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~120 Courses
~100 Instructors
70% PhDs or ScDs
97% have advanced degrees, including ALMs, FAIAs, JDs, MAs, MBAs, MEAs, MDs, MSJs, MPAs.

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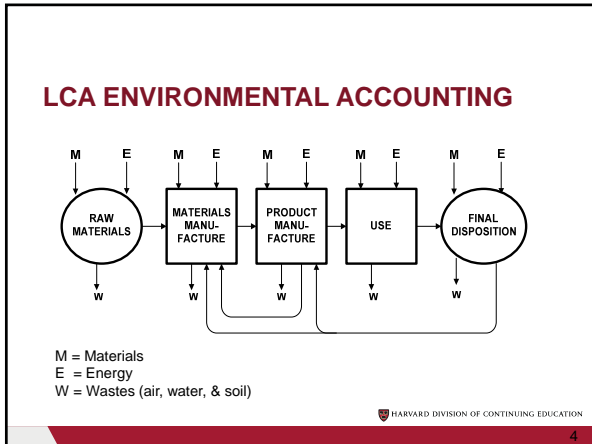
Key Learning Outcomes

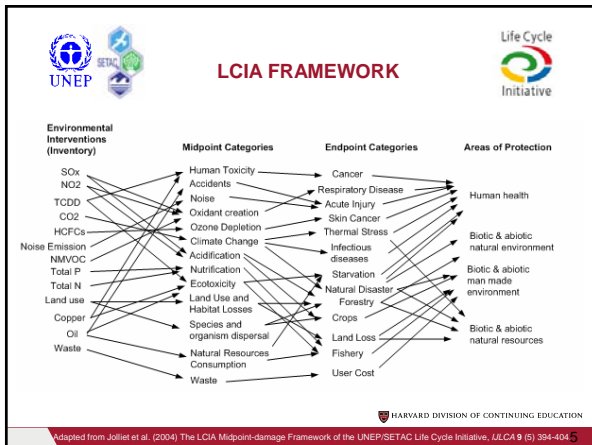


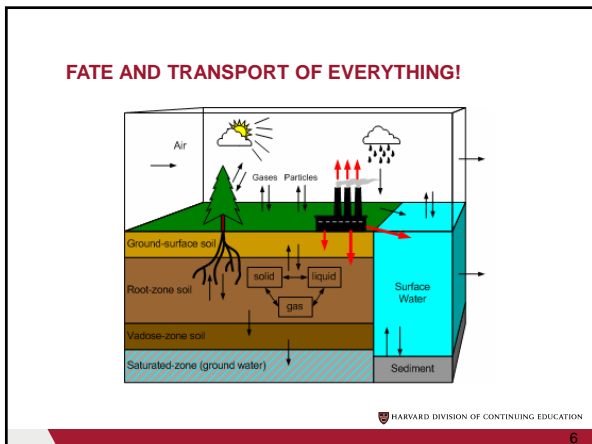
General understanding of:

- Approach to Life Cycle Impact Assessment (LCIA)
- Current Practice – USEtox
- Recent advancements - CLiCC
- Q & A

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MAPPING THE UNIVERSE!

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Princeton University; Sloan Digital Sky Survey www.sdss3.org

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IMPACT ASSESSMENT

Life Cycle Inventory	Classification	GWP Characterization (CO ₂ -e)	Human Health Toxicity (PAP.mg.day / kg emitted)	Ecological Toxicity (PAP.mg.day / kg emitted)
Resources		CO ₂ : 1		
XXX		CO ₂ : 1.53		
Airborne Emissions		CH ₄ : 28		
Carbon Dioxide		N ₂ O: 265		
Carbon Monoxide		CO ₂ : 1,730		
Methane		SF ₆ : 23,500		
Nitrous Oxide			CH ₄ : 2.11E-06	
Carbon Tetrachloride			CH ₄ : 2.09E-07	
Sulfur Hexafluoride			CH ₄ : 3.26E-09	
Benzene			CH ₄ : 3.80E-09	
Toluene				CO ₂ : 6.54E+01
Xylene				CH ₄ : 6.60E+01
XXX				CH ₄ : 5.69E+01
XXX				CH ₄ : 7.74E+01
Waterborne Emissions				
XXX				
XXX				
Soil Emissions				
XXX				

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STORY OF USETOX

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Westh et al. (2015) The USEtox story: a survey of model developer visions and user requirements. *ULCA* 20:299-310.

USETOX FRAMEWORK

FIGURE 3 Life cycle inventories systematically evaluate the relative impacts of chemical releases by modeling the fate of chemicals in air, water, and soil and their potential toxic effects on humans and other living organisms.

