Emissions Inventory Development through Computer Modeling

Abstract #476000

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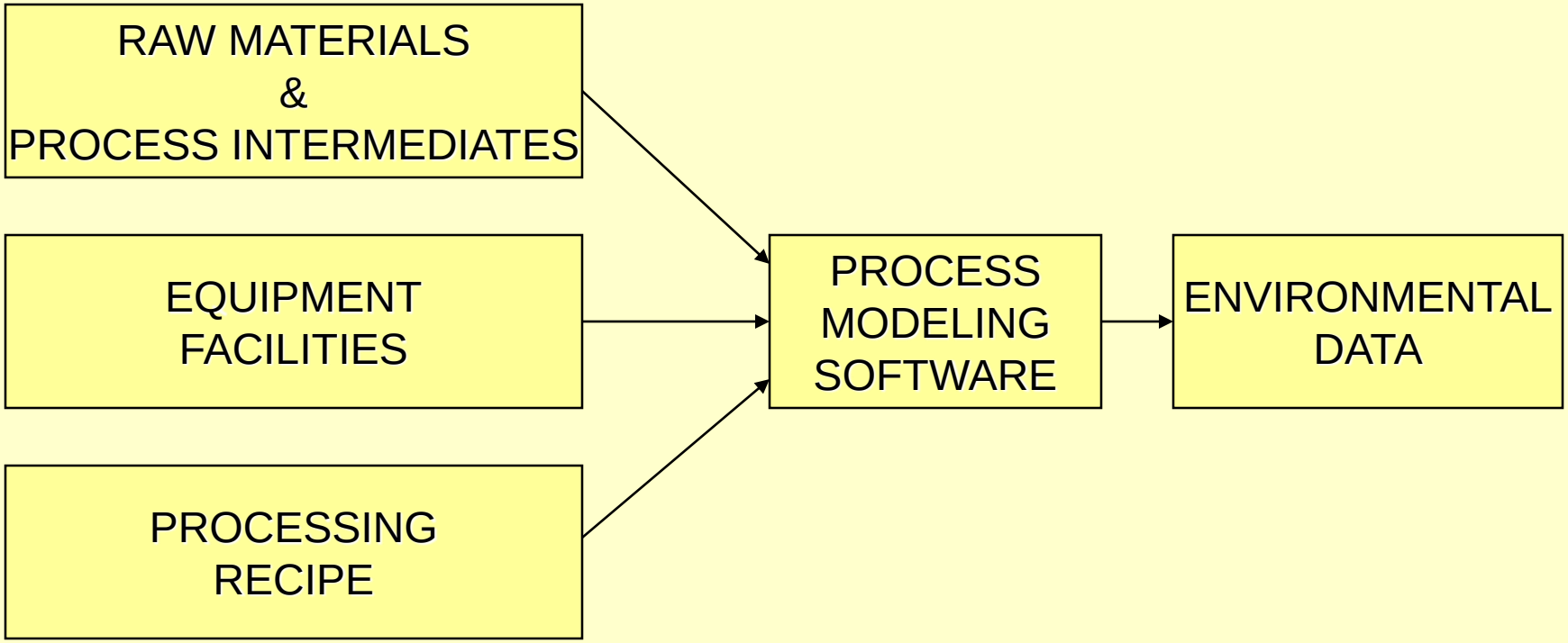
Process Modeling for Environmental Assessment



MANUFACTURING INFORMATION

SIMULATION

EVALUATION RESULTS (CALCULATED)

