WHAT IS A REFINERY ??

PETROLEUM REFINERY

Crude Oil → Equipments → Energy → Employees → ‘Marketable’ Products

REFINERY OVER VIEW

Corporate → Refinery Management

OM&S → Information Services

Maintenance/Inspection (Civil, Mechanical, Electrical, Metallurgy) → Process Section/Quality Control

Administration & Finance → Engineering Services

Stores & Materials → PRODUCTION
Refinery Types

- Each refinery has its own unique processing scheme
  - Product demand & specifications
  - Individual economic considerations
- Simple
  - Crude distillation, reforming, sulfur treating
  - Range of products is limited
- Complex
  - Simple + vacuum distillation, FCC, HCl, alkylation, gas recovery
- Integrated
  - Complex + recovery of material from VTB — coking
  - Full range of products
Complexity of a Refinery

The combination of refining processes and operations employed (complexity) varies from one refinery to another.

Factors deciding the complexity of a refinery:
- Nature/source of crude oils to be processed
- Demand pattern in the markets to be covered
- Product quality - current / future
- Production of feed stocks for downstream units
- Inter-fuel substitution
- Environmental stipulations

Crude Oil Characterization

By Gravity:

<table>
<thead>
<tr>
<th>Grade</th>
<th>°API</th>
<th>SG</th>
</tr>
</thead>
<tbody>
<tr>
<td>Light</td>
<td>&gt;35</td>
<td>&lt;0.85</td>
</tr>
<tr>
<td>Medium</td>
<td>26-35</td>
<td>0.85-0.8984</td>
</tr>
<tr>
<td>Heavy</td>
<td>10-26</td>
<td>0.8984-1.00</td>
</tr>
<tr>
<td>Extra Heavy</td>
<td>&lt;10</td>
<td>&gt;1.00</td>
</tr>
</tbody>
</table>

By Sulphur (%wt.):

<table>
<thead>
<tr>
<th>Type</th>
<th>%wt.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sweet</td>
<td>&lt;0.5</td>
</tr>
<tr>
<td>Medium sour</td>
<td>0.5-1.0</td>
</tr>
<tr>
<td>Sour</td>
<td>&gt;1.0</td>
</tr>
</tbody>
</table>
4 types of crude oils available to refiners around the world:

<table>
<thead>
<tr>
<th>Type</th>
<th>°API</th>
<th>Sulphur (% wt.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Light Sweet</td>
<td>30-40</td>
<td>&lt;0.5</td>
</tr>
<tr>
<td>Light Sour</td>
<td>30-40</td>
<td>0.5-1.5</td>
</tr>
<tr>
<td>Heavy Sour</td>
<td>15-30</td>
<td>1.5-3</td>
</tr>
<tr>
<td>Extra Heavy</td>
<td>&lt;15</td>
<td>&gt;3</td>
</tr>
</tbody>
</table>

*High Acid Crudes (HACs)*

- TAN (Total Acid Number) > 0.5mg KOH/gm Crude Oil

**PROFITABLE CRUDE**

- Crude Availability
- Crude Cost
- Desired Product Yield
- Refinery Complexity
- Environmental Constraints
CRUDE OIL SELECTION & OPTIMISATION IN REFINERIES

Depends on:

- Configuration of Refinery – what are the units present
- Metallurgy of refinery – particularly columns, piping to take care of acidic / corrosive crude
- Product demand in the region
- Netback/ GRM of a particular crude
- Availability of a particular crude at economic cost.

Crude Oil Selection

- Overall refinery economics depend on Crude cost + Processing Cost
- Lower the S, lower the SG
  - Higher is the crude price
  - Lower processing requirement
- HACs are normally cheaper
  - Higher neutralization cost
  - Refineries would like to handle crudes with TAN<0.5 & subsequent process streams containing TAN<1.5
**Crude Oil Selection**

- **Crude availability shifting from**
  - Light sweet $\rightarrow$ Heavy sour $\rightarrow$ Extra Heavy
- **HACs are opportunity crudes**

**New Refinery:**
- design to process Extra Heavy Crudes
- design to process HACs in admixture

**Major Refinery Products**

- LPG (Propane/Butane)/Propylene
- MS/Naphtha/Solvents/Benzene/Toluene
- ATF/SKO/MTO/LABFS
- HSD/LDO
- FO/LSHS/HPS/CBFS/PROCESS OILS
- Asphalts/Bitumen
- Lube Oil Base Stocks (GR-I & GR-2)
- RPC/CPC
- Slack Wax/MCW/Paraffin Wax
### Critical Quality Parameters of Products

<table>
<thead>
<tr>
<th>Sl.no</th>
<th>Product</th>
<th>Key Quality parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>LPG</td>
<td>Evaporation Temperature at 95 % Volume =&lt;2 deg C, Max Cu Corrosion = not worse than No.1. RVP =&lt;1050 KPa, Max</td>
</tr>
<tr>
<td>2.</td>
<td>Motor Spirit</td>
<td>Density =720-775 Kg/M3, RON =&lt;91 Min, Sulphur =&lt;150 ppm, Max, Benzene =&lt;1 Vol. %, Max</td>
</tr>
<tr>
<td>3.</td>
<td>ATF</td>
<td>Density =775-840 Kg/M3, Flash Point =&lt;38 deg c, Min, Sulphur =&lt;0.25 wt %, Max, Smoke Point =&lt;20 mm, Min</td>
</tr>
<tr>
<td>4.</td>
<td>SKO</td>
<td>Density =790-820 Kg/M3, Flash Point =&lt;35 deg c, Min, Sulphur =&lt;0.25 wt %, Max, Smoke point =&lt;18 mm, Min</td>
</tr>
</tbody>
</table>

### Critical Quality Parameters of Products

<table>
<thead>
<tr>
<th>Sl.no</th>
<th>Product</th>
<th>Key Quality parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.</td>
<td>Diesel</td>
<td>Density =820-845 Kg/M3, Sulphur =&lt;350 ppm, Cetane Number =&lt;51 Min, Recovery at 360 deg C =&lt;95 Min</td>
</tr>
<tr>
<td>6.</td>
<td>Fuel Oil</td>
<td>Kinematic Viscosity@ 50 deg c =0.125, Max (Winter) =0.180, Max (Summer), Sulphur =&lt;4 wt %, Max, Ash =&lt;0.1 wt %, Max</td>
</tr>
<tr>
<td>7.</td>
<td>Bitumen</td>
<td>Penetration at 25 deg c =&lt;60 (1/10mm), Min, Flash Point =&lt;175 deg C, Min, Softening Point =&lt;45-55 deg C</td>
</tr>
</tbody>
</table>
BUSINESS PROCESS FLOW

1. Crude evaluation & Procurement
   - BE/MOU/St Tar: Term contract crudes.
   - HLP: Spot procurement for next 3 months.

