Laboratory Waste Water Treatment by Supercritical Water Oxidation of Nitrobenzene

Vengdhanathan S. and P. R. Naren*

School of Chemical and Biotechnology, SASTRA Deemed to be University

Email ID: venkatsriba@gmail.com, prnaren@scbt.sastra.ac.in *

A. Background

Laboratory waste water can contain several organic as well as inorganic substances including heavy metals and several other toxic substances. This can be ejected from several educational as well as research institutes. The quantity as well as the quality of the waste water ejection from these places can vary from time to time. Hence an effective waste water treatment technique is necessary. Water at 374°C and 221 bar can form a miscible solution with both non polar as well as organic solvents. This water is called super critical water. Super critical water oxidation is widely explored to break down several organic and inorganic contaminants in waste water.

B. Process Flowsheet Description

The process flowsheet for Supercritical water oxidation of nitrobenzene is developed in DWSIM (ver 7.3.1) based on figure 2 from Dong et al.(2014). The Peng Robinson thermodynamic model is used for estimation of thermophysical properties. The nitrobenzene and water mixture at 20°C and 1 bar pressure enters a pump where its pressure is increased to 260 bar. This stream is now heated to 440°C to achieve the supercritical state. The decomposition of nitrobenzene to nitrogen, water vapour and carbon dioxide happens inside a reactor. In this flowsheet, a conversion reactor is used and the conversion is set at 85% based on Zhang et al.(2003). The entire vapour exiting from the reactor is then depressurised and cooled to ambient conditions and flashed to separate out the water, nitrobenzene and the gas streams.

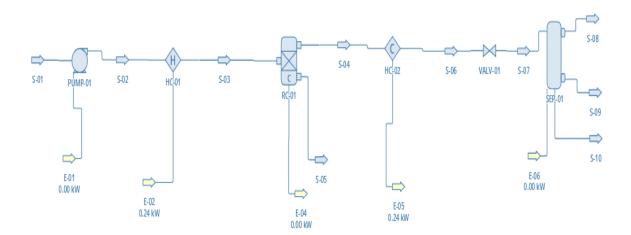


Figure 1. Supercritical oxidation of nitrobenzene.

C. Results and Discussion

Water with 99% purity is obtained, which is almost devoid of nitrobenzene. The results of the important streams are tabulated below in Table 1.

Variable	S-01	S-03	S-04	S-08	S-09	Units
Temperature	20	440	441.329	22.15	22.15	C
Pressure	1	260	260	1	1	bar
Mass Flow	0.3	0.3	0.3	0.00426451	0.295725	kg/h
Molar Flow	0.0165471	0.0165471	0.0165482	0.00013325	0.0164149	kmol/h
Molar Fraction Water	0.99208	0.99208	0.992109	0.0226771	0.999984	
Molar Fraction Carbon dioxide	0	0	0.000225305	0.0262681	1.39E-05	
Molar Fraction Nitrogen	0	0	1.88E-05	0.00233163	2.27E-10	
Molar Fraction Nitrobenzene	4.42E-05	4.42E-05	6.63E-06	0.00016851	1.26E-07	
Molar Fraction Oxygen	0.00787554	0.0078755	0.00764033	0.948555	2.22E-06	

Table 1. Results for important streams

D. Further Works

The heaters and coolers used in the simulation can be replaced with heat exchangers for energy optimisation. The conversion reactor used in the flowsheet can be replaced with a kinetic reactor (PFR/CSTR).

E. Reference

- 1. Dong X., Wang Y., Li X., Yu Y and Zhang M, Process Simulation of Laboratory Wastewater Treatment via Supercritical Water Oxidation, Ind. Eng. Chem. Res. 2014, 53, 7723–7729. dx.doi.org/10.1021/ie4044339.
- 2. Zhang G. and Hua I., Supercritical Water Oxidation of Nitrobenzene, Ind. Eng. Chem. Res. 2003, 42, 285-289. dx.doi.org/10.1021/ie010479j.