Module 6. Detailed design: Evaluation of maleic anhydride flowsheets

Green Engineering Short Course
Center for Environmentally Beneficially Catalysis
University of Kansas, Lawrence, KS
June 21-22 , 2004

David R. Shonnard
Associate Professor
Department of Chemical Engineering
Michigan Technological University

Presentation Outline

The last step for improving the environmental performance of a chemical process design is a detailed environmental impact assessment of a process flowsheet

- Pedagogical Approach - flowsheet Tier 3 assessment
  - » How to formulate environmental impact indicators
  - » How to "draw the boundaries" around the assessment - what to leave in - what to leave out
  - » A methodology to integrate emissions estimation, environmental fate and transport, and relative risk assessment
  - » Example application maleic anhydride production – comparison of benzene versus n-butane

Educational goals and topics covered in the module

Participants will:

- learn to apply a hierarchical approach to evaluate and improve the design of chemical processes
- use process diagnostic summary tables to identify pollution prevention opportunities

SCENE: A Software to integrate environmental and economic criteria with decision analysis

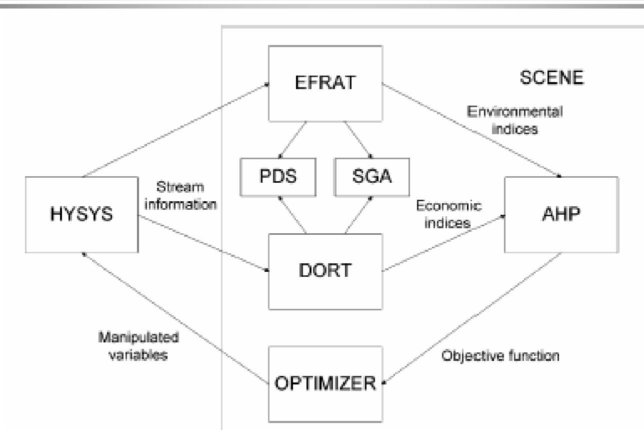
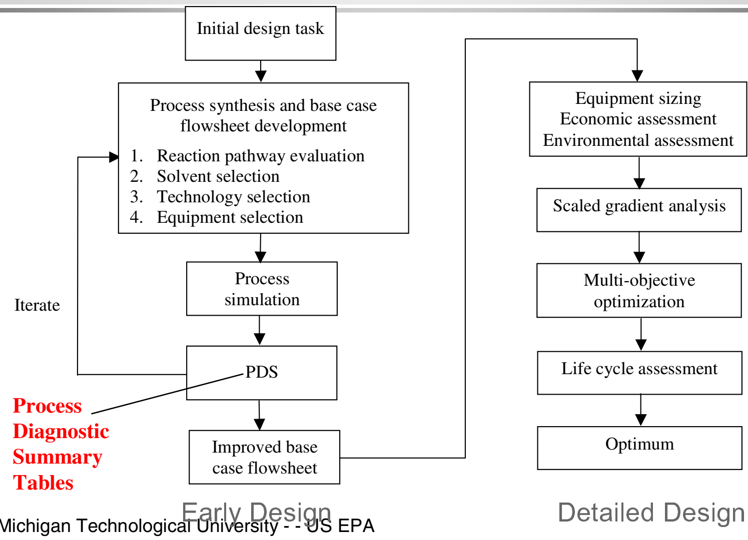


Figure 2. Structure of the software tool (SCENE).

*Chen, H. and Shonnard, D.R. Industrial and Engineering Chemistry Research, **43**, 535-552, 2004*

Early versus detailed design tasks

Chen, H., Rogers, T.N., Barna, B.A., Shonnard, D.R., *Environmental Progress*, 22(3), 147-160, 2003.

