Green Chemistry:
Evaluation of Alternative Reaction Pathways
Chapters 7 and 8

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Outline

The selection of a reaction pathway is the key step to establish the environmental performance of a chemical process, affecting the downstream separation units and their energy requirements, emissions, and impacts.

- Educational goals and topics covered in the module
- Green Chemistry (Chapter 7) and
- assessing potential environmental impacts based on limited information (Chapter 8)

Educational goals and topics covered in the module

Students will:

- understand a "Tier 1" approach for chemical process environmental evaluation
- learn qualitative and quantitative approaches to Green Chemistry
- be able to evaluate alternative reaction pathways; both economically and environmentally.

Education Goals and Topics Covered in the Module. In addition, students should be thinking about environmental issues at each stage of the design process.

Green Chemistry - Ch 7

- Guiding principles for Green Chemistry
  - » Maximum incorporation of raw materials into final products
  - » All chemicals should be nontoxic yet functional
  - » Auxiliary substances (solvents) should be nontoxic
  - » High energy efficiency
  - » Use of renewable resources is recommended
  - » Recyclable reagents and raw materials
  - » End products should not persist in the environment

Anastas, P.T. and Warner, J.C. 1998, Green Chemistry: Theory and Practice, Oxford University Press, New York

Green Chemistry -- Chapter 7. None.

Feedstocks and solvents

- Important considerations
  - » Human / ecosystem health properties
    - – Bioaccumulative?
    - – Persistent?
    - – Toxic?
    - – Global warming, Ozone depletion, Smog formation?
    - – Flammable or otherwise hazardous?
    - – Renewable or non renewable resource?
  - » Life cycle environmental burdens? - Ch 13, 14

Feedstocks and Solvents. Life cycle environmental burdens is a concept that as engineers we need to think about including the ultimate use and disposal of products.

Synthesis pathways

Reaction Type	*Waste Generation Potential*
Addition Reaction Isobutylene + methanol → methyl tert-butyl ether $C_4H_8 + CH_3OH \rightarrow (C_4H_9)\text{-}O\text{-}CH_3$	• completely incorporate starting material into product
Substitution Reaction Phenol + ammonia → analine + water $C_6H_5\text{-}OH + NH_3 \rightarrow C_6H_5\text{-}NH_2 + H_2O$	• stoichiometric amounts of waste are generated
Elimination Reaction Ethylbenzene → styrene + hydrogen $C_6H_5\text{-}C_2H_5 \rightarrow C_6H_5\text{-}C_2H_3 + H_2$	• stoichiometric amounts of waste are generated

Synthesis Pathways. Note: Different types of chemicals create different products and byproducts.

Atom and mass efficiency: *magnitude of improvements possible*

Atom Efficiency

- the fraction of starting material incorporated into the desired product -

C_6H_5-OH+ NH_3 $\rightarrow$ C_6H_5-NH_2 + H_2O

- Carbon - 100%
- Hydrogen - 7/9 x 100 = 77.8%
- Oxygen - 0/1 x 100 = 0%
- Nitrogen - 100%

Mass Efficiency (Basis 1 mole of product)

C_6H_5-OH+ NH_3 $\rightarrow$ C_6H_5-NH_2 + H_2O

Mass in Product = (6 C)(12) + (7 H)(1) + (0 O)(16) + (1 N)(14) = 93 grams

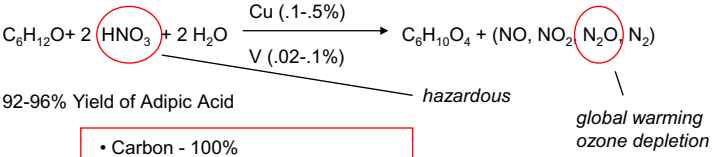
Mass in Reactants = (6 C)(12) + (9 H)(1) + (1 O)(16) + (1 N)(14) = 111 grams

Mass Efficiency = 93/111 x 100 = 83.8%

Atom and Mass Efficiency: Magnitude of Improvements Possible. Atom efficiency is a concept you see frequently in green chemistry, it is one way to look at efficiency but it is not the only way.

Chapter 7: Adipic Acid Synthesis
Traditional vs. New

Traditional Route - from cyclohexanol/cyclohexanone



92-96% Yield of Adipic Acid

- Carbon - 100%
- Oxygen - 4/9 x 100 = 44.4%
- Hydrogen - 10/18 x 100 = 55.6%
- Nitrogen - 0%

Product Mass = (6 C)(12) + (10 H)(1) + (4 O)(16) = 146 g

Reactant Mass = (6 C)(12) + (18 H)(1) + (9 O)(16) + (2 N)(14) = 262 g

Mass Efficiency = 146/262 x 100 = **55.7%**

Davis and Kemp, 1991, Adipic Acid, in Kirk-Othmer Encyclopedia of Chemical Technology, V. 1, 466 - 493

Chapter 7: Adipic Acid Synthesis
Traditional vs. New

New Route - from cyclohexene

$$C_6H_{10} + 4\ H_2O_2 \xrightarrow[[CH_3(n\text{-}C_8H_{17})_3N]HSO_4\ (1\%)]{Na_2WO_4 \cdot 2H_2O\ (1\%)} C_6H_{10}O_4 + 4\ H_2O$$

