Chapter 16: Methods for Estimating Air Emissions from Chemical Manufacturing Facilities

Mitchell Scientific, Inc.

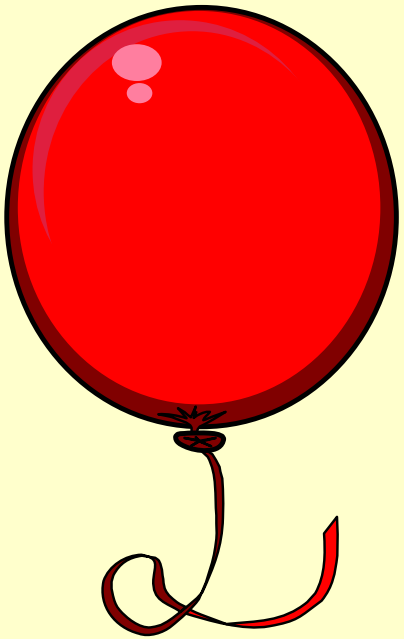
GUIDANCE DOCUMENT EVOLUTION

- 1978 CTG
- 1994 ACT
- 2007 CHAPTER 16

CHAPTER 16 BASIC PRINCIPLES

- APPLIES TO MOST CHEMICAL PROCESS OPERATIONS
- PROVIDES STANDARDIZED CALCULATIONS
- CONSERVATIVE ESTIMATES (WORST CASE)

IDEAL GAS LAW

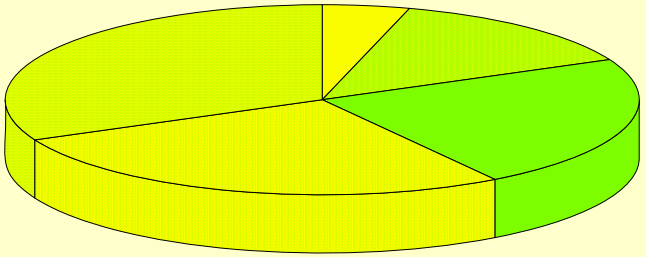


$$n = \frac{PV}{RT}$$

$$nRT = PV$$

DALTON'S LAW

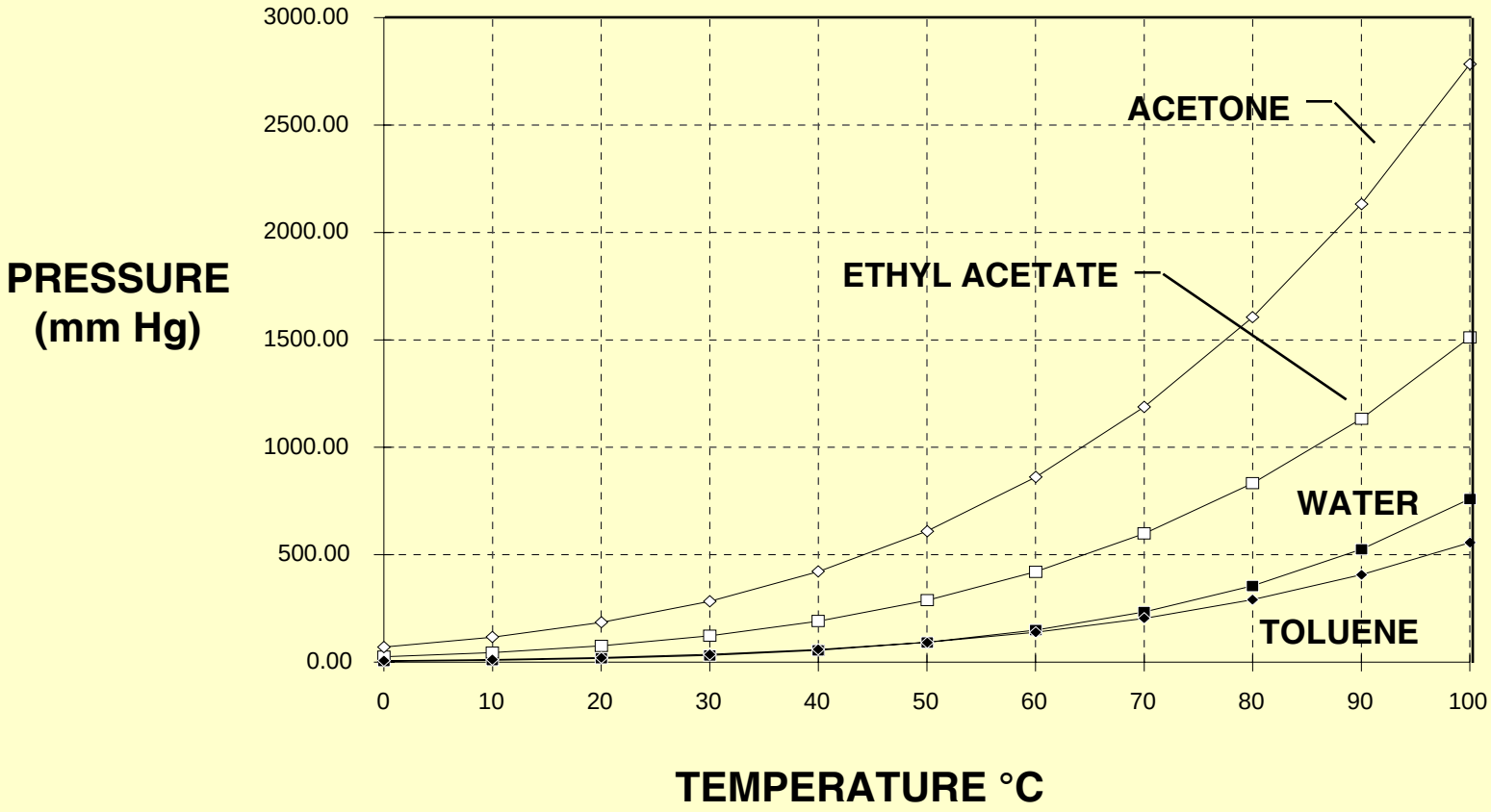
$$n_i = \frac{P_i V}{RT}$$



$$P_T = P_1 + P_2 + P_3 + \bullet\bullet\bullet + P_n$$

$$n_T = n_1 + n_2 + n_3 + \bullet\bullet\bullet + n_n$$

PURE COMPONENT VAPOR PRESSURE



Mitchell Scientific, Inc.