2. What and How to Feed
   - BE/MOU/St Tar
   - HLP

3. What & Where To Make
   - BE/MOU/St Tar
   - HLP

4. By Mktg

Demand Forecast

Distribution Planning

What to Store and where

BASIC REFINERY OPERATIONS

Hydrocarbon molecules in crude do NOT meet customer needs

1. SEPARATION PROCESSES
   (Primary Processes)
   - Segregate the molecules

2. CONVERSION PROCESSES
   (Secondary Processes)
   - Rearrange the molecules

3. FINISHING PROCESSES
   (Secondary Processes)
   - Remove Contaminants

MARKETABLE PRODUCTS
REFINERY SCHEME

Crude Pretreatment
- Desalting

Fractionation
- Atmospheric & Vacuum Distillation

Treatment
- Diesel Hydrodesulphurization
- Diesel Hydrotreatment
- Solvent Extraction (e.g. FEU)
- Catalytic Reforming

Conversion
- Fluidized-bed Catalytic Cracking
- Hydrocracking
- Delayed Coking
- Visbreaking /Coking

Formulation & Blending

Other Refinery Processes
a. Sour Water Stripping  b. Sulphur Recovery  c. Cooling Water Treatment

Processes in the oil refinery
### Processes in an Oil Refinery

<table>
<thead>
<tr>
<th>Physical processes</th>
<th>Chemical processes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distillation</td>
<td>Visbreaking</td>
</tr>
<tr>
<td>Solvent extraction</td>
<td>Delayed coking</td>
</tr>
<tr>
<td>Propane</td>
<td>Flexicoking</td>
</tr>
<tr>
<td>deasphalting</td>
<td>Hydrotreating</td>
</tr>
<tr>
<td>Solvent dewaxing</td>
<td>Catalytic reforming</td>
</tr>
<tr>
<td>Blending</td>
<td>Catalytic cracking</td>
</tr>
<tr>
<td></td>
<td>Hydrocracking</td>
</tr>
<tr>
<td></td>
<td>Catalytic dewaxing</td>
</tr>
<tr>
<td></td>
<td>Alkylation</td>
</tr>
<tr>
<td></td>
<td>Polymerization</td>
</tr>
<tr>
<td></td>
<td>Isomerization</td>
</tr>
</tbody>
</table>

### Market Demands

- Clean products (no S, N, O, metals, etc.)
- More gasoline (high octane number)
- More diesel (high cetane number)
- Specific products (Aromatics, alkenes, etc.)
- Less residue

**How to meet these demands?**

- More sophisticated distillation
- Physical separation steps
- Chemical conversion steps
# Refinery Operations

- PRIMARY PROCESSING UNITS
- SECONDARY PROCESSING UNITS

## Configuration of Refineries / Refining Processes

<table>
<thead>
<tr>
<th>Primary Units</th>
<th>Crude Distillation Unit (CDU) / Vacuum Distillation Unit (VDU)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Secondary Units</td>
<td>Fluid Catalytic Cracking Unit (FCCU), Hydro-Cracking Unit (HCU), Delayed Coker Unit (DCU), Visbreaker Unit (VBU)</td>
</tr>
<tr>
<td>Lube/Wax Producing Units</td>
<td>Furfural Extraction Unit (FEU) / NMP Extraction Unit, Solvent Dewaxing Unit (SDU), Catalytic Iso-Dewaxing Unit (CIDW), Wax Hydrotreating Unit (WHU), Hydro-Finishing Unit (HFU)</td>
</tr>
<tr>
<td>Treating Units</td>
<td>Catalytic Reforming Unit (CRU), Diesel Hydro-Treating Unit (DHDT), Diesel Hydro-Desulfurisation Unit (DHDS), Merox Unit, etc...</td>
</tr>
</tbody>
</table>
PRIMARY PROCESSING UNIT

The purpose of Primary unit is to separate the crude into different fractions by distillation.

Known as mother unit of the refinery, consist of:

- CRUDE DISTILLATION UNIT (CDU)
- VACUUM DISTILLATION UNIT (VDU)

Commonly referred as Atmospheric and Vacuum Distillation unit (AVU)

Separation
Heavy at the bottom, light on the top

The separation of crude oil by atmospheric and vacuum distillation into groups of hydrocarbon compounds of different boiling point ranges (called "fractions" or "cuts")

The first step in crude oil processing

The process unit where the first separation takes place is called Crude Distillation Unit (CDU), Atmospheric Unit (AU) or Atmospheric & Vacuum Unit (AVU)

This step is performed in all refineries: These units are called "Mother Units"

Typical products from CDU are: Gas, LPG, naphtha, SKO/ATF, HSD and RCO.

Vacuum Distillation of RCO produces VGO (or LOBS cuts) & VR

All products need further treatment/processing.
**Atmospheric & Vacuum Distillation**

- **Crude Stills**
  - Historically the oldest refining process
  - Only the first step in crude oil processing
- **Purpose**
  - To recover light materials
  - Fractionate into sharp fractions
- **Atmospheric**
  - Light gases
  - Straight run gasoline
  - Naphtha
  - Distillates
  - Atmospheric Gas Oil
  - Atmospheric Residuum
- **Vacuum**
  - Light & heavy vacuum gas oils
  - Vacuum Residue

---

**Crude Oil Refining**

<table>
<thead>
<tr>
<th>Distillate fraction</th>
<th>Boiling point (°C)</th>
<th>C-atoms/molecule</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gases</td>
<td>&lt;30</td>
<td>1-4</td>
</tr>
<tr>
<td>Gasoline</td>
<td>30-210</td>
<td>5-12</td>
</tr>
<tr>
<td>Naphtha</td>
<td>100-200</td>
<td>8-12</td>
</tr>
<tr>
<td>Kerosine (jet fuel)</td>
<td>150-250</td>
<td>11-13</td>
</tr>
<tr>
<td>Diesel, Fuel oil</td>
<td>160-400</td>
<td>13-17</td>
</tr>
<tr>
<td>Atmospheric Gas Oil</td>
<td>220-345</td>
<td></td>
</tr>
<tr>
<td>Gasoil</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heavy Fuel Oil</td>
<td>315-540</td>
<td>20-45</td>
</tr>
<tr>
<td>Atmospheric Residuum</td>
<td>&gt;540</td>
<td>&gt;30</td>
</tr>
<tr>
<td>Residue</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Vacuum Residue</td>
<td>&gt;615</td>
<td>&gt;60</td>
</tr>
</tbody>
</table>

*Middle Distillates*
Crude Oil

- Fractions of crude boil at different temperatures
- Components are separated by distillation and drawn off as they condense

Atmospheric & Vacuum Distillation Unit Flow Diagram
Hydrotreating Process (trickle bed)

Development of maximum Sulfur Content in automotive Diesel in Europe

Max S in Diesel ppm

Year

**Diesel Hydro-Desulphurisation Unit (DHDS)**

- **Objective**: To meet the EURO-II diesel quality requirement (<500 ppm S)
- **Feed**: Straight run diesel / FCC diesel component / Coker and Visbreaker diesel components.
- **Catalyst**: Ni-Mo oxides
DHDS Product Yields and Operating Conditions

1. Typical Product Yields

<table>
<thead>
<tr>
<th>SL no.</th>
<th>Products</th>
<th>Wt%</th>
<th>End Users</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Off Gas</td>
<td>1.36</td>
<td>Refinery Fuel gas system after Amine Wash</td>
</tr>
<tr>
<td>2.</td>
<td>Wild Naphtha</td>
<td>1.04</td>
<td>To Naphtha Pool after stabilisation</td>
</tr>
<tr>
<td>3.</td>
<td>Diesel</td>
<td>97.1</td>
<td>To Euro II Diesel Pool</td>
</tr>
</tbody>
</table>

2. Operating Conditions:
- Temperature range: 320-380 DEG C
- System Pressure: 30-40 kg/cm²(g)

Diesel Hydrotreating Unit (DHDT)
- Objective: To meet the Euro –III/IV diesel quality requirement (350/50 ppm ‘S’ and Min. 51 Cetane No.)
- Feed: Straight run diesel / FCC diesel component / Coker and Visbreaker diesel components
- Catalyst: Ni-Mo oxides
- Chemical reactions: Desulphurisation and Denitrification

\[
\text{Aromatic compound} + \text{H}_2 \rightarrow \text{Naphthene Compound}
\]
Diesel Hydrotreater unit Flow Diagram

DHDT Product Yields and Operating Conditions

1. Typical Product Yields

<table>
<thead>
<tr>
<th>Sl.no.</th>
<th>Products</th>
<th>Wt%</th>
<th>End Users</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Off Gas</td>
<td>2.65</td>
<td>Refinery Fuel gas system after Amine Wash</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Wild Naphtha</td>
<td>2.8</td>
<td>To Naphtha Pool after stabilisation</td>
</tr>
<tr>
<td>3</td>
<td>Diesel</td>
<td>96.1</td>
<td>To Diesel Pool</td>
</tr>
</tbody>
</table>

2. Operating Conditions:

- Temperature range: 320-380 DEG C
- System Pressure: 100-105 kg/cm²(g)
Upgrading Gasoline Blend Stocks

