UPDATES FROM ECOSAR 1.11 TO ECOSAR 2.2 (March 2022)

The following updates to ECOSAR version 1.11 occurred from November 2012 to March 2015, resulting in ECOSAR version 2.0 and 2.2.

1. **Ethoxylated Nonionic Surfactants Class**

Chronic value QSAR models have been developed for fish and daphnids and the relationships are log ChV = (- 0.3699 × log P) - 0.9480, and log ChV = (-0.4805 × log P) - 0.3460, respectively.

2. Alcohol Ethoxylates Nonionic Surfactants Class

A QSAR relationship for acute green algae 72-/96-hr ECb_{50} values (biomass) for alcohol ethoxylate nonionic surfactants has been developed. A combination of 13 PMN cases and 8 commercial surfactants were used in a training set to generate the following relationship: log (1/ ECb_{50}) = (0.5789 × log P) + 2.615. Use of this relationship for a validation set of 22 commercial surfactants gave predicted ECb_{50} values with a correlation coefficient R^2 of 0.90.

The acute algae QSAR is similar to those developed for daphnia 48 hr acute EC_{50} values [log (1/ EC_{50}) = (0.5767 × log P) + 2.672] and fish 96 hr acute LC_{50} values [log(1/ LC_{50}) = (0.4793 × log P) + 3.060], indicating that the mode of action of this surfactant class with biological membranes is similar for the three taxa.

3. Polymers Module

An ECOSAR module was developed for cationic polymers to provide aquatic toxicity predictions. In addition, user interface/dialog boxes were developed to upgrade the ECOSAR polymer module. A document describing the dispersibility behavior of polymers in water and a companion document on surfactant behavior and micelle formation to support the new Nonionic Surfactants are available in Appendix 2 of the ECOSAR 'Methodology Document' in the 'Helpful' files bundled with the ECOSAR version 2.2 executable. Appendix 2 also includes a narrative explanation on key points to aid users of the Polymers module, in particular with respect to the polymer compositional variables that users will input into the module to obtain toxicity prediction values.

4. ECOSAR Java Update

ECOSAR Java updates were completed for the new dyes, surfactants, and polymers modules. The K_{ow} values in the nonionic surfactant module was also updated.

The ECOSAR V2.0 user interface was updated using Java coding and JChemPaint for chemical structure viewing, drawing, and importing. In addition, several organic chemical classes were updated since ECOSAR V1.11. The chemical classes in ECOSAR V2.0 with updated QSARs based on new data or revised definition sheets are listed below:

ECOSAR V2.0 Updates

Class Name	ECOSAR V2.0 Updated QSARs	Update Details
Acrylates	X	
Aldehydes (mono)	X	
Amides	X	

Class Name	ECOSAR V2.0 Updated QSARs	Update Details
Anilines (hindered)	X	
Anilines (unhindered)	X	
Benzotriazoles	X	
Benzyl Halides	X	
Benzyl Nitriles	X	
Carbamate Esters	X	
Carbonyl Ureas	X	
Esters	X	
Esters, Dithiophosphate	X	
Esters, Monothiophosphate	X	
Esters, Phosphates-Inert Substitutions	X	New class: sub-classification of Esters, Phosphates class
Esters, Phosphates-Withdrawing Substitutions	X	New class: sub-classification of Esters, Phosphates class
Esters, Phosphinates	X	
Haloalcohols	Deleted	Measured data from this class will be moved to the Neutral Organics class in the next version update
Halo Ketones	X	
Hydrazines	X	
Imides	X	
Ketone Alcohols	X	
Methacrylates	X	
Nitro Alcohols	X	
Oxetanes	X	
Peroxides		Definition sheet updated
Peroxy Acids	X	Definition sheet updated
Peroxy Esters		Definition sheet updated
Polyaliphatic Nitriles	X	
Pyrroles/Diazoles	X	New class: combined Imidazoles & Pyrazoles-Pyrroles classes
Pyridine-α-acid	X	
Substituted Ureas	X	
Thiophenes	X	
Thiotetrazoles	X	
Thioureas	X	
Triazines, Aromatic	X	
Triazoles (non-fused)	X	
Vinyl/Allyl /Propargyl Alcohols Unhindered	X	New class: combined Unhindered Vinyl/Allyl Alcohols & Propargyl Alcohols
Vinyl/Allyl/ Propargyl Alcohols Hindered	X	New class: combined Hindered Vinyl/Allyl Alcohols & Propargyl Alcohols
Vinyl/allyl/Propargyl Aldehydes Hindered	X	New class: previously Vinyl/Allyl Aldehydes (split into hindered and unhindered)
Vinyl/allyl/Propargyl Aldehydes	X	New class: previously Vinyl/Allyl Aldehydes (split

