

Emissions Inventory Development through Computer Modeling

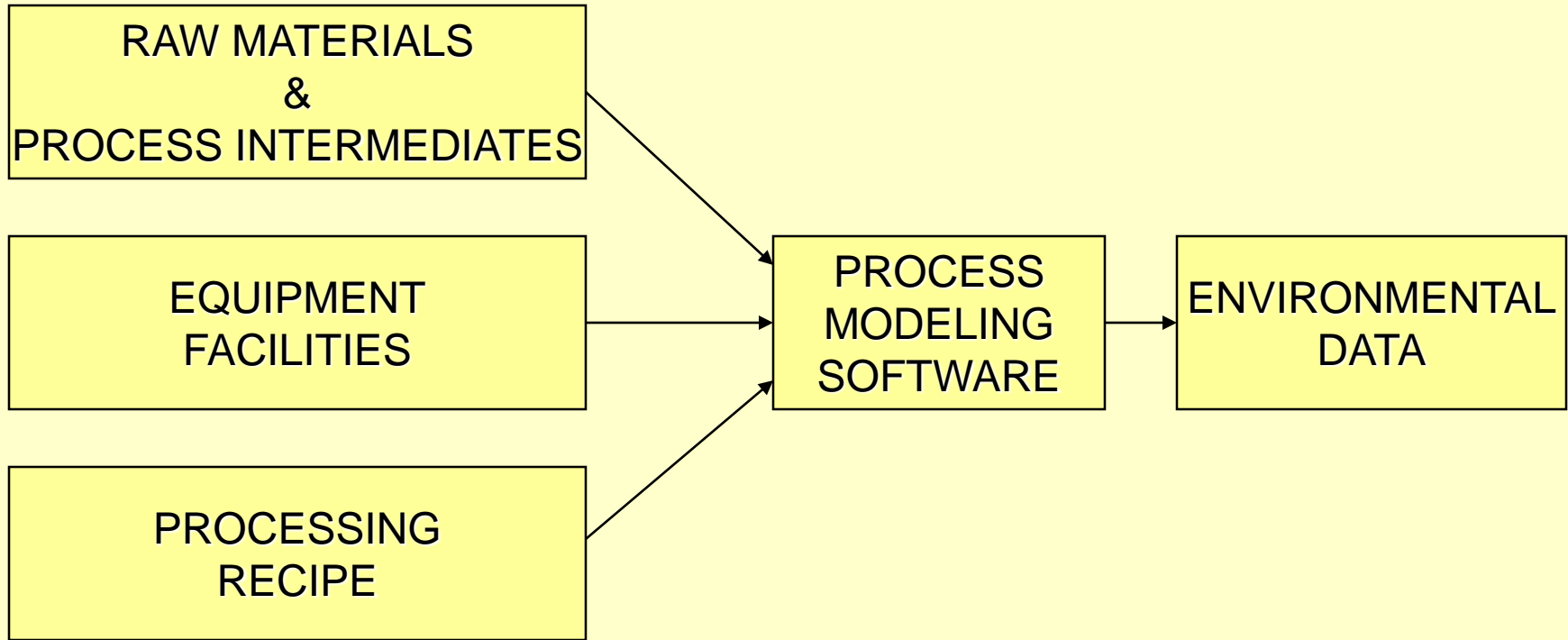
Abstract #476000

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*John Allen Hatfield
Mitchell Scientific, Inc.
www.MitchellScientific.com*



Process Modeling for Environmental Assessment



MANUFACTURING
INFORMATION

SIMULATION

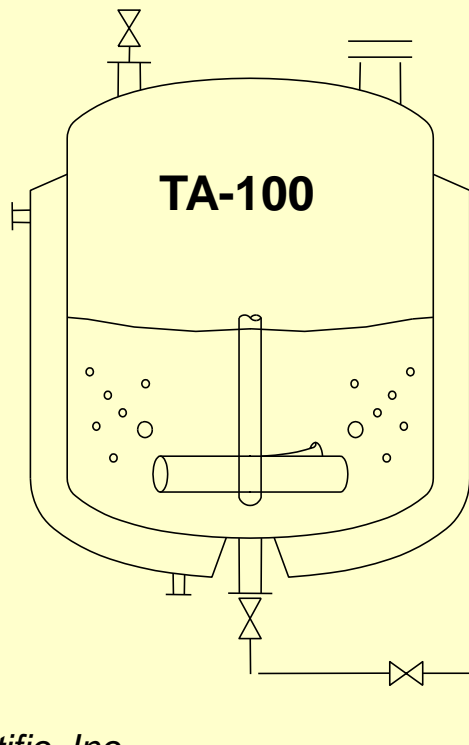
EVALUATION
RESULTS
(CALCULATED)

