Life Cycle Assessment Study For Two Different Phenol Production Processes

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Phenol is an important raw material in many branches of industry (petrochemical, pharmaceutical, plastic and pesticidal chemical industry). This research study on phenol production processes by using two different phenol production processes which are cumene oxidation (the Hock process) and toluene oxidation (the Dow process). In order to study in environmental impacts, Life Cycle Assessment (LCA) is applied to evaluate environmental impacts of phenol production processes. Environmental impacts are evaluated according to cradle-to-gate approach by using SimaPro 7.1 software for Life Cycle Assessment . Approach by IMPACT 2002+ . The result shows that cumene process is more environmentally favorable than toluene process.

Keywords: Phenol, Cumene, Toluene, Hock process, Dow process

1. Introduction

Life cycle assessment (LCA) methodology is used to evaluate the impact of processes or products on the environment. The inclusion of every stage of the process or product's life cycle is fundamental to this analysis. In the case of products, every stage from the production of the raw materials to the end of their useful lives and their use and maintenance should be included. Thus, all significant environment impact in their life cycle (cradle to grave) analysis is impossible and the analysis must terminate at an intermediate stage (gate to gate). [1]

Phenol, hydroxybenzene, carbolic acid (C_6H_5OH) discovered in 1834 by F.Runge, is the parent substance of a homologous series of compounds with the hydroxyl group bonded directly to the aromatic ring. Phenol occurs as a free component or as an addition product in natural products and organisms. For example, it is a component of lignin, from which it can be liberated by hydrolysis. As a metabolic product it is normally excreted in quantities of up to 40 mg/L in human urine. Higher quantities are formed in coking or low-temperature carbonization of wood, brown coal, or hard coal and in oil cracking. Initially phenol was extracted exclusively from hard coal tar, and only after consumption had risen significantly was it also produced synthetically. The earlier methods of synthesis have been replaced by modern processes, mainly by the Hock process starting from cumene. Phenol has achieve considerable importance as the starting material for numerous intermediates and finished products. [2]

Small quantities of phenol (cresylic acids) are isolate from tars and coking plant water produced in the coking of hard coal and the low temperature carbonization of brown coal as well as from the waste water from cracking plants. By far the largest proportion in obtained by oxidation of benzene or toluene. Although direct oxidation of benzene is in principle possible, the phenol formed in immediately oxidized further. Therefore, alternative routes must be chosen, e.g. via halogen compounds which are subsequently hydrolyzed or via cumene hydroperoxide which in then cleaved catalytically. The following processes were developed as industrial syntheses for the production of phenol:

1 Cumene oxidation(The Hock process).

2 Toluene oxidation (The Dow process).

2. Materials and Methods

2.1 Cumene oxidation (Hock process)

The cumene–phenol process is based on the discovery of cumene hydroperoxide and its cleavage to phenol and acetone published in the 1944 by H.HOCK and S.LANG. Cumene is produced commercially through the alkylation of benzene with propylene over an acid catalyst.

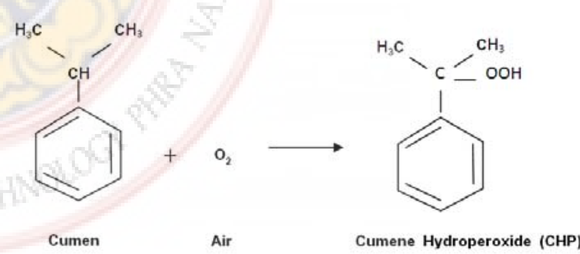

Figure 1. Oxidation of cumene to Cumene Hydroperoxide (CHP)

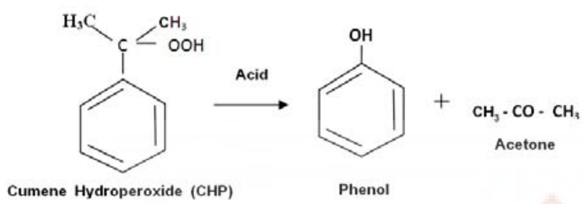

Figure 2. Reaction for phenol and acetone production

Table 1: Data in the SimaPro 7.1 software which the phenol product 1 kg**.** (Hock process)