Underlying Principles

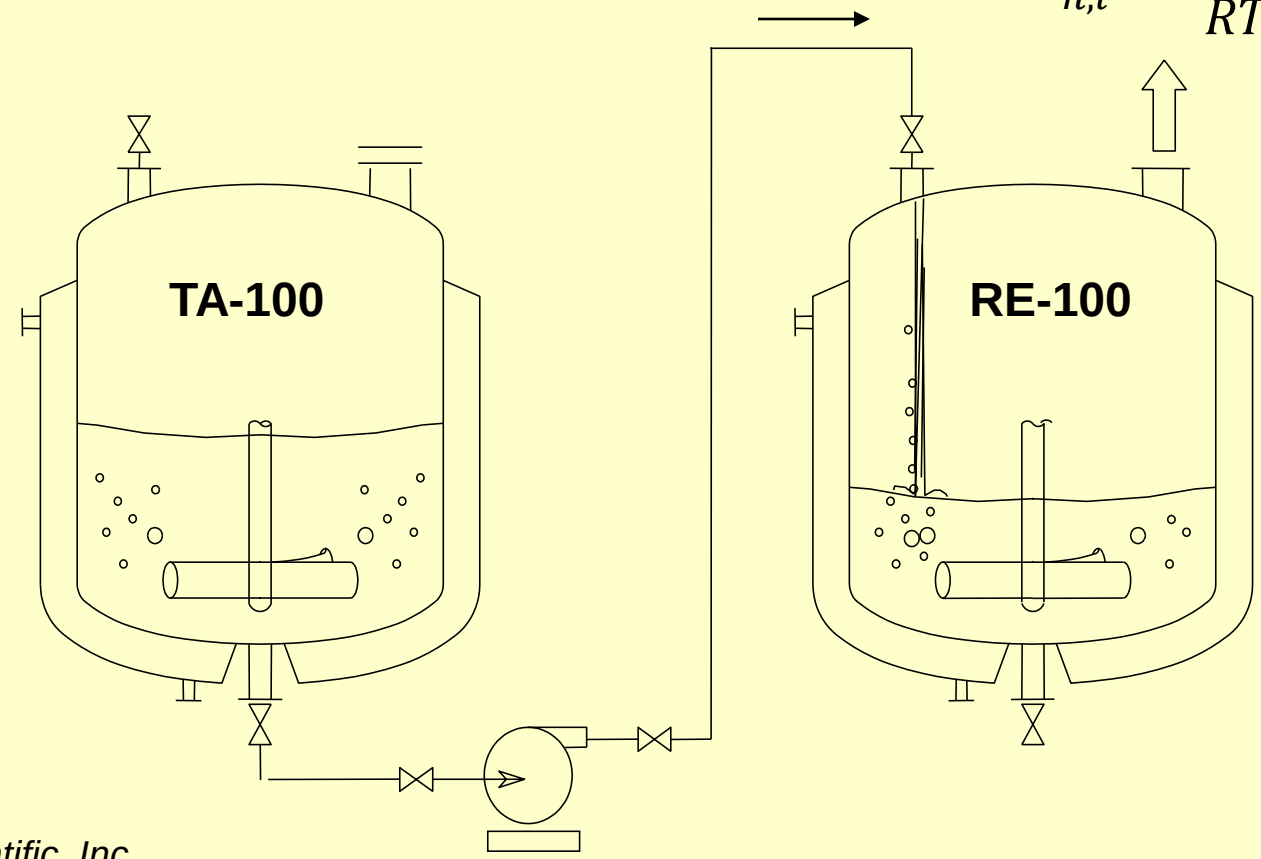
- *Ideal Gas Law*
- *Pure Component Vapor Pressures*
- *Raoult's Law of solution properties*
- *Activity Coefficients?*
- *Dalton's Law - Partial Pressures*
- *Vapor Space Composition*