Underlying Principles

- *Ideal Gas Law*
- *Pure Component Vapor Pressures*
- *Raoult's Law of solution properties*
- *Activity Coefficients?*
- *Dalton's Law - Partial Pressures*
- *Vapor Space Composition*

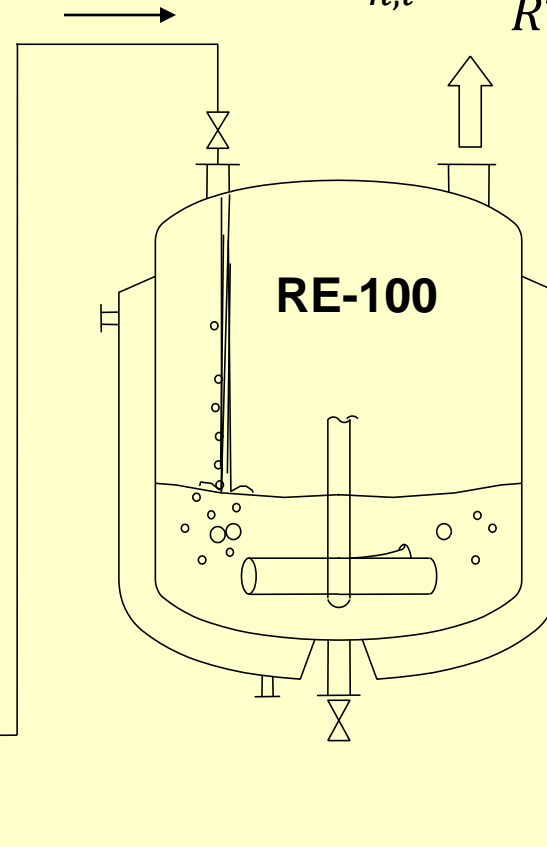
Above Surface Additions

Charges & Transfers



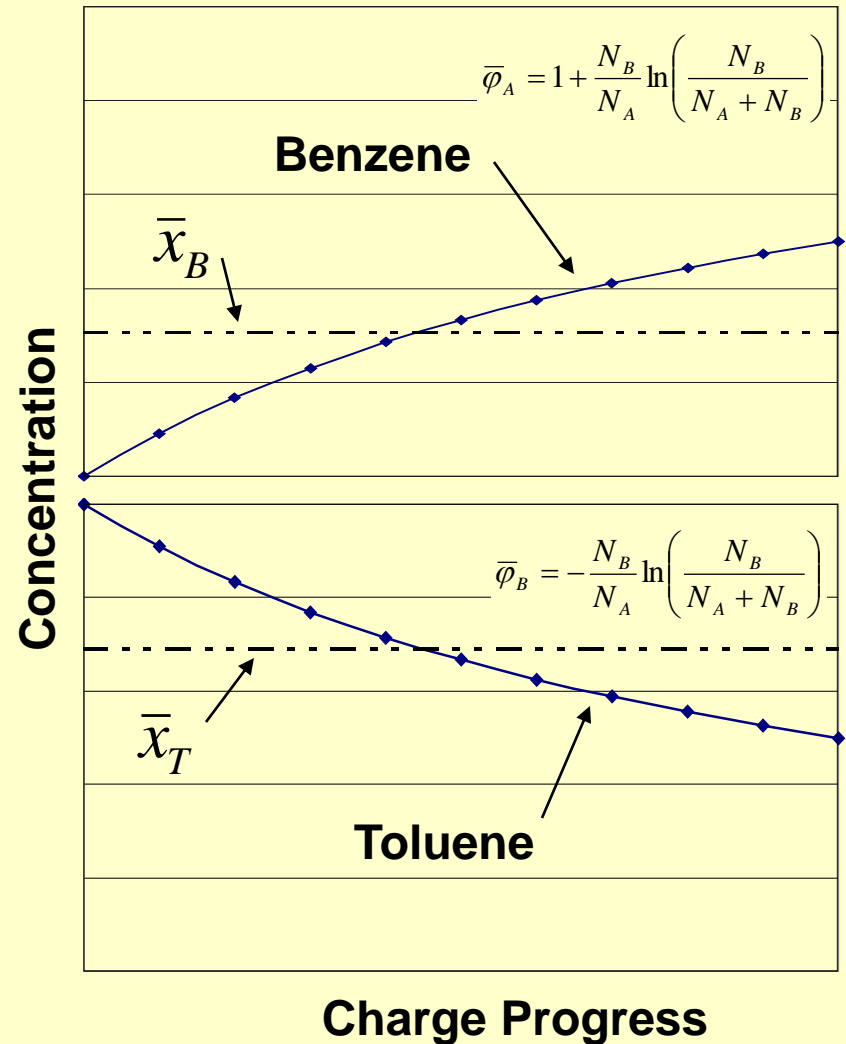
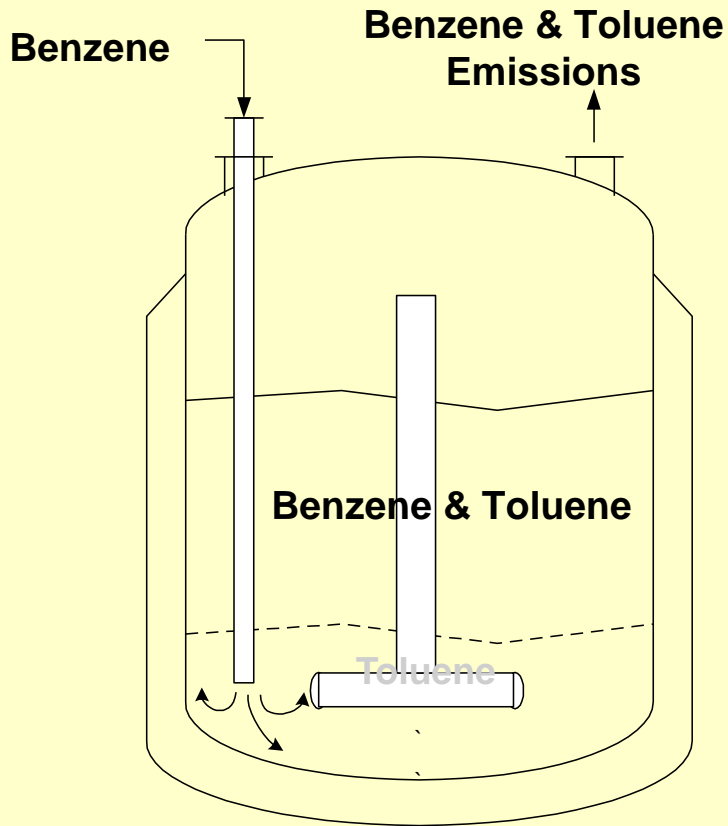
**Volatile Components
& Air, Nitrogen**