Data		*Name*	*Amount*	*Unit*
Input	*Cumene*		*1.340*	*kg*
	Oxygen		*0.358*	*kg*
Output	*Emission to air*	*Carbon dioxide*	*0.191*	*kg*
		Cumene	*0.002*	*kg*
		Heat (waste)	*1.200*	*MJ*
	Emission to water	*Water (waste)*	*10.000*	*mg*
		Cumene	*0.006*	*kg*

2.2 Toluene oxidation (Dow process).

The Dow phenol Process utilizes toluene as feedstock. In two separate steps, toluene is first oxidized to benzoic acid; thereafter benzoic acid is converted to phenol, using copper benzoate as the principal catalyst. In the first stage toluene is oxidized with atmospheric oxygen in the presence of a catalyst to benzoic acid in the liquid phase. In the second stage the benzoic acid isolated is decarboxylated catalytically in the presence of atmospheric oxygen to produce phenol.[3]

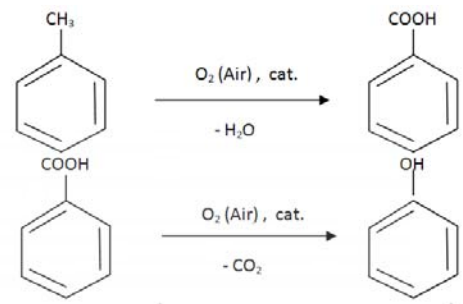

Figure 3. Reaction for phenol from toluene oxidation.

Table 2: Data in the SimaPro 7.1 software which the phenol product 1 kg**.** (Dow process)

Data		*Name*	*Amount*	*Unit*
Input	*Toluene*		*1.440*	*kg*
	Oxygen		*0.476*	*kg*
Output	*Emission to air*	*Carbon dioxide*	*10.300*	*mg*
		Carbon monoxide	*31.000*	*mg*
		Nitrogen dioxide	*1.900*	*g*
		Phenol	*22.000*	*mg*
		Toluene	*23.000*	*mg*
		Heat (waste)	*0.800*	*MJ*
	Emission to water	*Water (waste)*	*20.000*	*mg*
	Emission to soil	*Copper*	*322.000*	*mg*

3. Results and discussion

Evaluated the environmental impacts by SimaPro software. Life cycle assessment for Phenol production process from cumene or Hock process which use indicator IMPACT 2002+ .

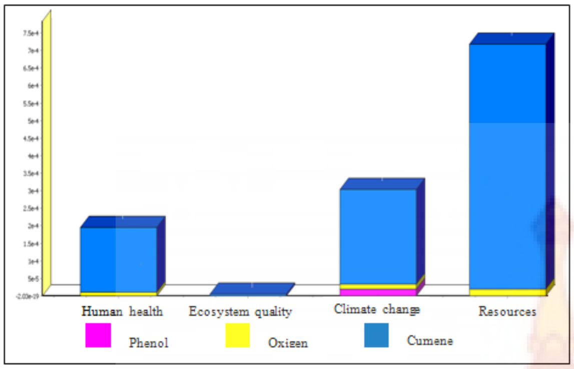

Figure 4. Life cycle assessment for phenol production process from cumene (Human health , Ecosystem, Climate change and Resources)

Table 3: Data in the SimaPro 7.1 software for Impact category of hock process

Impact category	Total	Phenol	Oxygen	Cumene
Carcinogens	4.95E-05	0.00E+00	1.69E-07	4.94E-05
Non-carcinogens	1.02E-05	5.93E-08	2.85E-07	9.87E-06
Respiratory inorganics	1.33E-04	0.00E+00	9.73E-06	1.23E-04
Ionizing radiation	9.84E-07	0.00E+00	3.57E-07	6.27E-07
Ozone layer depletion	7.37E-09	0.00E+00	1.04E-09	6.33E-09
Respiratory organics	1.47E-06	4.19E-07	3.91E-09	1.05E-06
Aquatic ecotoxicity	1.18E-07	0.00E+00	1.54E-08	1.03E-07
Terrestrial ecotoxicity	3.50E-06	0.00E+00	2.97E-07	3.20E-06
Terrestrial acid/nutri	2.42E-06	0.00E+00	1.33E-07	2.28E-06
Land occupation	2.42E-08	0.00E+00	7.62E-09	1.66E-08
Global warming	3.03E-04	1.93E-05	1.41E-05	2.69E-04
Non-renewable energy	7.18E-04	0.00E+00	1.93E-05	6.98E-04
Mineral extraction	1.92E-09	0.00E+00	1.53E-10	1.77E-09

Figure 4. show that phenol production process environmental impacts everyway as human health , Ecosystem quality, Climate change and Resources etc. Cumene more than phenol and oxygen in all way.