Above Surface Additions

Volatile Components & Air, Nitrogen

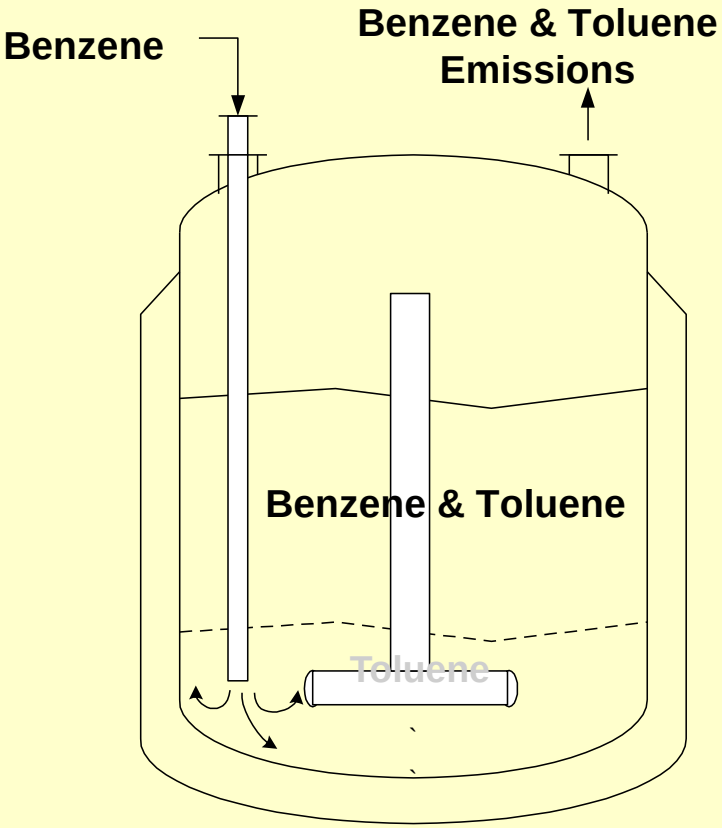
Charges & Transfers

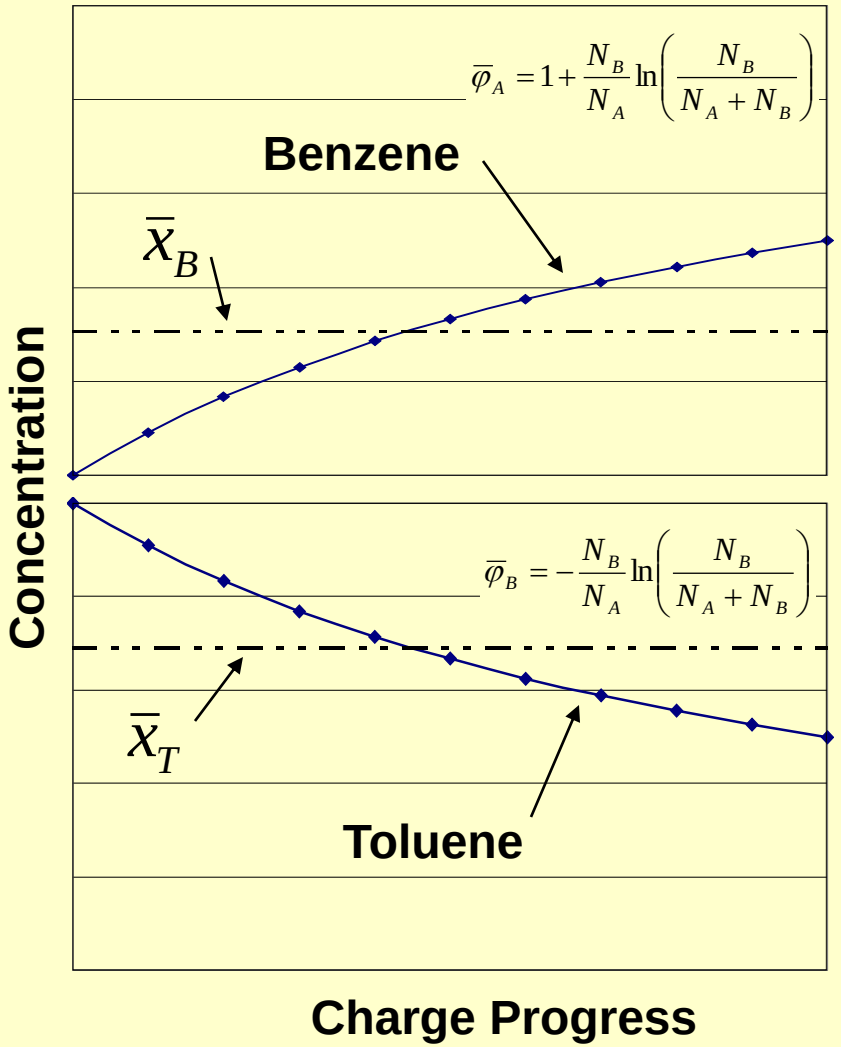
$$E_{n,i} = \frac{p_i \Delta V}{RT}$$



Subsurface Additions

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





