Economic and Environmental Impact Assessment of Alpha-Naphthol Production by Traditional and Biocataytic Routes

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ABSTRACT

Alpha-naphthol is an important industrial raw material used in the manufacture of insecticides, herbicides, drugs, and dye intermediates. Alpha-naphthol is produced via a Union Carbide patented process, as well as two other chemical predecessor process described in this work. In an effort to find "greener" approach to the conventional synthesis process, the Center of Environmental and Beneficial Catalysis, has proposed the use of a biocatalytic process. The experimental work preformed with computational simulation package have resulted in a process yield approximately 4.5 times higher the compared conventional process and 2.1 yield, with respect to the atom economy . The simulation methods used will also shown an increase in profitability as well as a definite positive environmental impact assessment of the biocatalytic process versus the conventional method.

INTRODUCTION

Reducing pollution has been a major concern leading to the development of a whole new mindset based on "green chemistry", that is, chemistry that is friendly to the environment, minimizes waste, reduces energy utilization and often favors renewable resources over petroleum-based feedstocks. Major goal, for research in the chemical industry is the development of processes and products that have high yield minimizes waste, and are profitable (New Biocatalysts, 2007).

The Center for Environmentally Beneficial Catalysis (CEBC) (Engineering Sustainable Chemicals, 2007) was started to impact and, over time, bring sustainable transformations to the chemical industry that faces many challenges as follows: increasing globalization, societal demands and governmental regulations for higher environmental performance; increased productivity and profitability to maintain global competitiveness; higher consumer expectations of product quality and a looming transition to renewal feedstocks and renewable energy. The perceived long-term outcome of the CEBC and parallel contributors with similar goals is a transformed chemical industry wherein pollution prevention and environmental sustainability replace waste production, pollution, regulation and remediation (The CEBC annual report, year 3 Vol.1).

This work reported here builds on methodology developed within the CEBC for chemical processes. The work then use the methodology to compare a traditional chemical production scheme with a proposed "greener" alternative based on a bio-catalytic route.

OBJECTIVES

In this thesis, several ways to improve environmental performance for chemical processes will be discussed, particularly alpha-naphthol production. These objectives can be achieved by:

a) Developing a baseline scenario for the production of alpha-naphthol based on a traditional chemical route, including process flow sheet, computer simulation, economic and environmental impact analysis.
b) Developing an alternative scenario for the production of alpha-naphthol using a bio-catalytic route, including process flow sheet, computer simulation, economic and environmental impact analysis.
c) Comparing the two alternative scenarios based on performance, cost and environmental impact.

To achieve these set objectives, flow sheets will be developed from technical information obtained from a thorough literature review. VISIO® is the software tool that will be used for the flow sheet representation. Computer simulations will be performed using HYSYS®, in order to obtain the performance specification for the processes described in a and b above. Economic and environmental impact analysis will be performed using SCENE® software.

PRODUCTION OF ALPHA NAPHTOL

There are 37 producers of alpha-naphthol worldwide. The locations of the producers are summarized in Figure 2.1. The figure was developed by the information presented in the directory of world chemical producers-2000 edition. The capacity produced in the western world was approximately over 15,000 tons per year of alpha-naphthol (Trofimov, 1973).

Alpha-naphthol was synthesized by three different ways historically. This includes the following methods.

a) Caustic fusion of naphthalene-1-sulfonic acid.
b) I.G Farbenindustrie process
c) Union Carbide process (Barmicki et.al., 1997).

The most important process to this thesis is the Union Carbide Process, because of its relevance to recent industrial practice. The only difference is in the starting material. Naphthalene is the starting material for the conventional chemical process while tetralin is the starting material for the Union carbide process. The detail description of the conventional chemical process and an alternative biocatalytic process are discussed in further detail elsewhere (Ajiboye 2007).