PURE COMPONENT VAPOR PRESSURE MODELS

- **Clapeyron Equation**
- **Antoine Equation**
- **Riedel Equation**
- **DIPPER Database Equation**

T = °K, °C, °F, °R, ???

(TYPICAL OF ALL VOLATILE ORGANIC COMPOUNDS)

RAOULT'S LAW

IDEAL MIXTURE

$$p_i = x_i P_i$$

NON IDEAL MIXTURE

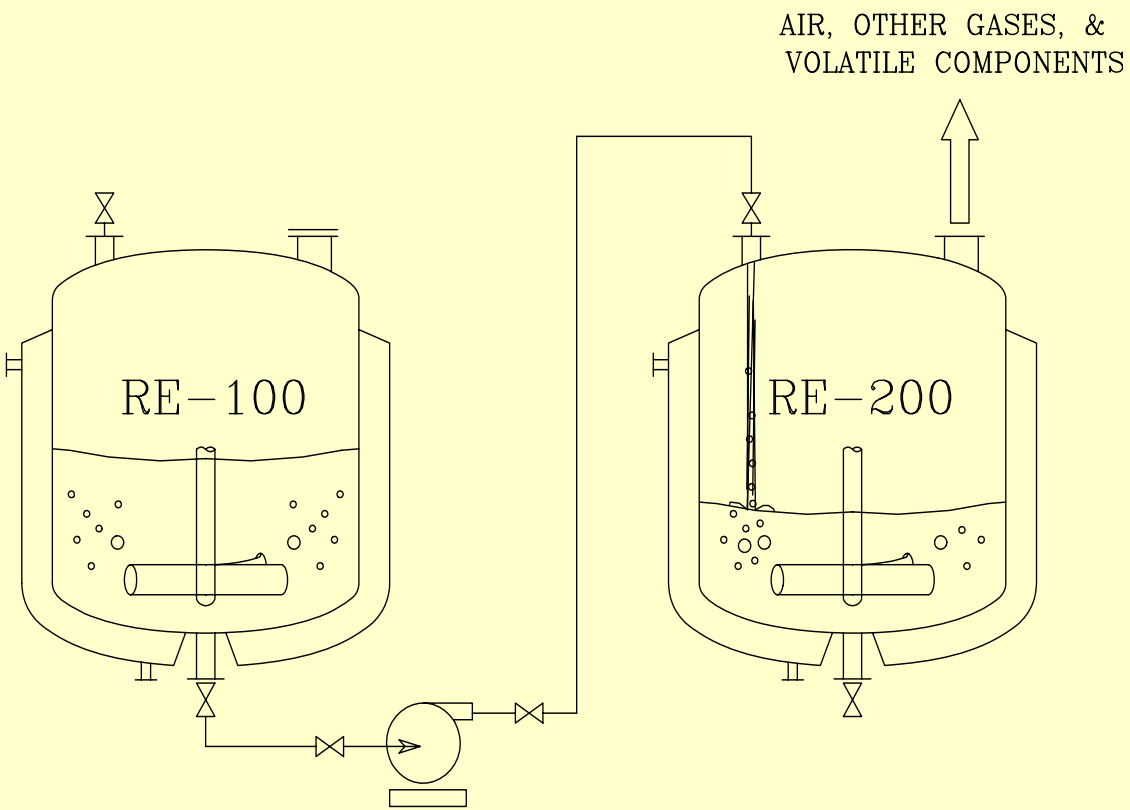
$$p_i = x_i \gamma_i P_i$$

Mole Fraction of Component 'i' in Gas Space

$$p_i = x_i \gamma_i P_i$$

$$y_i = \frac{p_i}{P_T}$$