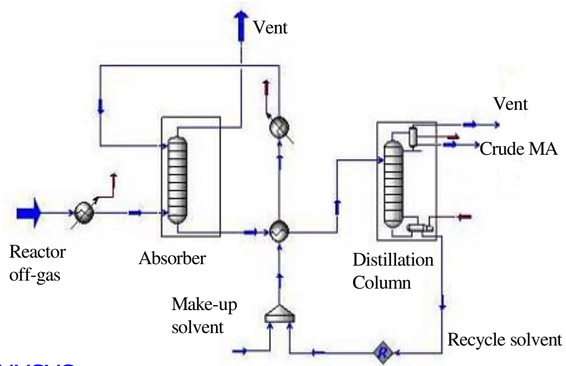


Case study: MA production

Level 3-8. Flowsheet Synthesis and Evaluation
"Tier 3" Environmental Impact Analysis

- Based on an initial process flowsheet created using "traditional" economic-based design *heuristics*.
- "tier 3" assessment
  - » Emissions estimation from units and fugitive sources
  - » Environmental fate and transport calculation
  - » Toxicity, other impact potentials, environmental fate and transport, and pollution control.

Absorber mass separating agent (MSA) for MA from n-C4



MA Data
b.p. 202°C

MSA
b.p. >222°C
m.p. < 35°C

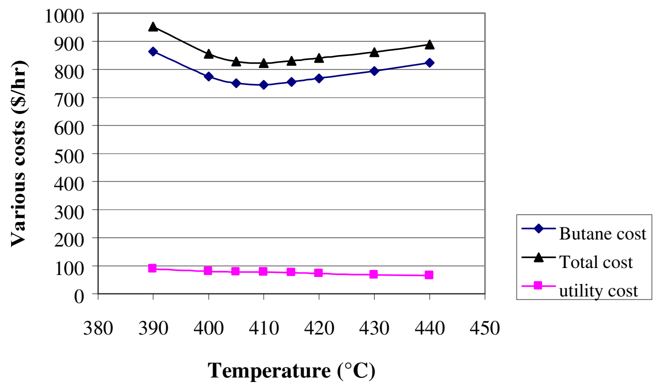
HYSYS
99% MA recovery in Absorber, 99.9% recovery of MA in distillation, 98% purity of MA.

Absorber mass separating agent (MSA) for MA from n-C4

	Benzene process			n-Butane process		
	TAC ($/yr)	I_{PC}	*AHP score*	*TAC* ($/yr)	I_{PC}	*AHP score*
Dibutyl phthalate	2.41E+06	6.59E-05	0.2319	2.80E+06	8.35E-05	0.4755
Dibutyl terephthalate	2.71E+06	1.41E-05	0.1636	3.12E+06	1.66E-05	0.1540
Dimethyl phthalate	2.12E+06	1.44E-05	0.5679	2.89E+06	2.13E-05	0.3244
Diisopropyl phthalate	3.00E+06	4.33E-04	0.0367	3.23E+06	5.08E-04	0.0461

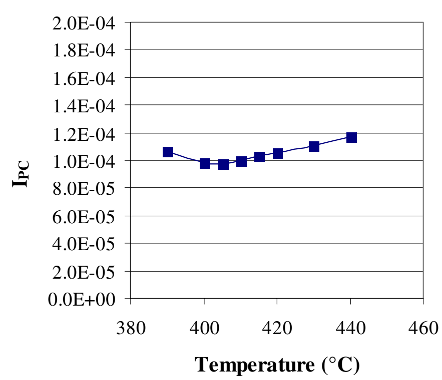
Chen, H., Environmental and Economic Assessments Applied to the Design and Optimization of Chemical Processes, Ph.D. Dissertation, MTU, 2002.