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Hauschild (2008) Building a Model Based on Scientific Consensus for Life Cycle Impact Assessment of Chemicals: The Search for Harmony and Consensus. ES&T 40:7032-7037

USETOX FRAMEWORK

Model component	Key factor	Parameter value (P) or algorithm choice (A)
Fate	Advection as a loss mechanism in some models	A
	Inclusion of the intermittent character of rain	A
	Residence times of media, particularly marine water, differ greatly	P
	Different algorithms used for estimation of partition coefficients	A
	Modeling of soil compartment: (i) homogeneous versus vertically layered soil compartment and (ii) generic versus division between agricultural, industrial and natural soils	A
Human exposure	Urban air compartment nested within continental air compartment	A
	Difference in population density on the urban and rural scale	P
	Different algorithms used for estimation of bio-transfer and bio-concentration factors (fish, meat, milk, vegetation)	A
Human toxic effects	Some models extrapolate between intake routes (inhalation, ingestion, dermal)	A
	Models use different effect indicators (TD ₅₀ , AD ₅₀ , TD ₁₀)	P
Ecosystem effects	Models use different effect indicators (PNEC, HC50)	P
	Oceans modelled as a sink only (no effects considered)	A
	Some models use acute ecotoxicity indicator	P

FIGURE 3 Life cycle inventories systematically evaluate the relative impacts of chemical releases by modeling the fate of chemicals in air, water, and soil and their potential toxic effects on humans and other living organisms.

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NESTED TRANSBOUNDARY MODEL

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<http://www.usetox.org/>

USETOX ACCEPTANCE & V.2 UPDATE

- Covers 3000+ ecotox and 1000+ HH Tox
- Endorsed by UNEP SETAC
- EC International Reference Life Cycle Data System
- US EPA TRACI Methodology
- Added for V2.1:
 - Residential and occupational indoor environments
 - Ionizing organic chemicals
 - Exposure to pesticides via food crop consumption
 - Generic freshwater ecotoxicity for metals
 - Continent (8) and sub-continent (17) specific landscape parameters

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USETox 2.0 Documentation v1

UNCERTAINTY & INTERPRETATION

- Characterization factors vary by 10^{15} magnitude
- Contributions of 1%, 5%, or 90% considered equal
- Very useful to identify the top 10 or 20 chemicals
- Chemicals contribution $> 1/1000^{\text{th}}$ to the total score
- "It is better to be vaguely right than exactly wrong" (Read 1920)

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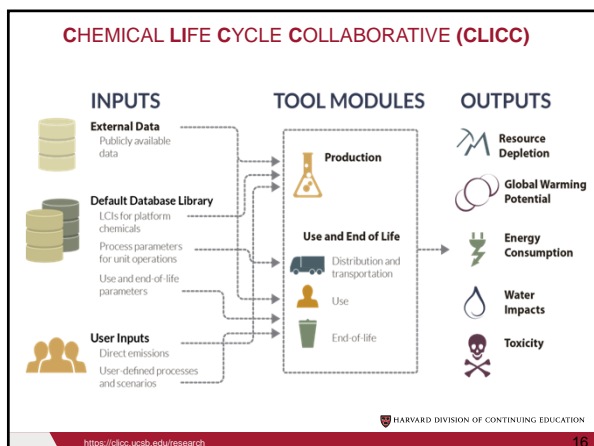
USETox 2.0 Documentation v1 & Read, C. (1920) Logic: Deductive and Inductive

