USEtox – characterizing human and ecotoxicological impacts of chemicals in LCA

Prof. Peter Fantke
Technical University of Denmark

Imperial Life Cycle Network Seminar Series
26-October-2021

http://doi.org/10.1039/D0GC01544J
## Main Application Areas of USEtox

Near-field/far-field USEtox framework is suitable for **comparative evaluation of chemicals** emitted along product life cycles and chemicals in various product applications. Primary application areas are (model already tested):

<table>
<thead>
<tr>
<th>Application area</th>
<th>Product types already covered in our framework (emissions already directly or indirectly included)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Product life cycle assessment (LCA)</td>
<td>Food contact materials</td>
</tr>
<tr>
<td>High-throughput exposure screening</td>
<td>Personal care products; food contact materials</td>
</tr>
<tr>
<td>High-throughput risk screening</td>
<td>Children toys; building materials; paints</td>
</tr>
<tr>
<td>Chemical exposure and risk prioritization</td>
<td>Household products (cleaning, personal care, and home maintenance products)</td>
</tr>
<tr>
<td>Chemical alternatives assessment (CAA) / chemical substitution</td>
<td>Building materials; personal care products; agricultural pesticides</td>
</tr>
</tbody>
</table>

[http://doi.org/10.1007/s11367-021-01889-y](http://doi.org/10.1007/s11367-021-01889-y)
What is USEtox?

- Global scientific consensus model
- Human toxicity & freshwater ecotoxicity
- Organic chemicals & metal ions

- Initiated by the UNEP-SETAC Life Cycle Initiative
- Used by European Commission and US EPA

http://vimeo.com/usetox/video
USEtox: the UNEP-SETAC toxicity model

USEtox: A parsimonious model to assess toxic impacts of chemicals on humans and ecosystems.
Now extended to chemicals in products

- **Parsimonious** – as simple as possible, as complex as necessary
- **Mimetic** – not differing more from the original models than these differ among themselves
- **Evaluated** – providing a repository of knowledge through evaluation against a broad set of existing models
- **Transparent** – being well documented, including the reasoning for model choices
USEtox characterization factors

- **Quantitatively** determine the impact score per impact category, in Comparative Toxic Unit (CTU): $\text{CTU}_{h\text{midpoint}} = \text{cases or incidences}$
- $\text{CTU}_{h\text{damage}} = \text{DALY} – \text{Disability Adjusted Life Years}$

\[
IS = \sum_i \sum_x CF_{x,i} \times m_{x,i}
\]

- **A characterization factor** is …
- A quantitative representation of the (relative) hazard potential of a specific emission per kg emitted,
- Expressed as absolute metric or relative to a reference substance.
- *Example*: Human toxicity characterization factor of benzene: $5.5E-07 \text{ CTU}_h/\text{kg}$ (cases per kg emitted to urban air (comparative toxic units = disease cases)
Impact Pathway: Ecotoxicity Impacts

**Emission**
Emission flow
\[ \text{kg}_{\text{emitted/d}} \]

**Fate**
Mass in environment
\[ \text{kg}_{\text{in compartment}} \]

**Exposure**
Dissolved mass fraction
\[ \text{kg}_{\text{bioavailable}} \]

**Effects**
Potential effects
\[ \text{PAF x m}^3 \]

**Fate factor, FF**
\[ \text{kg}_{\text{in compartment per kg}_{\text{emitted/d}}} \]

**Ecoexposure factor, XF**
\[ \text{kg}_{\text{bioavailable per kg}_{\text{in compartment}}} \]

**Effect factor, EF**
\[ \text{PAF x m}^3 \text{ per kg}_{\text{bioavailable}} \]
Impact Pathway: Human Toxicity Impacts

**Emission**
Emission flow \([\text{kg}_{\text{emitted}}/\text{d}]\)

**Fate**
Mass in environment \([\text{kg}_{\text{in compartment}}]\)

**Exposure**
Human intake \([\text{kg}_{\text{intake}}/\text{d}]\)

**Effects**
Potential effects \([\text{disease cases/d}]\)

**Fate factor, FF**
\([\text{kg}_{\text{in compartment}}/\text{kg}_{\text{emitted}}]\)

**Human exposure factor, XF**
\([\text{kg}_{\text{intake}}/\text{d}/\text{kg}_{\text{in compartment}}]\)

**Effect factor, EF**
\([\text{disease cases/d}/\text{kg}_{\text{intake}}]\)
Impact Pathway: Characterization Factors in USEtox