$$E_{n,i} = \frac{p_i \Delta V}{RT}$$



Subsurface Additions

$$E_{n,i} = \frac{p_i \Delta V}{RT}$$



Above Surface vs Subsurface

Above Surface Addition

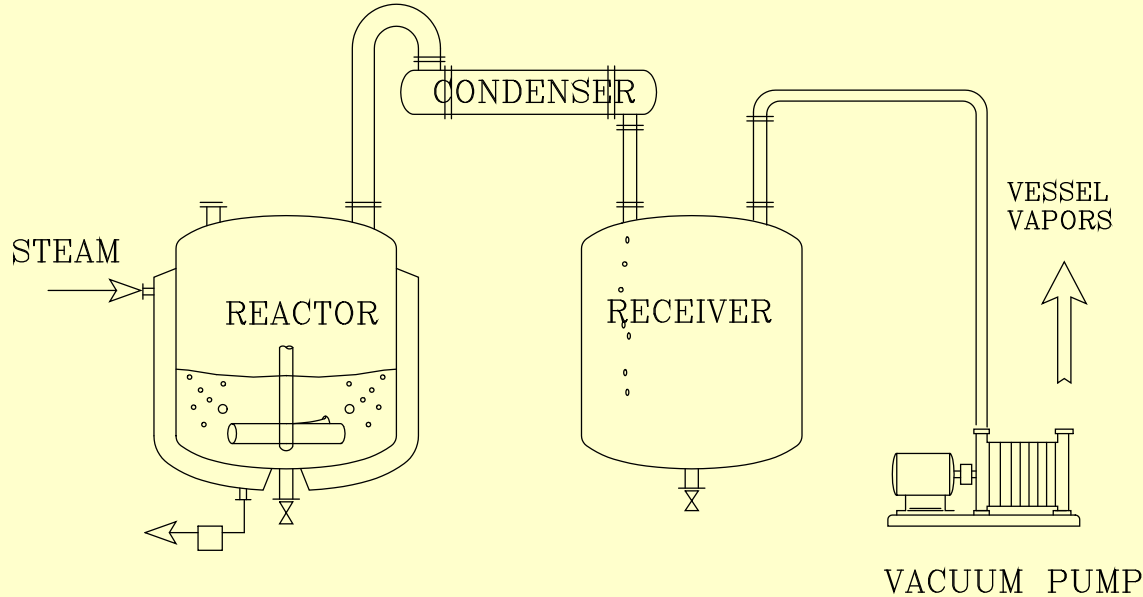
Inlet Stream	X_i	$\overline{\varphi_A}$ $\overline{\varphi_B}$	\overline{X}_i	$P_{i,mm\ Hg}$	$p_{i,mm\ Hg}$
Benzene	1.0	1.000	1.000	182.8	182.8
Toluene	1.0	0.693	0.693	59.2	41.0