<table>
<thead>
<tr>
<th>Purpose</th>
<th>Reforming</th>
<th>Isomerization</th>
<th>Alkylation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Create high octane gasoline blend stock</td>
<td></td>
<td></td>
<td>C4s (Butylene &amp; Isobutene)</td>
</tr>
<tr>
<td>Feedstock</td>
<td>Heavy Naphtha</td>
<td>Light Naphtha</td>
<td></td>
</tr>
<tr>
<td>Reactions</td>
<td>Dehydrogenation of Cycloparaffins</td>
<td>Isomerization of Straight Chain Paraffins</td>
<td>Combination of Smaller Molecules</td>
</tr>
<tr>
<td>Side Benefits</td>
<td>Make hydrogen for use elsewhere in the refinery</td>
<td>Use light olefins made in FCCU</td>
<td></td>
</tr>
</tbody>
</table>
Catalytic Reforming Unit (CRU)

- Objective: To Upgrade the Naphtha to High Octane MS Component (Reformate).
- Feed: 85-160 Deg C cut Naphtha / Visbreaker Naphtha
- Catalyst: Ni-Mo Oxides for NHTU Reactor
  Pt-Sn or Re for Reforming
Catalytic Reforming Unit

Main types of reformers are:

1. Semi-regenerative (SR)
   The reformer processes feedstock for a time and then shuts down for regeneration.

2. Cyclic
   Any reactor can be isolated for regeneration while the other reactors are in operation.

3. Moving bed or CCR
   Catalyst is moved continuous through the reactors, withdrawn from the last reactor, regenerated in regeneration section and returned to the first reactor as fresh catalyst.

Continuous Catalytic Reforming Unit Flow Diagram
CRU Product Yield and Operating Conditions

1. Typical Product Yields

<table>
<thead>
<tr>
<th>SL.no.</th>
<th>Products</th>
<th>Wt%</th>
<th>Quality</th>
<th>End Users</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H2 Rich gas</td>
<td>6.5-8.0</td>
<td>94% H2 gas</td>
<td>PSA Unit to recover H2</td>
</tr>
<tr>
<td>2</td>
<td>LPG</td>
<td>2.5-12</td>
<td>‘S’ free LPG</td>
<td>To MS Pool After catalytic Reforming</td>
</tr>
<tr>
<td>3</td>
<td>Reformate</td>
<td>80-91</td>
<td>RON-98, low ‘S’, High Bz.</td>
<td>To MS POOL after Reformate Splitter</td>
</tr>
</tbody>
</table>

2. Operating Conditions:

- Temperature range: 490-540 DEG C
- System Pressure: 2.0 - 30 kg/cm²(g)

Isomerisation Unit (PENEX-DIH)

- Objective: To Upgrade the Naphtha by increasing its Octane Number to Higher Octane/Low Benzene/Low Olefins MS Component (Isomerate) to Meet Euro III / IV MS Specifications.

- Feed: C5-85 Deg C cut Naphtha / FCC gasoline(70-90 deg C cut)/ Lt. Reformate

- Catalyst:
  - Co-Mo for Hydrotreater Reactor
  - Pt for Penex Reactor
  - Ni Based for Methanation
Isomerisation Unit Flow Diagram

ISOM Product Yield and Operating Conditions

1. Typical Product Yields

<table>
<thead>
<tr>
<th>Sl.no.</th>
<th>Products</th>
<th>Wt%</th>
<th>End Users</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Off gas</td>
<td>1.4</td>
<td>Refinery fuel gas System</td>
</tr>
<tr>
<td>2.</td>
<td>LPG</td>
<td>11.3</td>
<td>To LPG POOL</td>
</tr>
<tr>
<td>3.</td>
<td>Isomerate</td>
<td>87.3</td>
<td>To MS POOL</td>
</tr>
</tbody>
</table>

2. Operating Conditions:

Temperature range : 126- 145 DEG C
System Pressure   : 33.5 kg/cm²(g)
Cracking process

- Fluidized Catalytic Cracking Unit
- Hydro Cracker Unit
- Visbreaker Unit
- Coking unit

**TECHNOLOGICAL ASPECTS**

| FCCU / RFCCU | Heavier Hydro-Carbon molecules are cracked under severe operating conditions of Temp. (500 – 510 °C) and pressure (1.4 - 2.2 kg/cm²) to get Lighter Hydro-Carbons like LPG, MS & HSD components. Strict operating conditions are maintained to get on-specs. products.
| HCU / OHCU | Heavier Hydro-Carbon molecules are mixed with Hydrogen and the mixture is subjected to severe operating conditions of Temp. (380 - 400 °C) and pressure (165 - 185 kg/cm²) to get Lighter Hydro-Carbons like LPG, MS & HSD components. Strict operating conditions are maintained to get on-specs. products. All products are of Superior quality w.r.t. Sulfur content. |
Fluid Catalytic Cracking Unit (FCCU)

- **Objective**: To convert Heavy Vacuum Gas Oil to valuable distillates like LPG, Gasoline, Diesel by catalytic cracking in fluidized bed.
- **Feed**: VGO/RCO/VR/HydroCracker Bottom.
- **Catalyst**: Silica & Alumina Zeolite Structure

---

**Fluidized Bed Catalytic Cracking**

- Process gas oils using catalysts to crack the carbon-carbon bonds
  - Cracking lowers the average molecular weight & produces higher yields of fuel products
- Attractive feed characteristics
  - Small concentrations of contaminants
    - Poison the catalyst
  - Small concentrations of heavy aromatics
    - Crack & deposit coke on catalyst
- Products may be further processed
  - Further hydrocracked
  - Alkylated to improve gasoline anti-knock properties
## Yield Pattern of Various FCC Units

<table>
<thead>
<tr>
<th>Feed</th>
<th>VGO FCC</th>
<th>RFCC</th>
<th>INDMAX</th>
<th>PETROFCC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed Quality</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CCR, WT%</td>
<td>0.74</td>
<td>4.06</td>
<td>&lt;10</td>
<td>0.74</td>
</tr>
<tr>
<td>S*, WT%</td>
<td>3.4</td>
<td>3.59</td>
<td>&lt;4</td>
<td>3.4</td>
</tr>
<tr>
<td>VR Content, WT%</td>
<td>NIL</td>
<td>20 MAX</td>
<td>&lt;44</td>
<td>NIL</td>
</tr>
<tr>
<td>Product, WT %</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gas</td>
<td>1.47</td>
<td>3.00</td>
<td>10.44</td>
<td>8.80</td>
</tr>
<tr>
<td>LPG</td>
<td>8.68</td>
<td>8.79</td>
<td>16.80</td>
<td>21.00</td>
</tr>
<tr>
<td>Propylene</td>
<td>3.04</td>
<td>3.71</td>
<td>11.20</td>
<td>22.00</td>
</tr>
<tr>
<td>Gasoline</td>
<td>20.06</td>
<td>18.60</td>
<td>28.00</td>
<td>28.00</td>
</tr>
<tr>
<td>Diesel (TGO)</td>
<td>52.64</td>
<td>46.45</td>
<td>10.10</td>
<td>9.50</td>
</tr>
<tr>
<td>FO</td>
<td>7.98</td>
<td>10.82</td>
<td>8.60</td>
<td>5.00</td>
</tr>
<tr>
<td>Coke</td>
<td>5.00</td>
<td>7.43</td>
<td>13.80</td>
<td>5.50</td>
</tr>
</tbody>
</table>

## Product Key Properties

<table>
<thead>
<tr>
<th>Product</th>
<th>Gasoline : RON</th>
<th>Diesel</th>
<th>Coke</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gasoline</td>
<td>89</td>
<td>96</td>
<td>95</td>
</tr>
<tr>
<td>Diesel</td>
<td>92.9</td>
<td>30</td>
<td>30</td>
</tr>
</tbody>
</table>