FILLING OPERATIONS



Equations

$$E_n = \frac{PV}{RT}$$

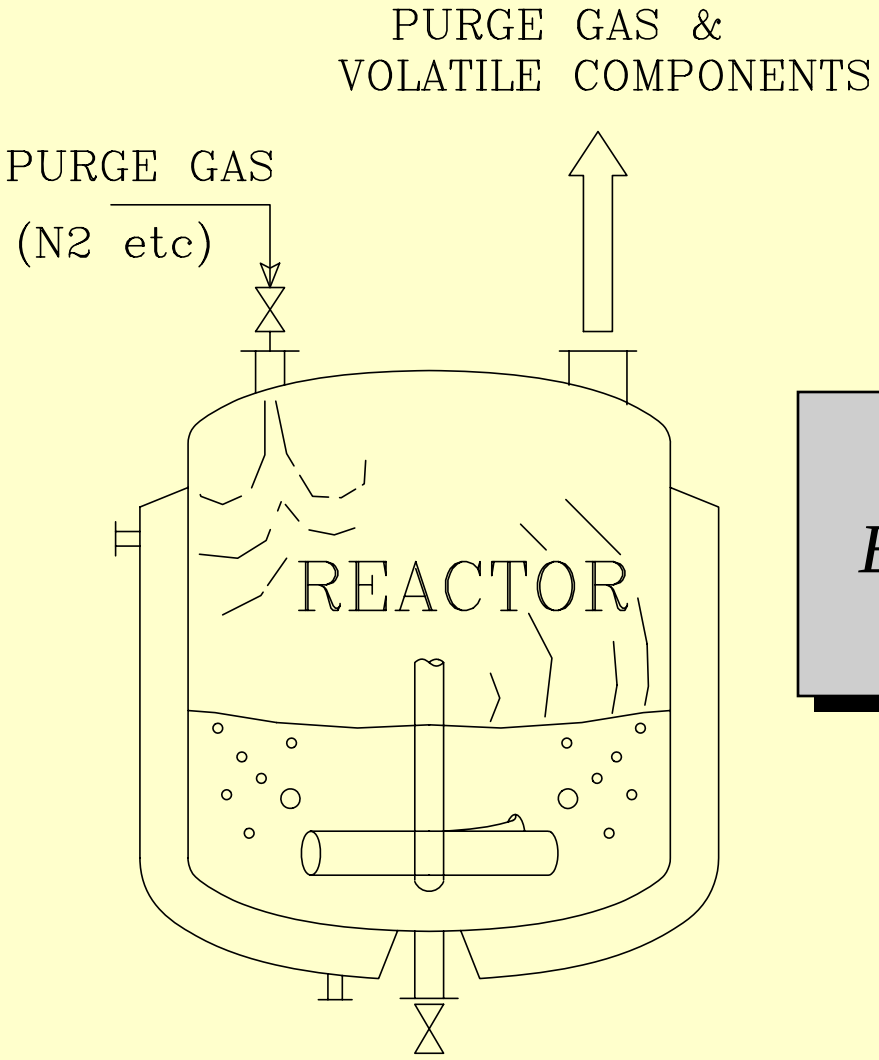
$$E_i = \frac{p_i V}{RT}$$

PARTIAL PRESSURE RATIO MODELS

$$\frac{n_i}{n_{nc}} = \frac{p_i}{p_{nc}}$$

$$n_i = n_{nc} \frac{p_i}{p_{nc}}$$

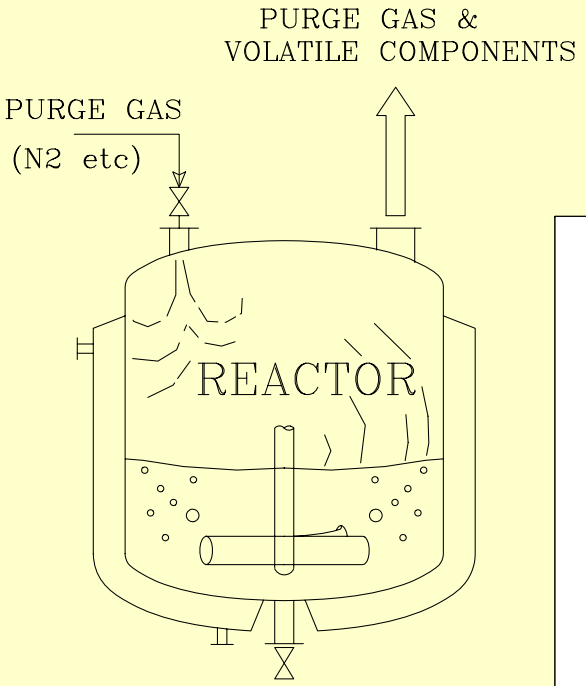
PURGE / SWEEP OPERATIONS

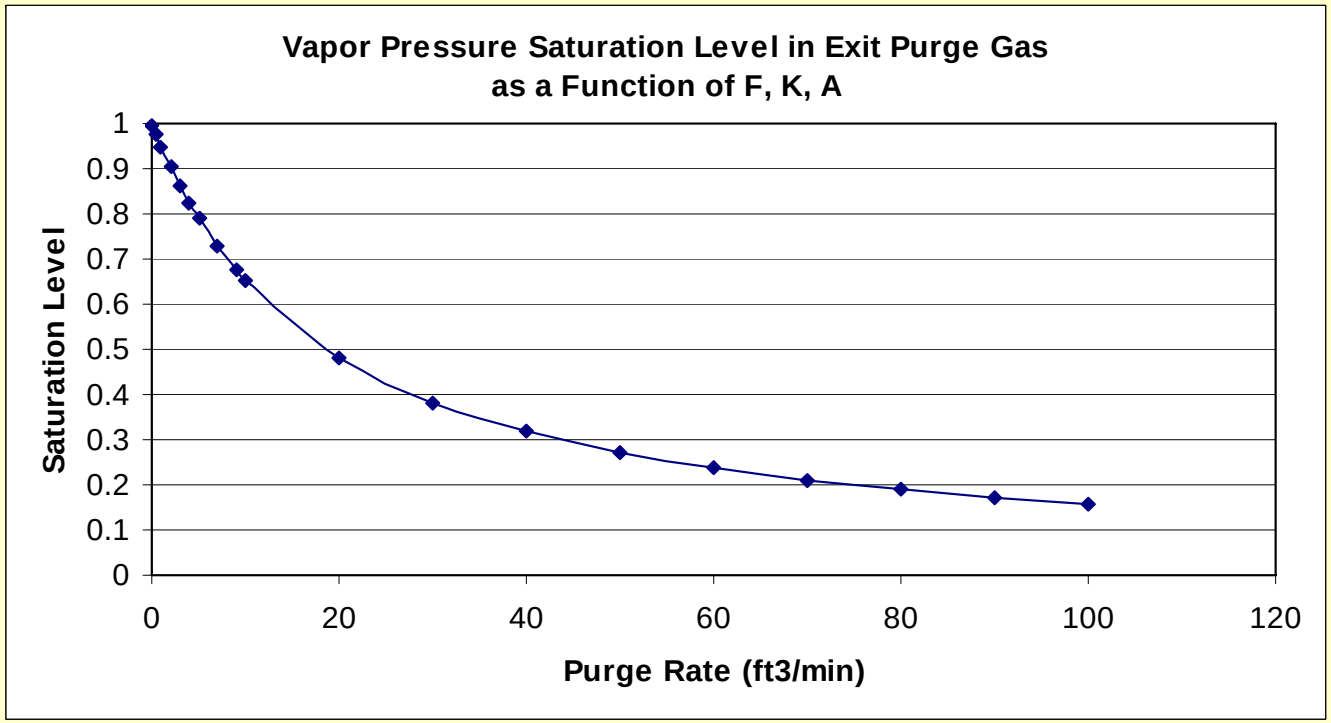


$$E_{R-i} = E_{R-nc}\frac{p_i}{p_{nc}} = E_{R-nc}S_i\frac{p_i^{sat}}{p_{nc}^{sat}}$$