Subsurface Addition

Benzene	1.0	0.307	0.307	182.8	56.1
Toluene	1.0	0.693	0.693	59.2	41.0

Temperature = 40°C

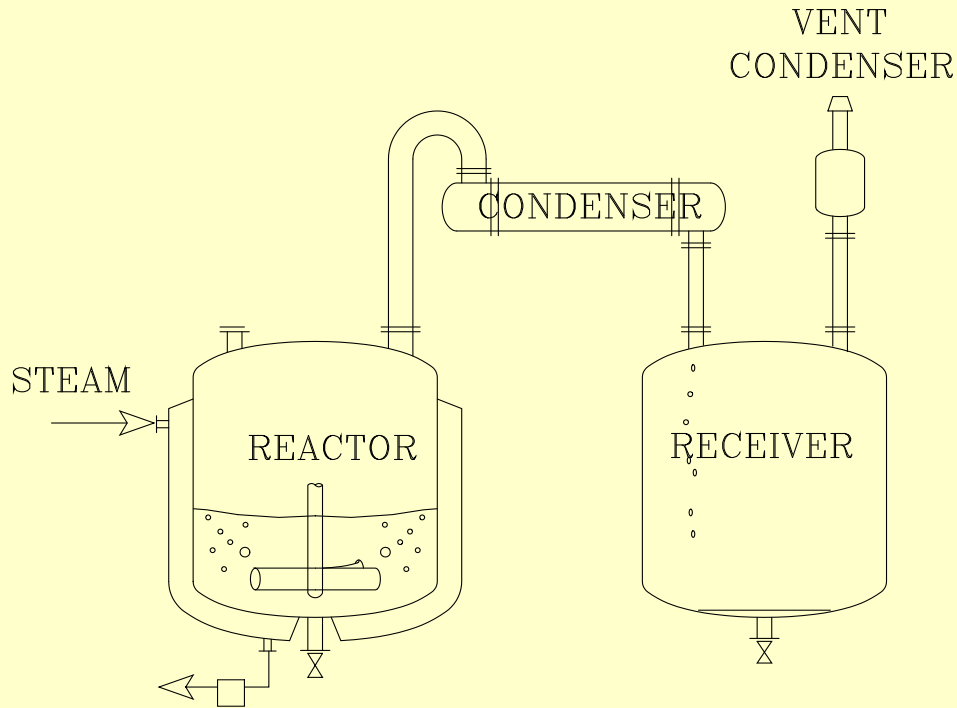
System Depressurization



$$n_{i,out} = N_{i,vessel} \ln \left(\frac{p_{nc,1}}{p_{nc,2}} \right)$$

1998 Equation (MACT)

Temperature Elevation

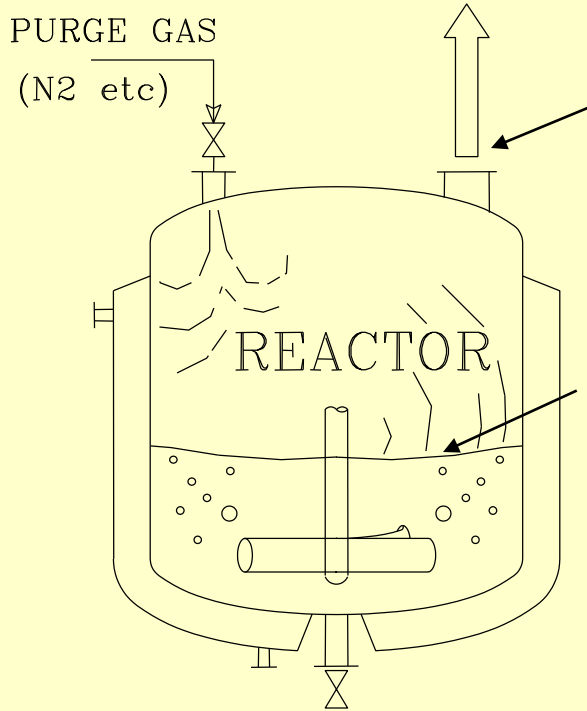


$$n_{i,out} = N_{avg} \ln \left(\frac{p_{nc,1}}{p_{nc,2}} \right) - (n_{i,2} - n_{i,1})_{headspace}$$