90% Yield of Adipic Acid

- Carbon - 100%
- Oxygen - 4/8 x 100 = 50%
- Hydrogen - 10/18 x 100 = 55.6%

Product Mass = (6 C)(12) + (10 H)(1) + (4 O)(16) = 146 g

Reactant Mass = (6 C)(12) + (18 H)(1) + (8 O)(16) = 218 g

Mass Efficiency = 146/218 x 100 = 67%

Sato, et al. 1998, A "green" route to adipic acid:…, Science, V. 281, 11 Sept. 1646 - 1647

Maleic anhydride (MA) synthesis: benzene vs butane - mass efficiency

Benzene Route (Hedley et al. 1975, reference in ch. 8)

$$2\ C_6H_6 + 9\ O_2\ (\text{air}) \xrightarrow[MoO_3]{V_2O_5} 2\ C_4H_2O_3 + H_2O + 4\ CO_2$$

70% Yield of Maleic Anhydride from Benzene in Fixed Bed Reactor

$$\text{Mass Efficiency} = \frac{2(4)(12)+3(2)(16)+2(2)(1)}{2(6)(12)+9(2)(16)+2(6)(1)}(100) = 44.4\%$$

Butane Route

$$C_4H_{10} + 3.5\ O_2\ (\text{air}) \xrightarrow{(VO)_2P_2O_5} C_4H_2O_3 + 4\ H_2O$$

60% Yield of Maleic Anhydride from Butane in Fixed Bed Reactor

$$\text{Mass Efficiency} = \frac{(4)(12)+(3)(16)+(2)(1)}{(4)(12)+3.5(2)(16)+(10)(1)}(100) = 57.6\%$$

Felthouse et al., 1991, "Maleic Anhydride, ..", in Kirk-Othmer Encyclopedia of Chemical Technology, V. 15, 893 - 928

Maleic Anhydride Synthesis Benzene vs. Butane – Mass Efficiency. Mass Efficiency is a green chemistry concept; you can also calculate atomic efficiency. There is no single "correct" measurement of efficiency.

Maleic anhydride (MA) synthesis: benzene vs butane - summary table

Chapter 8 Material	Stoichiometry [1]	$/lb [2]	TLV [3]	TW [4]	Persistence [5] Air (d)	Persistence [5] Water (d)	log BCF [5]
Benzene Process							
Benzene [71-43-2]	-1.19	0.184	10	100	10	10	1.0
Maleic Anhydride	1.00	0.530	0.25	----	1.7	$7x10^{-4}$	----
Butane Process							
Butane [106-97-8]	-1.22	0.141	800	----	7.25	----	----
Maleic Anhydride	1.00	0.530	0.25	----	1.7	$7x10^{-4}$	----

1 Rudd et al. 1981, "Petroleum Technology Assessment", Wiley Interscience, New York
2 Chemical Marketing Reporter (Benzene and MA 6/12/00); Texas Liquid (Butane 6/22/00)
3 Threshold Limit Value, ACGIH - Amer. Conf. of Gov. Indust. Hyg., Inc. , www.acgih.org
4 Toxicity Weight, www.epa.gov/opptintr/env_ind/index.html and www.epa.gov/ngispgm3/iris/subst/index.html
5 ChemFate Database - www.esc.syrres.com, EFDB menu item

Maleic Anhydride Synthesis Benzene vs. Butane – Summary Table. Think of the reaction pathways based on persistence, bioaccumulation, and toxicity (PBT). At this point the students have the group data necessary to calculate persistence and bioaccumulation, recommend providing data sources for toxicity.

Maleic Anhydride Synthesis:

Butane: 53% converted to MA and 30% Cox, 17% not converted

Main $C_4H_{10} + 3.5O_2 \rightarrow C_4H_2O_3 + 4 H_2O$

Side $C_4H_{10} + 6.5 O_2 \rightarrow 4 CO_2 + 5 H_2O$

Side $C_4H_{10} + 4.5 O_2 \rightarrow 4CO + 5 H_2O$

Benzene: 72% converted to MA and 26% converted to CO & CO_2, 2% not converted

$C_6H_6 + 4.5O_2 \rightarrow C_4H_2O_3 + 2H_2O + 2CO_2 + 2H_2O$

Side $C_6H_6 + 7.5O_2 \rightarrow 6 CO_2 + 3 H_2O$

Side $C_6H_6 + 4.5O_2 \rightarrow 6CO + 3H_2O$

Maleic anhydride (MA) synthesis: benzene vs butane - tier 1 assessment

(TLV Index)

$$\text{Environmental Index (non-carcinogenic)} = \sum_i |\nu_i| \times (\text{TLV}_i)^{-1}$$

Benzene Route

$$\text{TLV Index} = (1.19)(1/10) + (1.0)(1/.25) = 4.12$$

Butane Route

$$\text{TLV Index} = (1.22)(1/800) + (1.0)(1/.25) = 4.00$$

Where ν_i is the overall stoichiometric coefficient of reactant or product *i*

Maleic Anhydride Synthesis Benzene vs. Butane -- Tier 1 Assessment. None.

