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PII: S0960-8524(16)31655-8
DOI: http://dx.doi.org/10.1016/j.biortech.2016.12.004
Reference: BITE 17380

To appear in: *Bioresource Technology*

Received Date: 25 September 2016
Revised Date: 30 November 2016
Accepted Date: 1 December 2016

Please cite this article as: Wang, S., Xia, Z., Hu, Y., He, Z., Bernard Uzoejinwa, B., Wang, Q., Cao, B., Xu, S., Co-pyrolysis Mechanism of Seaweed Polysaccharides and Cellulose Based on Macroscopic Experiments and Molecular Simulations, *Bioresource Technology* (2016), doi: http://dx.doi.org/10.1016/j.biortech.2016.12.004

Co-pyrolysis Mechanism of Seaweed Polysaccharides and Cellulose Based on Macroscopic Experiments and Molecular Simulations

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Abstract: Co-pyrolysis conversion of seaweed (*Enteromorpha clathrat* and *Sargassum fusiforme*) polysaccharides and cellulose has been investigated. From the Py-GC/MS results, *Enteromorpha clathrata* (EN) polysaccharides pyrolysis mainly forms furans; while the products of *Sargassum fusiforme* (SA) polysaccharides pyrolysis are mainly acid esters. The formation mechanisms of H_2O, CO_2, and SO_2 during the pyrolysis of seaweed polysaccharides were analyzed using the thermogravimetric-mass spectrometry. Meanwhile the pyrolysis of seaweed polysaccharide based on the Amber and the ReaxFF force fields, has also been proposed and simulated respectively. The simulation results coincided with the experimental results. During the fast pyrolysis, strong synergistic effects among cellulose and seaweed polysaccharide molecules have been simulated. By comparing the experimental and simulation value, it has been found that co-pyrolysis could increase the number of molecular fragments, increase the pyrolysis

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