



**Short Communication**

**ECOSAR- A Tool for Analyzing Toxicity of Pollutants to Aquatic Life**

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Available online at: [www.ijrce.org](http://www.ijrce.org)

(Received 1<sup>st</sup> October 2011, Accepted 31<sup>st</sup> October 2011)

**Abstract** - ECOSAR is a program that has been designed for the expert user. It is a menu driven and contains many functions to assist the user. The acute toxicity of a chemical to fish fresh water and salt water, water fleas and green algae has been the focus of the ECOSAR. Hence even before commencing the project if the chemical composition of the waste is known or studied, the impact of waste will be known to everyone. The process may be altered if the waste is harmful to aquatic life or ECOSAR even is able to help to post monitoring of the project within the frame. Environmental assessors, chemical manufacturers, chemical suppliers and other regulatory agencies have used ECOSAR to develop quantitative screening level toxicity profiles for fish, aquatic invertebrates, and green algae. The paper aims at presenting case study, how the aquatic life gets affected due to let out of pollutants from paper industries situated at Chandrapur, district of Maharashtra.

**Keywords:** ECOSAR, Pollutants, Paper industry, Aquatic life.

### Introduction

The ECOSAR analysis is currently practiced by the office of pollution prevention and toxics, USA. The program has been designed for the expert user. It is a menu driven and contains many functions to assist the user. The user has to enter the structure activity relationship, SAR, to the software which is used to predict the aquatic toxicity of chemicals based on their similarity of structure. SMILES are an acronym for Simplified Molecular Input Line Entry System. It is a chemical notation system used to represent a molecular structure by a linear string of symbols. SMILES notations are comprised of atoms (designated by atomic symbols), bonds, parentheses (used to show branching) and numbers (used to designate ring opening and closing positions). The SMILES notation system was specifically designed for computer use by chemists. The encoding rules for SMILES can be learned quickly and easily by anyone with any type of chemistry background. Learning to write a SMILES notation for most chemicals is not difficult. However, writing a SMILES notation for a complicated ring system can be tricky and time-consuming. The CAS Number Data Base (available from Syracuse Research Corporation (SRC) as an add-on product) is extremely helpful and time-efficient in obtaining SMILES notations. After SMILES and CAS one important factor is Kow. The octanol/water partition coefficient (Kow) is defined as the ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of a two-phase octanol/water system.  $Kow = \frac{\text{Concentration in octanol}}{\text{Concentration in aqueous phase}}$

phase / Concentration in aqueous phase. Values of Kow are thus unitless. Measured values of Kow for organic chemicals have been found as low as  $10^{-3}$  and as high as  $10^7$ , thus encompassing a range of ten orders of magnitude. Hence, it is possible to calculate the Kow by using software tools.<sup>[4]</sup>, by drawing a structure of particular chemicals.

### Case Study

Chandrapur district consist of about 18 big and 1205 small industries situated in 10,490 Sq. Km. The city also boasts of having the largest paper manufacturing unit of Ballarpur Paper Industry (BILT), largest manufacturer and exporter of paper in India, Integrated paper mill with a 350 TPD capacity releases wastewater @ 55,000 m<sup>3</sup> per day. Paper and pulp industry contributes large number of pollutants to water resources, mainly, sulphur containing compounds from different processes. Sulfur-based compounds are used in both the Kraft process and the sulfite process for making wood pulp. Sulfur is generally recovered, with the exception of ammonia-based sulfite processes, but some is released as sulfur dioxide during combustion of black liquor, a byproduct of the kraft process, or "red liquor" from the sulfite process. The kraft/sulphate process is used for the conversion of wood into wood pulp consists of pure binded cellulose fibers. In the process, wood chips treated with mixture of sodium hydroxide and sodium sulphide called as white liquor are used to break bonds between cellulose fibers. Large amount of sulphur

compound mainly  $\text{Na}_2\text{S}$  is feed to the rivers in the form of water waste. If the process of disposing the waste continuous, the river water in near future will be fully polluted. Therefore, it was intended to find out the effects of

pollutants on the aquatic life. When the toxicity of  $\text{Na}_2\text{S}$  is calculated by using ECOSAR software, it gives following results.

