QSAR TOOLS IN ENVIRONMENTAL ANALYSIS FOR THE SEMICONDUCTOR INDUSTRY

Sarah Boyd
Sponsored by: UC Berkeley Toxic Substances Research and Teaching Program

ABSTRACT

Semiconductor manufacturing and process design is driven to change rapidly by technology demands and competition. Incorporating environmental considerations into this process requires decision tools which will generate environmental analyses in as short a turn-around as possible. The predictive capability of QSAR methods are investigated and U.S. government QSAR software tools are surveyed for their applicability to environmental decision analysis in semiconductor equipment design.

PROBLEM STATEMENT

Pollution prevention and environmental decision-making is particularly difficult in the case of semiconductor manufacturing because the decision-space for manufacturing choices is limited, and the stakeholders and decisions are distributed over time and space. Chemical suppliers perform fundamental research in the early stages of process design, and restrict the material options of equipment designers. Equipment suppliers, in turn, design process machinery around these chemicals which determine the options of semiconductor designers and manufacturers.

In order to best incorporate environmental considerations into this design process, impact metrics for process and material options should be applied as early in the decision chain as possible, in this case at the point of chemical and equipment manufacturers who perform basic research on semiconductor process design. With regard to these demands, data on chemicals must be aggregated as quickly as possible.

INVESTIGATION

In current practice, the results of acute toxicological bioassays are used to create a human health impact metric for environmental decision support in semiconductor equipment design (Thurwachter, 2000; Krishnan, 2003). However, in many cases, toxicological endpoints for process chemicals have not yet been determined. Of 110 standard semiconductor chemicals surveyed, only 38 are profiled in RTECs, and 17 in IRIS. Basic chemical descriptors are not required for permission to manufacture or import a new chemical, as regulated by the EPA. Only 19 of this representative are tracked through the EPA's High Production Volume chemical management system, and are subject to bi-annual review through the Inventory Update Rule.

Quantitative structure activity techniques are notable as a tool for prediction of human toxicity and environmental fate, as QSAR results are immediate, as compared to results from bioassays. QSAR tools are used routinely by numerous government agencies to manage chemicals and direct chemical policy in the absence of toxicological data and chemical descriptors such as octcanol-water coefficient, boiling point, or solubility. EPA-developed QSAR tools are investigated because, in addition to being publicly available, they are subject to public review and criticism.

CONCLUSION

ECOSAR is determined to be the best available QSAR tool in terms of predictability, applicability, size of domain, and ease of integration through software with current environmental analysis tools.

REFERENCES

Thurwachter, S. (2000), "Environmental Value Analysis: Evaluating Manufacturing Product and Process Design Trade-Offs," Dissertation, University of California, Berkeley, Spring 2000.

Krishnan, N. (2003), “Design for Environment (DFE) in Semiconductor Manufacturing,” Dissertation, University of California Berkeley, Spring 2003.