### Fluid Catalytic Cracking Flow Diagram
### FCCU Product Qualities & End Users

<table>
<thead>
<tr>
<th>Sl.No</th>
<th>Product</th>
<th>Qualities</th>
<th>End Users</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.</td>
<td>LPG</td>
<td>H2S, Mercaptans, olefins like Propylene/Butylene</td>
<td>To LPG Pool/ Petrochemical feedstock</td>
</tr>
<tr>
<td>3.</td>
<td>Gasoline</td>
<td>High Octane No. and high Olefin contents</td>
<td>MS Pool</td>
</tr>
<tr>
<td>5.</td>
<td>CLO</td>
<td>High Aromatics, Good Cutter Stock</td>
<td>Fuel Oil</td>
</tr>
</tbody>
</table>

### Hydrocracker Unit

- **Objective**: To convert Heavy Vacuum gas oil to valuable distillates like LPG, Naphtha, ATF, Kerosene and Diesel.
- **Feed**: VGO / Coker Products
- **Catalyst**: Ni/Mo oxides for Dematalisation & Hydrotreating  
  Ni/Mo/W(Tungsten) for Hydrocracking
Hydrocracking Process

**Feedstock:** VGO

**Products & Yields:**
- Gas: 2.5%
- LPG: 2.5%
- Naphtha: 8%
- SKO/ATF: 25%
- HSD: 22%
- Unconverted: 40%

Good process for increasing distillates and producing finished products.

Existing at Gujarat, Mathura, and Panipat refineries.

---

<table>
<thead>
<tr>
<th></th>
<th>HCU</th>
<th>OHCU</th>
</tr>
</thead>
<tbody>
<tr>
<td>FEED</td>
<td>VGO</td>
<td>VGO</td>
</tr>
<tr>
<td>FEED QUALITY</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CCR, WT% MAX</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>S, WT%, MAX</td>
<td>2.8</td>
<td>2.8</td>
</tr>
<tr>
<td>N, PPM, MAX</td>
<td>800</td>
<td>800</td>
</tr>
<tr>
<td>Ni+V, PPM, MAX</td>
<td>1.25</td>
<td>1.25</td>
</tr>
<tr>
<td>SODIUM, PPM</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>PRODUCTS, WT %</td>
<td></td>
<td></td>
</tr>
<tr>
<td>GAS</td>
<td>2.52</td>
<td>3.27</td>
</tr>
<tr>
<td>LPG</td>
<td>4.57</td>
<td>1.95</td>
</tr>
<tr>
<td>NAPHTHA</td>
<td>11.33</td>
<td>9.13</td>
</tr>
<tr>
<td>KEROSENE</td>
<td>39.58</td>
<td>12.00</td>
</tr>
<tr>
<td>DIESEL</td>
<td>41.81</td>
<td>50.65</td>
</tr>
<tr>
<td>BOTTOM</td>
<td>0.00</td>
<td>25.00</td>
</tr>
</tbody>
</table>
PRODUCT KEY PROPERTIES

**NAPHTHA:**
- RON: 72 HCU, 72 OHCU
- S', PPM, MAX: 10 HCU, 10 OHCU

**KEROSENE:**
- SMOKE POINT, MM: 22-23 HCU, 22-23 OHCU
- FREEZING POINT, °C: < 60 HCU, < 60 OHCU

**DIESEL:**
- CETANE INDEX: 62 HCU, 56 OHCU
- S', PPM: < 10 HCU, < 10 OHCU
- POUT POINT, °C: - 12 HCU, - 12 OHCU

**Various configurations of Hydrocraker Units**

1. **Single stage Once through Hydrocraker unit (SSOT):**
   - a. Feed and Hydrogen is passed through reactors only once for 60-80% of partial conversion.
   - b. Unconverted Oil is sent to FCCU.

2. **Single stage recycle (SSRec):**
   - a. Unconverted oil is recycled back to feed for 100% conversion.

3. **Two stage Hydrocraker Unit:**
   - a. Unconverted Oil of SSOT is sent to another reactor for 100% conversion.
1) Single Stage in Blue
2) Two Stage is Blue and Green Combined
Hydro Cracker Unit Flow Diagram

HCU Product Qualities & End Users

<table>
<thead>
<tr>
<th>Sl.No</th>
<th>Product</th>
<th>Qualities</th>
<th>End Users</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.</td>
<td>LPG</td>
<td>H2S Contents</td>
<td>To LPG Pool after caustic wash</td>
</tr>
<tr>
<td>3.</td>
<td>Naphtha</td>
<td>low Octane No. and low ‘S’ contents</td>
<td>To Gasoline Pool / Hydrogen unit Feed</td>
</tr>
<tr>
<td>4.</td>
<td>ATF / Kero</td>
<td>Low ‘S’ and Low Aromatics</td>
<td>To ATF/ kero, Pool</td>
</tr>
<tr>
<td>5.</td>
<td>Diesel</td>
<td>Low ‘S’ and High Cetane</td>
<td>EURO – III Diesel</td>
</tr>
<tr>
<td>6.</td>
<td>Unconverted Oil</td>
<td>Low ‘S’, High Saturates</td>
<td>FCCU FEED</td>
</tr>
</tbody>
</table>
**Visbreaker Unit (VBU)**

- **Objective**: To reduce viscosity of Heavy Ends i.e. RCO/Vacuum residue by Thermal Cracking.
- **Feed**: RCO/Vacuum residue/Asphalts
- **Typical Operating Conditions**:
  - Temperature Range: 450-470 Deg C
  - Pressure: 9-14 kg/cm²(g)
- **Viscosity**:
  - Viscosity of Feed: 500-3000 cst at 100 Deg C
  - Viscosity of Product (VBtar): 50 – 300 cst at 100 deg C
**Visbreaker Unit Flow Diagram**

**Visbreaking Process**

**Feedstock**: Vacuum Residue

**Products & Yields:**

- Gas+loss 3%
- Naphtha 2%
- Gas oil 2%
- FO 93%

Good for FO production. Other products unstable and need further treatment.

Existing at Gujarat, Haldia, Mathura & Panipat refineries.
VBU Product Yield/Qualities & End Users

<table>
<thead>
<tr>
<th>Sl.No</th>
<th>Product</th>
<th>Yield</th>
<th>Qualities</th>
<th>End Users</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Gas</td>
<td>1.82</td>
<td>H2S rich Off. Gas</td>
<td>Refinery Fuel gas System after Amine Wash</td>
</tr>
<tr>
<td>2.</td>
<td>VB Naphtha</td>
<td>3.12</td>
<td>H2S, Mercaptans, high olefins</td>
<td>To FCCU or CRU</td>
</tr>
<tr>
<td>3.</td>
<td>VB Gas Oil</td>
<td>13.9</td>
<td>Low Cetane no, Highly unsaturated</td>
<td>To DHDS or Fuel Oil</td>
</tr>
<tr>
<td>4.</td>
<td>VB Tar</td>
<td>81.16</td>
<td>Lower Viscosity than feed</td>
<td>Fuel Oil</td>
</tr>
</tbody>
</table>

Delayed Coker

- **Objective**: To produce valuable distillate from Heavy ends by thermal cracking.
- **Feed**: RCO/Vacuum Residue/other heavy ends or residues
- **Typical Operating Conditions**:
  - Temperature Range: 495-505 Deg C
  - Pressure: 2-3 kg/cm²(g)
Delayed Coking Process

- **Feedstock**: Vacuum Residue / VGO
- **Products & Yields**:
  - Gas + Loss: 10%
  - LPG: 4%
  - Naphtha: 5%
  - Gas Oil: 53%
  - FO: 11%
  - RPC: 17%
- Good process for increasing distillates and minimising black oil production. Gas oil & Naphtha need further treatment.
- Existing at Barauni, Guwahati & Digboi refineries and under commissioning at Panipat.