Maleic anhydride (MA) synthesis: benzene vs butane - tier 1 assessment

EPA Index

Environmental Index (carcinogenic) = $\sum_i |\nu_i| \times$ (Maximum toxicity we

Benzene Route

$$\text{EPA Index} = (1.19)(100) + (1.0)(0) = 119$$

Butane Route

$$\text{EPA Index} = (1.22)(0) + (1.0)(0) = 0$$

Maleic Anhydride Synthesis Benzene vs. Butane -- Tier 1 Assessment. None.

A More Detailed Analysis of MA Production

Level 1. Input / Output Information

Benzene Process

V_2O_5-MoO_3

$$2C_6H_6 + 9O_2 \rightarrow 2C_4H_2O_3 + 4CO_2 + 4H_2O$$

$$2C_6H_6 + 9O_2 \rightarrow 12CO + 6H_2O$$

$$2C_6H_6 + 15O_2 \rightarrow 12CO_2 + 6H_2O$$

$$C_4H_2O_3 + O_2 \rightarrow 4CO + H_2O$$

$$C_4H_2O_3 + 3O_2 \rightarrow 4CO_2 + H_2O$$

Benzene conversion, 95%
MA Yield, 70%
Air/Benzene, ~ 66 (moles)
Temperature, 375°C
Pressure, 150 kPa

n-Butane Process

VPO

$$2C_4H_{10} + 7O_2 \rightarrow 2C_4H_2O_3 + 8H_2O$$

$$2C_4H_{10} + 9O_2 \rightarrow 8CO + 10H_2O$$

$$2C_4H_{10} + 13O_2 \rightarrow 8CO_2 + 10H_2O$$

$$C_4H_2O_3 + 3O_2 \rightarrow 4CO_2 + H_2O$$

$$C_4H_2O_3 + O_2 \rightarrow 4CO + H_2O$$

n-butane conversion, 85%
MA Yield, 60%
Air/n-butane, ~ 62 (moles)
Temperature, 400°C
Pressure, 150 kPa

Shown are the major reactions for product and byproduct generation, with expected conversions, yields, and reaction conditions (temperature, pressure, etc.) for MA production from either benzene or n-butane. Most MA production has migrated from benzene to n-butane, and this represents one of the earliest examples of Green Chemistry making a significant change in chemical production.

Maleic anhydride (MA) production: Costs

Level 1. Input / Output Information
"Tier 1" Economic analysis (raw materials costs only)

Benzene Process

1 mole/(0.70 mole) × (78 g/mole) × (0.00028 $/g) = 0.0313 $/mole of MA

MA Yield | Bz MW | Benzene cost

N-butane process has lower cost

n-Butane Process

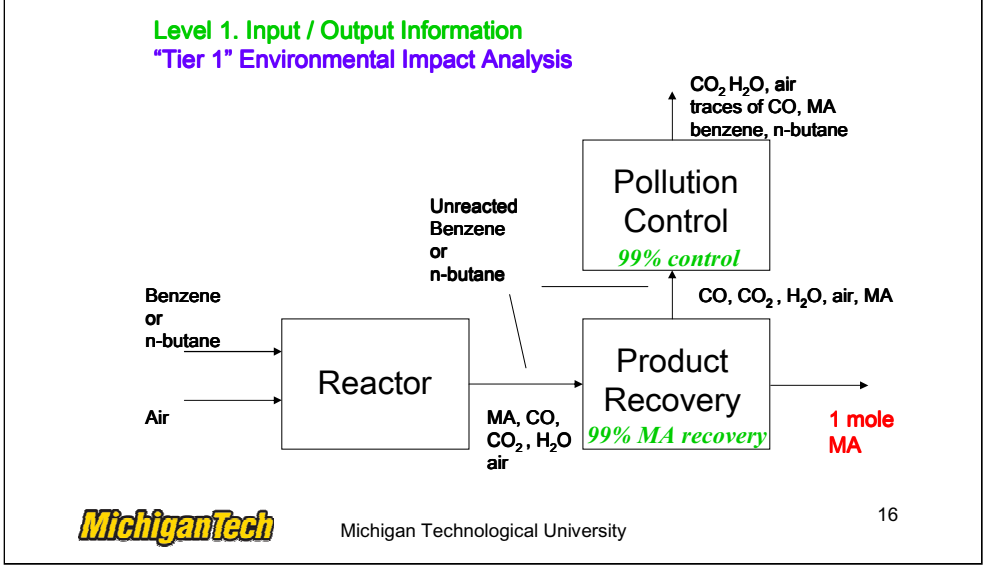
1mole/(0.60 mole) × (58 g/mole) × (0.00021 $/g) = 0.0203 $/mole of MA

MA Yield | nC4 MW | nC4 cost

Assumption: raw material costs dominate total cost of the process

Using this input / output information for the reaction step, we can compute raw material costs for each reaction route for MA production. n-butane is superior to benzene with regard to raw material costs, even when the benzene route exhibits higher conversions and yields compared to n-butane. One reason is because 2 of the carbons on the benzene molecule are not incorporated into the final product, MA.

MA production: IO assumptions



A production rate of 1 mole of MA is chosen as the basis for this impact analysis. Shown also are estimated recoveries and pollution control efficiency for the chemicals in the process.