Class Name	ECOSAR V2.0 Updated QSARs	Update Details
Unhindered		into hindered and unhindered)
Vinyl/Allyl/Propargyl Esters	X	New class: previously Vinyl/Allyl Esters
Vinyl/Allyl/Propargyl Ethers	X	New class: combined Vinyl/Allyl Ethers & Propargyl Ethers
Vinyl/Allyl/Propargyl Halides	X	New class: combined Vinyl/Allyl Halides & Propargyl Halides
Vinyl/allyl/Propargyl Ketones	X	New class: previously Vinyl/Allyl Ketones
Vinyl/Allyl/ Propargyl Aromatic Amines	X	New class: previously Vinyl/Allyl Pyrazoles-Pyrroles
Vinyl/Allyl/ Propargyl Nitriles	X	New class: previously Vinyl/Allyl Nitriles
Vinyl/Allyl/Propargyl Sulfones	X	New class: previously Vinyl/Allyl Sulfones
Special Classes		
Surfactants, nonionic	X	
Polymers, nonionic	X	
Polymers, anionic	X	
Polymers, cationic	X	
Polymers, amphoteric	X	

ECOSAR V.2.2 Updates

1. Added user input of MP, Log K_{OW} and water solubility to the search screen for the organic module and added user input of these properties in Excel format in the batch search function.

2. In Batch Mode:
    a. ECOSAR will now enumerate the output so that it can be matched to the input.

    b. Images are not loaded for batch processes with greater than 20 input structures (to speed up the batch processing). For batch processes up to 20 input structures, the images are retained.

    c. The 'Submit' button is available for batch inputs of up to 20 chemicals. For batches greater than 20 chemicals, only the 'Report' enabled. Batch results for up to 20 selected chemicals are displayed individually, as in the organic module. Batch results greater than 20 chemicals are exported to Microsoft Excel.

    d. For SMILES entries with more than one chemical output, the user selects the desired chemical from the list that pops up in the Batch Chemical Input window.

    e. Increased JVM/heap memory when running batch files to allow the application to run through longer before timing out.

3. Added the Neutral Organics class output for each chemical for a baseline to compare chemical class endpoint values.

4. Chemical class QSAR equations and associate training data set, the ECOSAR Methodology Manual and the Operation Manual are now packaged with the ECOSAR v.2.2 download in a separate 'Helpful' folder.

5. Corrected QSAR equation and output issues identified in version 2.0 by Proctor & Gamble Company in the table below:

Class Name	Change noted in What's new in ECOSAR V2.0			2.0 Manual matches 1.1 Manual for all endpoints	2.0 output matches predicted from 2.0 Manual	Notes
	Updated definition	Deleted or merged class	New class			
Esters	x					manual changed but output did not
Esters, Dithiophosphate	x					manual changed but output did not
Esters, Monothiophosphate	x					manual changed but output did not
Esters, Phosphate		x				class should be split (see next two classes) but still present with 1.11 QSAR
Esters, Phosphates - Inert Substitutions	x		x			new class and QSAR that is not being used
Esters, Phosphates - Withdrawing Substitutions	x		x			new class and QSAR that is not being used
Phenol Amines				x		QSARs in 1.11 and 2.0 match but output is different
Phenols				x		QSARs in 1.11 and 2.0 match but output is different
Vinyl/Allyl/Propargyl Alcohols - hindered	x		x	N/A		Propargyls are correct; vinyls and allyls have incorrect class and output
Vinyl/Allyl/Propargyl Aldehydes - hindered	x		x	N/A		new QSAR not being used. Class not correctly updated (no distinction between hindered and unhindered) or aldehyde, mono for propargyls
Vinyl/Allyl/Propargyl Aldehydes - unhindered	x		x	N/A		new QSAR not being used. Class not correctly updated (no distinction between hindered and unhindered) or aldehyde, mono for propargyls
Vinyl/Allyl/Propargyl Aromatic Amines	x		x	N/A		propargyls not coming up correctly
Vinyl/Allyl/Propargyl Esters	x		x	N/A		propargyls not coming up correctly
Vinyl/Allyl/Propargyl Ethers	x		x	N/A	x	Note that for propargyls information is repeated (listed twice)

Class Name	Change noted in What's new in ECOSAR V2.0			2.0 Manual matches 1.1 Manual for all endpoints	2.0 output matches predicted from 2.0 Manual	Notes
	Updated definition	Deleted or merged class	New class			
Vinyl/Allyl/Propargyl Halides	x		x	N/A		new class but QSARs from previous classes (comes up twice for propargyls)
Vinyl/Allyl/Propargyl Ketones	x		x	N/A		new class but QSARs from previous class and propargyl not classified correctly
Vinyl/Allyl/Propargyl Nitriles	x		x	N/A		propargyls not coming up correctly
Vinyl/Allyl/Propargyl Sulfones	x		x	N/A		propargyls not coming up correctly