

MODELING APPROACHES FOR NANOMANUFACTURING RISK ASSESSMENT



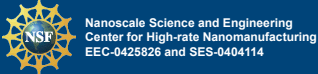
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QPL

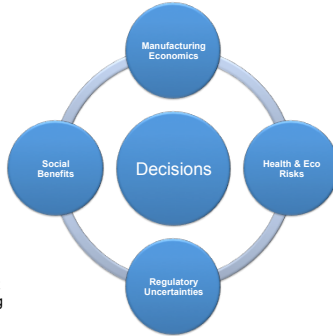
Quality & Productivity Laboratory



BACKGROUND

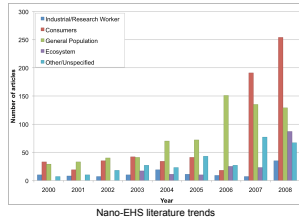
Problem

- High commercialization of nanotechnology in numerous application areas ranging from medicine to electronics
- Uncertainty exists in:
 - Environmental, health and safety (EHS) risks of nanotechnology
 - Full-scale nanomanufacturing economics
 - Possible future regulatory standards
- Risk – benefit tradeoff assessment difficult given limited understanding of possible risks



Significance

- Growing nano-EHS concerns – published studies have increased 600% since 2000
- Until sufficient EHS data become available, a great need exists to help inform decision making under uncertainty for a wide range of industrial / commercial applications and nanomanufacturing processes



Approach

- Identified and piloted most promising modeling approaches for nanotechnology risk assessment

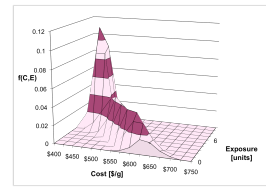
Method	Advantages & Disadvantages	Contexts
Monte Carlo simulation	+ Allows modeling uncertainty – No tradeoff framework	Random sampling for output distribution
Multi-criteria decision making	+ Tradeoff frontiers – Deterministic	Tradeoff or compromise solutions
Stochastic programming	+ Allows stochastic parameters – Computational time	Probabilistic constraints or objectives
Desirability	+ Can compare discrete alternatives, robust – Abstract approach, arbitrary weights	Balance weighted total multi-criteria

- Monte Carlo models were developed to assess cost-exposure trade-offs in high pressure carbon monoxide (HiPCo) processes
- Goal programming was applied to a multi-criteria optimization problem to balance three criteria in a nanomanufacturing process – reliability, throughput, and workplace exposure
- Stochastic programming models were developed to minimize cost while meeting exposure, reliability, and throughput targets with set probabilities of a nanomanufacturing process
- Desirability functions were used to balance weighted total multi-criteria for selection among nanotechnology laboratory equipment and fume hood design

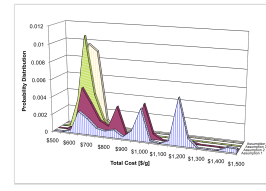
MODELING APPROACHES

Monte Carlo Models

- Inherent tradeoffs between HiPCo production cost and exposure and multi-modality in total cost function
- High amount of uncertainty in costs, exposure, dose response, and regulatory environments translates to excessive variability in output with overlapping distributions



Example of joint HiPCo cost-exposure density



Example of probability distribution of total (manufacturing & exposure) cost for 4 EHS scenarios

Multi-criteria Models

- Many multi-criteria methods available that are applicable to a wide range of nanomanufacturing applications
- Goal programming example:
 - Objective: To minimize deviations from set goals for reliability, production rate, and workplace exposure
 - Decision variables: pH (x_1), conductivity (x_2), temperature (x_3)

Problem formulation:

$$\text{lexmin} \{d_i^+, d_i^-\} \text{ is equivalent to}$$

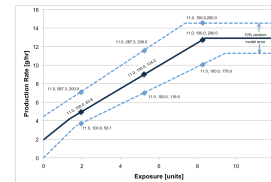
$$\text{min } Md_i^+ + Sd_i^- + 3d_i^-$$

$$\text{s.t. } 0.098x_1 + 0.00014x_2 - 0.0004x_3 + d_1^+ \geq 90\%$$

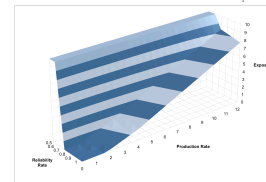
$$0.27x_1 - 0.0167x_2 + 0.058x_3 + d_1^- \geq 10$$

$$-0.01x_2 + 0.047x_3 - d_2^+ \leq 5$$

$$7 \leq x_1 \leq 11, 100 \leq x_2 \leq 1000, 50 \leq x_3 \leq 200 \text{ all } d_i \geq 0$$