PURGE / SWEEP OPERATIONS

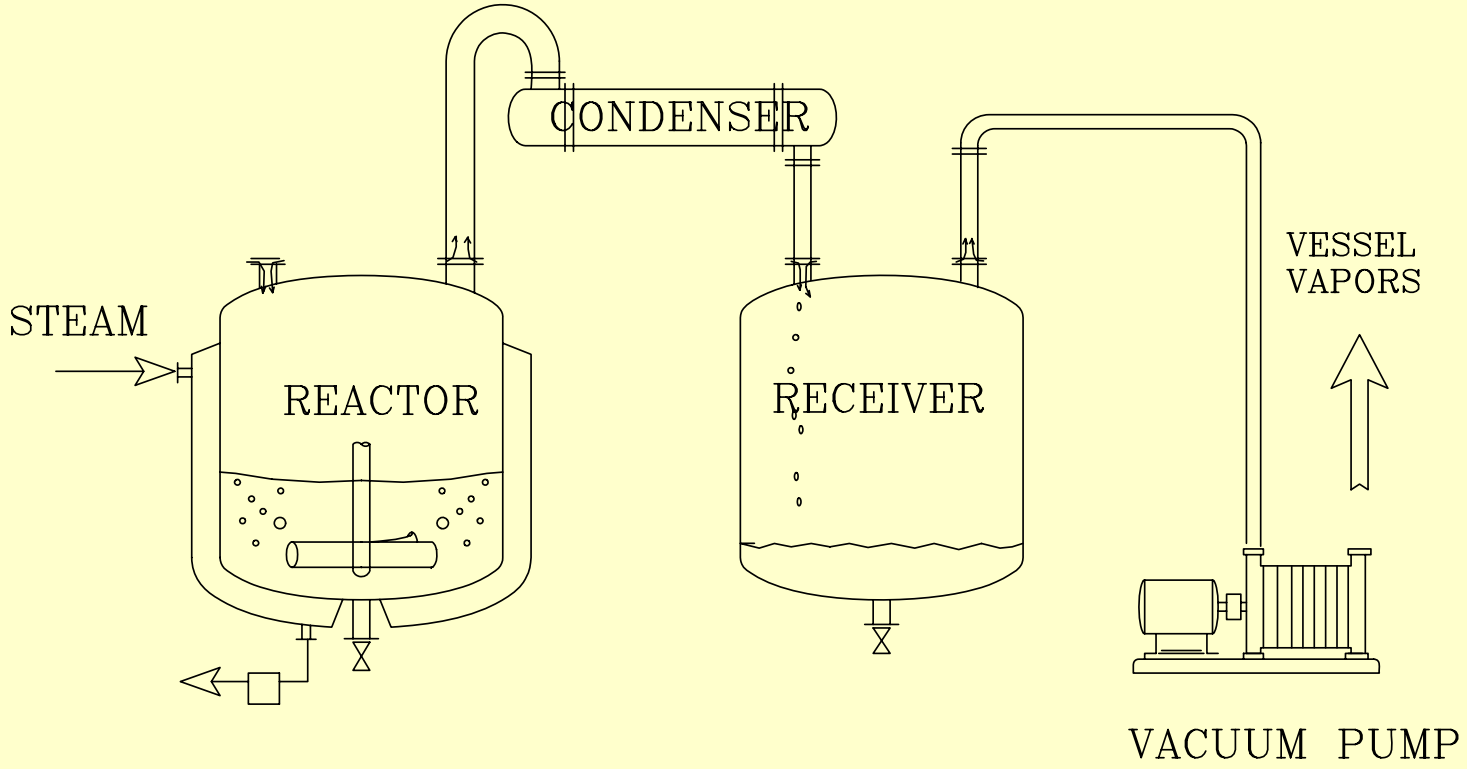
$$S_i = \frac{p_i}{P_i^{Sat}} = \frac{KA}{F + KA}$$





Mitchell Scientific, Inc.

VACUUM OPERATION

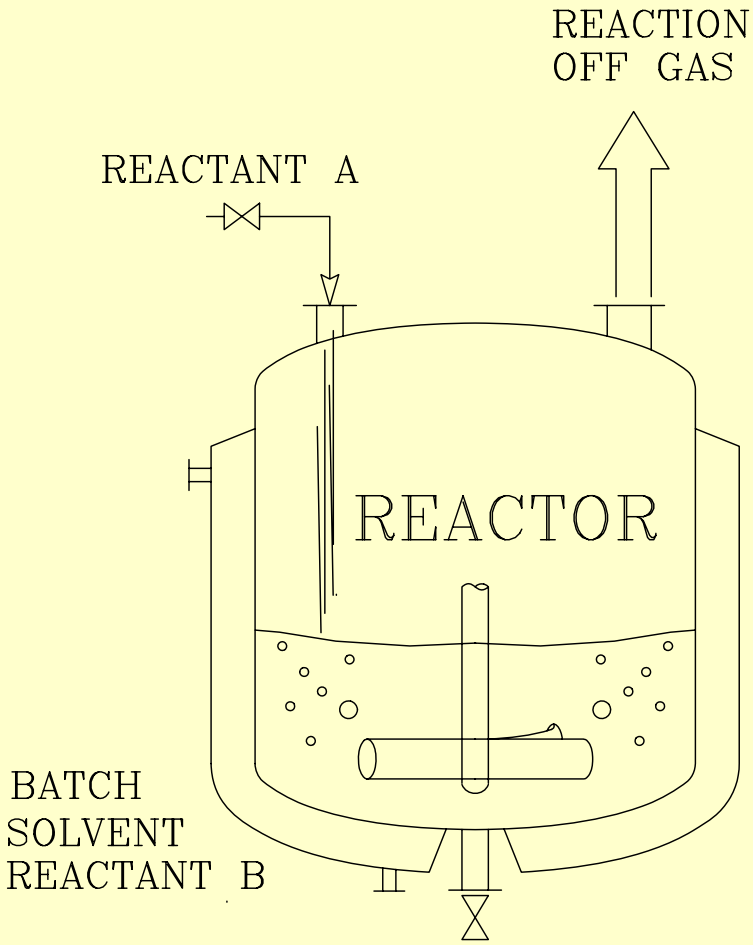


Equation

$$E_i = E_{nc} \frac{p_i}{p_{nc}}$$

Mitchell Scientific, Inc.

