Extending ProScale to Far-Field Human Exposure: The Indirect Exposure (IE) Module

Efstathios Reppas-Chrysovitsinos[1], Pernilla Andersson[1], Amanda Lundberg[1], Maja Halling[1], Rosella Telaretti Leggieri[1], Therese Kärnman[1], Ioannis Liagkouridis[1], and Tomas Rydberg[1]

[1.] IVL Swedish Environmental Research Institute

INTRODUCTION

Chemical footprinting links chemical use and release to potential toxicity impacts from a life-cycle perspective. Existing approaches often fall between two extremes:

- Hazard screening, which identifies intrinsic concern but does not account for release, fate, exposure relevance, or mass flow
- Higher-tier fate – exposure – effect models which are powerful but may require data and modelling effort not available in early-stage SSbD assessment.

Indirect human exposure can arise when chemicals released during production, use, recycling, or end-of-life enter environmental compartments and later reach humans. This creates a need for a Tier-1, regulatory-aligned, LCA-compatible screening-level method for human-via-environment toxicity potential.

Here we introduce **ProScale-IE**, a ProScale module for assessing indirect human toxicity potential from environmental releases in product systems.

Aim and objectives

Aim

To introduce ProScale-IE, a ProScale module for assessing screening-level indirect human toxicity impact potential mediated by environmental releases.

Objectives

1. Define the role of ProScale-IE within the ProScale Suite.
2. Develop a module-specific characterization factor for indirect exposure.
3. Implement **route-specific** scoring for inhalation, drinking water, and food consumption.
4. Provide conservative rules for uncertain release compartments and missing data.
5. Support chemical footprinting and Tier-1 SSbD prioritization.

Materials and methods

The ProScale approach is focused on utilizing existing regulatory data. The table below presents the main data source for each of the ProScale-IE factors.

Factor	Main data source
$HF_{H,i,r}$	GHS H-phrases + OELs/DNELs
$ERF_{i,u,c}$	ECHA Environmental Release Categories (ERCs)
DF_i	OECD biodegradation tests + REACH/SDS persistence data
$E_{i,r}$	Physicochemical properties from REACH/SDS: vapor pressure, H', K_{OW}, K_{OC}, water solubility, BCF/BAF

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Generic ProScale structure

All ProScale modules follow the same accounting logic:

$$PS = MF \times CF$$

where:

- PS is the ProScale score
- MF is the chemical mass flow associated with the functional unit, and
- CF is the module-specific characterization factor

For ProScale-IE

For chemical i, unit process u, exposure route r, and release compartment c:

$$CF_{IE,i,u,r,c} = HF_{H,i,r} \times ERF_{i,u,c} \times DF_i \times E_{i,r}$$

and thus:

$$PS_{IE,i,u,r,c} = MF_{i,u} \times CF_{IE,i,u,r,c}$$

The ProScale-IE score is a characterized mass-based toxicity potential.

Factor	Meaning	Role in ProScale-IE
$MF_{i,u}$	Chemical mass flow	Links the substance to the functional unit
$HF_{H,i,r}$	Human-health hazard factor	Route-relevant toxicological concern
$ERF_{i,u,c}$	Environmental release factor	Potential release to air, water, or soil
DF_i	Degradation factor	Persistence-related exposure opportunity
$E_{i,r}$	Exposure-route relevance factor	Physicochemical relevance for indirect human exposure

Results and Discussion

Module output

ProScale-IE delivers route-specific scores for human-via-environment exposure through inhalation, drinking water, and food. These can be reported separately or aggregated into an overall human-via-environment toxicity potential:

$$PS_{IE,total} = PS_{IE,inh} + PS_{IE,drink} + PS_{IE,food}$$

High scores can be decomposed to identify whether concern is driven by hazard, release, persistence, route relevance, or mass flow.

Screening logic

ProScale-IE applies conservative Tier-1 rules:

- high $E_{i,r}$ if any high-relevance criterion is met
- low $E_{i,r}$ only when available indicators consistently support low relevance
- missing or conflicting data default to the more conservative band
- uncertain release compartments are handled using a bounding approach

Interpretation

A high ProScale-IE score can be decomposed into its drivers: hazard (HF), environmental release (ERF), persistence (DF), route relevance (E), or mass flow (MF). This helps distinguish whether concern should be addressed through substitution, emission reduction, improved degradation profile, additional data collection, or higher-tier modelling.

CONCLUSIONS

- ProScale-IE translates regulatory information on **hazard**, **environmental release**, **degradation/persistence**, and **route relevance** into an LCA-compatible chemical footprint score for human-via-environment toxicity potential.
- The module delivers route-specific screening results for **inhalation**, **drinking water**, and **food**, helping identify whether concern is driven by hazard, release, persistence, route relevance, or mass flow.
- ProScale-IE supports **Tier-1 SSbD** screening, hotspot identification, and prioritization, while indicating when higher-tier modelling, substitution, emission reduction, or redesign may be needed.

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Presenter: Efstathios Reppas-Chrysovitsinos, Ph.D. Tel: +46 76 1423047 Email: Stathis.Reppas@ivl.se