Emission  Fate  Exposure  Effects  Damage

Fate factor  Exposure factor  Effect factor  Damage factor

[Midpoint characterization factor, \( CF_{\text{midpoint}} \) [impacts/kg_{emitted}]]

[Damage characterization factor, \( CF_{\text{damage}} = XF \times FF \times ERF \times SF \) [damage/kg_{emitted}]]
USEtox far-field environmental fate assessment
Impact Pathway: Environmental Fate

Emission
Emission flow
\[ \text{kg}_\text{emitted/d} \]

Fate
Mass in environment
\[ \text{kg}_\text{in compartment} \]

Exposure
Dissolved mass fraction
\[ \text{kg}_\text{bioavailable} \]

Effects
Potential effects
\[ \text{PAF} \times \text{m}^3 \]

Fate factor, FF
\[ \frac{\text{kg}_\text{in compartment}}{\text{kg}_\text{emitted/d}} \]
Defining the «Fate Factor»

- Links the chemical mass in a given compartment to the quantity released into any compartment
- Accounts for multimedia & spatial transport between environmental media (e.g. air, water, soil, etc.)
- Can be interpreted as the «increase of chemical mass in compartment \( i \) [kg] due to an emission into compartment \( j \) [kg/day]».
Chemical Partitioning: Main Phases

- Air
  - Kaw (air/water partition coefficient)
  - Koa (octanol/air partition coefficient)

- Water
  - Kow (octanol/water partition coefficient)

- Lipid

Technical University of Denmark (DTU) | University of Michigan
Chemical Partitioning: Why Multimedia?

Multimedia partitioning:
Bennett et al. 2002
USEtox: Environmental Fate System

USEtox: UNEP-SETAC scientific consensus model for characterizing human toxicity and ecotoxicity in LCA and comparative risk screening

Boxes = compartments
Arrows = processes

USEtox documentation
Main Environmental Fate Processes

Degradation processes
→ Chemical decomposition (photochemical decomposition, photolysis, hydrolysis)
→ Biodegradation/bio-transformation (metabolism)

Transport removal processes
→ Sorption
→ Sedimentation

Transport to other media (diffusion and advection)
→ Deposition
→ Evaporation
→ Air flow
→ Volatilization
→ Re-suspension

Rate constants: $k_{w,tot} = k_{deg} + k_{sed} + k_{w>a} + \ldots$
Mass Balance Modeling: Residence Time (Fate Factor)

**Steady state:** inflow = outflow $\rightarrow \frac{dm}{dt} = 0$

Emission source rate: $s$ [kg/d]

Mass in compartment: $m$ [kg]

Removal rate coefficient: $k$ [1/d]

(mass eliminated per day; $t_{1/2}$ : half-life [d])

Residence time: $\tau$ [d]

$$\tau \triangleq m/(k \times m) = 1/k$$
**K matrix of rate constants [1/day]**

Expresses how many times per day is the chemical removed from the media and/or directly transferred to another media or to humans.

The diagonal is equal to minus the total removal rate:

\[ k_{ia,tot} = k_{ia,deg} + k_{ia,sorption} + k_{oa\leftarrow ia} + k_{inh\leftarrow ia} + k_{derm\leftarrow ia} \]

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USEtox far-field human exposure and intake
Impact Pathway: Human Exposure

Emission
Emission flow \([kg_{\text{emitted}}/d]\)

Fate
Mass in environment \([kg_{\text{in compartment}}]\)

Exposure
Human intake \([kg_{\text{intake}}/d]\)

Effects
Potential effects \([\text{disease cases}/d]\)

Exposure factor, \(XF\)
\([kg_{\text{intake}}/d \text{ per } kg_{\text{in compartment}}]\)
Exposure

Defining Exposure:

«Contact between stressors and receptors, and the associated sources, pathways and processes.» (Fantke et al. 2020)

Contact takes place at an exposure surface (mouth, skin, eyes) over an exposure period.