GAS EVOLUTION



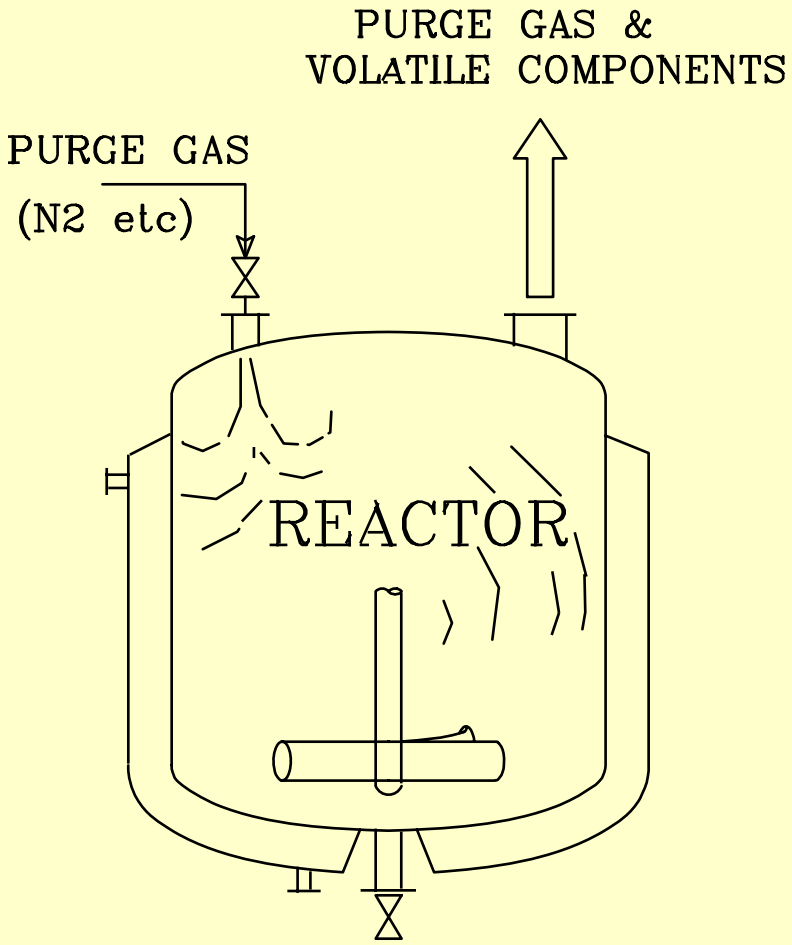
Equation

$$E_i = E_{rxn} \frac{p_i}{p_{rxn}}$$

DYNAMIC CHANGING CONDITION MODELS

- EMPTY VESSEL PURGE
- DEPRESSURIZATION
- HEATING

EMPTY VESSEL PURGE

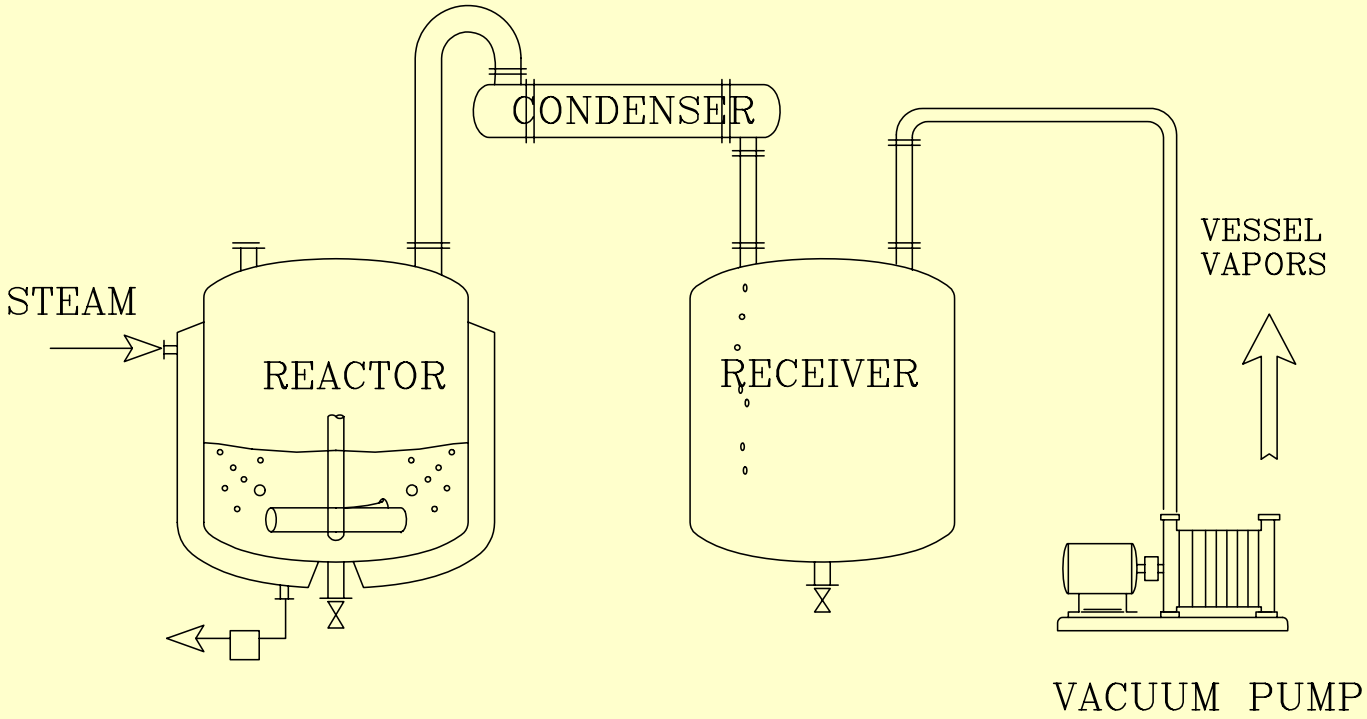


Equations

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

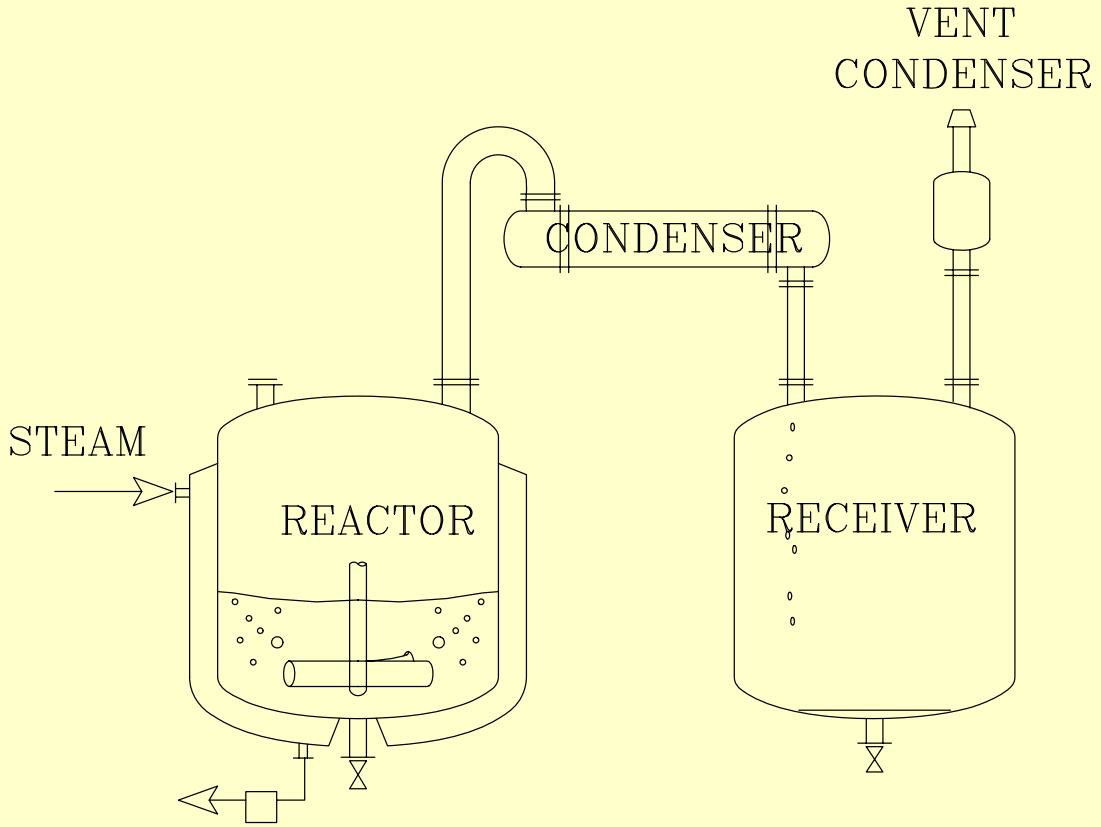