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Above Surface vs Subsurface

Above Surface Addition

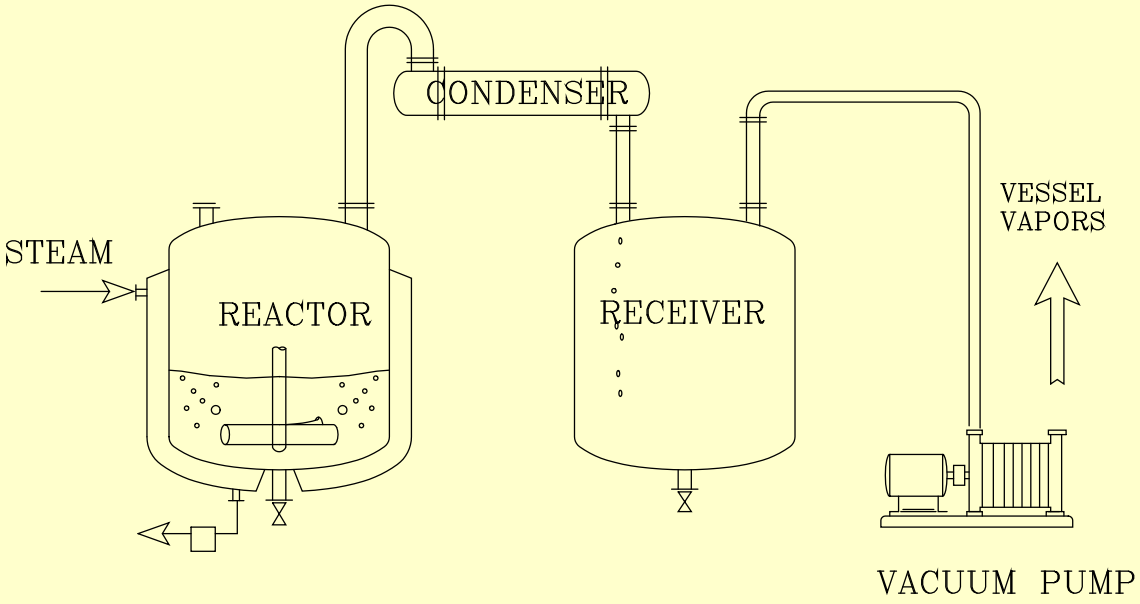
Inlet Stream	X_i	$\overline{\varphi_A}$ $\overline{\varphi_B}$	$\overline{X}_i$	$P_{i,mm\ Hg}$	$p_{i,mm\ Hg}$
Benzene	**1.0**	**1.000**	**1.000**	**182.8**	**182.8**
Toluene	**1.0**	**0.693**	**0.693**	**59.2**	**41.0**