→ Contact with air, water, soil, food, or consumer products containing potentially harmful substances

Exposure Assessment

The process of estimating or measuring the magnitude, frequency and duration of exposure to an agent, along with the number and characteristics of the population exposed. Ideally, it describes the sources, pathways, routes, and the uncertainties in the assessment.
Human Exposure Pathways

What is the total chemical mass taken in by the human population via all exposure pathways?
Human Exposure Factors (XF)

Direct exposure: \( X_{F_{k,i}}^{\text{direct}} \)

The exposure factor for direct exposure is the rate coefficient for transfer of contaminants in compartment \( k \), through consumption of drinking water or inhalation of air to humans. Here, \( TF_{k,i} = C_i/C_k = 1 \), since \( i = k \), meaning that we interpret the compartment \( k \) is directly taken in:

\[
X_{F_{\text{air,inhalation}}}^{\text{direct}} = \frac{IR_{\text{inhalation}} \left[ \text{m}^3/\text{d} \right] \times n_{\text{persons}}}{V_{\text{air}} \left[ \text{m}^3 \right]}
\]

\[
X_{F_{\text{water,ingestion}}}^{\text{direct}} = \frac{IR_{\text{water ingestion}} \left[ \text{m}^3/\text{d} \right] \times n_{\text{persons}}}{V_{\text{water}} \left[ \text{m}^3 \right]}
\]

Residence time

The inverse of the direct exposure factor is the residence time, reflecting the average time required for the population in compartment \( k \) to take in the volume of the respective compartment (inhale the volume of air or drink the volume of water).
Human Exposure Factors (XF)

Indirect exposure: $XF_{k,j}^{\text{indirect}}$

The exposure factor for direct exposure is the rate coefficient for transfer of contaminants in compartment $k$, through consumption of an exposure medium $j$ that was contaminated from compartment $k$ – additional fraction of $V_k$ taken in every day:

$$XF_{k,j}^{\text{indirect}} = \frac{TF_{k,j} \text{[kg/kg]} \times IR_j \text{[kg/d]} \times n_{\text{persons}}}{\rho_k \text{[kg/m}^3\text{]} \times V_k \text{[m}^3\text{]}}$$

$TF_{k,j}$ quantifies the transfer efficiency for a contaminant from an environmental compartment $k$ to an exposure medium $j$. Various definitions and measures are used to model it, which can be found in literature. Examples:

Bioconcentration factor at steady-state, $BCF_{k,j} = \frac{C_j \text{ (conc. in exposure medium } j)}{C_k \text{ (conc. in compartment } k)}$

Bioaccumulation factor at steady-state, $BAF_{k,j} = BCF_{k,j} \times f_{\text{uptake from diet}}$
Impact Pathway: Human Intake Fraction

Emission
Emission flow \([\text{kg}_{\text{emitted}}/\text{d}]\)

Fate
Mass in environment \([\text{kg}_{\text{in compartment}}]\)

Exposure
Human intake \([\text{kg}_{\text{intake}}/\text{d}]\)

Effects
Potential effects \([\text{disease cases}/\text{d}]\)

Fate factor
Exposure factor
Intake fraction, \(iF\)
Human Intake Fraction (iF)

308 Compounds Evaluated

- Inhalation Dominant
- Multipathway
- Ingestion Dominant

Number of compounds

iF (total, air) [unitless]

- 308 Compounds Evaluated
- 0 to 10^2
- 10^-8 to 10^-2
- 10^-7 to 10^-6
- 10^-5 to 10^-4
USEtox human toxicity and ecotoxicity effects
Dose Response Models

**Effect dose:** $ED_x$ (lifetime) dose generating an **additional risk of x%** over background.

e.g. 50% over background for $ED_{50}$

**Dose-response Assessment:** Defines the quantitative relationship between the **dose** of a chemical received and the **incidence** of adverse health **effects** in the exposed population.
Dose Response in LCIA: Curve

Via inhalation / ingestion exposure

Cancer / non-cancer effects

Life time disease probability

Life time dose (kg intake per life time)
**Human Toxicity Effect Factor (EF)**

Incremental risk = Intake dose $\times \frac{0.5}{\text{Life time dose generating 50\% of additional risk}}$