$$E_{n-i} = \frac{p_{i,1} V}{RT}\left(1 - e^{-Ft/V}\right)$$

DEPRESSURIZATION



$$n_{voc,out} = n_{voc,vsl} \ln\left(\frac{P_{nc,1}}{P_{nc,2}}\right)$$

HEATING



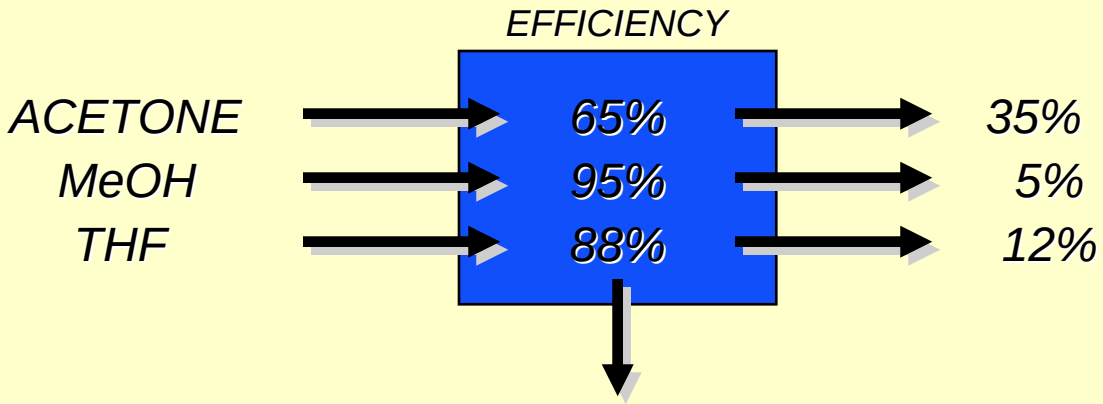
$$n_{voc,out} = N_{avg} \ln\left(\frac{p_{nc,1}}{p_{nc,2}}\right) - \left(n_{voc,2} - n_{voc.1}\right)_{headspace}$$