PROCESS ANALYSIS

<u>Conventional Process</u>

Figure 1 shows a flow diagram for the process of synthesizing alpha-naphthol from naphthalene using the conventional chemical process. Naphthalene enters the hydrogenation reactor at 617°F and 1102 psia in the presence of CoMo-Al_2O_3 catalyst where it is converted to tetralin (Krichko et. al., 1969). Tetralin is then contacted with oxygen entering the oxidation reactor at 188°F and 68 psia where it is converted to tetralin-hydroperoxide (Yamauchi et. al., 1981) as intermediate, which immediately decomposes into alpha-tetralone and alpha-tetralol, and modeled in the decomposition reactor at 122°F and 58 psia. The alpha-tetralone and alpha-tetralol have close boiling points and was separated by fractional distillation. The dehydrogenation reaction takes place in the vapor phase at 716°F, and 40 psia in the presence of a catalyst to produce alpha-naphthol (Kudo et. al., 1976).

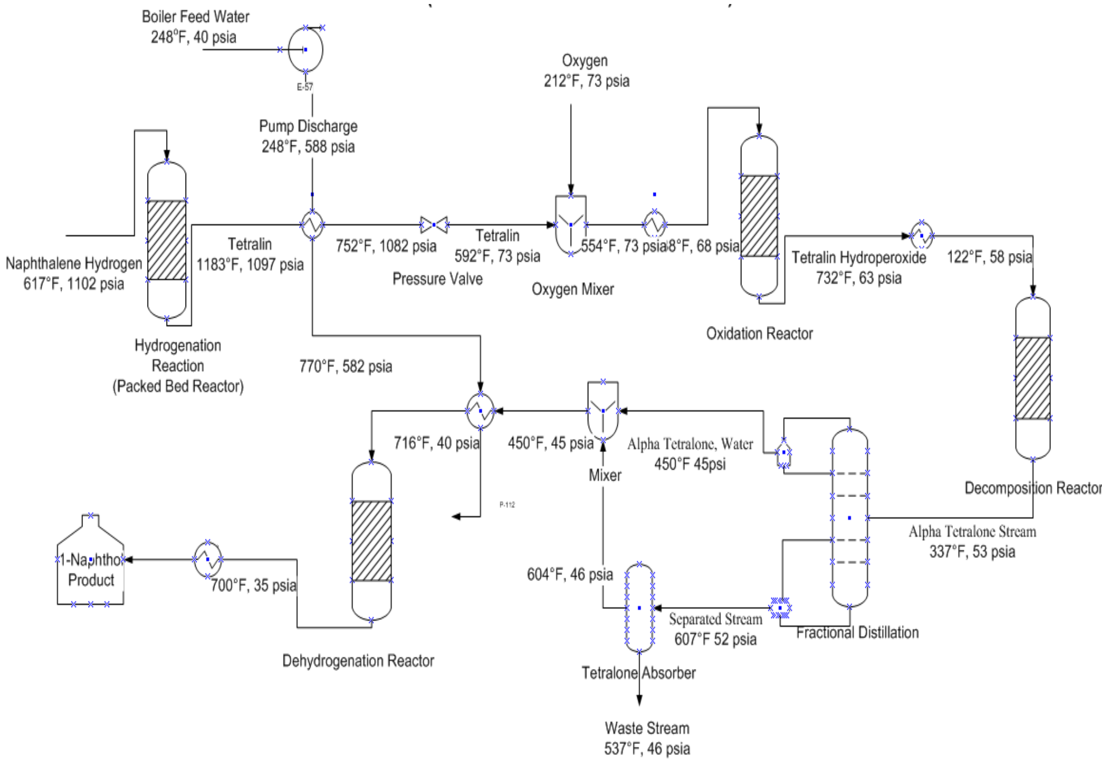

Figure 1 Process flow diagram using Microsoft VISIO®, used as a basis for HYSYS® simulation of the conventional alpha-naphthol production process form naphthalene.