DELAYED COKING UNIT FLOW DIAGRAM
## Delayed Coker Product Yield/Qualities & End Users

<table>
<thead>
<tr>
<th>Sl.No</th>
<th>Product</th>
<th>Qualities</th>
<th>End Users</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Gas</td>
<td>H₂S rich Off. Gas</td>
<td>Refinery FG after Amine Wash</td>
</tr>
<tr>
<td>2.</td>
<td>LPG</td>
<td>Mercaptans, unsaturates</td>
<td>To LPG after Merox/Caustic wash</td>
</tr>
<tr>
<td>3.</td>
<td>Naphtha</td>
<td>Low Octane, High Olefins</td>
<td>To FCC or CRU</td>
</tr>
<tr>
<td>4.</td>
<td>Kerosene</td>
<td>High unsaturates</td>
<td>To DHDT Feed</td>
</tr>
<tr>
<td>5.</td>
<td>Gas Oil</td>
<td>Low Cetane No. and high unsaturates</td>
<td>To DHDT &amp; HCU feed</td>
</tr>
<tr>
<td>6.</td>
<td>Fuel Oil</td>
<td>Good cutter stock</td>
<td>Fuel Oil</td>
</tr>
</tbody>
</table>

## Treating Process
- Caustic wash
- Merox Unit
Treating Process

1. **Caustic Washing** for removing H2S and light Mercaptans and suitable for LPG and Naphtha

2. **Merox Process**
   a. Extractive Merox: Suitable for Lighter fractions
   b. Sweetening Merox: Suitable for boiling range upto 350 Deg C

Chemical Reaction:

\[
2RSH + \frac{1}{2} O_2 \xrightarrow{\text{Amb.Temp.}} RSSR + H_2O
\]

Iron group metal chelates

After Treatment:

The treated stream is given water wash, followed by sand Bed Coalescer or salt drier for removing entrained water.

Production of Lubricating Oil Base Stock
Lube Base Oil Processing

- Crude Selection
- Multi-step manufacturing process

Lube Base Oils - Key Properties:
- Viscosity
- Viscosity Index
- Pour point
- Colour
- Flash point
- Volatility
- Oxidative & Thermal Stability
API Base Oil Characterization Groups

<table>
<thead>
<tr>
<th>Group</th>
<th>Viscosity Index</th>
<th>Saturates % wt</th>
<th>Sulphur %wt</th>
</tr>
</thead>
<tbody>
<tr>
<td>GROUP I</td>
<td>80-120</td>
<td>&lt;90</td>
<td>&gt;0.03</td>
</tr>
<tr>
<td>GROUP II</td>
<td>80-120</td>
<td>&gt;90</td>
<td>&lt;0.03</td>
</tr>
<tr>
<td>GROUP III</td>
<td>&gt;120</td>
<td>&gt;90</td>
<td>&lt;0.03</td>
</tr>
<tr>
<td>GROUP IV</td>
<td>Poly Alpha Olefins (Synthetic Oils)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>GROUP V</td>
<td>All other base oils</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Lube Base Oil Processing Philosophy

Properties controlled by Process Units:
-KV, Flash Point
-VI, CCR
-Pour Point
-Colour & Stability

Crude oil ➔ Atmospheric distillation ➔ Vacuum distillation ➔ Solvent Extraction (Furfural & NMP) ➔ Solvent Dewaxing Unit ➔ Hydrofinishing ➔ Group I LOBS

Crude oil ➔ Atmospheric distillation ➔ Vacuum distillation ➔ Solvent Extraction (Furfural & NMP) ➔ Solvent Dewaxing Unit ➔ Catalytic Dewaxing Unit ➔ Group II LOBS
API Gr I and Gr II Processing Schemes

<table>
<thead>
<tr>
<th>Solvent Extraction</th>
<th>Solvent De-waxing</th>
<th>Hydro-finishing</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solvent Extraction</td>
<td>Hydro Treating</td>
<td>Wax Isomerisation</td>
</tr>
<tr>
<td>Hydro-finishing</td>
<td></td>
<td>Hydro-finishing</td>
</tr>
</tbody>
</table>

Group I

Group II

Other Process Units

- Hydrogen Generation Unit
- Bitumen Blowing Unit
- Sulphur Recovery Unit
Hydrogen Generation Unit (HGU)

- Objective: To Meet the Hydrogen requirement for DHDS/DHDT/OHCU/ISOM/Reforming Units and Other Hydrotreaters.

- Feed: Natural Gas / Naphtha

- Catalyst:
  - Co-Mo for Hydrotreater
  - ZnO/K2Co3 for H2S and Chloride adsorber
  - NiO for Preformer
  - Ni for Reformer
  - CuO for HT/LT Shift reactors
  - Adsorbents for PSA Adsorbers

HGU Product Purity and Operating Conditions

1. HGU Product is 99.99% Pure Hydrogen

2. Operating Conditions:
   - Temperature range: 860-870 Deg C
   - System Pressure: 23-26 kg/cm2(g)
Objective: To produce different grades of Bitumen by air blowing of vacuum residue at high temperature.

Bitumen is colloidal solution of asphaltenes and high molecular gums in the medium formed by oils and low molecular gums.

Feed: Vacuum Residue
BBU yield /quality and Operating Conditions

1. Typical Product Quality

<table>
<thead>
<tr>
<th>SL no.</th>
<th>Products</th>
<th>Wt%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Off gas</td>
<td>0.86</td>
</tr>
<tr>
<td>2.</td>
<td>Recovered liquid cut (FLO)</td>
<td>0.26</td>
</tr>
<tr>
<td>3.</td>
<td>Finished Bitumen</td>
<td>98.88</td>
</tr>
</tbody>
</table>

2. Typical Operating Conditions of Bitumen Blowing Unit:

- **Temperature Range**: 230-260 Deg C
- **Pressure**: 0.5 kg/cm²(g)

Bitumen Blowing Unit Flow Diagram
**Sulphur Recovery Unit**

- **Objective**: To Reduce the SO2 emission from the Refinery by recovering Sulphur from Amine Acid and Sour Gases produced during various Hydrotreating Process.

- **Feed**: Amine Acid gases and Sour acid gases

**Sulphur Recovery Unit Flow Diagram**

- Rich amine
- Lean amine
- H₂S / NH₃ gas
- Sour water
- Stripped water
- Claus Reactors 1/2/3
- T = 135-110 Deg C
- A/R
- Off-gas incineration
  - T = 730 Deg C
- To stack
- Process gas
- T = 220 deg C
- Sulphur degasification
- Strpped water
- Product sulphur handling
SRU Product Yield and Operating Conditions

1. Typical Product Yields

<table>
<thead>
<tr>
<th>Sl.no.</th>
<th>Products</th>
<th>Wt%</th>
<th>End Users</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Off gas</td>
<td>0.1</td>
<td>To Stack after incineration</td>
</tr>
<tr>
<td>2.</td>
<td>Sulphur</td>
<td>99.9</td>
<td>Sulphur Yard for Dispatch</td>
</tr>
</tbody>
</table>

 Typical Operating Conditions:

- Temperature Range: 195-320 Deg C
- Pressure: 0.56 kg/cm²(g)

Other refinery Processes/operations

- Steam & Power generation
- Process and DM water systems
- Hydrogen, nitrogen and air systems
- Flares and relief systems
- Sulfur recovery system
- Waste water treatment systems
- Safety & fire fighting systems
- Quality control, maintenance and administrative systems
Energy consumption differs in different refineries due to:

- Refinery configuration / complexity
- Crude oil composition
- Technology / Equipments efficiency
ENVIRONMENTAL CONCERNS

- SULPHUR in PRODUCTS
- BENZENE in PRODUCTS
- EFFLUENT WATER QUALITY
  - SOx, NOx, H2S, Toxic Gases
- OTHER WASTE

MINIMIZING POLLUTION

- **Operate Furnaces Efficiently**
- Unrecovered Light Ends burnt in flare Stack
- Avoid Spills & Accidental Releases
- Special Treatment of Sewer Water
MINIMIZING POLLUTION

FACILITIES TO BE IMPROVISED AT DESIGN STAGE

• Adequate Stack height for better dispersion of pollutants
• Desulphurisation of fuel gas
• Provision of a Sulphur recovery unit
• Provision of continuous SO2 analyzers in all stacks
• Providing Air monitoring stations
• Efficiently running Effluent Treatment Plants
• New Unit / Up-to-date technology for producing Ultra low Sulphur and benzene free fuels.