EF = \frac{0.5}{\text{ED50}_{\text{human}} \times 365 \frac{d}{\text{yr}} \times 70 \text{ kg}_{\text{bodyweight}} \times 70 \text{ yr}_{\text{lifetime}} \times 10^{-6} \frac{\text{kg}}{\text{mg}}}$

EF = \frac{0.5}{\text{ED50}_{\text{human}} \times \left[ \frac{\text{cases}}{\text{kg intake}} \right]}$

**EF** : Substance-specific human toxicity effect factor [incidence risk / kg intake]

**ED50_{human}** : Effect dose inducing a response over background of 50\% for humans [mg/kg/d]

**ED50_{lifetime}** : Effect dose inducing a response over background of 50\% in humans over lifetime [kg intake over lifetime]

0.5 : Response level corresponding to the ED50 [lifetime incidence risk]
Aquatic Ecosystem Species Network

Who is exposed e.g. in an aquatic ecosystem? Species with different sensitivities!
Aquatic Ecosystem Exposure Assessment

Exposure factors for aquatic ecotoxicity represent the fractions of a chemical dissolved in contaminated aquatic compartment, calculated by:

\[
X_F_{\text{aquatic}} = \frac{m_{\text{dissolved}}}{m_{\text{total}}} = \frac{1}{1 + (K_P \times \text{SUSP} + K_{\text{doc}} \times \text{DOC} + BCF_{\text{fish}} \times \text{BIO})}
\]

where

- \(K_P\): partition coefficient between water and suspended solids [l/kg]
- \(\text{SUSP}\): suspended matter concentration in freshwater [kg/l]
- \(K_{\text{doc}}\): partitioning coefficient between dissolved organic carbon and water [l/kg]
- \(\text{DOC}\): dissolved organic carbon concentration in freshwater [kg/l]
- \(BCF_{\text{fish}}\): bioconcentration factor in fish [l/kg]
- \(\text{BIO}\): concentration of biota in water [kg/l]
Potentially Affected Fraction (PAF) of Species

\[ PAF = \frac{1}{1 + e^{-\log C - \alpha}} \]

with

\[ \alpha = \log HC50 \]

\[ = \frac{1}{n_{\text{species}}} \sum_{i=1}^{n} \log EC50_{\text{species}} \]

\[ \beta = \frac{\sqrt{3}}{\pi} \times \sigma_{\log EC50} \]
Ecotoxicity Effect Factor (EF)

\[ EF = \frac{\Delta PAF}{\Delta C} = \frac{0.5}{HC50} \]

HC: Hazard concentration = concentration at which the indicated % of species is affected above their individual EC

\[ \Delta PAF = 0.5 \]

\[ \Delta C = HC50 = 1 \text{ kg/m}^3 \]
Integration of USEtox far-field and near-field environments
Integration of far-field and near-field in USEtox

Emission flow [kg$_{emitted}$/d]
Emission mass [kg$_{emitted}$]
Mass in environment [kg$_{in\ compartment}$]
Time-integrated mass [kg$_{in\ compartment\ d}$]
Exposure level [kg$_{intake}$/d] [kg$_{dissolved}$]
Toxicity impacts [cases/d] [PAF m$^3$]
Health damage [DALY/d] [PDF m$^3$]

Fate factor
$FF = -K^{-1}$

Exposure factor
$XF$

Effect factor
$EF$

Severity factor
$SF$

Transfer fractions
$TF = (k_{x}/k_{\Sigma x})^{-1}$

Midpoint characterization factor, $CF_{\text{midpoint}}$ [impacts/kg$_{emitted}$]

Damage characterization factor, $CF_{\text{damage}} = XF \times FF \times ERF \times SF$ [damage/kg$_{emitted}$]
Near-Field Consumer Exposure to Chemicals in Toys

Far-field points of entry
- Ambient Air
- Water
- Soil
- Landfill

Near-field points of entry
- Object interior
- Food & beverage
- Object surface (dry or wet)
- Skin surface (dry or wet)
- Dust
- Skin surface (dry or wet)
- Indoor or near-person air

