Low Temperature Catalytic Oxidation of Phenol Wastewater Stream

Background

Phenol is one of the most common organics contained in waste streams originating in the chemical process industries. In addition to being suspected carcinogens, phenol and some of its derivatives have also been shown to be either toxic or lethal to aquatic life. It is also well known that even low phenol levels, in the parts per billion range, impart to water a disagreeable taste and odor. Therefore, it is necessary to eliminate as much of the phenol from the stream before discharging. In this process, the phenol concentration in water is 6.8 wt%, a typical value for steel coking facilities. The target concentration for effluent water is 39 ppb.

Low-temperature, aqueous-phase heterogeneous catalytic oxidation of dissolved organic compounds is a potential means for remediation of contaminated ground and surface waters, industrial effluents, and other wastewater streams. The ability for operation at substantially milder conditions of temperature and pressure, in comparison to supercritical water oxidation and wet air oxidation, is achieved through the use of an extremely active bi-metallic noble metal catalyst.

Environmental Significance

Treatment of a waste stream

Process Description

The PFD is attached. In the process, the wastewater stream, containing 6.8 wt% phenol, is fed into the system as Stream 2. This stream is then pumped, by P-901 A/B, and heated with low-pressure steam, in E-901, up to the necessary pressure and temperature. Stream 1 contains 200% excess O_2. An alternative design would consider

air as the source of oxygen. Stream 1 is compressed in C-901 and then mixed with the wastewater stream before entering the reactor, R-901. In the reactor, it is assumed that the water stream is always saturated with oxygen. How to accomplish this is an interesting mass transfer problem associated with the reactor design. Some type of sparged reactor would probably be required. Stream 7, exiting the reactor, contains only water, oxygen and carbon dioxide, with virtually no phenol. The effluent stream is then enters the flash vessel, V-901, where the off-gas is separated from the purified water.

Necessary Information and Simulation Hints

The overall reaction for the complete oxidation of phenol to inorganic products is:

$$C_6H_5OH + 7\ O_2 \rightarrow 6\ CO_2 + 3\ H_2O$$

Reaction rate constants have been determined for phenol disappearance using pseudo-first-order kinetics in phenol concentration (mol/L) over a range of temperatures[1]. The dissolved oxygen concentration is assumed to be at saturation. The results are:

Arrhenius activation energy: 33.8 kJ/mol

Pre-exponential factor: 61.70 s^{-1}

All simulations were run using SRK for *K* values for the compressor (C-901), pump (P-901 A/B), and heater (E-901) and Henry's Law for *K* values for the reactor (R-901) and flash vessel (V-901). SRK was used for the enthalpy model on all simulations.

References

1. Atwater, James E., James R. Akse, Jeffrey A. McKinnis and John O. Thompson. "Low Temperature Aqueous Phase Catalytic Oxidation of Phenol," *Chemosphere*, Vol. 34, No. 1, pp 203-212, 1997.