REFINERY OPERATIONS – HAZARDS

Fouling and Corrosion

Low Flash Point

Low Explosivity Limits

Develop Static Charge

Low self ignition temperatures

Carcinogenic

Pyrophoric

Toxic
TECHNOLOGY ADOPTION IN REFINERIES

- Desulfurization of fuel products for reduction in Sulfur- DHDS unit, Kero-HDS unit, DHDT
- Conversion processes for bottom of the barrel upgradation - FCC, Hydrocracker, DCU etc.
- Quality Improvement to meet environment norm- Cetane improvement in Diesel; Benzene, Olefin, Aromatics & Sulfur reduction in Motor Spirit.
- Adoption of catalytic-dewaxing technology for Quality Lube.

CHALLENGES TO OIL INDUSTRY

- Environmental pressure- key factor in development & acquisition of new technology
- Sophistication in equipment design- demands for high performance products.
- Adoption of Euro norms for environment friendly transport fuels production, viz., Gasoline & Diesel.
- Demand for environment friendly, high quality LOBS- API class-II/ III.
- Cost Intensive Refining Technology.
CONSTRAINTS TO MEET THE CHALLENGES

- Crude oil sourcing - Indigenous production is only about 30% of the total requirement.
- Sharp fall in the availability of low Sulfur crude oil and even to the extent lighter crude oil.
- Hence refineries are forced to process wide variety of crude oil including high sulfur crude.
- Selection of suitable technology having enough flexibility.

EMERGENCE OF COST INTENSIVE REFINING TECHNOLOGY

- Switch over to Automation & Advance Controls
- Upgradation of the bottom of the barrel
- Efficiency Improvement thru’ debottlenecking / low cost revamps etc.
- Environment friendly processes for pollution abatement
- Stringent quality products manufacture & QC.
FUTURE CHALLENGES

- Total Deregulation
- Competition from Private Refining Companies
- Product Quality – Stringent
- Market Dynamics
- Margin Pressure
- Customer Focus

STRATEGIES

- Value addition
- Capacity Saturation
- Quick Response – Quality / Quantity
- Cost Reduction
- Effective Manning
- Integration – Forward/Backward/Lateral
Refining Vision

- Refinery Capacity
- Refinery Margins
- Product Quality
Phase Equilibria in Refinery Processes

Ratan Mohan

Department of Chemical Engineering
I.I.T. Delhi, New Delhi
Thermodynamic data needs in process simulation

Phase equilibria

Stream properties; enthalpy, entropy

Reaction equilibria; Gibb’s free energy of rxn, Eq. constt.
Basic Phase Equilibrium equation:

\[ f_i^v = f_i^l \]  \hspace{1cm} (1)

Where:

\[ f_i^v = \text{Fugacity of component } i \text{ in the vapor phase} \]
\[ f_i^l = \text{Fugacity of component } i \text{ in the liquid phase} \]

Applied thermodynamics provides two methods for representing the fugacities from the phase equilibrium relationship in terms of measurable state variables, the equation-of-state method and the activity coefficient method.

**In the equation of state method:**

\[ f_i^v = \phi_i^v y_i p \]  \hspace{1cm} (2)
\[ f_i^l = \phi_i^l x_i p \]  \hspace{1cm} (3)

With:

\[ \ln \phi_i^\alpha = -\frac{1}{RT} \int_{\infty}^{V_\alpha} \left[ \left( \frac{\partial \rho}{\partial n_i} \right)_{T,V,n_\text{eq}} - \frac{RT}{V} \right] dV - \ln Z_m^\alpha \]  \hspace{1cm} (4)

Hence,

\[ \phi_i^v y_i = \phi_i^l x_i \]
Property Calculations:

- Fugacity coefficient:
  \[ f_i^y = \varphi_i^y \gamma_i p \]  (13)

- Enthalpy departure:
  \[ (H_m - H_m^{ig}) = -\int_{\infty}^{V} \left( p - \frac{RT}{V} \right) dV - RT \ln \left( \frac{V}{V_m^{ig}} \right) + T \left( S_m - S_m^{ig} \right) + RT (Z_m - 1) \]  (14)

- Entropy departure:
  \[ (S_m - S_m^{ig}) = \int_{\infty}^{V} \left[ \left( \frac{\partial p}{\partial T} \right)_V - \frac{R}{V} \right] dV + R \ln \left( \frac{V}{V_m^{ig}} \right) \]  (15)

- Gibbs energy departure:
  \[ (G_m - G_m^{ig}) = -\int_{\infty}^{V} \left( p - \frac{RT}{V} \right) dV - RT \ln \left( \frac{V}{V_m^{ig}} \right) + RT (Z_m - 1) \]  (16)

- Molar volume:
  Solve \( p(T, V_m) \) for \( V_m \).
Activity Coefficient method:

\[ \varphi_i x_i y_i \rho = x_i \gamma_i f_{i,l}^* \]

where

The liquid phase reference fugacity \( f_{i,l}^* \) is computed as:

\[ f_{i,l}^* = \varphi_i^* \gamma_i^* \left( T, p_{i,l}^* \right) p_{i,l}^* \theta_{i,l}^* \]

For non-condensing gaseous components:

\[ \varphi_i x_i y_i \rho = x_i \gamma_i^* H_i \]
Liquid property calculations:

**Liquid phase:** Liquid mixture enthalpy is computed as:

\[ H_m^l = \sum_i x_i (H_i^{*,v} - \Delta_{vap} H_i^*) + H_{m}^{E,l} \]  \hspace{1cm} (34)

Where:

- \( H_i^{*,v} \) = Pure component vapor enthalpy at T and vapor pressure
- \( \Delta_{vap} H_i^* \) = Component vaporization enthalpy
- \( H_{m}^{E,l} \) = Excess liquid enthalpy

Excess liquid enthalpy \( H_{m}^{E,l} \) is related to the activity coefficient through the expression:

\[ H_{m}^{E,l} = -RT^2 \sum_i x_i \frac{\partial \ln \gamma_i}{\partial T} \]  \hspace{1cm} (35)

Liquid mixture Gibbs free energy and entropy are computed as:

\[ S_m^l = \frac{1}{T} \left( H_m^l - G_m^l \right) \]  \hspace{1cm} (36)

\[ G_m^l = G_m^v - RT \sum_i \ln \varphi_i^{*,l} + G_{m}^{E,l} \]  \hspace{1cm} (37)

Where:

- \( G_{m}^{E,l} = RT \sum_i x_i \ln \gamma_i \)  \hspace{1cm} (38)

Liquid density is computed using an empirical correlation.
**Equations of State:**

**Cubic EOS:**

<table>
<thead>
<tr>
<th>Redlich-Kwong(-Soave) based</th>
<th>Peng-Robinson based</th>
</tr>
</thead>
<tbody>
<tr>
<td>Redlich-Kwong</td>
<td>Standard Peng-Robinson</td>
</tr>
<tr>
<td>Standard Redlich-Kwong-Soave</td>
<td>Peng-Robinson</td>
</tr>
<tr>
<td>Redlich-Kwong-Soave</td>
<td>Peng-Robinson-MHV2</td>
</tr>
<tr>
<td>Redlich-Kwong-ASPN</td>
<td>Peng-Robinson-WS</td>
</tr>
<tr>
<td>Schwartzentruber-Renon</td>
<td></td>
</tr>
<tr>
<td>Redlich-Kwong-Soave-MHV2</td>
<td></td>
</tr>
<tr>
<td>Predictive SRK</td>
<td></td>
</tr>
<tr>
<td>Redlich-Kwong-Soave-WS</td>
<td></td>
</tr>
</tbody>
</table>