Product life cycle
- Chemical mass in product
- Product usage
- Chemical content

Direct points of entry
- Epidermis
- Gastrointestinal tract
- Respiratory tract

Fantke et al. 2018. Environ Health Perspect 126: 125001
Near-Field Consumer Exposure to Chemicals in Toys

Far-field points of entry

- Ambient Air
- Water
- Soil
- Landfill

Near-field points of entry

- Object interior
- Inside enclosed devices
- Dust
- Indoor or near-person air

Direct human points of entry

- Epidermis
- Gastrointestinal tract
- Respiratory tract

1. Chemical mass in product
2. Product usage
3. Chemical content

Product life cycle

Fanke et al. 2018. Environ Health Perspect 126: 125001
K matrix of rate constants [1/day]

Expresses how many times per day is the chemical removed from the media and/or directly transferred to another media or to humans

The diagonal is equal to minus the total removal rate:

\[ k_{ia,tot} = k_{ia,deg} + k_{ia,sorption} + k_{oa\leftarrow ia} + k_{inh\leftarrow ia} + k_{derm\leftarrow ia} \]

\[
\begin{pmatrix}
-k_{ia,tot} & k_{ia\leftarrow oa} & 0 & k_{ia\leftarrow inh} & 0 \\
k_{oa\leftarrow ia} & -k_{oa,tot} & k_{oa\leftarrow w} & k_{oa\leftarrow inh} & 0 \\
0 & k_{w\leftarrow oa} & -k_{w,tot} & 0 & k_{w\leftarrow ing&derm} \\
k_{inh\leftarrow ia} & k_{inh\leftarrow oa} & 0 & -k_{inh,tot} & 0 \\
k_{derm\leftarrow ia} & k_{derm\leftarrow oa} & k_{ing\leftarrow w} & 0 & -k_{ing&derm,tot}
\end{pmatrix}
\]

How can we determine the chemical fraction transferred from e.g. indoor to outdoor air?
### Direct Transfer Fractions matrix $T$ $[\text{--}]$

Diagonals: 100% entry in compartments, non-diagonals: transfers to other compartments

\[ t_{oa\leftarrow ia} = k_{oa\leftarrow ia} / -k_{ia,tot} \]

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<tbody>
<tr>
<td>indoor air</td>
<td>1</td>
<td>$-\frac{k_{ia\leftarrow oa}}{k_{oa,tot}}$</td>
<td>0</td>
<td>$-\frac{k_{ia\leftarrow inh}}{k_{inh,tot}}$</td>
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Near-field sub-models in USEtox

USEtox base model + 6 sub-models for 10000 chemicals in ~500 products

→ customized to particular applications + developed necessary QSARS for high throughput determination

Direct environmental emission

Skin surface

Article interior (with indoor sorption)

Food contact materials

Object surface

Pesticide residue
Article Interior Sub-Model (emission from solid products)

Transfer from product to air:

Diffusion-limited:

\[
TF_{\text{diffusion-limited}}^{\text{product} \rightarrow \text{air}} = \alpha \times (1 - e^{-\beta_1 D_m t}) + (1 - \alpha) \times (1 - e^{-\beta_2 D_m t})
\]

Partition-limited:

\[
TF_{\text{partition-limited}}^{\text{product} \rightarrow \text{air}} = 1 - (v_1 e^{\lambda_1 t} + v_2 e^{\lambda_2 t})
\]

Criteria for applying these two models:

\[
\begin{align*}
D - \text{limited: } & K_{ma} < 0.4 \cdot D_m^{-0.61} \\
K - \text{limited: } & K_{ma} > 0.4 \cdot D_m^{-0.61}
\end{align*}
\]

Key parameters: solid-phase diffusion coefficient \(D_m\) (m\(^2\)/s), solid material-air partition coefficient \(K_{ma}\)

Transfer via dermal contact:

\[
TF_{\text{direct dermal}}^{\text{product} \rightarrow \text{skin}} = \frac{1}{m_0} \times N_{\text{persons}} \times FQ_{\text{contact}} \times f_{\text{home}} \times A_{\text{contact}} \times \frac{K_{p-aq}}{K_{ma} \times K_{aw}} \times \int_{t_1}^{t_2} C_m(d_m, t) \, dt
\]

(Assumes equilibrium between skin surface and material surface)

