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## From Incremental to Fundamental Chemical Substitution: Addressing the Lock-In Problem

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# ABSTRACT BOOK



**BUZZING WITH SCIENCE**  
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methodologies for completing AAs according three separate frameworks: sequential, simultaneous, and hybrid. In order to evaluate the effectiveness of the Guide, the Washington Dept. of Ecology funded a project to conduct AAs using each framework described in the IC2 Guide. The primary objective of this project was to evaluate the IC2 Guide and provide feedback on usability and recommendations for improvements, but a secondary objective was to develop a basis for a future assessment of alternatives to copper anti-fouling paint, which is scheduled to be phased out in WA by 2020. Under Task 1 of the project, ToxServices conducted GreenScreen® Chemical Hazard Assessments to create a Uniform Data Set (UDS) depicting hazards posed by individual chemicals in paint formulations identified in reports by CalEPA and USEPA. Under Tasks 2-4, a team led by ToxServices (ToxServices, Massachusetts Toxics Use Reduction Institute (TURI), and Abt Associates) completed three independent AAs using each framework described in the IC2 Guide and referring only to the common UDS and performance, cost/availability, and exposure data drawn from the CalEPA and USEPA reports. Under Task 5 of the project, the organizations met to share results and challenges and collaborated to offer recommendations for improving the IC2 Guide. While the organizations came to similar conclusions following the performance, cost/availability, and exposure assessment modules, implementation of the hazard module required additional decision-making rules and approaches varied by assessor. In addition, each assessor handed data gaps differently, which lead to different outcomes between the frameworks. The report for this project discusses shared challenges encountered by assessors, including a lack of guidance on decision-making strategies and how to interpret hazard data, address incomplete formulations, and conduct a product-level AA. It also describes module and framework-level challenges and recommendations to improve readability of the IC2 Guide. While using the IC2 Guide requires some expertise, it is valuable and flexible resource that meets the needs of a range of users.

#### **425 From Incremental to Fundamental Chemical Substitution: Addressing the Lock-In Problem**

*M. Scheringer, Leuphana Univ of Lüneburg; P. Fantke, Technical Univ of Denmark / Quantitative Sustainability Assessment Division; R. Weber, POPs Environmental Consulting*

Large-scale screening studies have shown that there may be hundreds of chemicals with hazardous properties among the several tens of thousands of chemicals in commercial use. Hence, several chemicals in consumer products are subject to binding or voluntary phase-out agreements. To facilitate an actual phase-out process, alternatives assessment is commonly applied as emerging approach to identify potential chemical and non-chemical alternatives serving as substitutes. However, there are different challenges in assessing and evaluating chemical alternatives. These challenges are mainly related to similarity in chemical structures and, hence, similar hazard profiles between phase-out and substitute chemicals, leading to a rather incremental than fundamental substitution. Further challenges are related to a hampered phase-out process and the lack of implementing Green Chemistry principles in chemicals design and lack of Sustainable Chemistry aspects in industrial processes design. We illustrate the various aspects and challenges of the phase-out agreement process and of the process of assessing and evaluating alternatives with focus on chemical-by-chemical substitution as currently the most widely applied option in alternatives assessment of hazardous chemicals. We discuss in which cases the problem of incremental substitution is likely to occur and how to strive toward more fundamental changes in chemical structures without the risk of burden shifting to facilitate a successful substitution of hazardous chemicals in consumer products. We explored possible solutions to address the various challenges in chemical substitution and propose an integrated approach of all stakeholders involved toward more fundamental and function-based substitution by greener and more sustainable chemicals and non-chemical alternatives. For hazardous chemicals for which (currently) no alternatives exist, we propose that an adequate end-of-life management is ensured. Our recommendations finally constitute a starting point for identifying further research needs and for improving current alternatives assessment practice.

#### **426 Methylene Chloride Paint Strippers Alternatives Analysis: Hazard Screening Using GreenScreen® for Safer Chemicals**

*B. Wang, ToxServices LLC; M. Jacobs, Univ of Massachusetts Lowell / Lowell Center for Sustainable Production; M. Rossi, Clean Production Action*

Methylene chloride-containing paint or varnish strippers are listed as one of the three Priority Products proposed by California's Dept of Toxic Substances Control (DTSC) that require alternatives analysis (AA) to inform rule-making that leads to elimination/reduction of exposure. The BizNGO Alternatives Assessment Working Group conducted a demonstration project of the first stage of the AA required by the CA Safer Consumer Product Regulations to identify potential alternatives and to evaluate challenges with compliance to the Regulation. Twelve alternative paint stripper chemicals were identified, including ten solvents, one acid and one base. Initial hazard assessment of these alternatives along with methylene chloride were achieved with the GreenScreen® for Safer Chemicals tool, which is a chemical hazard assessment methodology that is built on the 12 Principles of Green Chemistry and USEPA's Design for the Environment (DfE) alternatives assessment method. It evaluates eighteen endpoints covering human health, environmental toxicity and fate and physical hazards based primarily on criteria set forth in Globally Harmonized System of Classification and Labelling of Chemicals (GHS). The GreenScreen® assessments for two of the chemicals are publicly available through the Interstate Chemicals Clearinghouse (IC2) hazard assessment database and ToxServices evaluated the rest of these alternatives. Although these chemicals are "data-rich", many of them lack data on critical human health and/or environmental toxicity and fate endpoints. ToxServices used a variety of SAR and QSAR tools to fill the data gaps or to produce supportive evidence in hazard assignments. Two alternatives, methanol and toluene are GreenScreen Benchmark™ 1 chemicals ("Avoid – Chemicals of High Concern") along with methylene chloride based primarily on their carcinogenicity, reproductive toxicity and/or developmental toxicities. Therefore, these chemicals are excluded from further analyses. The Benchmark scores for most of the other chemicals are 2 ("Use but Search for Safer Substitutes"). DMSO has the highest Benchmark score of 3 ("Use but Still Opportunity for Improvement"). However, it is known to promote the dermal absorption of other substances, and this should be considered in the AA. Although limitations exist, GreenScreen® is in general a useful tool in AA for assessors with and without extensive knowledge in toxicology.

#### **427 Multi-Criteria Decision Analysis methods as a framework for comparative risk assessment and in the case of insecticide use in pome fruit production**

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Selection among multiple alternatives often involves a trade-off among risks as well as benefits. The pesticides used in pome fruit production are an illustrative example of a system of alternatives. The registration withdrawal of one previously popular chemical, azinphos methyl, contributed to recent disruptions of this system. The currently available insecticides for codling moth control belong to many different chemical classes and occupational exposures to them may be associated with a variety of potential health impacts, as assessed by a battery of toxicological studies performed during registration. The selection criteria that drive the use of each pesticide vary among available alternatives, and there are a number of environmental and situational constraints on the selection. This pest control system is therefore a good candidate for the use of decision analysis methods in the estimation of relative popularity of insecticide classes and for the quantification of risk-benefit tradeoffs between pesticide alternatives. Interviews were conducted with crop protection specialists involved in the recommendation of pesticides for codling moth in central Washington. In these interviews, the criteria and limiting factors important to pesticide choice were discussed and assigned weights, and preference thresholds were explored for each criterion. The specialists were also asked to assign relative values to the