PROCESS OPERATIONS

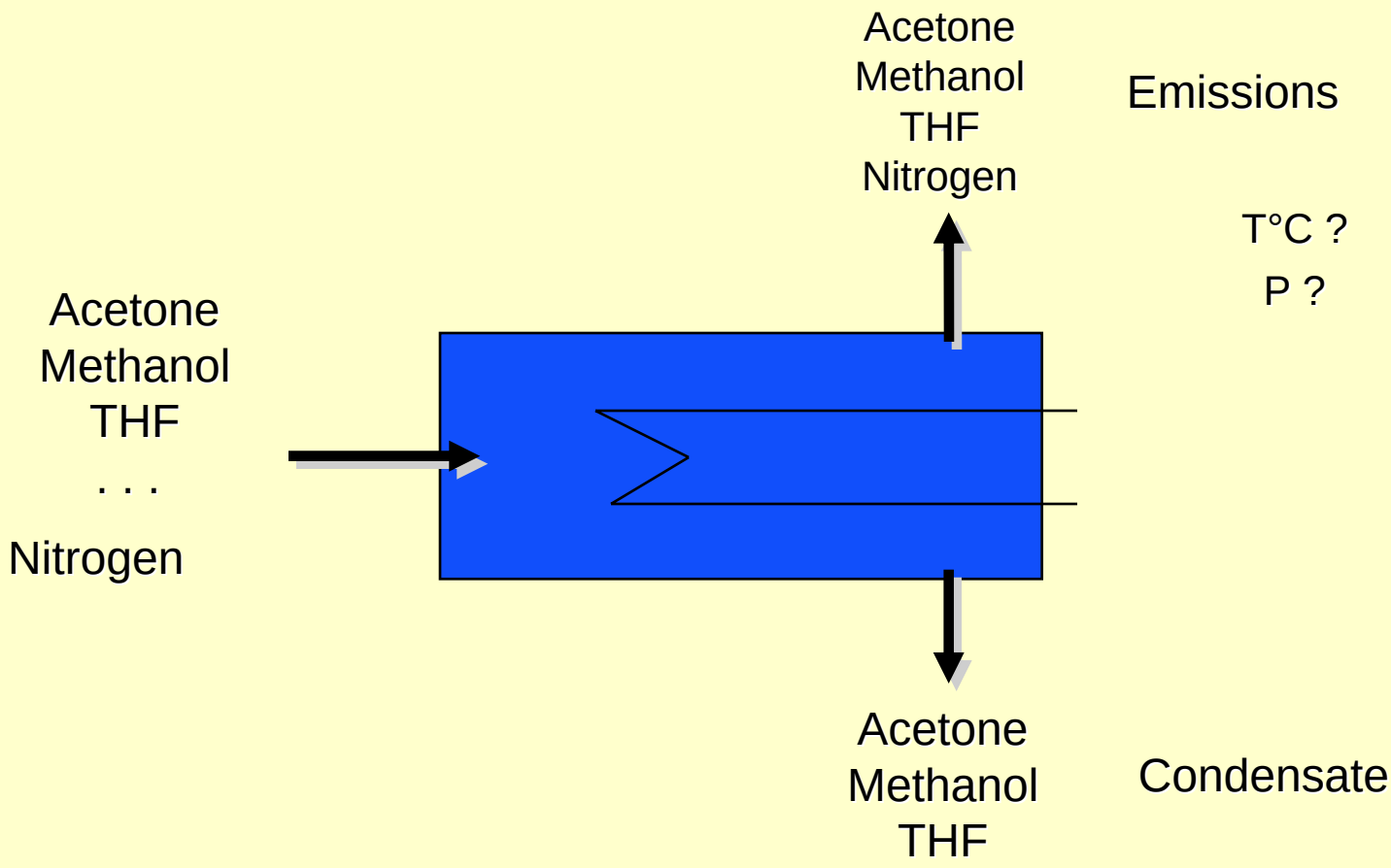
- **LIQUID TRANSFERS / FILLING OPERATIONS**
- **FILLED VESSEL PURGE OPERATIONS**
- **GAS SWEEP MODEL**
- **SEMI-CONTINUOUS VACUUM OPERATIONS**
- **GAS EVOLUTION**
- **EMPTY VESSEL PURGE**
- **TEMPERATURE ELEVATION**
- **SYSTEM DEPRESSURIZATION**
- **OTHER ACTIVITIES . . .**