An example of this class of equations is the Soave-Redlich-Kwong equation of state (Soave, 1972):

\[
p = \frac{RT}{(V_m - b)} - \frac{a(T)}{V_m (V_m + b)}
\]

\[
a = \sum_i \sum_j x_i x_j (a_i a_j)^{\frac{1}{2}} (1 - k_{a,ij})
\]

\[
b = \sum_i x_i b_i = \sum_i \sum_j x_i x_j \left(\frac{b_i + b_j}{2}\right)
\]
Activity Coefficient Models:

Van Laar
Scatchard-Hildebrand
Margules
Redlich Kister
Wilson
NRTL
UNIQUAC
UNIFAC
Non Random Two Liquid (NRTL) Model:

- applicable to partially miscible as well as completely miscible systems
- The NRTL equation for the excess Gibbs energy
  \[
  \frac{g^E}{RT} = \sum_i x_i \sum_j x_j G_{ij} \tau_{ji}
  \]

- Activity coefficient in its \textit{generalized form} is given by
  \[
  \ln \gamma_i = \left[ \frac{\partial (\alpha G^E / RT)}{\partial n_i} \right]_{P,T,n_j}
  \]
  \[
  \ln \gamma_i = \frac{\sum_j \tau_{ji} G_{ji} x_i}{\sum_k G_{ki} x_k} + \sum_j \frac{x_j G_{ji}}{\sum_k G_{ki} x_k} \left( \frac{\sum_i x_i \tau_{ji} G_{ij}}{\sum_k G_{ki} x_k} \right)
  \]

\textbf{contd...}

- where: \(i, j, k = 1, 2, \ldots c\); 
  \[
  \tau_{ij} = \frac{(g_{ji} - g_{ij})}{RT} ;
  \]
  \[
  G_{ji} = \exp(-\alpha_{ji} \tau_{ji}) ;
  \]

- \(\tau_0\)'s \& \(\alpha_{ij}\) are NRTL model parameters

- where \(\tau_0 \neq \tau_{ij}\)
  \[
  \alpha_y = \alpha_j = 0.2 \quad \text{...for liquid – liquid system}
  \]
UNIFAC (Universal Functional Activity Coefficient) method

- estimates activity coefficients based on the group contribution concept
- Excess Gibbs energy (and logarithm of the activity coefficient) as a combination of 2 effects:
  1. combinatorial term
  2. residual term

\[
\ln \gamma_i^c = \ln \frac{\varphi_i}{x_i} + \frac{z}{2} q_i \ln \left( \frac{\theta_i}{\varphi_i} \right) + l_i - \frac{\varphi_i}{x_i} \sum_{j=i}^{NOG} \chi_j l_j
\]

where

\[
\varphi_i = \frac{x_i r_i}{\sum_{j=i}^{NOG} x_j r_j} ; \quad \theta_i = \frac{x_i q_i}{\sum_{j=i}^{NOG} x_j q_j} ; \quad l_i = \frac{z}{2} (r_i - q_i) - (r_i - l_i)
\]

\[
\ln \gamma_i^c = \ln \gamma_i^C + \ln \gamma_i^R
\]

\[
\ln \gamma_i^R = \sum_{k=1}^{NOG} v_i^k \left( \ln \Gamma_k - \ln \Gamma_i^k \right)
\]

where

- \( \Gamma_k \) = residual activity coefficient of group \( k \) in the mixture
- \( \Gamma_i^k \) = residual activity coefficient of group \( k \) in a reference solution containing only molecules of type \( i \).

- The parameters \( \Gamma_k \) and \( \Gamma_i^k \) are defined by:

\[
\ln \Gamma_i = \sum_{k=1}^{NOG} v_i^k \left( 1 - \ln \sum_{m=1}^{NOG} \tau_{mm} - \frac{\theta_i}{\sum_{m=1}^{NOG} \theta_i \tau_{mm}} \right)
\]

\[
\theta_i = \frac{x_i Q_i}{\sum_{m} X_m Q_m} ; \quad \tau_{mm} = e^{-\theta_m / T}
\]

\( X_i \) is the group mole fraction of group \( k \) in the liquid:

\( X_i = \frac{\sum_{j=1}^{NOG} \chi_{ij} x_j}{\sum_{j=1}^{NOG} \chi_{ij} x_j} \)
Property methods for Petroleum mixtures:

**Liquid Fugacity and K-Value Models**

<table>
<thead>
<tr>
<th>Property Method Name</th>
<th>Models</th>
</tr>
</thead>
<tbody>
<tr>
<td>BK10</td>
<td>Braun K10 K-value model</td>
</tr>
<tr>
<td>CHAO-SEA</td>
<td>Chao-Seader liquid fugacity, Scatchard-Hildebrand activity coefficient</td>
</tr>
<tr>
<td>GRAYSON/GRAYSON2</td>
<td>Grayson-Streed liquid fugacity, Scatchard-Hildebrand activity coefficient</td>
</tr>
<tr>
<td>MXBONNEL</td>
<td>Maxwell-Bonnell liquid fugacity</td>
</tr>
</tbody>
</table>

**Petroleum-Tuned Equations of State**

<table>
<thead>
<tr>
<th>Property Method Name</th>
<th>Models</th>
</tr>
</thead>
<tbody>
<tr>
<td>PENG-ROB</td>
<td>Peng-Robinson</td>
</tr>
<tr>
<td>RK-SOAVE</td>
<td>Redlich-Kwong-Soave</td>
</tr>
<tr>
<td>SRK</td>
<td>Soave-Redlich-Kwong</td>
</tr>
</tbody>
</table>

Eqn of State property methods for hydrocarbons at high pressure:

<table>
<thead>
<tr>
<th>Property Method Name</th>
<th>Models</th>
</tr>
</thead>
<tbody>
<tr>
<td>BWR-LS</td>
<td>BWR-Lee-Starling</td>
</tr>
<tr>
<td>BWRS</td>
<td>Benedict-Webb-Rubin-Starling</td>
</tr>
<tr>
<td>LK-PLOCK</td>
<td>Lee-Kesler-Plöcker</td>
</tr>
<tr>
<td>PR-BM</td>
<td>Peng-Robinson-Boston-Mathias</td>
</tr>
<tr>
<td>RKS-BM</td>
<td>Redlich-Kwong-Soave-Boston-Mathias</td>
</tr>
</tbody>
</table>
• Peng-Robinson (PR)
  
  – Most enhanced model in Aspen HYSYS
  – Largest applicability range in terms of T and P
  – Special treatments for some key components
  – Largest binary interaction parameter database

• PRSV
  
  – Modified PR model
  – Better representation of vapor pressure of pure components and mixtures
  – Extends applicability of the original PR model to moderately non-ideal systems

• SRK
  
  – Modified RK model
  – Can provide comparable results to PR in many cases, but with a lot less enhancement in Aspen HYSYS

• PR-Twu

• SRK-Twu

• Twu-Sim-Tassone (TST)
  
  – Modified equations of state models for hydrocarbon systems-non ideal systems (used for glycol package)

• Generalized Cubic Equation of State (GCEOS)
  
  – Provides a framework which allows users to define and implement their own generalized cubic equation of state including mixing rules and volume translation

• MBWR
  
  – Modified BWR model
  – Having 32 parameters, this model works extremely well with a number of pure components within specified T and P ranges

• Lee-Kesler-Plöcker
  
  – Also a modified BWR model for non-polar substances and mixtures

• BWRS
  
  – Modified BWR to handle multi components
  – Requires experimental data
• Zudkevitch Joffee
  – Modified RK model with better prediction of VLE for hydrocarbon systems, and systems containing hydrogen

• Kabadi-Danner
  – Modified SRK model with the enhancement to improve the VLE calculations for H2O-hydrocarbon systems, particularly in dilute regions

• Sour PR/Sour SRK
  – Used for sour water systems containing H2S, CO2, and NH3 at low to moderate pressures

Semi-empirical Models :

• Chao-Seader model
  – Applicable to hydrocarbon systems in the range of T=0-500°C, and P<10,000 kPa