Maleic Anhydride Synthesis
Benzene vs Butane - Tier 1 Assessment

Benzene Exiting Reactor :

$$(1\,\text{mole}/((0.70)(.99)) \times (1 - 0.95) = 0.0722\ \text{mole benzene/mole of MA}$$

Benzene Emission from Pollution Control :

$$(0.01) \times (0.0722\ \text{mole/mole of MA}) = \boxed{7.22 \times 10^{-4}}\ \text{mole benzene/mole of MA}$$

n-Butane Exiting Reactor :

$$(1\,\text{mole}/((0.60)(.99)) \times (1 - 0.85) = 0.2525\ \text{mole n-butane/mole of MA}$$

n-Butane Emission from Pollution Control :

$$(0.01) \times (0.2525\ \text{mole/mole of MA}) = \boxed{2.53 \times 10^{-3}}\ \text{mole n-butane/mole of MA}$$

Maleic Anhydride Synthesis
Benzene vs Butane - Tier 1 Assessment

Benzene Process : CO Exiting Reactor :

$$(1\,\text{mole}/((0.70)(.99)) \times (0.95 - 0.7) \times \frac{6}{2} = 1.082\ \frac{\text{mole CO}}{\text{mole MA}}$$

Benzene Process : CO Emission from Pollution Control :

$$(0.01) \times (1.082\ \text{mole/mole of MA}) = 1.08\text{x}10^{-2}\ \frac{\text{mole CO}}{\text{mole MA}}$$

n-Butane Process : CO Exiting Reactor :

$$(1\,\text{mole}/((0.60)(.99)) \times (0.85 - 0.6) \times \frac{4}{2} = 0.842\ \frac{\text{mole CO}}{\text{mole MA}}$$

n-Butane Process : CO Emission from Pollution Control :

$$(0.01) \times (0.842\ \text{mole/mole of MA}) = 8.42\text{x}10^{-3}\ \frac{\text{mole CO}}{\text{mole MA}}$$

Chapter 8: Maleic Anhydride Synthesis
Benzene vs Butane - Tier 1 Assessment

Benzene Process: CO_2 Exiting Reactor:

$$(1\,\text{mole MA})\left(\frac{2\,\text{mole } CO_2}{\text{mole MA}}\right)+(1\,\text{mole}/((0.7)(.99))\times(0.95-0.7)\times\frac{6}{2}=3.082\,\frac{\text{mole } CO_2}{\text{mole MA}}$$

Benzene Process: CO_2 Emission from Pollution Control:

$$(3.082)+(0.99)(1.082)+(0.99)(0.0722)(6)+(0.01)(0.99)(4)=\boxed{4.622\,\frac{\text{mole } CO_2}{\text{mole MA}}}$$

n-Butane Process: CO_2 Exiting Reactor:

$$(1\,\text{mole}/((0.60)(.99))\times(0.85-0.6))\times\frac{4}{2}=0.842\,\frac{\text{mole } CO_2}{\text{mole MA}}$$

n-Butane Process: CO_2 Emission from Pollution Control:

$$(0.842)+(0.99)(0.842)+(0.99)(0.25)(4)+(0.01)(0.99)(4)=\boxed{2.705\,\frac{\text{mole } CO_2}{\text{mole MA}}}$$

MA production: Flows/Emissions for process streams

Benzene process					
	Flow Rates/Emissions (kg/mole of MA)				
	Benzene	CO	CO_2	Maleic anhydride	Total
Reactor inlet	1.13E-01	0.00E+00	0.00E+00	0.00E+00	1.13E-01
Reactor outlet	5.63E-03	3.03E-02	1.36E-01	9.90E-02	2.71E-01
Separation unit (w/pollution control)	5.63E-05	3.03E-04	2.03E-01	9.90E-06	2.03E-01
n-Butane process					
	Flow Rates/Emissions (kg/mole of MA)				
	n-Butane	CO	CO_2	Maleic anhydride	Total
Reactor inlet	9.76E-02	0.00E+00	0.00E+00	0.00E+00	9.76E-02
Reactor outlet	1.46E-02	2.36E-02	3.71E-02	9.90E-02	1.74E-01
Separation unit (w/pollution control)	1.46E-04	2.36E-04	1.19E-01	9.90E-06	1.19E-01

This table summarizes the rates of reactants, products, and byproduct entering and leaving the reactor as well as the emission of pollutants from the pollution control equipment to the environment. These emission estimates are the basis for calculating environmental impact indicators.

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	n-Butane	CO	CO_2	Maleic anhydride	Total
Reactor inlet	9.76E-02	0.00E+00	0.00E+00	0.00E+00	9.76E-02
Reactor outlet	1.46E-02	2.36E-02	3.71E-02	9.90E-02	1.74E-01
Separation unit (w/pollution control)	1.46E-04	2.36E-04	1.19E-01	9.90E-06	1.19E-01

This table summarizes the rates of reactants, products, and byproduct entering and leaving the reactor as well as the emission of pollutants from the pollution control equipment to the environment. These emission estimates are the basis for calculating environmental impact indicators.