SINGLE STAGE VENT DEVICES

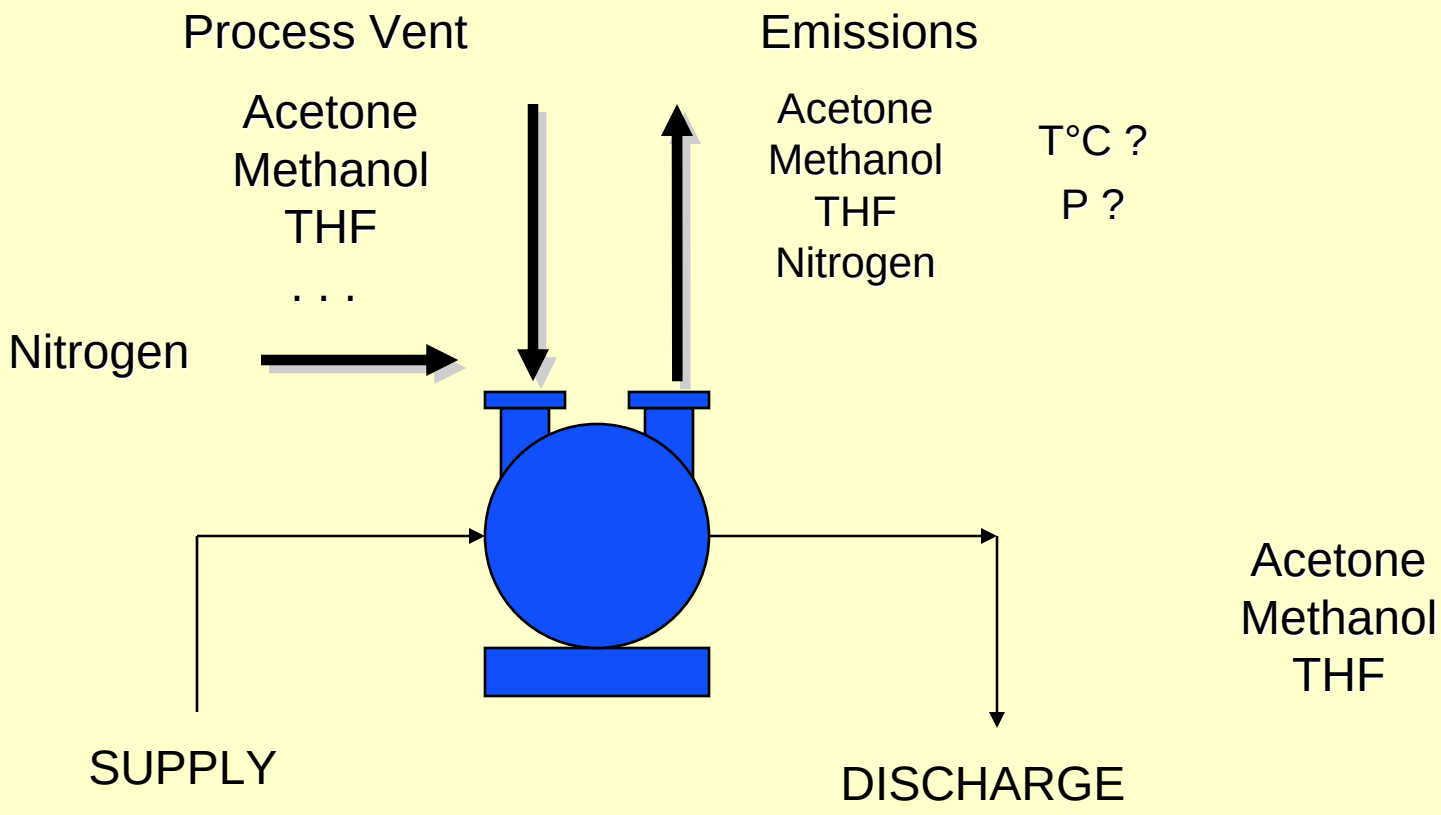
- *VENT CONDENSERS*
- *LIQUID RING VACUUM PUMPS*
- *VACUUM STEAM JETS*



CONDENSERS


Acetone
Methanol
THF
Nitrogen
Emissions
T°C ?
P ?
Acetone
Methanol
THF
. . .
Nitrogen
Acetone
Methanol
THF
Condensate

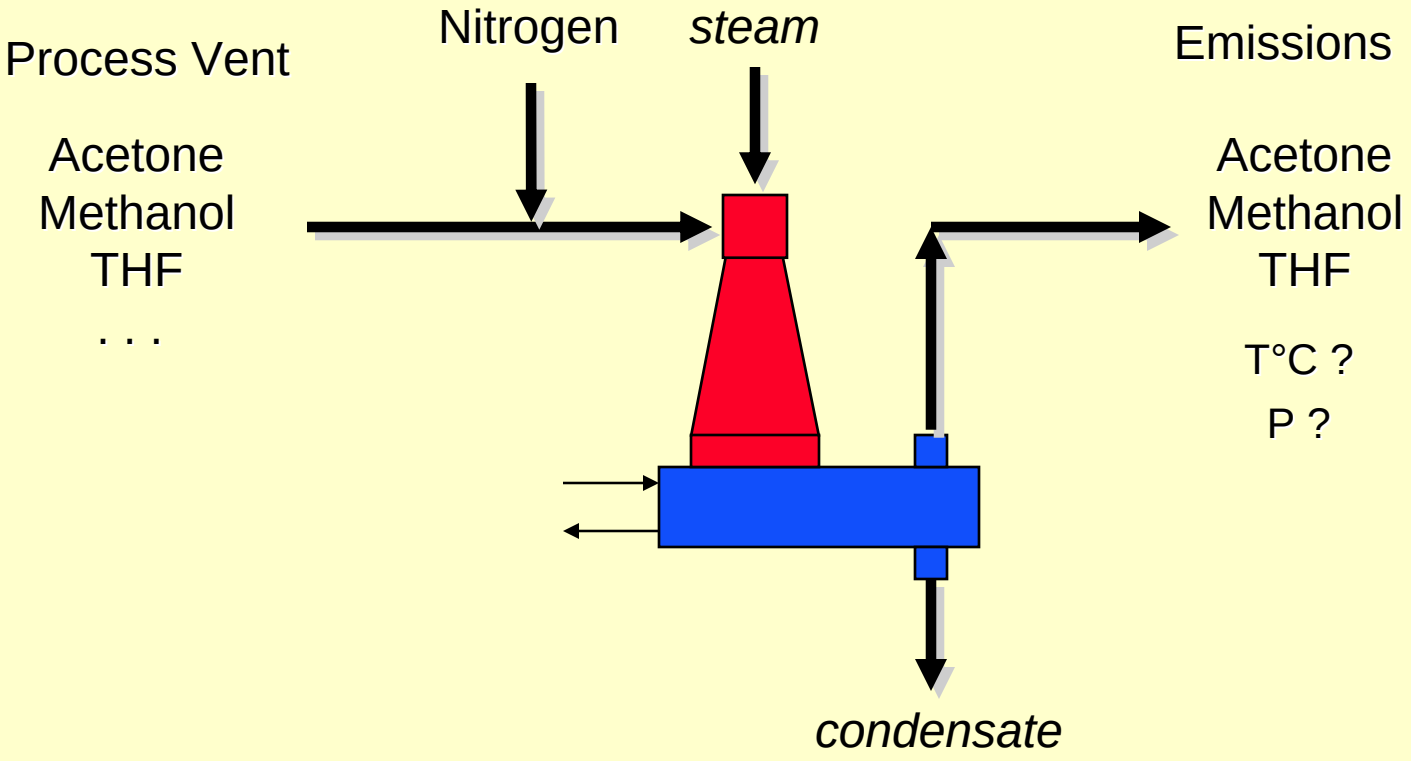
VACUUM PUMP



LIQUID RING VACUUM PUMP

Mitchell Scientific, Inc.

VACUUM STEAM JET



Mitchell Scientific, Inc.

SINGLE STAGE VENT DEVICES

Modified Rachford-Rice Equation

$$f\left(V/F\right) = \sum_{i=1}^{C_{cond}} \frac{\left(K_i - 1\right) z_i}{1 + \left(K_i - 1\right) V/F} + \sum_{i=1}^{C_{nc}} \frac{z_i}{V/F} = 0 \qquad K_i = \frac{y_i}{x_i}$$

Partial Pressure Correction Method

$$n_{i,L,k+1} = n_{i,L,k} - \frac{f\left(n_{i,k}\right)}{f'\left(n_{i,k}\right)} \qquad f\left(n_i\right) = p_{i,L} - p_{i,V}$$

Partial Pressure Correction Method

$$n_{i,L,k+1} = \frac{n_{i,L,k}}{\phi_{i,k}} \qquad \phi_i = \frac{n_{i,L} + n_{i,V}}{n_{i,F}}$$