1998 Equation (MACT)

Gas Sweep Operations

**Volatile Components
& Air, Nitrogen**



$$Q_v = \frac{M_i F p_i}{RT}$$

Vent Losses

$$Q_m = \frac{M_i K_i A}{RT} (p_i^{Sat} - p_i)$$

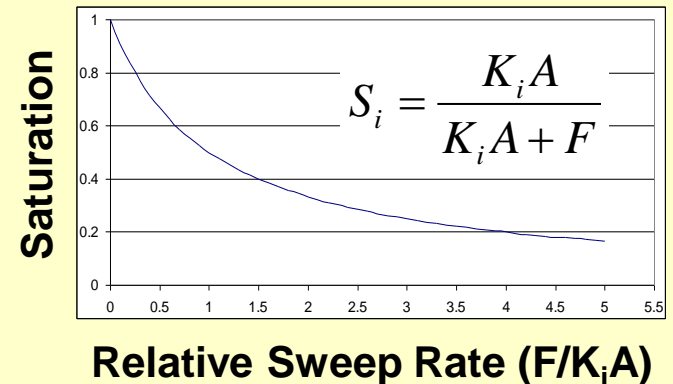
Evaporation Losses

$$Q_m = Q_v$$

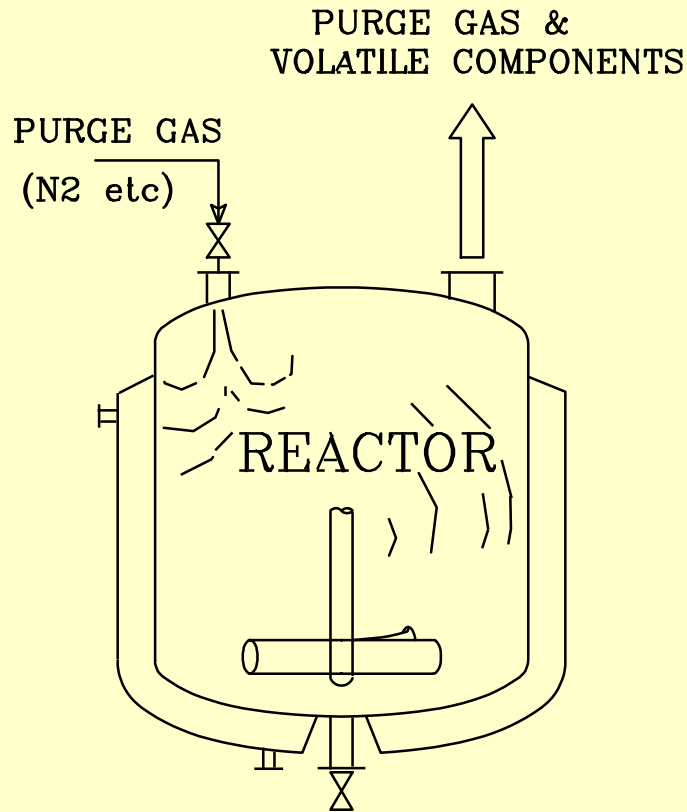
$$\frac{M_i K_i A}{RT} (p_i^{Sat} - p_i) = \frac{M_i F p_i}{RT}$$