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

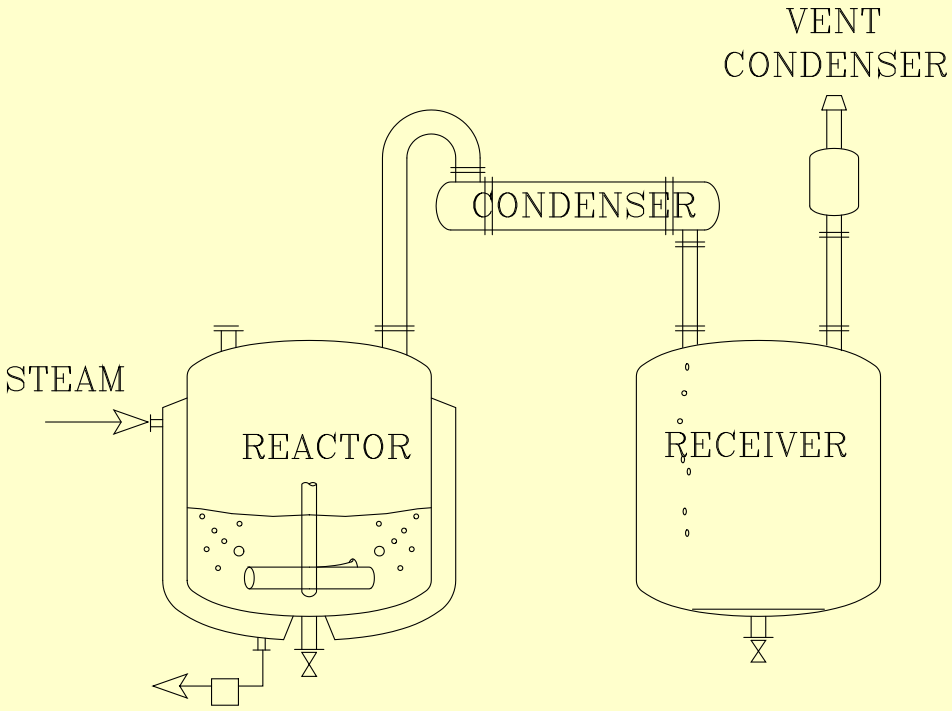
System Depressurization



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

1998 Equation (MACT)

Temperature Elevation

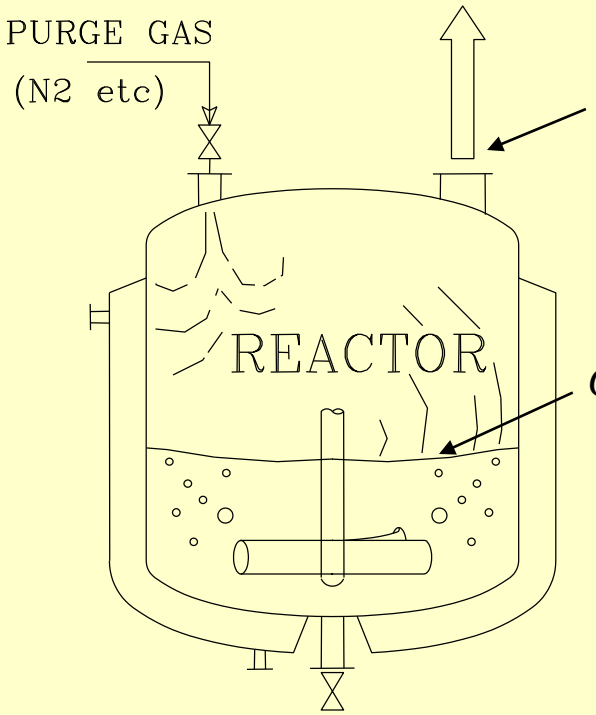


$$n_{i,out} = N_{avg} \ln\left(\frac{p_{nc,1}}{p_{nc,2}}\right) - \left(n_{i,2} - n_{i,1}\right)_{headspace}$$