Emission Factors - for major equipment

Page 223 of textbook

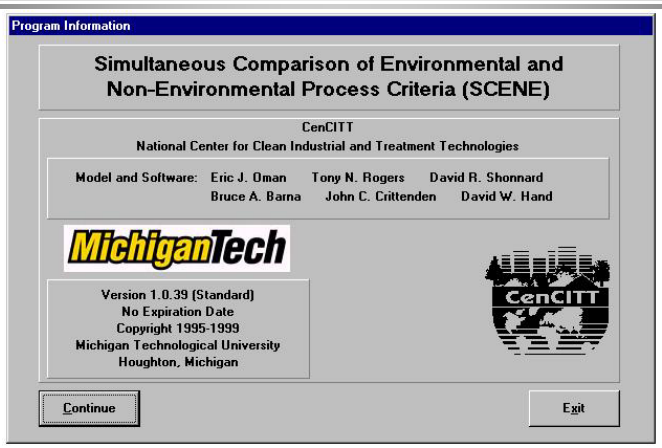
$E = m_{VOC}\, EF_{av}\, M$ Equation 8-4

Average Emission Factors for Chemical Process Units Calculated from the US EPA L&E Database

Process Unit	EF_{av} (kg emitted/10^3 kg throughput)
Reactor Vents	1.50
Distillation Columns Vents	0.70
Absorber Units	2.20
Stripping Columns	0.20
Sumps/Decanters	0.02
Dryers	0.70
Cooling Towers	0.10

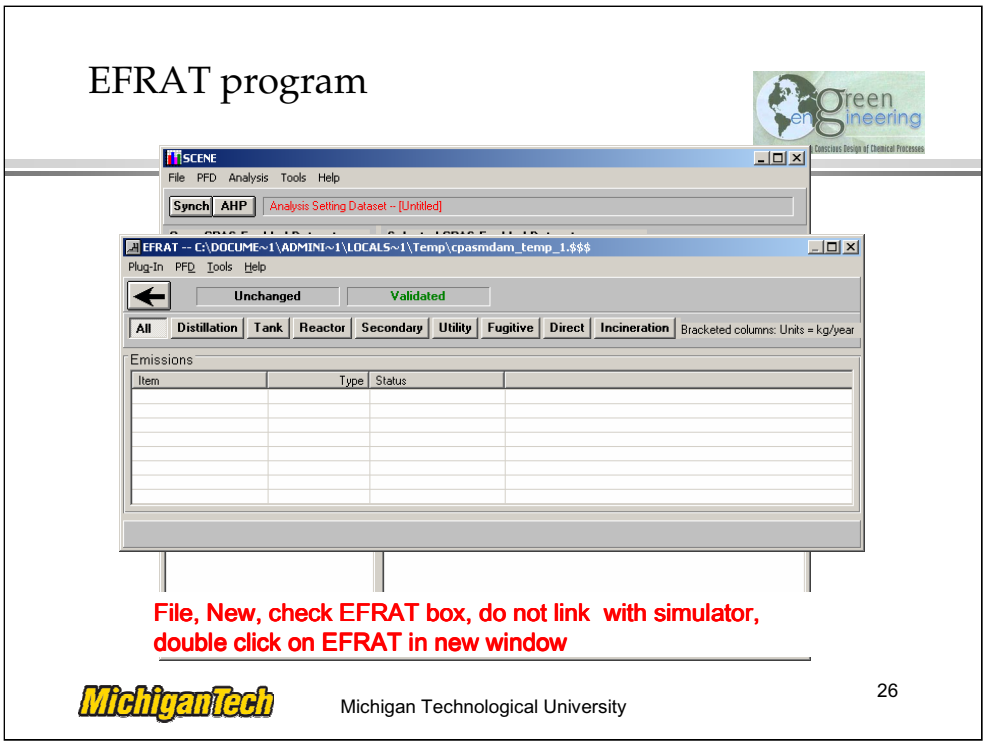
Now that we have estimated direct emissions from the stream exiting the process, we can estimate emissions of chemicals from major pieces of equipment. For this we use the equipment input/out mass flow rates, concentrations, and emission factors from the US EPA. These emission factors were obtained by averaging the factors over a number of case studies involving a number of process flowsheets.

SCENE program



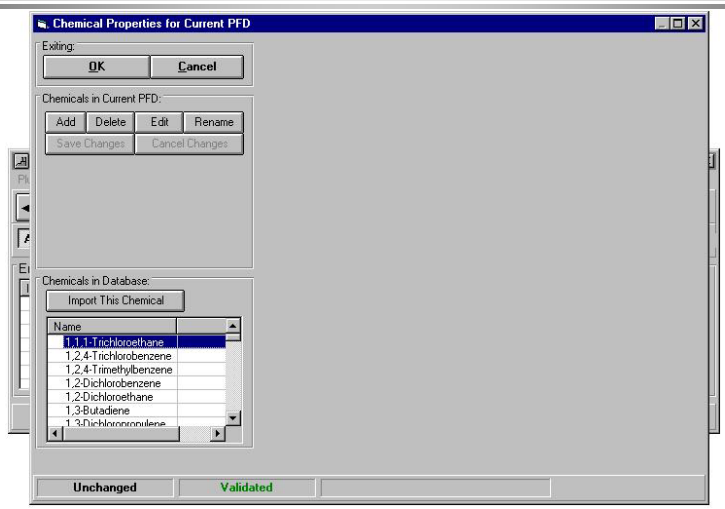
Start, Programs, CPAS Programs, SCENE

The SCENE software is used to estimate emissions from process equipment using emission factors listed previously, it calculates environmental fate using a "Level I" multimedia compartment model (partitioning among air, water, soil, and sediment), and calculates nine impact indices, similar to those listed in the previous slides. We will calculate environmental indices using the emissions estimated for the MA process in the previous table.