Simulation of Reactor temperature for MA from n-C4



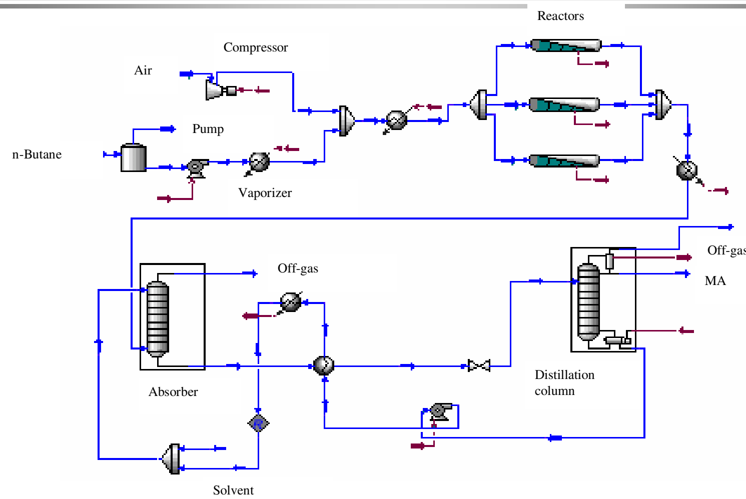
Chen, H., Environmental and Economic Assessments Applied to the Design and Optimization of Chemical Processes, Ph.D. Dissertation, MTU, 2002.

Simulation of Reactor temperature for MA from n-C4



Chen, H., Environmental and Economic Assessments Applied to the Design and Optimization of Chemical Processes, Ph.D. Dissertation, MTU, 2002.

Initial flowsheet for MA from n-C4



Process diagnostic summary tables: Energy input/output for nC4 process

Stream	Available temperature (In,Out)(°F)	Available Pressure (In,Out)(psia)	Energy flow (MM Btu/hr)	% of total energy
		Input		
Air	77	14.696	0.0000	0.00%
n-Butane	50	22.278	-0.0424	-0.11%
Make-up solvent	95	18.13	0.0004	0.00%
Solvent pump	472.87~472.96	1.2505~18.13	0.0107	0.03%
Air compressor	77~167.18	14.696~22.278	3.9588	9.92%
n-Butane vaporizer	50~50.004	22.278	1.0059	2.52%
Reactor feed heater	160.62~770	22.278	29.8800	74.90%
Reboiler	472.87	1.2505	5.0774	12.73%
Total			39.8908	100.00%
		Output		
Absorber off-gas	120.53	18.275	2.0033	1.80%
Distillation off-gas	95.043	0.3897	0.0002	0.00%
Crude MA	95.043	0.3897	0.0368	0.03%
Reactor 1	770		23.6340	21.29%
Reactor 2	770		23.6340	21.29%
Reactor 3	770		23.6340	21.29%
Reactor off-gas cooler	770~230	18.943	26.8940	24.23%
Solvent subcooler	234.95~95	18.13	7.1588	6.45%
Condenser	95.043	0.3897	4.0202	3.62%
Total			111.0153	100.00%

Process diagnostic summary tables: Manufacturing profit and loss, nC4

	Name	Total ($/yr)	% of total cost
Revenue			
	Maleic anhydride	21,258,236	100.00%
	Total Sales Revenue	**21,258,836**	**100.00%**
Manufacturing Expenses			
	Raw Materials		
	n-Butane cost	4,760,866	55.80%
	Make-up solvent	81,343	0.95%
	Utilities		
	Cooling water (tower)	159,913	1.87%
	Electricity (on site)	679,014	7.96%
	Steam (50 psig)	58,014	0.68%
	Steam (600 psig)	580,303	6.80%
	Natural gas	2,212,796	25.93%
	Total Manufacturing Expenses	**8,532,249**	**100.00%**