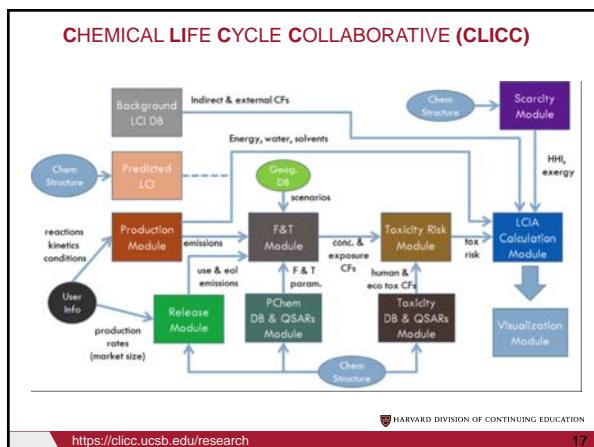
REGISTERED CHEMICALS CONTINUE TO GROW

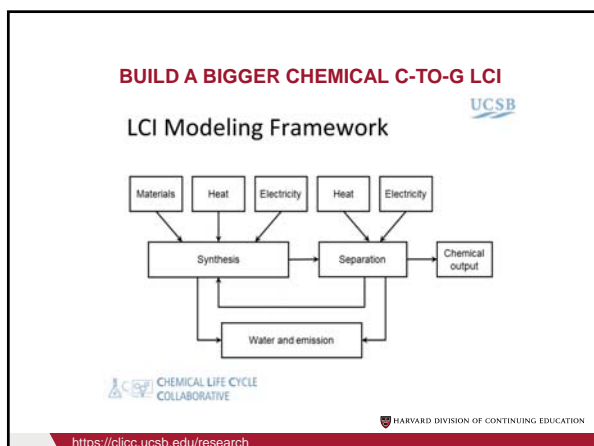
~15,000 Chemicals per day

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<http://www.cas.org/news/media-releases/100-millionth-substance>








BUILD A BIGGER CHEMICAL C-TO-G LCI

UCSB

Link to Cradle-to-Gate LCI

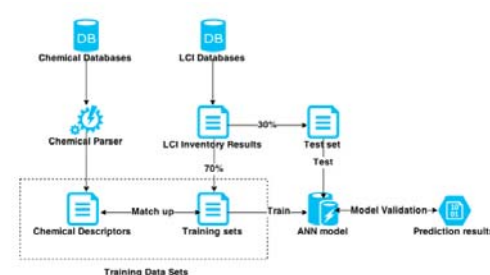
- Users would only able to input **unit process information**.
- We build a background database to generate chemical LCI.
- More than **1,000 common chemicals** unit process information are collected and linked.
- Cutted off at basic "building block" chemicals where we have accurate LCI.
- LCIs are calculated under **three different scenarios** according to user's inputs.



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https://clicc.ucsb.edu/sites/clicc.ucsb.edu/files/assets/2016_clicc_webinar_1.pdf

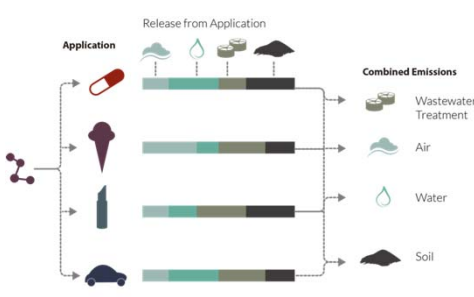
PREDICTIVE LIFE CYCLE INVENTORY MODULE



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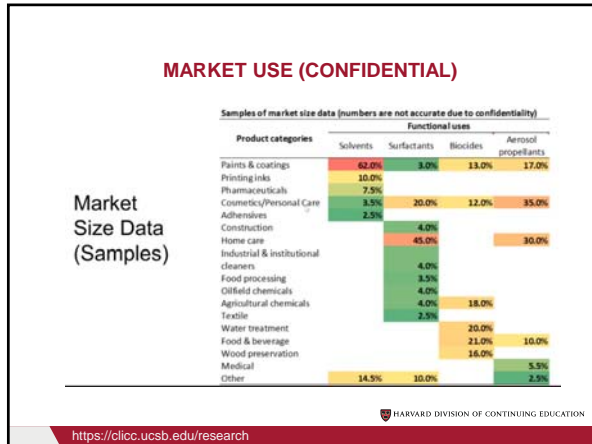
<https://clicc.ucsb.edu/research>

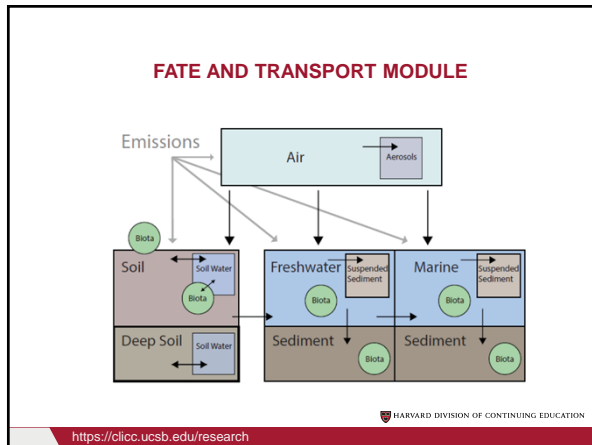
CHEMICAL RELEASE MODULE



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<https://clicc.ucsb.edu/research>





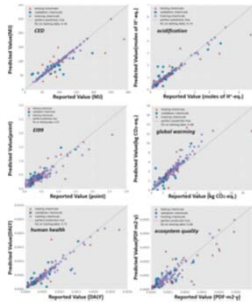
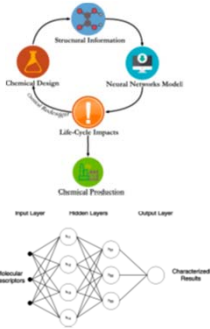
FATE AND TRANSPORT MODULE