Transfer via dust ingestion:

\[
TF_{\text{dust ingestion}}^{\text{product} \rightarrow \text{GI tract}} = \frac{1}{m_0} \times f_{\text{home}} \times f_{\text{dust,ingested}} \times \frac{IR_{\text{ing}}}{K_{md} \times \rho_{\text{dust}}} \times \int_{t_1}^{t_2} C_m(d_m, t) \, dt
\]

(Assumes dust ingested is related to hand contact frequency)

USEtox overall framework and interpretation
**USEtox Impact Pathway Framework: Ecotoxicity**

- **Ecotoxicological effect factor matrix** $EF_{eco}$ [PAF m$^3$/kg]:
- **Midpoint ecotox characterization factor matrix** $CF_{eco}$ [PAF m$^3$/kg emitted]:
- **Endpoint ecotox characterization factor matrix** $CF_{eco}$ [PDF m$^3$/kg emitted]:

---

**EF_{eco}**

<table>
<thead>
<tr>
<th>Emission compartment</th>
<th>freshwaat</th>
<th>occ util</th>
<th>attU</th>
<th>attC</th>
<th>fl waterC</th>
<th>sea waterC</th>
<th>net solC</th>
<th>agr solC</th>
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<tbody>
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<td>0</td>
<td>1.46</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<tr>
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**CF_{eco}**

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Uncertainty, variation, and discerning power

• Uncertainties are important for interpretation and typically capture only precision when quantified, not accuracy
• Comparing uncertainties of CFs from different impact categories? Consider how much of the impact pathway they capture
• Toxicity impacts can be caused by 1000’s of substances
• Overall variation of CFs from most to least toxic substances ranges 11-20 orders of magnitude with uncertainties in the range of 2 to 4 orders of magnitude
• Discerning power of toxicity CFs still meaningful and comparable to other impact categories
Key Information of USEtox

- Initial model differences were considerably reduced by harmonisation, as their sources were identified.
- Relative accuracy of the new CFs is within a factor of
  - $100-1’000$ for human health
  - $10-100$ for freshwater ecotoxicity
  - compared to 12 orders of magnitude variation between CFs
- USEtox falls within range of the other models, emulating their results, but avoiding their complexity and their pitfalls.
- Characterisation factors are available for:
  - Human toxicity: $1’000$ recommended + $100$ indicative CFs (= $1’100$ substances covered)
  - Ecotoxicity: $1’184$ recommended + $1’335$ indicative CFs (= $2’519$ substances covered)
How to interpret and apply USEtox CFs in LCA

- Always show and compare toxicity scores in log-scale
- Always include **ALL** available characterization factors including “indicative” – consider higher uncertainty
- Identify **10-20** most contributing substances
- Ignore the ranking among them
- Identify most contributing processes
- Check sensitivity of conclusions to choice of LCIA model

http://doi.org/10.1007/s11367-021-01889-y
USEtox Deliverables and publications: Further Reading

- Rosenbaum et al. (2008) → general model
- Hauschild et al. (2008) → consensus process
- Henderson et al. (2011) → ecotoxicity
- Rosenbaum et al. (2011) → human toxicity
- Special issue ‘LCIA of impacts on human health and ecosystems’
- Rosenbaum et al. (2015) → indoor settings
- Westh et al. (2015) → user requirements survey
- Fantke et al. (2021) → near-field/far-field model

- USEtox is used by U.S. EPA for screening of chemicals
- USEtox is recommended by the EC for PEF and by ILCD
- USEtox is endorsed by the UNEP/SETAC Life Cycle Initiative
USEtox future development: UNEP GLAM

• 1992-1999 SETAC LCIA working groups (Society for environmental toxicology chemistry): Assessment framework → LCIA ISO recommendations

• 1999: contacted UNEP → 2 weeks in Paris
  2002 Launch of the UNEP-SETAC Life cycle Initiative!


• 2012-2019 GLAM Phase 1 & 2: Consensus finding for environmental assessment indicators and methods in multiple impact categories → Pellston workshop™ 1 (January 2016) & 2 (June 2018, Valencia)

• 2019-2023 Phase 3: Dissemination and stewardship
  Creation of a Global LCIA method
  https://www.lifecycleinitiative.org/applying-lca/lcia-cf/