

PetroTox Release notes - version 4.01

PetroTox has been developed and improved by Dr. Aaron Redman (HydroQual Inc.) on behalf of Concawe up to version 3.06. Improvements from version 3.07 to 4.0 have been implemented by Mr. Nikola Loncar and Mr. Borja Serrano (Penman Consulting Ltd.) on behalf of Concawe. Improvements from 4.01 and above have been implemented by Dr. Yves Verhaegen (Concawe).

Version 1.02 January 9, 2007: Previous release version 1.01 had a few errors related to reported dissolved phase LC50s instead of product loadings (e.g., LL50) and was mislabelled as Model LL50 (mg/L water) in addition to a bug in the species selection menu and mapping functions. They are corrected in Version 1.02. The Version 1.02 reports the product loading (g product / L water) instead of total dissolved hydrocarbons at the LL50. Another error was identified in the reporting of inputted loads during dose-response calculations whereas instead of the inputted load being printed on the output sheets the dissolved phase concentration was reported in its place. This has been corrected to report the loads instead of dissolved phase concentrations in the user-defined and normal versions of PetroTox. The User-Defined model had an error occur whenever the user-defined species was selected for toxicity calculations. There was an error in the mapping of orphan blocks (assigned mass without corresponding structures in database) that has been corrected.

Version 1.03 March 12, 2007: The previous version of the default and user-defined models had an error associated with the use of chemical activity in the headspace partitioning calculation. The manuals have been updated to reflect these changes. This has been corrected and, generally, the results (e.g., LL50s) are higher by about a factor of 2 over the previous calculations, please see previously released 'SampleDatasets_060127.xls' and the current release of 'SampleDatasets_070112.xls' for an example of the magnitude of these changes. The updated model results are in slightly better agreement with observed LL50's. In the user-defined model, the polyaromatic chemical class was set as the default condition to ensure a conservative model result. Previous versions of the UDM used the aliphatic chemical class as the default condition. Also, a few compounds were removed from the hydrocarbon physicochemical properties database since certain of their properties (e.g., $\log(K_{ow})$, Henry's Law constant) were considered to be outliers. These are the compounds that were removed:

ID in v1.02	Name
686	n-phenylcyclohexane
1433	Cyclopropylbenzene
1442	2-methyloctyl-hexadecahydricene
1461	Diadamantane
1462	1-methyldiadmantane

Version 2.01 October 12, 2007: This version of the model has been modified from v1.03 with a new membrane-water cut-off point at a $\log(Kow)$ of 6.0, instead of the previous value of 5.5. This change was made to reflect recent experimental toxicity data for high $\log(Kow)$ compounds¹. Also, the spreadsheet models were modified so that the user can select to perform calculations with the default membrane-water cut-off (6.0) or a user-defined option. This feature is available in both the default and user-defined models on the 'CTLBB' spreadsheet. See the manuals for additional information. Also, the HC5 parameters were updated to be consistent with McGrath and Di Toro 2006 (TLM update) and McGrath et al 2004 (original TLM-HC5 derivation).

¹ The rationale for this change and the data were later published in: Redman, A.D.; Parkerton, T. F.; Leon Paumen, M.; Butler, J.D.; Letinski, D. J. and Den Haan, K. (2017) "A re-evaluation of PETROTOX for predicting acute and chronic toxicity of petroleum substances", Env. Tox. and Chemistry, Vol. 36, 8, 2245-2252.

Version 2.02 August 2008: This version of the model has been modified from v2.01 with a modified mass distribution algorithm for low resolution calculations only. The new mass allocation method increases mass to PAH structures by about 3 times only at BP > 350 °C. Mass to other structures and chemical classes is scaled down proportionately to preserve the overall mass distribution. This modification was implemented to better match the mass allocation in heavy fuel oils and to improve consistency between the high and low resolution predictions for the same. A few data fields and titles were modified for consistency with model operations and documentation, these changes were minor.

The CONCAWE database was updated and finalized with a few additional structures and from the most recent SPARC model (v4.2) run in batch mode for consistency.

Version 3.01 October 2008: This version has a more streamlined output and allows the user to enter custom parameters for the membrane-water partition coefficient. Also, the High-Resolution input was re-fitted to accept compositional information as a function of actual carbon number instead of boiling point in order to be more consistent with the analytical results from the 2D GC method. Also, diadamantane and methyladamantane were removed as outliers from the database based on their Henry's Law constants that were several orders of magnitude different than other naphthenic compounds with similar BP or logKow.

Version 3.01 April 2009: The following changes were made:

- PNEC output by chemical class consistent with input resolutions (High vs Low)
- Expanded entries up to n=100
- Detailed results are printed in 'DetailedOut' to show how compounds are assigned to HB

Version 3.02 May 2009: HC5 updated to be consistent with McGrath and Di Toro 2009.

Version 3.03 May 2009: Fixed minor error in Bioavailability UserForm that is linked to drop-down menu. Fixed Avg Kow and PNEC reporting error.

Version 3.04 September 1, 2009: Removed adamantane structures from database

Version 3.05 October 28, 2009: Correctly reassigned phenyl-cyclohexane as naphthenic mono aromatic. Password protected code and Library sheets.

Version 3.06 October 2011: Compatible with MS Office 2010. ACR changed from 4.5 (McGrath et al 2004) to 3.8 consistent with TLM application to hydrocarbon-only subset (McGrath and Di Toro 2009). Added additional CTLBBs to list. Chart function does not work in low-res mode. The toxicity cut-off is now consistent with the latest iteration (Parkerton et al 2012).

Version 4.0 November 2019: Translation of PetroTox implementation in Excel to implementation in KNIME. Added possibility to select specific classes and/or structures for representing the user-defined compositional input. 2 additional options to compensate for missing compositional information (spread missing concentration to highest blocks or to lowest blocks). An alternative HC5-based calculation of the PNEC can be chosen, based on K_{TLW} instead of K_{OW} . Revamped manual. Correction of typographical errors.

Version 4.01 February 2025: Limited re-organisation of nodes, metanodes and output format. Nodes which were incompatible with (or incorrectly translated to) KNIME version 5.2.6 were corrected.