1998 Equation (MACT)

Gas Sweep Operations

Volatile Components & Air, Nitrogen



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

Vent Losses

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

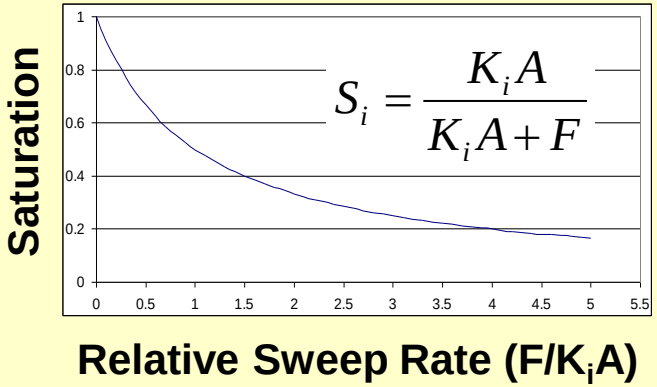
Evaporation Losses

$$Q_m = Q_v$$

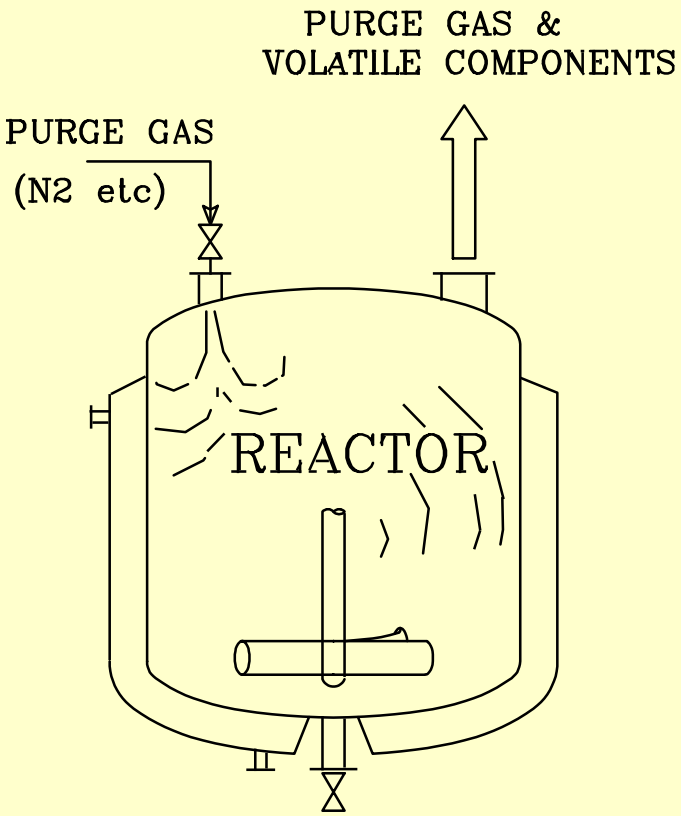
$$\frac{M_i K_i A}{RT}\left(p_i^{Sat} - p_i\right) = \frac{M_i F p_i}{RT}$$

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

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



Empty Vessel Purge



Equations

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

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

$$weight(i) = MWt_i n_i$$

Processing Operations

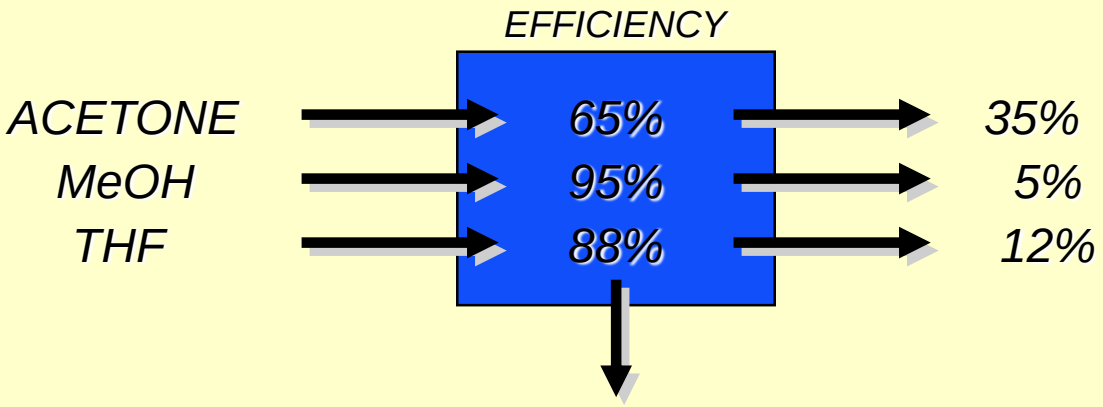
- ***FILLING OPERATIONS / LIQUID TRANSFERS***
- ***FILLED VESSEL PURGE OPERATIONS***
- ***TEMPERATURE ELEVATION***
- ***SYSTEM DEPRESSURIZATION***
- ***VACUUM OPERATIONS***
- ***GAS EVOLUTION***
- ***EMPTY VESSEL PURGE***