<u>Bio-catalytic Process Development</u>

In 2003, following the challenges indicated by VISION 2020, in a workshop "New Biocatalyst" an alternative approach for alpha-naphthol production, by a greener bio-catalytic method was suggested. The process (see Fig. 2) involved naphthalene oxidation by wild type toluene ortho-monooxygenase with E-coli to perform stereo- and enantiospecific reactions. High selectivity of enzymes reduces the formation of unwanted by-products thereby increasing the atom-economy and efficiency factor (Olivo et.al, 2003). Alpha-naphthol is produced when naphthalene is biodegraded to alpha-naphthol at 30°C; this is a bi-phasic reaction that can be used industrially. (Janardhan, et.al. 2007)

The product is absorbed in both phases and the solvent and organic compounds that contain mainly the makeup stream and naphthalene is recycled back into the feed mixer. This process was chosen as an alternative, because of the promising results obtained by researchers from the University of Iowa, and anticipated to be a good substitute to the conventional chemical process.

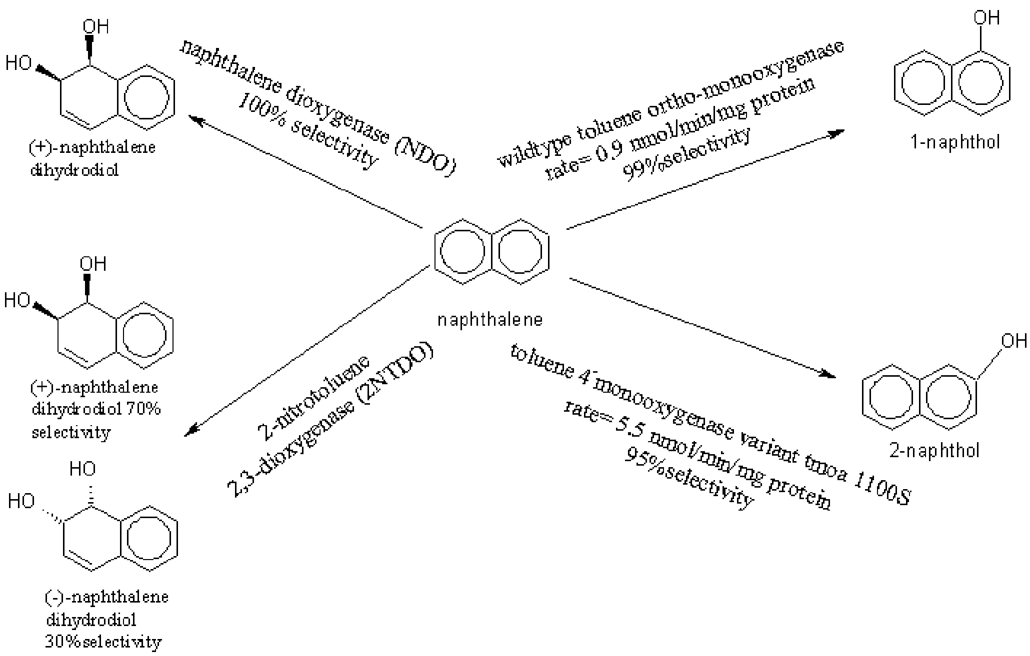

Figure 2. Alternative processes for the production of alpha naphthol. Naphthalene oxidation by wild type toluene ortho-monooxygenase with E-coli (Janardhan et.al., 2007).

Information gathered from the study carried out by researchers at The University of Iowa, on bio-oxidation of naphthalene to alpha-naphthol by the use of ortho-monooxygenase with E-coli, was used in the development of the process flow diagram for the alternative bio-catalytic process as represented on VISIO® by Figure 3.