1. Open SCENE and then open the EFRAT main window (Figure 2-13 of Tutorial).

EFRAT program: Add chemicals



2. Add chemicals: benzene, CO, CO_2 and maleic anhydride.

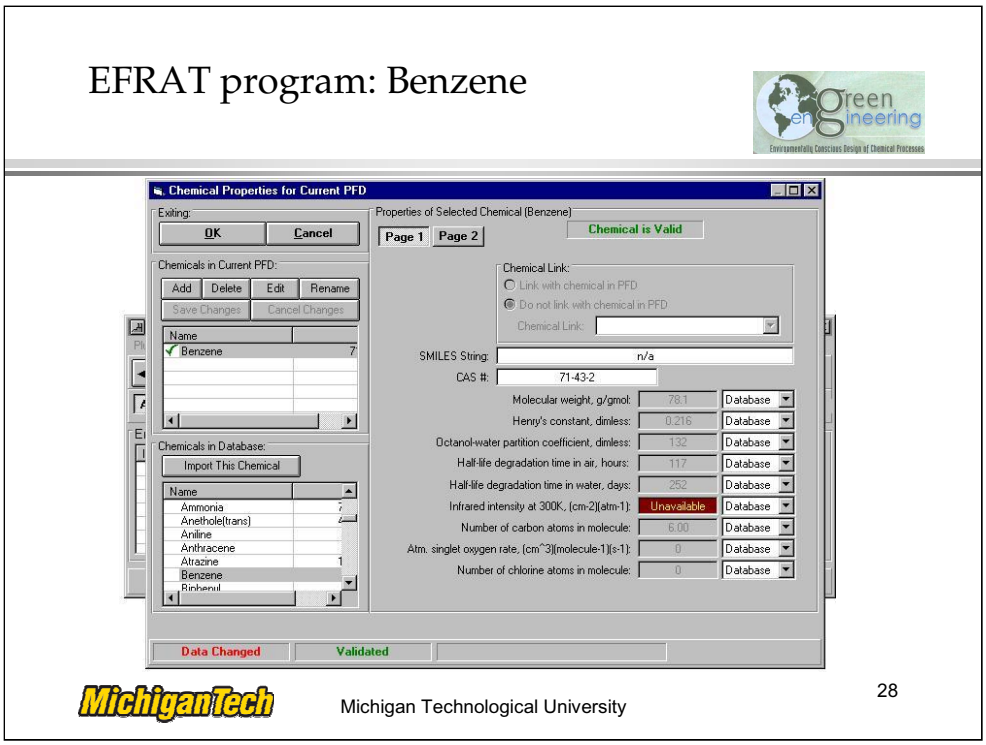
- Open 'PFD' menu, select 'chemical list' and then open the following window (Figure 3-2 of Tutorial).

This window contains a list of 'Chemicals in Database'. You can choose chemicals from this list and import them to the list of 'Chemicals in Current PFD'.

- Find chemical benzene. Use the vertical scroll bar of the chemical list to move down the list until benzene becomes visible, then highlight it.

- Import chemical benzene. Click 'Import This Chemical' button. Benzene will appear in the list of 'Chemicals in Current PFD' (Figure 3-3 of Tutorial).

On the right side of this window, it displays two pages of 'Properties of Selected Chemical (Benzene)'. If there are some data unavailable for one chemical, the data cell will display 'Unavailable' and will be highlighted.



