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# Green chemical applications: Highly efficient process on selective formation of industrial materials

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**A B S T R A C T**

Green industrial aspects about processes of important materials such as synthesis of lubricating oils which indeed it has a long-term service life and significantly high oxidation stability under severe temperature conditions (Yoshida and Yokohama, 1988). One of these lubricates oil as the main component, 2-*tert*-amylnaphthalene derived from direct *tert*-amylation reaction of naphthalene over *tert*-amyl alcohol and zeolite of H-mordenite using an autoclave as closed system. The zeolites can be easily regenerated by heating and then reused (Keith Smith *et al.*, 2012). Its eco-friendly process and obeyed the 12th applied principles of green chemistry by measuring of some parameters specific for the environmental efficiency. These parameters are including: Atom Economy, Selectivity, Yield, E-Factor, Environmental Quotient, and Effective Mass Yield (EMY), as a comparison between these two processes. The service life at oxidation test for the compound of 2-*tert*-amylnaphthalene was (400.0 h) and the yield was over than 76% at both processes approximately.

## Introduction

Recently, more than 10 years ago from the discovery, the science of green chemistry defines as a group of several modern techniques and industrial processes for chemical reactions that distinguished with efficient energy. It can serve to reduce or prevent formation of undesired by-products, prevent using reagents or toxic solvents, use renewable resources and avoid use of these non renewable materials before their depletion in the nearest future, e.g. oil and coke (Mike Lancaster, 2002).

The 12$^{th}$ applied principles of green chemistry are aimed to make the chemical reactions eco-friendly for environment and human, safer and not harmful, more efficiently and cleanly (Al-Khalaf, 2012), and reduce or prevent use or produce the toxic and dangerous materials on these steps: design, industry, application of chemicals and ability of its degradation (Anastas and Warner, 1998). There are some important principles of green chemistry such as:

## Atom economy

This concept is considered as a design tool for the chemical reactions that refers to numbers of reactant atoms that corporate to form the desired product and the numbers of other reactant atoms to form by-product as the following equation depending on the original chemical equation and the same regarding with parameters of selectivity and yielding of product:

$$\text{Atom Economy} = \frac{\text{Molecular mass of product}}{\text{Molecular mass of all reagents}} \times 100\% \quad (1)$$

$$\text{Selectivity} = \frac{\text{Yield of desired product}}{\text{Amount of substrate converted}} \times 100\% \quad (2)$$

$$\text{Yield} = \frac{\text{Actual quantity of products achieved}}{\text{Theoretical quantity of products achievable}} \times 100\% \quad (3)$$

## E-Factor

This concept can be defined as the ratio between the waste amounts and the amounts of the desired product as the following equation:

*E-factor = [Raw Materials (Total input)-Product]/Product* (4)

This parameter is a good tool used to show the dilemma of the waste that accompanied with production of desired material. However, all the amounts of used chemicals in the chemical reaction from the starting to the ending including the water used in washing and purification processes. The consumption of large amounts of these benign waste such water, diluted ethanol, acetic acid, and low concentrations of inorganic salts will make the environmental factor seem to be worse than the truth. Table 1 showed the annual production, total waste, and values of E-factor for the industry segments (Sheldon, 1992)

## Environmental quotient

It is a multiple of E-factor by the factor of undesired by-products (Q-factor). E.g. Q equal to 100 for salts of heavy metal and equal to 1 for NaCl as the following equation:

$$EQ = \text{E-factor} \times \text{Q-factor} \qquad (1)^{(5)}$$

## Effective Mass Yield (EMY)

This is the ratio between the amount of desired product and amount of non-benign material used. However, this parameter treats the problem of calculating the benign waste in law of E-factor. The environmental benign waste like water will be taken in account as in below:

$$EMY = \frac{\text{Mass of Product}}{\text{Mass of non-benign material used}} \times 100\% \quad (6)$$

The two processes of synthesis of lubricating oils as a case study have differences in relating with the yield of products and amount of produced wastes through the calculated parameters in order to detect which process is greener and applicable easily (Jaleel *et al.*, 2013).

## Results and Discussion

From data of Keith Smith *et al* (2012) which used in measurements of the following parameters as in Table 2, depending on the chemical equation of synthesis of 2-*tert*-amylnaphthalene as lubricating oil:

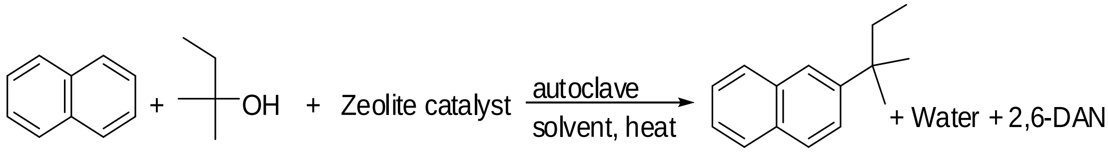


**Table.1** Values of E-factor for the different types of industry

| Type of industry | Annual production (ton) | Total waste (Ton;approx.) | E-factor |
|---|---|---|---|
| Pharmaceuticals | $10\text{-}10^3$ | $10^3$ | 25->100 |
| Fine chemicals | $10^2\text{-}10^4$ | $10^4$ | 5->50 |
| Bulk chemicals | $10^4\text{-}10^6$ | $10^5$ | <1-5 |
| Oil refining | $10^6\text{-}10^8$ | $10^6$ | 1.0 |