Process diagnostic summary tables: Environmental impacts, nC4

Normalization

$$I_N^k = \frac{I_k}{\hat{I}_k}$$

I_k — Process Index

$\hat{I}_k$ — National Index

Chemical	I_{FT}	I_{ING}	I_{INH}	I_{CING}	I_{CINH}	I_{OD}	I_{GW}	I_{SF}	I_{AR}
Sulfur dioxide	0.00E+00	0.00E+00	1.49E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.35E+02
TOC	1.36E-02	1.49E-02	6.62E+01	0.00E+00	0.00E+00	0.00E+00	4.11E+03	4.24E+02	0.00E+00
Carbon dioxide	4.36E+02	0.00E+00	8.91E+01	0.00E+00	0.00E+00	0.00E+00	6.09E+07	0.00E+00	0.00E+00
Carbon monoxide	1.90E-01	0.00E+00	1.65E+07	0.00E+00	0.00E+00	0.00E+00	2.33E+05	2.03E+03	0.00E+00
Dibutyl phthalate	7.70E+01	1.00E+02	3.01E+00	0.00E+00	0.00E+00	0.00E+00	2.56E+02	0.00E+00	0.00E+00
Maleic Anhydride	5.10E+02	7.27E+05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.49E+04	0.00E+00	0.00E+00
n-Butane	6.98E-02	0.00E+00	2.38E+05	0.00E+00	0.00E+00	0.00E+00	6.97E+04	0.00E+00	0.00E+00
Nitrogen dioxide	2.10E-01	0.00E+00	2.89E+03	0.00E+00	0.00E+00	0.00E+00	4.09E+06	0.00E+00	7.16E+04
Totals	1.02E+03	7.27E+05	1.67E+07	0.00E+00	0.00E+00	0.00E+00	6.54E+07	2.46E+03	7.17E+04
Contribution to I_{PC}	1.55%	0.34%	86.63%	0.00%	0.00%	0.00%	4.85%	0.14%	6.50%
I_{PC}	6.13E-04								

Process composite index

$$I_{PC} = \sum_k (I_N^k \times W_k)$$

Weighting Factors

global warming	2.5
ozone depletion	100
smog formation	2.5
acid rain	10
carcinogenic	5
noncarcinogenic	5
ecotoxicity	10

Source: Eco-Indicator 95 framework for life cycle assessment, Pre Consultants, http://www.pre.nl

Process diagnostic summary tables: Environmental impacts, nC4

By Emission Sources

Table 6. Risk Index of Each Emission Source for the *n*-Butane Process as Shown in Figure 4[a]

	n-butane tank	solvent tank	MA tank	reactors	*n*-butane vaporizer	feed heater	reboiler
I_{FT}	1.09×10^{-4}	6.46×10^{-7}	2.44	4.46×10^{2}	4.30	1.28×10^{2}	2.17×10^{1}
I_{ING}	0.00	8.40×10^{-7}	3.44×10^{3}	6.34×10^{5}	3.21×10^{-4}	9.54×10^{-3}	1.62×10^{-3}
I_{INH}	3.73×10^{2}	2.53×10^{-8}	3.01×10^{-2}	1.26×10^{6}	2.73×10^{4}	8.12×10^{5}	1.38×10^{5}
I_{CING}	0.00	0.00	0.00	0.00	0.00	0.00	0.00
I_{CINH}	0.00	0.00	0.00	0.00	0.00	0.00	0.00
I_{OD}	0.00	0.00	0.00	0.00	0.00	0.00	0.00
I_{GW}	1.09×10^{2}	2.15×10^{-6}	1.66×10^{2}	1.14×10^{5}	7.07×10^{5}	2.10×10^{7}	3.57×10^{6}
I_{SF}	0.00	0.00	3.59×10^{-6}	1.31×10^{2}	1.25×10^{1}	3.72×10^{2}	6.33×10^{1}
I_{AR}	0.00	0.00	0.00	0.00	1.86×10^{3}	5.52×10^{4}	9.40×10^{3}
I_{PC}	1.19×10^{-8}	6.00×10^{-15}	3.26×10^{-8}	4.60×10^{-5}	2.27×10^{-6}	6.73×10^{-5}	1.15×10^{-5}

[a] All values are in units of kg/year, excluding I_{PC}, which is unitless.

*Chen, H. and Shonnard, D.R. Industrial and Engineering Chemistry Research, **43**, 535-552, 2004*