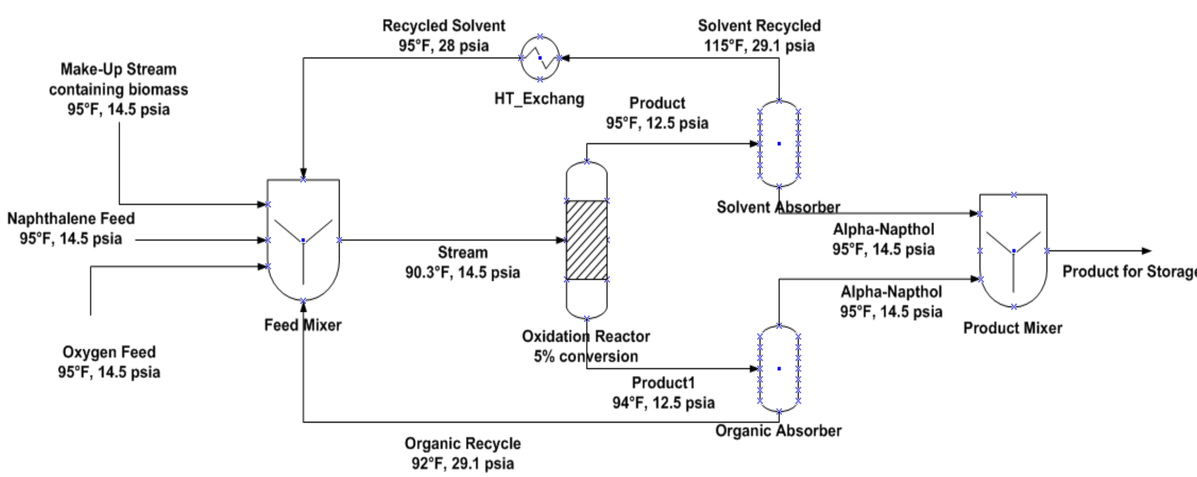

Figure 3. Flow flow diagram of process to be used as a basis for HYSYS® simulation of the alpha-naphthol production process from naphthalene, by bio-catalysis.

PERFORMANCE INDICATORS

The evaluation will be based on comparison of performance indicators 1) yield and 2) atom economy, plus cost and environmental impact. The yield and atom economy are discussed in detail elsewhere (Ajiboye 2007).

COST ESTIMATION

The cost was estimated based on the life cycle cost for a plant, based on major components. The major segments are addressed in the categories of pre-production cost and production cost. The post production costs are assumed to be similar for conventional and alternative processes and hence, are not discussed. Definition of the major elements used in the pre-production cost estimation is discussed in detail elsewhere (Ajiboye 2007).

Environmental Impact Assessment Using SCENE

This study used a simulation software tool called SCENE® to evaluate environmental issues that can be encountered in a manufacturing facilities. The tool introduced nine key environmental indices as explained below. The simulation tool synchronizes with HYSYS® to capture information on the amount of the emissions leaving the process boundary. The chemicals emitted are categorized as to the risk they pose to the environment and the process indices are reported numerically for comparison of process scenarios. Further details of the environmental impact analysis are reported elsewhere (Ajiboye 2007).

RESULTS

Material flows for the two scenarios were determined using HYSYS, which enabled the yield estimates. Similarly, atom economy was determined by material flows for the conventional chemical process and the bio-catalytic alternative. Comparisons of yield and atom economy are presented in Table 1.

Table 1. Comparison of performance Indicators based on the conventional chemical process and alternative bio-catalytic process for synthesizing alpha-naphthol.

Performance Indicators		
	Conventional Chemical Process	**Bio-Catalytic Alternative**
Yield	21.2%	95.7%
Atom Economy	46.5%	100%
Product Mass Flow Alpha-Naphthol	15,000 ton/year	

Life cycle cost was estimated based on the most important elements. Cost for the conventional chemical process and the alternative bio-catalytic process in the categories of pre-production cost, and production cost were determined to produce estimates of plant investment costs, revenue and profitability for values of plant life ranging from 10 to 50 years. These are summarized in Figs. 4 and 5.