Other Operations

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

Control Devices

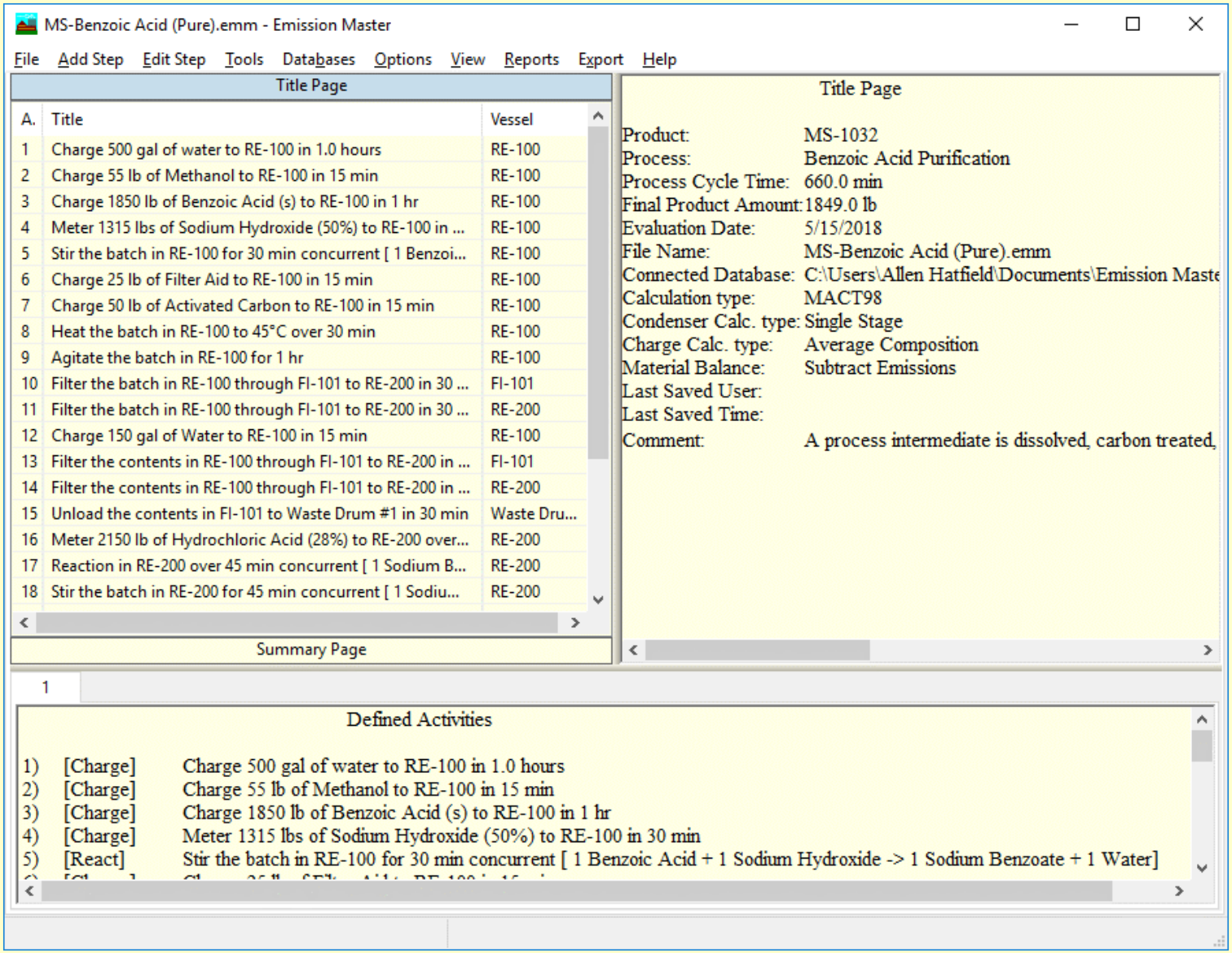
- *CONDENSERS*
- *SCRUBBERS*
- *CARBON ADSORPTION*
- *THERMAL OXIDIZERS*



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



