The updated and consolidated ProScale-E: Ecotoxicity potential scoring method for chemical footprint, LCA and SSbD assessment

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INTRODUCTION

Based on a collaborative effort between ProScale consortium members and the ECETOC Task Force on Evaluation of a comparative safety assessment approach for products in the SSbD context, the ProScale-E method has now been revised in order to align the ProScale and ECETOC Task Force approaches [3]. Results from the update are shown in this presentation.

The ambition for the current ProScale-E model was to a) obtain a model analogous to ProScale-H:

a) as far as possible aligned with REACH, straightforward to use, easy to understand, require little to moderate substance data and still provide meaningful results for substances classified according to ecotoxicity (hazard classes in the H400 family) thereby accounting for the severity of impacts,

b) accounting for potency of substances, and

c) facilitating inclusion of fate and degradation of substances.

Simplification to ecotoxicity and degradation factors only, was supported by previous research on ecotoxicity models for LCA [4].

ProScale-E model

ProScale-E ecotoxicity characterisation factors (CF), based on the CLP environmental hazard classification for both acute and chronic effects, potency via M-factors, as well as biodegradability properties based on tests reported in the European Chemicals Agency (ECHA) chemicals database, are calculated according to the following formula, where HF is the hazard factor, and DF is the degradation factor, for a substance:

$$CF = HF_e \times DF$$

Harmonisation work procedure

A detailed analysis of the criteria for hazard classification of ecotoxicity was carried out by the ECETOC task force and discussed with experts from member companies of the ProScale consortium. In summary, the Task Force has worked through a series of meetings organised with 2-4 weeks interval and with various aspects of the model elaborated in between these meetings. Beyond the Task Force itself, Task Force representatives have discussed with internal experts in order to come up with an agreeable classification and scoring scheme, covering environmental transformation and fate as well as environmental hazard.

Results – updated & harmonized factors

Hazard factors

ProScale-E hazard class	H-phrases according to GHS/CLP	ProScale hazard score
E	EUH440, EUH441, EUH450, EUH451, EUH430 H410RD (M = 1000)	100 000 *(highest hazard)*
D	EUH431 H400RD, H410NRD (M = 1000) H410RD (M = 100)	 10 000
C	H400NRD (M = 1000) H400RD, H410NRD (M = 100) H410RD (M = 10)	 1 000
B	H400NRD (M = 100) H400RD, H410NRD (M = 10) H410RD (M = 1)	 100
A	H400NRD (M = 10) H400RD, H410NRD (M = 1) H411_RD	 10
AA	H400NRD (M = 1) H411NRD, H412RD	 1
AAA	 H412NRD, H413	0.1 *(lowest hazard)*

Hazard scoring system (above) and degradation factor (below) for ecotoxicity impact potentials in ProScale, based on the consolidated analysis [3] of hazard phrases and M-factors in CLP (EU Regulation No. 1272/2008), and degradation factors. The denotations RD and NRD stand for rapidly degrading and not rapidly degrading respectively

Degradation factor

Degradability statement	Criteria	Degradability factor
Very persistent/Persistent /Not biodegradable	P or vP according to Annex XIII / No pass OECD 301 or OECD 302	1
Rapidly degradable /Inherently degradable	OECD 302 pass	0.1
Readily degradable	OECD 301/310 pass	0.01

Results – differences compared to previous version

Chemical Name	CAS No	ProScale-E 2.0	ProScale-E 1.0	Ratio
Bisphenol A (BPA)	80-05-7	1000	1000	1
Methylisothiazolinone	2682-20-4	10	1000	100
Ammonia	7664-41-7	10	1000	100
Cyclohexane	110-82-7	1	10	10
Hydrogen peroxide	7722-84-1	1	100	100
Toluene diisocyanate/Toluene, 2,4-diisocyanate	584-84-9	0.1	100	1000
Octadecane -1-ol ethoxylated	9005-00-9	0.1	10	100
Cumene	98-82-8	0.1	10	100
Flumexol WDN	126-71-6	0.01	1	100
Monoethanolamine	141-43-5	0.01	1	100
Benzene	71-43-2	0.01	1	100

CONCLUSIONS AND OUTLOOK

- Assigning significance to the M-factor is a key aspect of ProScale-E, as the M-factor is based on EC50 values and therefore introduces the potency of a substance into the scoring. As comparison, in ProScale-H [1] the potency is accounted for by adjusting the hazard factor with respect to the OEL or DNEL. Substances having more than one H4XX-phrase (e.g. classified as both acute and chronic) will be assigned to the highest ProScale-E hazard class among the ones relevant to the classification for that substance.
- In the hazard classificaiton in CLP; degradability plays a role in the sense that rapidly degrading substances are classified differently from non-rapidly degradeable ones.However, the scoring system has been designed to break out the degradation from the hazard score. Instead, ProScale-E introduces a similar but slightly more granular approach to degradation, in which readily degradable is further distinguished, and an intermediate degradability class is defined for 1) rapidly (but not readily) degradable substances and 2) inherently degradable substances.
- Prediction tools based on, e.g., QSAR algorithms, can be used for estimating the relevant hazard class for new substances, not yet classified in CLP. Still, further work will be carried out to strengthen strategies to address data gaps and to further advance *in silico* prediction tools.
- Comparing ProScale-E 2.0 with its predecessor, it is evident that the update is relevant, due to the span of ratios (Table 1) for even this small sample of substances.
- ProScale-E appears to be an easy-to-use approach for screening level ranking/prioritization of ecotoxicity impact potentials. Development of characterization factors and validation is in progress, as is application in actual assessments, and implementation in regular LCA databases.

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