Main impacts in table 3 are cumenae impacts to Non-renewable energy, Global warming, Respiratory inorganics and Carcinogens respectively. Oxygen in process impacts to Global warming, Non-renewable energy and Respiratory inorganics respectively. Phenol impacts to Global warming .

Evaluated the environmental impacts by SimaPro software. Life cycle assessment for Phenol production process from toluene or Hock process which use indicator IMPACT 2002+ method.

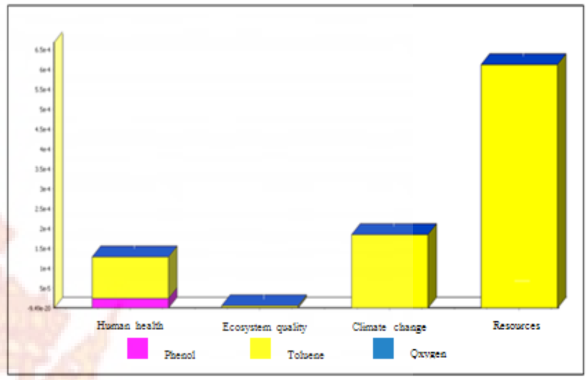

Figure 5. Life cycle assessment for phenol production process from toluene (Human health , Ecosystem, Climate change and Resources)

Table 4: Data in the SimaPro 7.1 software for Impact category of dow process

Impact category	Total	Phenol	Toluene	Oxygen
Carcinogens	2.63E-05	1.85E-13	2.63E-05	2.25E-13
Non-carcinogens	1.25E-06	2.15E-09	1.25E-06	3.79E-13
Respiratory inorganics	1.00 E-04	2.39E-05	7.66E-05	1.29E-11
Ionizing radiation	5.91E-10	0.00E+00	5.91E-10	4.74E-13
Ozone layer depletion	9.91E-12	0.00E+00	9.91E-12	1.39E-15
Respiratory organics	5.00E-07	4.41E-09	4.96E-07	5.20E-15
Aquatic ecotoxicity	7.43E-08	2.41E-08	5.02E-08	2.04E-14
Terrestrial ecotoxicity	2.95E-06	1.29E-06	1.66E-06	3.95E-13
Terrestrial acid/nutri	2.28E-06	7.92E-07	1.49E-06	1.77E-13
Land occupation	2.46E-09	0.00E+00	2.46E-09	1.01E-14
Global warming	1.85 E-04	1.05E-09	1.85 E-04	1.87E-11
Non-renewable energy	6.11 E-04	0.00E+00	6.11 E-04	2.56E-11
Mineral extraction	5.50E-10	0.00E+00	5.50E-10	2.04E-16

Figure 5 main impact to environment as human health , Ecosystem quality, Climate change and Resources etc. Toluene impact to everyway more than phenol and oxygen.

Table 4 show that toluene impacts to Non-renewable energy, Global warming, Respiratory inorganics and Carcinogens respectively.

Oxygen in process impacts to Non-renewable energy, Global warming, Respiratory inorganics and Carcinogens respectively. And phenol impacts to Respiratory inorganics .

4. Conclusions

Environmental impacts are evaluated according to cradle-to-gate approach by using SimaPro 7.1 software for Life Cycle Assessment . Approach by IMPACT 2002+ . The result shows that cumene process is more environmentally favorable than toluene process which main impacts are Non-renewable energy, Global warming, Respiratory inorganics and Carcinogens etc show that in figure 4 and figure 5.

So phenol production process will be better off toluene process or dow process but in Thailand has cumene process which impacts to environment very much so be using Life Cycle Assessment for decreasing environment impacts.

5. References

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[3] Schmidt, R. "Industrial catalytic processes phenol production." 19 October (2005): 89–1