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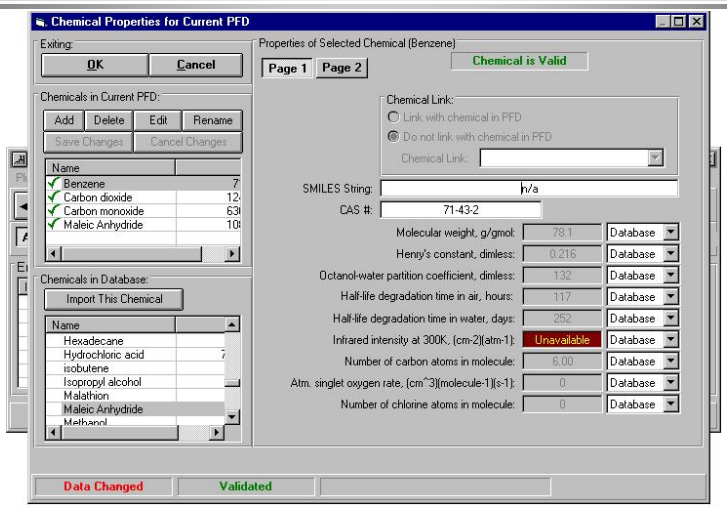
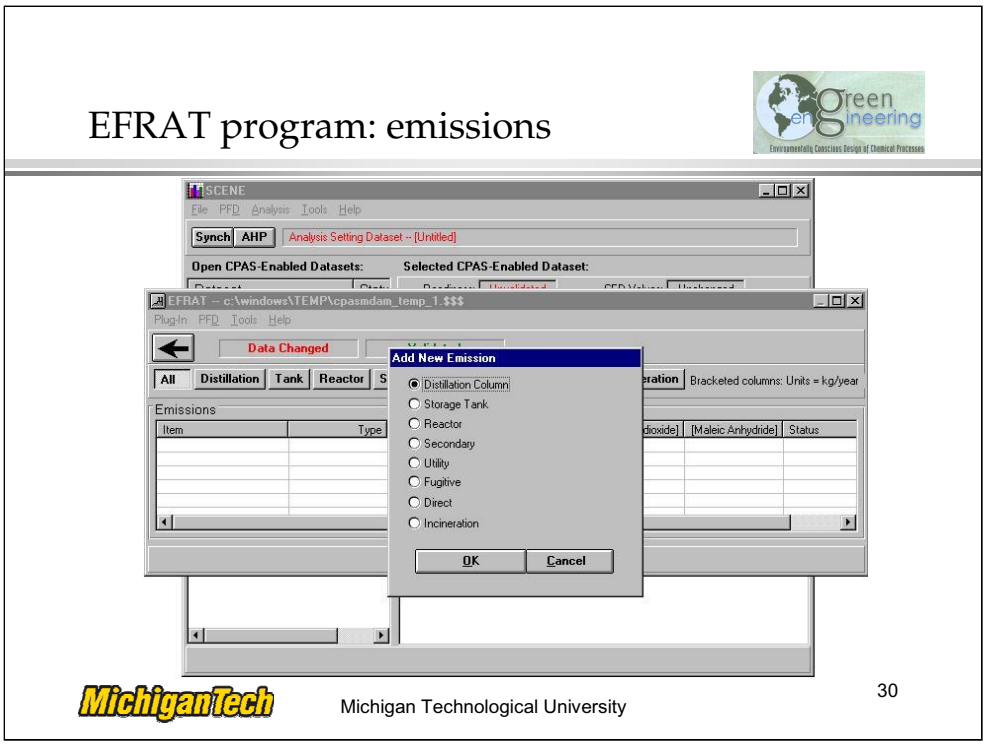
EFRAT program: All chemicals added



- Import chemicals CO, CO_2, and maleic anhydride following the same procedures as benzene (Figure 3-4 of Tutorial).
- Click ‘OK’, exit this window and return to the EFRAT main window, or click ‘Cancel’ to abandon these changes.



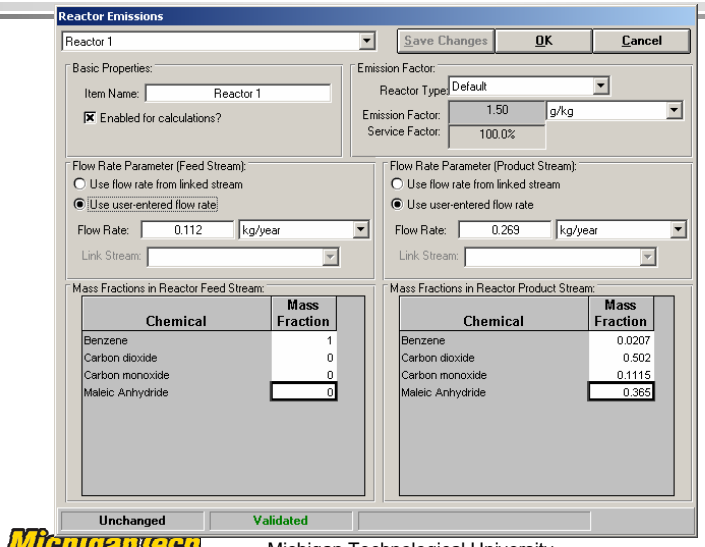
3. Add reactor emission.

- Open ‘PFD’ menu, select ‘Emissions’ and then click ‘Add New Emission…’. You can choose to add emissions from eight different sources (Figure 3-5 of Tutorial).

- Select ‘Reactor’, then click ‘OK’ and enter into the reactor emissions window (Figure 3-6). EFRAT gives this emission a default name, ‘Reactor 1’. You can rename it by activating ‘Item Name’ field and inputting a new name.

- Input total feed flow rate and total product flow rate from Table 3-2. Please note that the unit of the flow rate in this evaluation is kg/mole of MA. However, in EFRAT, this unit does not exist. We can use the unit of flow rate as ‘kg/yr’ and then substitute it with ‘kg/mole of MA’ in the final results.