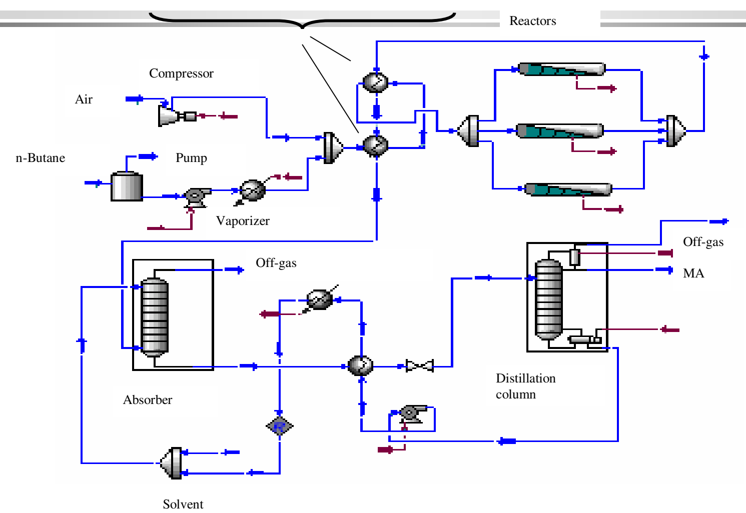
Process diagnostic summary tables: Environmental impacts, nC4

By Emission Sources (cont. from previous slide)

	solvent pump	air compressor	absorber	distillation	total
I_{FT}	1.22×10^{-1}	4.51×10^{1}	3.72×10^{2}	5.30	1.02×10^{3}
I_{ING}	9.13×10^{-6}	3.37×10^{-3}	8.20×10^{4}	7.03×10^{3}	7.27×10^{5}
I_{INH}	7.03×10^{2}	2.60×10^{5}	1.42×10^{7}	2.02×10^{3}	1.67×10^{7}
I_{CING}	0.00	0.00	0.00	0.00	0.00
I_{CINH}	0.00	0.00	0.00	0.00	0.00
I_{OD}	0.00	0.00	0.00	0.00	0.00
I_{GW}	1.79×10^{4}	6.59×10^{6}	3.33×10^{7}	5.13×10^{4}	6.54×10^{7}
I_{SF}	3.47×10^{-1}	1.28×10^{2}	1.75×10^{3}	2.49×10^{-1}	2.46×10^{3}
I_{AR}	1.40×10^{1}	5.17×10^{3}	0.00	0.00	7.17×10^{4}
I_{PC}	3.95×10^{-8}	1.46×10^{-5}	4.71×10^{-4}	1.57×10^{-7}	6.13×10^{-4}

*Chen, H. and Shonnard, D.R. Industrial and Engineering Chemistry Research, **43**, 535-552, 2004*

Flowsheet for MA production from n-C4: with heat integration.



Flowsheet for MA production from n-C4: with heat integration.

		Unit	n-Butane		Benzene	
Economic performance	NPV	$		3,044,252		2,561,415
	CI	$		19,472,756		16,081,942
	OC	$/yr		13,049,907		14,211,938
	RC	$/yr		5,274,830		6,809,811
Environmental performance			Value	Contribution to I_{PC}	Value	Contribution to I_{PC}
	I_{FT}	kg/yr	9.05E+02	1.554%	1.80E+03	0.016%
	I_{INH}	kg/yr	1.59E+07	93.933%	4.26E+06	0.133%
	I_{ING}	kg/yr	7.53E+05	0.404%	7.94E+06	0.002%
	I_{CINH}	kg/yr	0.00E+00	0.000%	4.27E+04	49.912%
	I_{CING}	kg/yr	0.00E+00	0.000%	4.27E+04	49.912%
	I_{GW}	kg/yr	4.08E+07	3.438%	4.61E+07	0.021%
	I_{AR}	kg/yr	5.28E+03	0.543%	3.77E+03	0.002%
	I_{SF}	kg/yr	2.03E+03	0.127%	6.37E+03	0.002%
	I_{OD}	kg/yr	0.00E+00	0.000%	0.00E+00	0.000%
	I_{PC}	unitless		5.40E-04		1.02E-01

*Chen, H. and Shonnard, D.R. Industrial and Engineering Chemistry Research, **43**, 535-552, 2004*

Recap

- Pedagogical Approach - flowsheet Tier 3 assessment
  - » How to formulate environmental impact indicators
  - » How to “draw the boundaries” around the assessment - what to leave in - what to leave out
  - » A methodology to integrate emission estimation, environmental fate and transport, and relative risk assessment
  - » The Tutorial on the Short Course CD contains detailed instructions on how to combine HYSYS and SCENE to generate the results shown here.