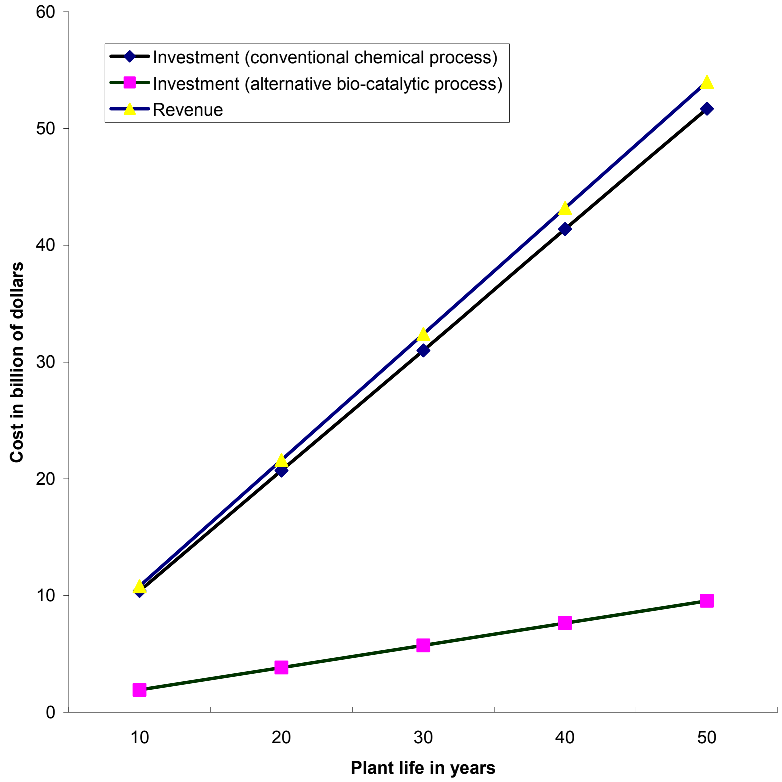

Figure 4 Comparison of variation in total investment and revenue with plant life for conventional chemical process and bio-catalytic process.

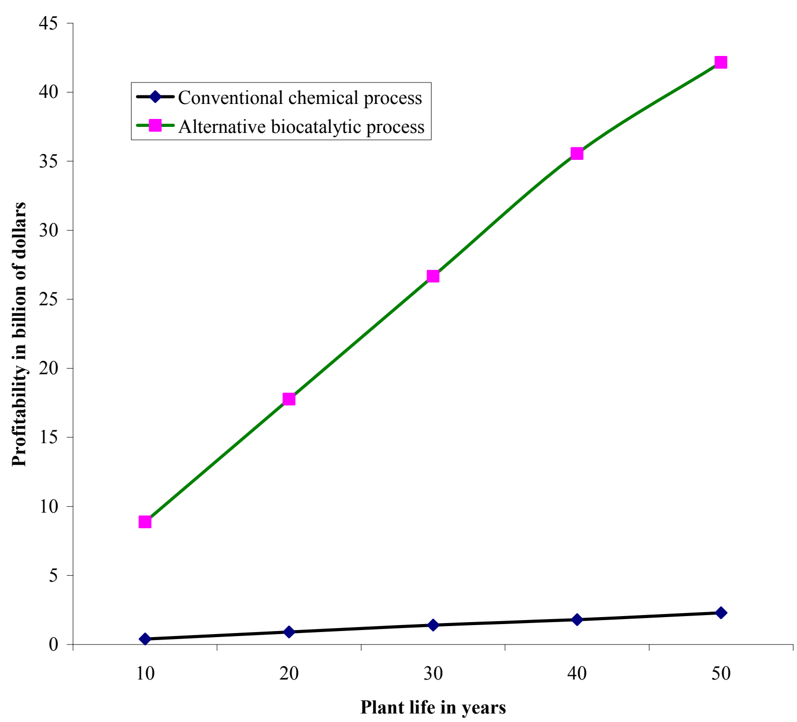

Figure 5. Comparison of profitability with plant life for conventional chemical process and bio-catalytic process.

