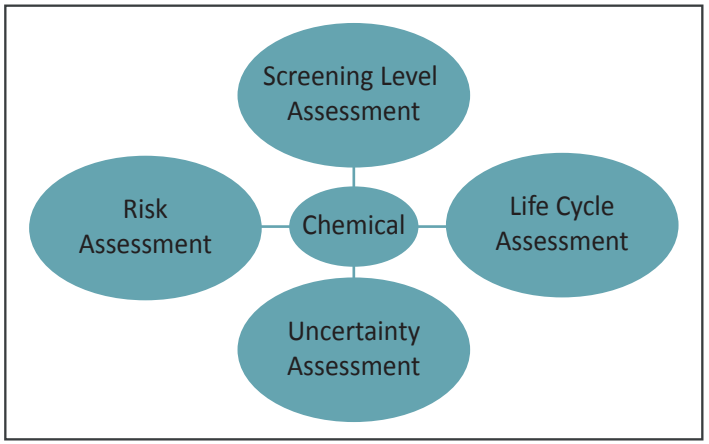
Chemical Life Cycle Collaborative

Introduction to CLiCC

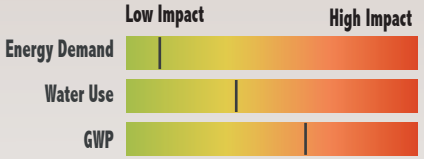
The Chemical Life Cycle Collaborative (CLiCC) Tool is a suite of models that performs early assessment of the life cycle impacts of novel chemicals and materials. The CLiCC Tool can also be used to fill-in data gaps in the prediction of life cycle impacts for existing chemicals with large data gaps or new chemicals with no available data. The CLiCC Tool is composed of four distinctive goals that address the different needs of a user: 1) Screening Level Assessment, 2) Life Cycle Assessment, 3) Risk Assessment, and 4) Uncertainty Assessment. They can be used either independently for specific purposes or together to gain a more holistic view.

The CLiCC Tool is designed with the purpose of providing rapid assessments with minimum *a priori* information on chemicals to face the challenge of the ever increasing number of chemicals used in our society. Nevertheless, customizations on numerous input parameters are available for more sophisticated users wishing to adapt the tools for more specific scenarios. The tools are based on state-of-the-art science, in support of early decision-making, but more detailed work may be needed for regulatory or compliance purposes.



Screening Level Assessment

Select a chemical and generate predicted impact scores relative to other chemicals using the ***Screening Level Scorecard***.



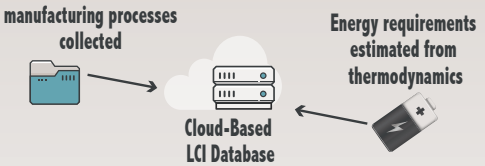
Safety Data Sheet (SDS) support is provided for parameters related to Section 9 (physical and chemical properties), Section 11 (toxicological information), and Section 12 (ecological information).

More than 60 ***Chemical Properties*** are available, including physico-chemical properties, waste water treatment efficiency, and human and ecological toxicity. Data are collected from publicly available databases and/or predicted using QSAR models.

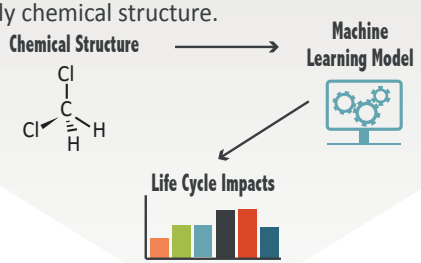
Methylene Chloride → List of available experimental and predicted properties

Life Cycle Assessment

CLiCC has developed one of the largest ***Life Cycle Inventory*** databases available for organic chemicals using stoichiometry and thermodynamics to complete predictions. These results are fully customizable.

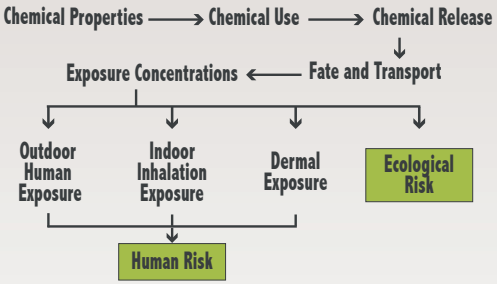


Machine learning techniques are used to estimate the ***Life Cycle Impacts*** of organic chemicals at a screening level. The Artificial Neural Networks models can predict up to six impact categories for the input chemical, using only chemical structure.



Risk Assessment

Risk assessment is designed to estimated potential human and ecological health implications from using chemicals is various products. CLiCC provides access to data and predictive models that allow for rapid assessment. The CLiCC risk assessment section can be customized to allow a more detailed analysis than the more general LCA tools.

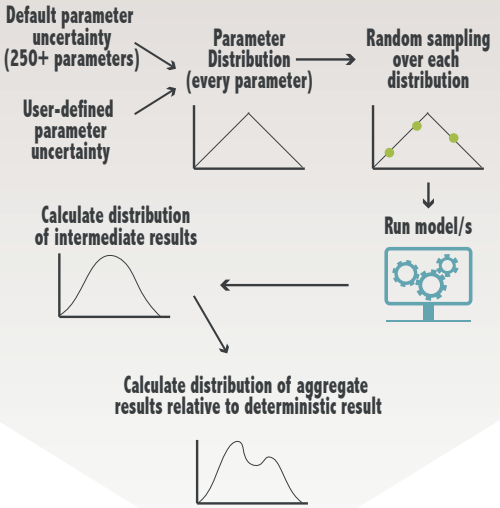


Risk quantification includes both cancer and non-cancer human risk and ecological risk.

Quantified Risk

Uncertainty Assessment

While basic uncertainty is associated with all results in the previous tools, CLiCC also provides access to an ***Extended Uncertainty Analysis*** that uses a Monte Carlo Simulation method to aggregate uncertainty for the Life Cycle Impact Assessment and the entire Risk Assessment tool.



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