**Table.2** Parameters of the environmental efficiency for the process of synthesis (2)*

| Parameters of Environ. Efficiency | Product | 'Greenness' |
|---|---|---|
| Atom economy | 92.0 | Quite good |
| Yield (%) | 80.0 | OK |
| Selectivity (%) | 80.0 | Quite good |
| E-Factor | 1.0 | Quite good |
| E-quotient | 1.0 | Quite good |
| EMY (%) | Maximum value | Excellent |

* Water is considered as a benign waste; Q equal 1.

The Table 2 shows the values of environmental efficiency parameters for the reaction of direct *tert*-amylation of naphthalene to produce main product of 2-*tert*-amylnaphthalene, along with the traces products of 2,6-dialkylnaphthalenes (2,6-DAN) which is useful in polymers industry (Keith Smith *et al.*, 2012), and that also affected on the percentage of yield and selectivity. The atom economy (%) of the main product is 91.66 and other percentage for released molecule of water as by-product and can be easily recycled. So, synthesis process of 2-*tert*-amylnaphthalene is clean, economic, efficient, and eco-friendly process. In addition to the other related parameters as E-factor, E-quotient, and EMY (%) which are actually depends on the released benign wastes like water and no wastes were appeared. The catalyst of zeolite can be easily regenerated by heating and then reused.

While in contrast, the other process of synthesis of lubricating oils, from the data of Yoshida and Watanabe (1988) which used in measurements of the following parameters as in Table 3, depending on the chemical equation of synthesis of 2-*tert*-amylnaphthalene as lubricating oil by using naphthalene with suitable alkene (2-methyl-2-butene) through reflux process:

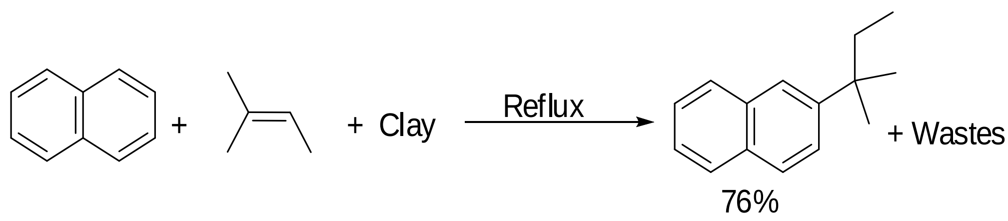


**Table.3** Parameters of the environmental efficiency for the process of synthesis (1)*

| Parameters of environ. Efficiency | Product | 'Greenness' |
|---|---|---|
| Atom economy | 100.0 | Quite good |
| Yield (%) | 76.0 | OK |
| Selectivity (%) | Not clear | — |
| E-Factor | 32.0 | Not |
| E-quotient | >>32.0 | Not |
| EMY (%) | 25.0 | Not |

* 2-methyl-2-butene is not benign waste; Q will absolutely not equal 1.

**Table.4** Service life of prepared lubricating oils at oxidation test (1)

| Tested compounds | Service life at oxidation test (h) |
|---|---|
| 2-*tert*-amylnaphthalene | 400.0 |
| 2-(1,1-dimethyloctyl) naphthalene | 250.0 |
| 2-(1,1-dimethylhexyl) naphthalene | 250.0 |
| 2-(1,1-dimethyldecyl) naphthalene | 230.0 |

The Table 3 shows the values of environmental efficiency parameters for the reaction of synthesis of 2-*tert*-amylnaphthalene by using 2-methyl-2-butene and naphthalene through reflux process, along with the unknown products (waste product). The atom economy (%) of the main product is 100. So, synthesis process of 2-*tert*-amylnaphthalene is not clean, not economic and efficient process depending on the related parameters as E-Factor, E-quotient which is depending on the released non benign wastes like 2-methyl-2-butene and its possible derivatives.

The produced material by two processes has high oxidation level (Yoshida and Yokohama, 1988), through the prepared materials were subjected to high-temperature oxidation tests where the test conditions were as follows:

Test temperature: 170°C; Flow of oxygen: 31/h; Catalyst: Copper wire 1mmΦ × 80 cm.

The test evaluation was found by measuring how long each of tested compound to be resistant in acid value (until to reach 1.0 mg KOH/g) and the time was belongs to be service life at oxidation test. The results of that test are as in the Table 4.

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