The environmental impact assessment was made based on results obtained from the simulation tool SCENE.® The results are based on emission of chemicals and risk index summary for the conventional chemical process and the alternative bio-catalytic process. The comparison of the environmental indicators is presented in Fig. 6.

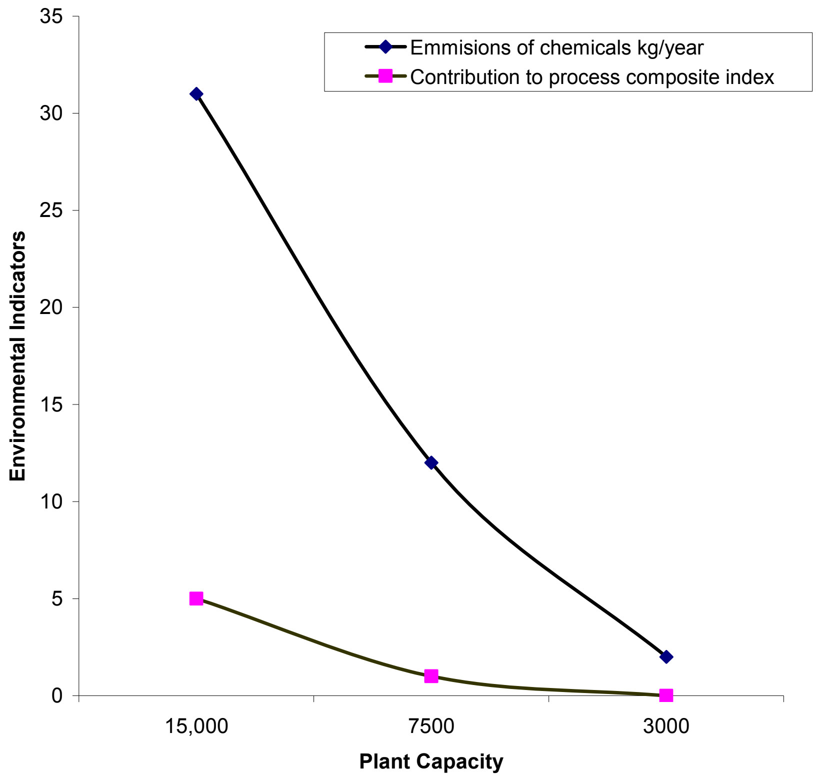

Figure 6. Variation of environmental indicators for conventional chemical process for different plant capacities. Emission of chemicals and risk index summary for the bio-catalytic alternative is negligible (SCENE is only concerned with chemical emission rather than biological waste).

CONCLUSIONS

The need for a greener process development is of recognized importance. This work has made an evaluation of an alternative bio-catalytic process for the synthesis of alpha-naphthol in comparison to a conventional chemical process. The methods used to determine the performance indicators necessary for the comparison use several computer modeling tools such as HYSYS,® CAPCOST,® EPI Suite,® and SCENE® to arrive at results that formed the basis for comparison. Results were presented with comparisons on the basis of performance, life cycle cost and environmental impact assessment.

In term of performance, the conventional chemical process have a yield of 21.2% and an atom economy of 46.5% while in the other hand, the alternative bio-catalytic process have a yield of 95.7% and an atom economy of 100%. In term of yield the alternative process is 74.5% better than the conventional chemical process and 53.5% better in term of atom economy. Based on the result obtained, the alternative bio-catalytic process is a better alternative to the conventional chemical process.

Environmental indicators compared impact based on emission and risk index, it is also very noticeable too that the alternative bio-catalytic process is very green and the waste generated from the process poses no threat to the environment because it is non-toxic, "when it is biological waste is not considered" on the other hand, the conventional chemical process pose a significant threat level. The choice based on environmental impact favors the alternative chemical process because it is greener than the conventional chemical process.

Following the trend of results reported here, the alternative bio-catalytic process appears to be the better choice, because it has a better performance, is more profitable and is greener than the conventional chemical process for the synthesis of alpha naphthol.

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