$$S_i = \frac{p_i}{p_i^{Sat}} = \frac{K_i A}{K_i A + F}$$

$$E_i = E_{nc} \frac{S_i p_i^{sat}}{p_{nc}}$$



Empty Vessel Purge



Equations

$$p_{i,2} = p_{i,1}e^{-Ft/V} = p_{i,1}e^{-\tau}$$

$$n_i = (p_{i,1} - p_{i,2}) \left[\frac{V}{RT} \right]$$

$$\text{weight}(i) = MWt_i n_i$$

Processing Operations

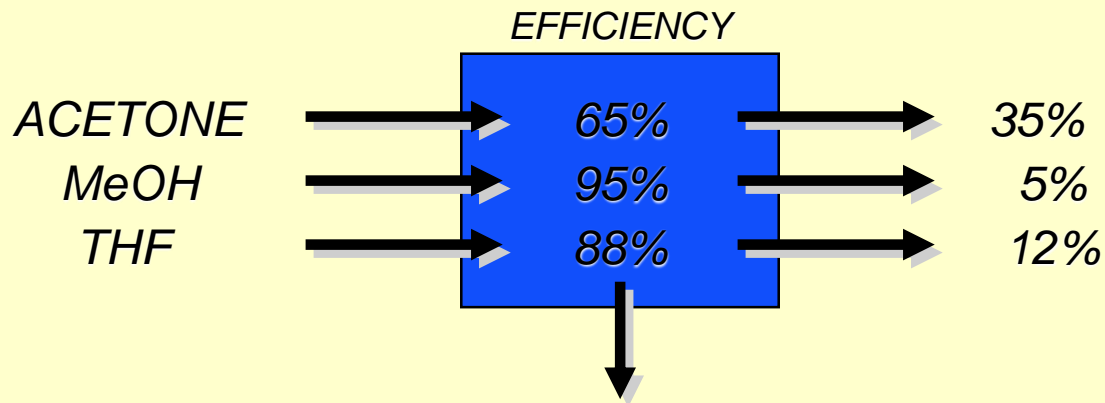
- ***FILLING OPERATIONS / LIQUID TRANSFERS***
- ***FILLED VESSEL PURGE OPERATIONS***
- ***TEMPERATURE ELEVATION***
- ***SYSTEM DEPRESSURIZATION***
- ***VACUUM OPERATIONS***
- ***GAS EVOLUTION***
- ***EMPTY VESSEL PURGE***

Other Operations

- **PRODUCT DRYING OPERATIONS**
- **Distillation**
- **REACTIONS**
- **COMBUSTION (boilers, generators, thermal oxidizers)**
- **FUGITIVE EMISSIONS**
- **STORAGE TANK OPERATIONS**
 - **Fixed Roof**
 - **Floating Roof**