Examples of optimal tradeoff frontiers/surfaces for exposure, yield, throughput



Stochastic Programming

Chance-constrained Models

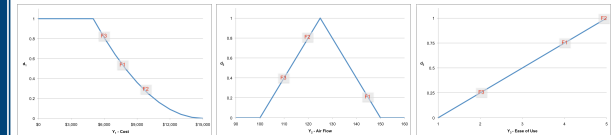
- Objective: Minimize cost while satisfying reliability, production rate, and workplace exposure constraints with some specified probability
- Decision variables: pH (x_1), conductivity (x_2), temperature (x_3), occupational health protection level (x_4)
- Problem formulation: Minimize $\$6.5x_1 + \$0.7x_2 + \$3.25x_3 + \$10x_4$
 - subject to $P(0.137x_1 + 0.007x_2 - 0.0023x_3 + 0.033x_4 \geq 60\%) \geq 0.95$
 - $P(1.82x_1 - 2.34x_2 + 7.1x_3 - 1x_4 \geq 10) \geq 0.90$
 - $P(0.94x_1 - 0.0043x_2 + 0.13x_3 - 10x_4 \leq 2) \geq 0.95$
 - $7 \leq x_1 \leq 11, 100 \leq x_2 \leq 1000, 50 \leq x_3 \leq 200, 1 \leq x_4 \leq 4$
 - $x_1, x_2, x_3, x_4 \geq 0$, and x_4 integer
- Optimal solution: x_1 (pH) = 11, x_2 (conductivity) = 292.5, x_3 (temperature) = 97.9, x_4 (occupational health protection level) = 3, and Cost = \$624.57

Multi-period Recourse Models

- Objective: Minimize total expected costs (i.e., the cost of the first-stage decisions, x , and also the expected recourse cost of the second-stage problem)
- Model scenario:
 - First Stage
 - Second Stage (Levels 0-5)
- Optimal solution:
 - Cost = \$443.33
 - $x=3, y_{20}=0, y_{21}=0, y_{22}=0, y_{23}=0, y_{24}=1, y_{25}=2$

Desirability Functions

- Choose between a finite number of alternatives (e.g., fume hood selection) or identify the optimal settings of process variables (e.g., flow rate, hood height, solution concentration)
- Fume hood selection example:
 - Criteria: air flow (Y_1), cost (Y_2), and ease of use (Y_3)



Fume hood desirability curves for cost (left), air flow (center), ease of use (right)

Candidate Fume Hood	Individual Criteria and Desirabilities (d_i)			Overall Desirability D (w_1, w_2, w_3)		
	Cost	d_1	Effectiveness	d_2	Ease of Use	d_3
F1	\$7,500	0.56	145	0.2	4	0.75
F2	\$9,500	0.30	120	0.8	5	1
F3	\$6,000	0.81	110	0.4	2	0.25

CONCLUSIONS

- Inherent tradeoffs and enormous uncertainty exist for nanomanufacturing economics and workplace exposure
- Until sufficient toxicology and other studies progress, these type of risk assessment models can help decision-makers with the difficult task of identifying appropriate or optimal process design, equipment selection, and regulatory policy decisions
- Experimental design can be used to identify important model parameters and interactions

PUBLICATIONS

- Ok, Z. D., J. C. Benneyan, and J. A. Isaacs. (2008). "Risk Analysis Modeling of Production Costs and Occupational Health Exposure of Single-Wall Carbon Nanotube Manufacturing." *Journal of Industrial Ecology* 12(3): 411-434.
- Ok, Z. D., J. A. Isaacs, and J. C. Benneyan. (2008). Probabilistic and Monte Carlo Risk Models for Carbon Nanomaterial Production Processes. *IEEE International Symposium on Electronics and the Environment*, San Francisco, CA, United States: 1-6.
- Ok, Z. D., J. A. Isaacs, and J. C. Benneyan. (2008). Risk Analysis of Carbon Nanotube Production Processes Under Uncertain Occupational Health Risks and Regulatory Standards. *Industrial Engineering Research Conference*, Vancouver, BC, Canada: 1712-1717.
- Ok, Z. D., J. A. Isaacs, and J. C. Benneyan. (2008). Monte Carlo Multi-criteria Risk Analysis of Single Wall Carbon Nanotube Production Processes Under Uncertain Manufacturing Costs, Occupational Health Risks, and Regulatory Standards. *NSTI Nanotechnology Conference and Trade Show*, Boston, MA, United States. 2: 153-156.
- Ok, Z. D., J. C. Benneyan, and J. A. Isaacs. (2007). Modeling Production Costs for SWNT Manufacturing Given Uncertain Health and Safety Standards. *IEEE International Symposium on Electronics and the Environment*, Orlando, FL, United States: 85-90.