Equipment Descriptions

C-901 Oxygen Compressor

P-901 A/B Wastewater Pumps

E-901 Wastewater Heater

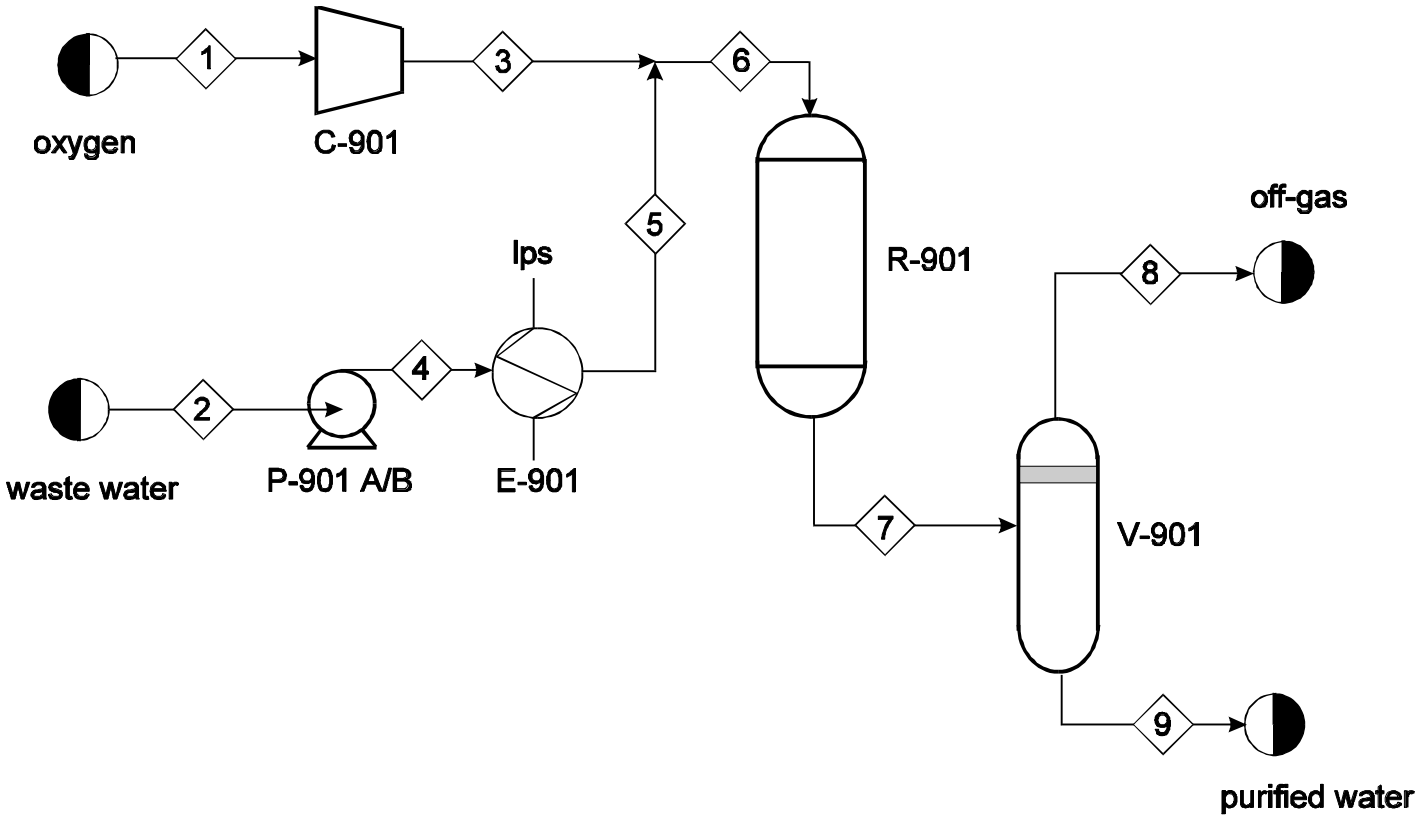
R-901 Reactor

V-901 Flash Vessel

Low Temperature Catalytic Oxidation Stream Table

Stream No.	1	2	3	4	5	6
Temperature (°C)	20.00	20.00	96.79	20.04	74.19	60.00
Pressure (bar)	1.01	1.01	2.00	2.34	2.00	2.00
Phase	vapor	liquid	vapor	liquid	liquid	V/L mix
Total Flow (kg/h)	5212.32	10730.00	5212.32	10730.00	10730.00	15942.32
Total Flow (kmol/h)	162.89	562.85	162.89	562.85	562.85	725.74
Component Flowrates (kmol/h)						
Water	--	555.09	--	555.09	555.09	555.09
Phenol	--	7.76	--	7.76	7.76	7.76
Carbon Dioxide	--	--	--	--	--	--
Oxygen	162.89	--	162.89	--	--	162.89

Stream No.	7	8	9
Temperature (°C)	60.00	30.00	30.00
Pressure (bar)	1.66	1.66	1.66
Phase	V/L mix	vapor	liquid
Total Flow (kg/h)	15942.32	5589.71	10352.61
Total Flow (kmol/h)	733.50	159.06	574.44
Component Flowrates (kmol/h)			
Water	578.36	4.09	574.28
Phenol	--	--	--
Carbon Dioxide	46.54	46.39	0.15
Oxygen	108.59	108.58	0.01



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