CLICC Fate & Transport Model	Other Models
<ul style="list-style-type: none"> • Mass balance model <ul style="list-style-type: none"> – Non-steady state model 	<ul style="list-style-type: none"> • Steady-state
<ul style="list-style-type: none"> • Predicts time-dependent <u>daily</u> concentrations 	<ul style="list-style-type: none"> • Output is average value at steady state
<ul style="list-style-type: none"> • Uses regionally specific climate data 	<ul style="list-style-type: none"> • Low resolution
<ul style="list-style-type: none"> • Release scenario is fully customizable 	<ul style="list-style-type: none"> • Rigid structure

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<https://clicc.ucsb.edu/research>

RAPID LCIA SCREENING – ARTIFICIAL NEURAL NETWORKS



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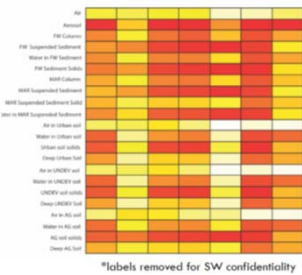
EXAMPLE OUTPUT

Average Chemical Concentration in the U.S. (kg/m³)

Average Concentration in the U.S. (kg/m³)

Average Concentration in the U.S. Region of chemicals in environmental compartments. Values are calculated as the average concentration of a chemical across six locations: Los Angeles, CA; San Francisco, CA; Salem, OR; New York City; St. Louis, Missouri, IL.

PM: Particulate Matter; MMB: Methylmercury; URBAN: Urban; SW: Surface Water; UNINVESTIGATED SW: Uninvestigated Surface Water; Agricultural SW: Agricultural Surface Water.

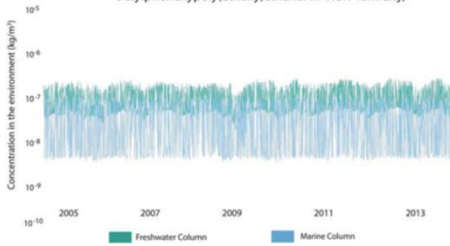


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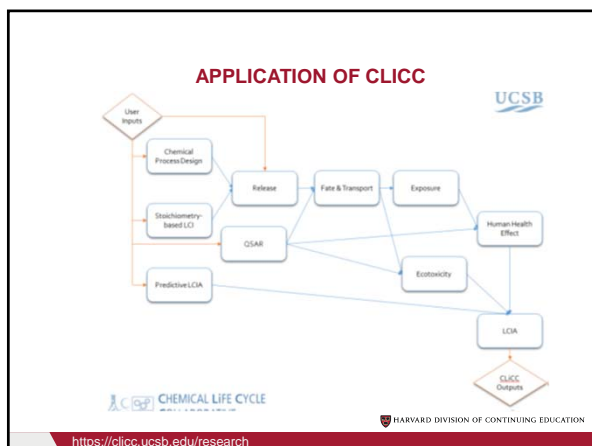
EXAMPLE OUTPUT

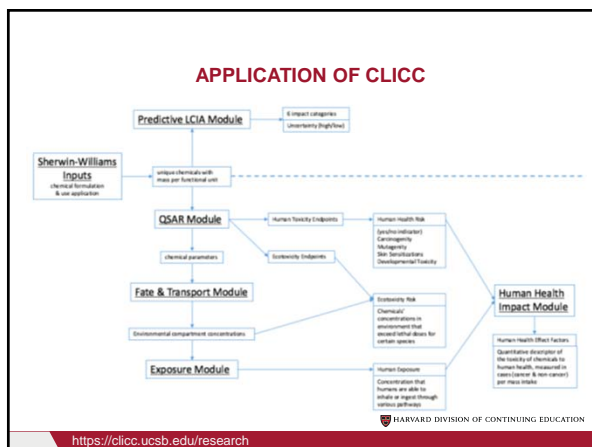
Daily concentration of Octylphenoxypoly(ethoxy)ethanol in New York City.



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<https://clicc.ucsb.edu/research>





SUMMARY

- USEtox most widely used toxicity model in LCA
 - Consensus approach
 - Continue to update
- Growing number of chemicals
 - Lack of CtG information
 - Lack of LCIA CF information
- CLiCC
 - Advancing LCI coverage
 - Dynamic Fate and Transport model
 - Advancing LCIA coverage (not just tox)
 - Imbedding uncertainty & sensitivity

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