters and reaction rate of organic chemicals in Fenton process in temperature range of 15.8 °C - 60 °C

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ABSTRACT:

In order to have a better prediction for the degradation reaction rate constant of organic compounds in Fenton process at different temperatures. A partial least squares (PLS) model was established based on 116 lg*k* values for 24 organic compounds and quantum chemical parameters, some basic information of molecules as well as the temperature of reaction system. The optimal model was demonstrated as stable, robust and had good predictive ability, with the associate statistical indices of adjusted squared correlation coefficient was 0.722, internal validation was 0.652, external validation was 0.512, cumulative cross-validation coefficient was 0.635, the criterions indicated the developed model could be used to estimate the reaction rate of organic compounds in Fenton process at different temperature. The model contains three components, the most significant descriptors explaining the reaction rate are T and $^1/_T$ for component 1, the maximum charge in a carbon atom and minimum charge for nucleophilic attack for component 2, the charge in a hydrogen atom, maximum charge for hydroxyl radical attack and minimum value of bond order for component 3. The applicability domain (APD) of the proposed model was

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