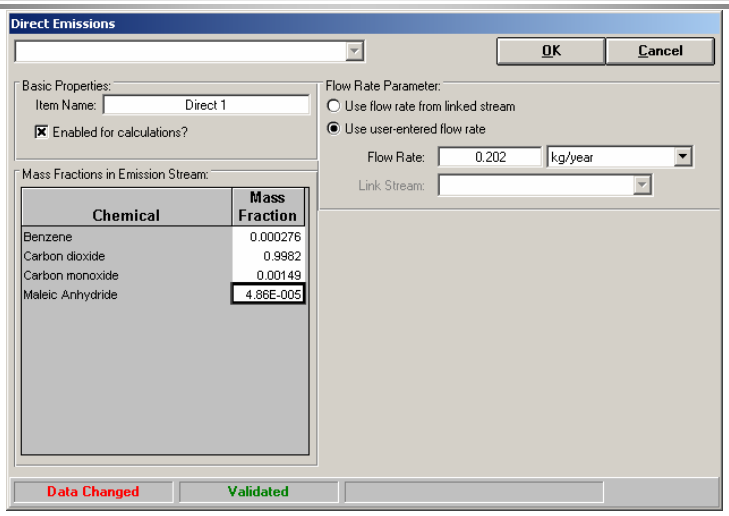
EFRAT program: Reactor Emission



3. Add reactor emission.

- Select ‘Reactor’, then click ‘OK’ and enter into the reactor emissions window (Figure 3-6 of Tutorial). EFRAT gives this emission a default name, ‘Reactor 1’. You can rename it by activating ‘Item Name’ field and inputting a new name.
- Input total feed flow rate and total product flow rate from Table 3-2 of Tutorial. Please note that the unit of the flow rate in this evaluation is kg/mole of MA. However, in EFRAT, this unit does not exist. We can use the unit of flow rate as ‘kg/yr’ and then substitute it with ‘kg/mole of MA’ in the final results.
- Input mass fraction of each chemical in both feed and product streams. These can be calculated from Table 3-2 by dividing the flow rate of one chemical by the total flow rate.
- Click ‘OK’ to save the changes and return to the EFRAT main window, or click ‘Cancel’ to abandon these changes.

EFRAT program: Direct Emission

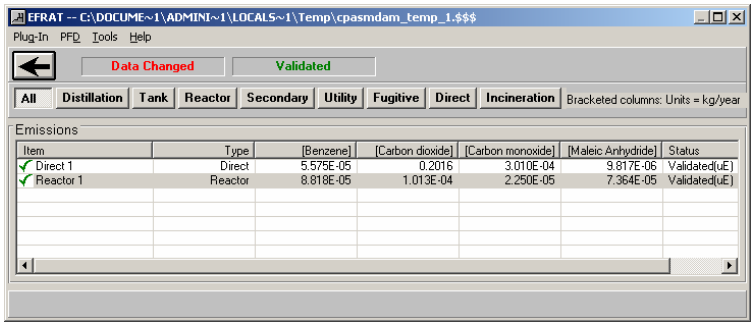


4. Add direct emission.

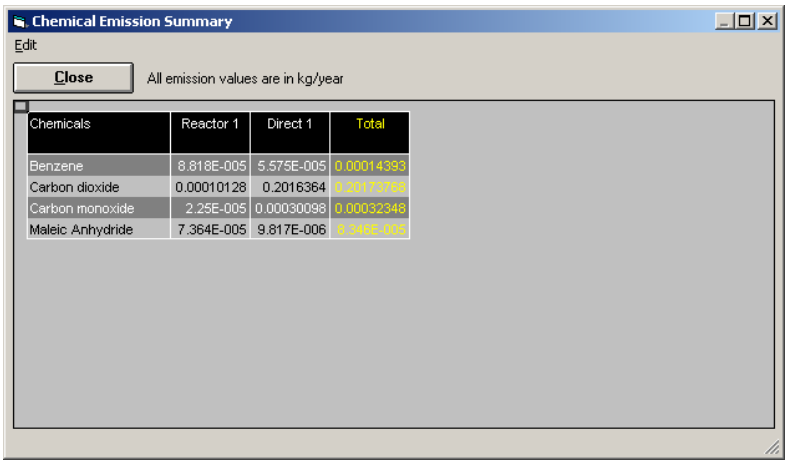
- Open ‘PFD’ menu, select ‘Emissions’ and then click ‘Add New Emission…’ (Figure 3-5 of Tutorial).
- Select ‘Direct’, then click ‘OK’ and enter into the direct emissions window (Figure 3-7 of Tutorial).
- Input total flow rate and mass fraction of each chemical, calculated from Table 3-2 of Tutorial.
- Click ‘OK’ to save the changes and return to the EFRAT main window, or click ‘Cancel’ to abandon these changes.

Now the EFRAT main window shows two emissions (Figure 3-8 of Tutorial).

EFRAT program: Emissions Window



EFRAT program: Viewing Results
Emission Summary



5. View the results.

Open menu ‘PFD’ and select ‘Emission Summary…’ to view the results.

This table can be pasted into MS Excel by clicking ‘Edit’ menu and then selecting its submenu.

- Click ‘Close’ and return to the EFRAT main window.

Recap

Green Chemistry concepts and Atom Economy are useful for designing more environmentally beneficial reaction pathways. Early design Green Engineering analysis methods for environmental impacts of alternatives.

- Educational goals and topics covered in the module
- Green Chemistry (Chapter 7) and assessing potential impacts based on limited information (Chapter 8)
- Estimating emissions from processes in early design.