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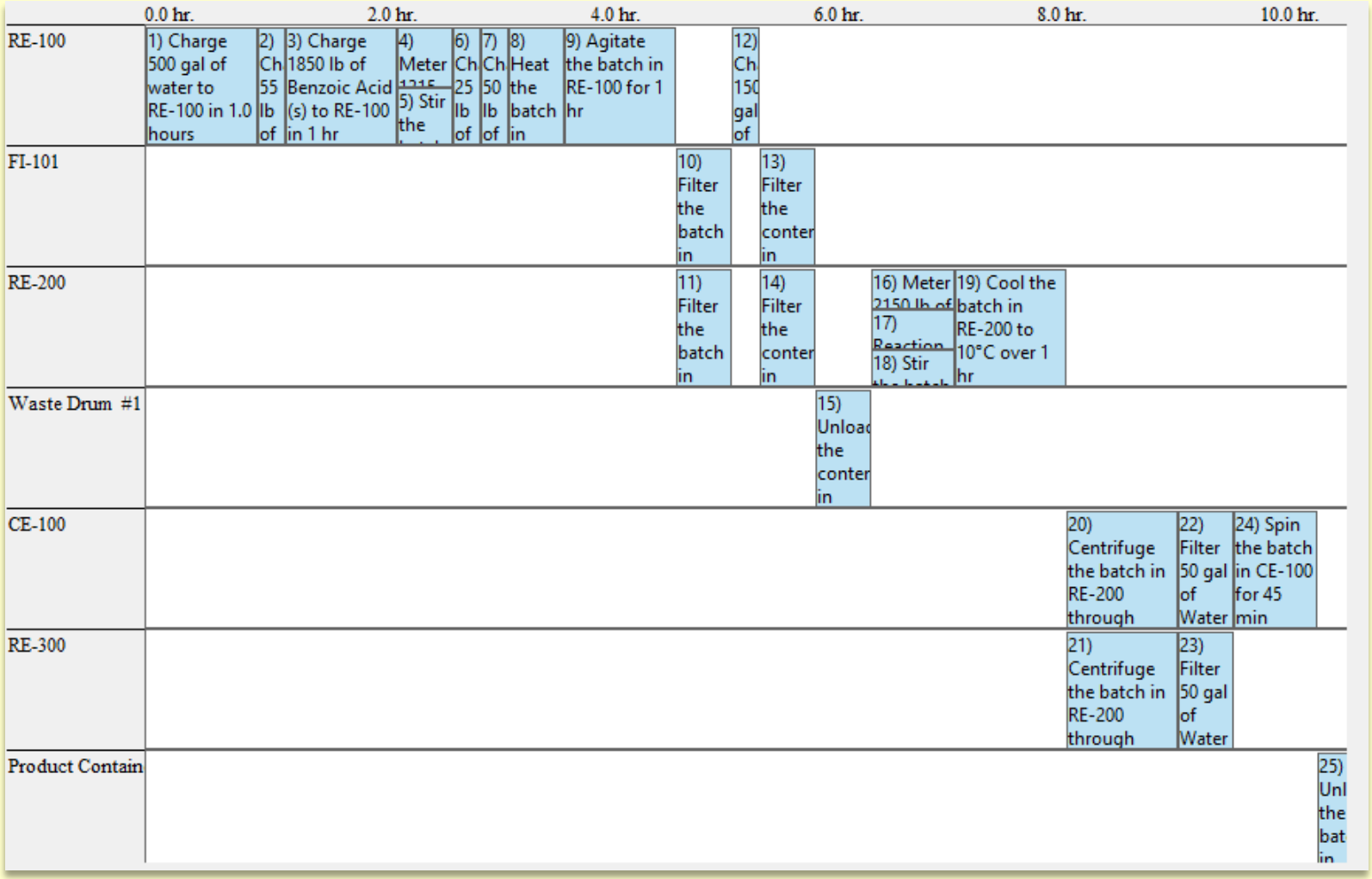
Process Gantt Chart



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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.