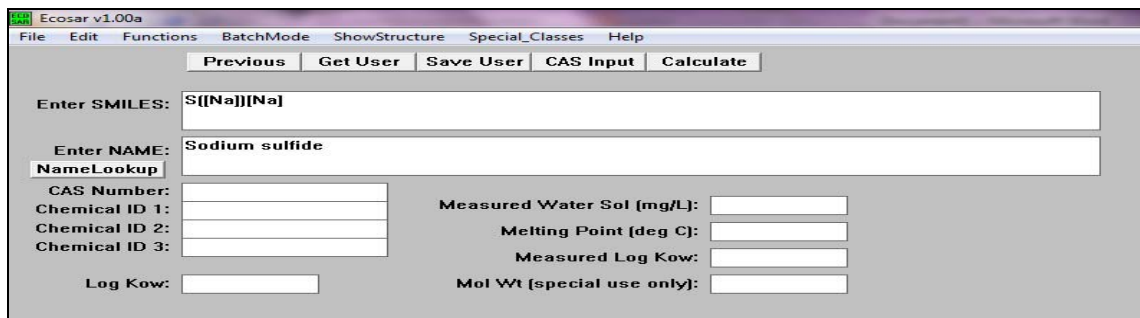


Figure: 1 Starting window of Toxicity analysis of  $\text{Na}_2\text{S}$  by using ECOSAR

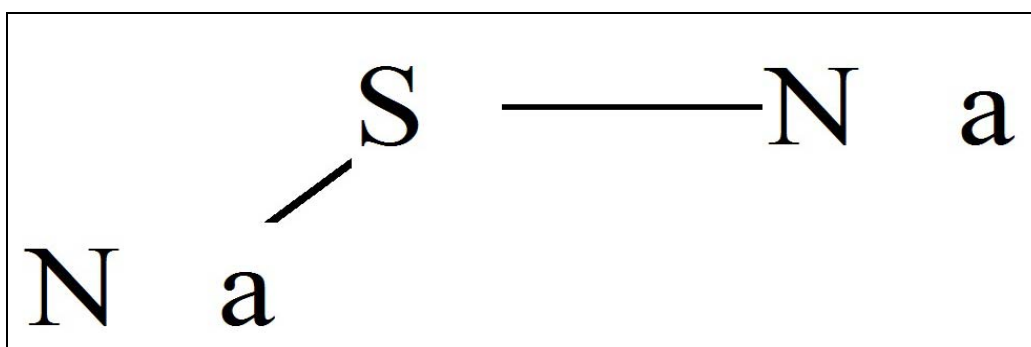


Figure: 2 Structure window of  $\text{Na}_2\text{S}$ .

ECOWIN Results

Print Save Results Copy Remove Window Help

SMILES : S[[Na]][Na]  
 CHEM : Sodium sulfide  
 CAS Num: 001313-82-2  
 ChemID1:  
 ChemID2:  
 ChemID3:  
 MOL FOR: S1 Na2  
 MOL WT : 78.04  
 Log Kow: -4.23 (KowWin estimate)  
 Melt Pt:  
 Wat Sol: 1.86E+005 mg/L (experimental database)

ECOSAR v1.00a Class(es) Found

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organics	: Fish	96-hr	LC50	1.81e+007 *
Neutral Organics	: Fish	14-day	LC50	1.65e+007 *
Neutral Organics	: Daphnid	48-hr	LC50	4.06e+006 *
Neutral Organics	: Green Algae	96-hr	EC50	1.29e+005
Neutral Organics	: Fish	30-day	ChU	1.24e+006 *
Neutral Organics	: Daphnid		ChU	1.76e+005
Neutral Organics	: Green Algae		ChU	17470.285
Neutral Organics	: Fish (SW)	96-hr	LC50	4.03e+007 *
Neutral Organics	: Mysid Shrimp	96-hr	LC50	1.53e+009 *
Neutral Organics	: Fish (SW)		ChU	73527.141
Neutral Organics	: Mysid Shrimp (SW)		ChU	8.36e+008 *
Neutral Organics	: Earthworm	14-day	LC50	599.928

Note: \* = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Neutral Organics:

For Fish LC50 (96-h), Daphnid LC50, Mysid: If the log Kow is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

For Fish LC50 (14-day) and Earthworm LC50: If the log Kow is greater than 6.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Figure: 3 Result window of Toxicity analysis of  $\text{Na}_2\text{S}$  by using ECOSAR

## **Results and Discussion**

The calculated toxicity for fish is found to be high. If the toxicity remains for a duration of 96hr, it is dangerous for aquatic life. LC50 indicates the "Lethal Concentration". LC values usually refer to the concentration of a chemical in air but in environmental studies it can also mean the concentration of a chemical in water. For inhalation experiments, the concentration of the chemical in air that kills 50% of the test animals in a given time (usually four hours) is the LC<sub>50</sub> value. Even it can be predicted that the insoluble chemical is carried by water body, which may danger the life of those using the water on down-stream.

## **Conclusion**

ECOSAR software was used to find out, how pollutants let out from paper industries in Chandrapur district of Maharashtra are harmful to aquatic life when disposed in water. A case study is presented to know the effects of chemicals on aquatic life which can disturb the ecological balance. The chemical is also carried away by the stream in the form of insoluble chemical, which affects all those using

it. Hence the people should be made aware about the ill effects of let out pollutants to human life as well as aquatic life.

## **References**

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