Control Devices

- *CONDENSERS*
- *SCRUBBERS*
- *CARBON ADSORPTION*
- *THERMAL OXIDIZERS*



Manufacturing Recipe

	Product: MS-1032.
	Process: Benzoic Acid Purification.
	Production: 1849 lb.
	Vent RE-100 to CN-100 to CN-143 at 5 C to Vent ID 1012A.
	Vent RE-200 to CN-200 to CN-210 at 5 C to Vent ID 1012A.
	Recipe Step Dissolution.
1	Charge 500 gal of water to RE-100 in 1.0 hours; 5 scfh Nitrogen sweep.
2	Charge 55 lb of Methanol to RE-100 in 15 min; 5 scfh Nitrogen sweep.
3	Charge 1850 lb of Benzoic Acid (s) to RE-100 in 1 hr.
4	Meter 1315 lbs of Sodium Hydroxide (50%) to RE-100 in 30 min.
	Stir the batch in RE-100 for 30 min concurrent; 1 Benzoic Acid + 1 Sodium Hydroxide -> 1 Sodium Benzoate + 1 Water.
	Recipe Step Carbon Treatment.
5	Charge 25 lb of Filter Aid to RE-100 in 15 min.
6	Charge 50 lb of Activated Carbon to RE-100 in 15 min.
7	Heat the batch in RE-100 to 45°C over 30 min.
8	Agitate the batch in RE-100 for 1 hr.
9	Filter the batch in RE-100 through FI-101 to RE-200 in 30 min; wet cake LOD 30%.
10	Charge 150 gal of Water to RE-100 in 15 min.
11	Filter the contents in RE-100 through FI-101 to RE-200 in 30 min; wet cake LOD 30%.
12	Unload the contents in FI-101 to Waste Drum #1 in 30 min.
	Recipe Step Crystallization.
13	Meter 2150 lb of Hydrochloric Acid (28%) to RE-200 over 45 min.
	Reaction in RE-200 over 45 min concurrent; 1 Sodium Benzoate + 1 Hydrogen Chloride -> 1 Benzoic Acid (s) + 1 Sodium Chloride.
	Stir the batch in RE-200 for 45 min concurrent; 1 Sodium Hydroxide + 1 Hydrogen Chloride -> 1 Sodium Chloride + 1 Water.
14	Cool the batch in RE-200 to 10°C over 1 hr.
	Recipe Step Centrifugation.
15	Centrifuge the batch in RE-200 through CE-100 to RE-300 for 1 hr; wet cake LOD 12%.
16	Filter 50 gal of Water at 10 C through CE-100 to RE-300 in 30 min; wet cake LOD 12%.
17	Spin the batch in CE-100 for 45 min.
18	Unload the batch in CE-100 to Product Containers during 30 min.

Process Modeling Software

The screenshot displays the 'Emission Master' software interface for a process named 'MS-Benzoic Acid (Pure).emmm'. The window title is 'MS-Benzoic Acid (Pure).emmm - Emission Master'. The menu bar includes 'File', 'Add Step', 'Edit Step', 'Tools', 'Databases', 'Options', 'View', 'Reports', 'Export', and 'Help'. The main window is divided into three sections: 'Title Page', 'Summary Page', and 'Defined Activities'.

Title Page

A.	Title	Vessel
1	Charge 500 gal of water to RE-100 in 1.0 hours	RE-100
2	Charge 55 lb of Methanol to RE-100 in 15 min	RE-100
3	Charge 1850 lb of Benzoic Acid (s) to RE-100 in 1 hr	RE-100
4	Meter 1315 lbs of Sodium Hydroxide (50%) to RE-100 in ...	RE-100
5	Stir the batch in RE-100 for 30 min concurrent [1 Benzoic...	RE-100
6	Charge 25 lb of Filter Aid to RE-100 in 15 min	RE-100
7	Charge 50 lb of Activated Carbon to RE-100 in 15 min	RE-100
8	Heat the batch in RE-100 to 45°C over 30 min	RE-100
9	Agitate the batch in RE-100 for 1 hr	RE-100
10	Filter the batch in RE-100 through FI-101 to RE-200 in 30 ...	FI-101
11	Filter the batch in RE-100 through FI-101 to RE-200 in 30 ...	RE-200
12	Charge 150 gal of Water to RE-100 in 15 min	RE-100
13	Filter the contents in RE-100 through FI-101 to RE-200 in ...	FI-101
14	Filter the contents in RE-100 through FI-101 to RE-200 in ...	RE-200
15	Unload the contents in FI-101 to Waste Drum #1 in 30 min	Waste Dru...
16	Meter 2150 lb of Hydrochloric Acid (28%) to RE-200 over...	RE-200
17	Reaction in RE-200 over 45 min concurrent [1 Sodium B...	RE-200
18	Stir the batch in RE-200 for 45 min concurrent [1 Sodi...	RE-200

Summary Page

Defined Activities

- 1) [Charge] Charge 500 gal of water to RE-100 in 1.0 hours
- 2) [Charge] Charge 55 lb of Methanol to RE-100 in 15 min
- 3) [Charge] Charge 1850 lb of Benzoic Acid (s) to RE-100 in 1 hr
- 4) [Charge] Meter 1315 lbs of Sodium Hydroxide (50%) to RE-100 in 30 min
- 5) [React] Stir the batch in RE-100 for 30 min concurrent [1 Benzoic Acid + 1 Sodium Hydroxide -> 1 Sodium Benzoate + 1 Water]

Title Page

Product: MS-1032
Process: Benzoic Acid Purification
Process Cycle Time: 660.0 min
Final Product Amount: 1849.0 lb
Evaluation Date: 5/15/2018
File Name: MS-Benzoic Acid (Pure).emmm
Connected Database: C:\Users\Allen Hatfield\Documents\Emission Master
Calculation type: MACT98
Condenser Calc. type: Single Stage
Charge Calc. type: Average Composition
Material Balance: Subtract Emissions
Last Saved User:
Last Saved Time:
Comment: A process intermediate is dissolved, carbon treated,

Process Gantt Chart

	0.0 hr.	2.0 hr.	4.0 hr.	6.0 hr.	8.0 hr.	10.0 hr.
RE-100	1) Charge 500 gal of water to RE-100 in 1.0 hours	2) Charge 1850 lb of Benzoic Acid (s) to RE-100 in 1 hr	3) Charge 1850 lb of Benzoic Acid (s) to RE-100 in 1 hr	4) Meter 25 lb of 5) Stir the batch in	6) Charge 25 lb of 7) Charge 50 lb of 8) Heat the batch in	9) Agitate the batch in RE-100 for 1 hr
FI-101				10) Filter the batch in	13) Filter the container	
RE-200				11) Filter the batch in	14) Filter the container	16) Meter 2150 lb of 17) Reaction 18) Stir the batch 19) Cool the batch in RE-200 to 10°C over 1 hr
Waste Drum #1					15) Unload the container	
CE-100					20) Centrifuge the batch in RE-200 through	22) Filter 50 gal of Water 24) Spin the batch in CE-100 for 45 min
RE-300					21) Centrifuge the batch in RE-200 through	23) Filter 50 gal of Water
Product Contain						25) Unload the batch in

Emissions Analysis

The batch is then precipitated and isolated using a centrifuge				
Compound	Activities Emitting	Emissions Uncontrolled (lb)	Emissions Controlled (lb)	Emissions Percent Removal
Benzoic Acid	11	1.259E-05	1.240E-05	1.510
Carbon	8	0	0	
Hydrogen Chloride	12	0.0107	0.0077	28.129
Methanol	27	0.0678	0.0538	20.667
Nitrogen	34	53.0820	53.0820	0
Silicon Dioxide	9	0	0	
Sodium Benzoate	13	0	0	
Sodium Chloride	10	0	0	
Sodium Hydroxide	16	0	0	
Water	29	0.9891	0.7938	19.743
Compound	Process Cycle Average (lb/hr)	Compound Emission Hours	Compound Emission Average (lb/hr)	Max Rate (lb/hr) Within 1 hour
Benzoic Acid	1.127E-06	5.999	2.067E-06	1.024E-05
Carbon	0	3.249	0	0
Hydrogen Chloride	6.979E-04	4.498	1.707E-03	7.481E-03
Methanol	4.891E-03	9.747	5.520E-03	3.088E-02
Nitrogen	4.8256	10.996	4.8273	21.4267
Silicon Dioxide	0	3.499	0	0
Sodium Benzoate	0	4.249	0	0
Sodium Chloride	0	4.499	0	0
Sodium Hydroxide	0	4.748	0	0
Water	0.07217	10.997	0.07219	0.5015
(1) Process Cycle Average = Compound emission quantity / Total process cycle time in hours.				
(2) Compound Emission Average = Compound emission quantity / Compound emission time in hours.				