• Grayson-Streed model
  – An extension to the Chao-Seader model with special emphasis on H2
  – Recommended for heavy hydrocarbon systems with high H2 content, such as hydrotreating units
• Hydrocarbon systems up to distillate range hypo components
  – PR, SRK or any other EOS*

• Vacuum columns – GS, PR or BK10

• Sour gas sweetening with Amines

• Sour water treatment process – Sour PR/SRK

• Clean fuels for sulfur components and hydrocarbons

• High H2 content systems – GS, PR

• Utility systems using H2O – Steam Table
### Refinery Processes:

<table>
<thead>
<tr>
<th>Application</th>
<th>Recommended Property Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low pressure applications (up to several atm)</td>
<td>Petroleum fugacity and K-value correlations (and assay data</td>
</tr>
<tr>
<td>Vacuum tower</td>
<td>analysis)</td>
</tr>
<tr>
<td>Atmospheric crude tower</td>
<td></td>
</tr>
<tr>
<td>Medium pressure applications (up to several tens</td>
<td>Petroleum fugacity and K-value correlations</td>
</tr>
<tr>
<td>of atm)</td>
<td>Petroleum-tuned equations of state (and assay data analysis)</td>
</tr>
<tr>
<td>Coker main fractionator</td>
<td></td>
</tr>
<tr>
<td>FCC main fractionator</td>
<td></td>
</tr>
<tr>
<td>Hydrogen-rich applications</td>
<td>Selected petroleum fugacity correlations</td>
</tr>
<tr>
<td>Refiner</td>
<td>Petroleum-tuned equations of state (and assay data analysis)</td>
</tr>
<tr>
<td>Hydrocracker</td>
<td></td>
</tr>
<tr>
<td>Lube oil unit</td>
<td>Petroleum-tuned equations of state (and assay data analysis)</td>
</tr>
<tr>
<td>De-asphaltng unit</td>
<td></td>
</tr>
<tr>
<td>Gas Processing</td>
<td></td>
</tr>
<tr>
<td>Application</td>
<td>Recommended Property Method</td>
</tr>
<tr>
<td>Hydrocarbon separations</td>
<td>Equations of state for high pressure hydrocarbon applications</td>
</tr>
<tr>
<td>Demethanizer</td>
<td>(with kij)</td>
</tr>
<tr>
<td>C3-splitter</td>
<td></td>
</tr>
<tr>
<td>Cryogenic gas processing</td>
<td>Equations of state for high pressure hydrocarbon applications</td>
</tr>
<tr>
<td>Air separation</td>
<td>Flexible and predictive equations of state</td>
</tr>
<tr>
<td>Gas dehydration with glycols</td>
<td>Flexible and predictive equations of state</td>
</tr>
<tr>
<td>Acid gas absorption with</td>
<td>Flexible and predictive equations of state</td>
</tr>
<tr>
<td>Methanol (rectisol)</td>
<td></td>
</tr>
<tr>
<td>NMP (purisol)</td>
<td></td>
</tr>
<tr>
<td>Acid gas absorption with</td>
<td>Electrolyte activity coefficients</td>
</tr>
<tr>
<td>Water</td>
<td></td>
</tr>
<tr>
<td>Ammonia</td>
<td></td>
</tr>
<tr>
<td>Amines</td>
<td></td>
</tr>
<tr>
<td>Amines + methanol (amisol)</td>
<td></td>
</tr>
<tr>
<td>Caustic</td>
<td></td>
</tr>
<tr>
<td>Lime</td>
<td></td>
</tr>
<tr>
<td>Hot carbonate</td>
<td></td>
</tr>
<tr>
<td>Claus process</td>
<td>Flexible and predictive equations of state</td>
</tr>
</tbody>
</table>
Scope of Optimization in Refining Operation

The Presentation Structure

- Basics of Optimization
- Optimization within Refinery
- Optimization among Refineries
- Petroleum Supply Chain Optimization
A process to achieve best solution / performance within defined constraints

**Profit Maximization**
- Throughput maximization within hardware constraints
- Maximize equipment life through optimum usage

---

**Basics of Optimization**

![Graph showing month average crude price & cracks](image)
Basics of Optimization

- Optimization
  - Profit Maximization
  - Throughput maximization within hardware constraints
  - Maximize equipment life through optimum usage

- Ref. Profit = Prod. Realization - Input Cost - Operating cost
  = \( \sum (Q_i \times P_i) \) - \( \sum (C_i \times p_i) \) - \( \sum (F_i \times U_i) \) - Losses

- \( Q_i \) (Prod. qty) = f (Type of crude, Process Configuration, Demand Pattern)
  => Under Control

- \( P_i \) (Prod. Price) = f (Demand -> domestic, International)
  => Little control

- \( p_i \) (Crude Cost) = f (Global demand (Premium/Disc), Location of Ref. & Crude source)
  => No control

- \( C_i \) (Crude Type) = f (Production rate, Global demand, Political scenario)
  => Under control
Basics of Optimization

- Optimization within Refinery

**Product Mix Optimization**
- Naphtha / MS / Pet-chem
- ATF / SKO
- ATF / SKO / HSD
- FO / Bitumen
Optimization within Refinery

**Functional Objective**
- Maximize Gross Refinery Margin
  - Input cost reduction
  - Maximize capacity utilization to reduce operating cost
  - Maximize value added products
    - Swing Operation in FCCU
    - Optimum utilization of VBU / BBU
  - Minimize low value products irrespective of demand
- Operational Efficiency improvement
  - Fuel & Loss, R&M cost, Quality give-away etc.

Net Margin = Products sold * Transfer Price - Crude process * Crude cost at Refinery - Operating Cost

**Margins**
- Function of
  - Demand pattern
  - Products Prices
  - Product pattern of refinery & its flexibility / Optimization
  - Refinery configuration
  - Logistic Infrastructure availability

- Optimization
  - LPG Vs Propylene (PRU)
  - Naphtha Vs MS (CCRU, FCCU, Isom, Crude type)
  - SKO Vs ATF
  - SK Vs HSD
  - FO / LSHS Vs HSD
  - FO Vs Bitumen
Optimization within Refinery

**On-line Optimization**
- Advanced Process Control
  - CDU Pressure minimization subject to constraints
  - CDU COT maximization subject to constraints
  - FCC Severity maximization / optimization
  - Value added product maximization subject to property constraints
    - Inferential properties prediction
    - Constraint controller
    - Multi-variable predictive control
    - On-line Optimizer
  - Offsite blend optimization

Optimization within Refinery - Offline

**Product pattern Optimization**
- Secondary units availability
  - FCC / RFCC
  - HCU / OHCU
  - Coker / VBU / BBU
  - Naphtha cracker
- Type of crude processing
  - LS / HS / Hy. crude
    - Refinery operating cost
- Flexibility of swinging product pattern
  - Demand pattern
    - Seasonal demand (Naphtha, ATF, Bitumen)
    - Prod. Price difference (FO / HSD, LDO/ HSD, Naphtha vs Nat. Gas)
  - RTPs of products
Optimization within Refinery

**Product Pattern Optimization**

- **Secondary Units- FCC / RFCC**
  - MS / LPG maximization
  - Suitable for higher UOP K VGO feed
  - Medium investment
  - Medium Op. cost
    - CCR limitation
    - Metal limitation
    - Lower Cetane of TCO

- **Secondary Units- HCU / OHCU**
  - SK / ATF / HSD maximization without any treatment
  - Lower UOP K VGO feed can be processed
  - High investment
  - High Op. cost
    - Nitrogen limitation

**Optimization within Refinery**

- **Product pattern Optimization**
  - **Secondary Units- Coker**
    - Residue up-graduation
    - Facilitates Hy. Crude processing
    - Relatively low investment
    - Relatively low Op. cost
      - Around 30% coke generation
      - HPS vs Coke price deciding factor
      - Cracked products needs treatment
      - HCGO needs reprocessing in HCU / FCCU
Optimization within Refinery

Product Pattern Optimization

- **Secondary Units- VBU**
  - Viscosity breaking to produce FO
  - Lower cutter stock requirement
  - Low investment
  - Low Op. cost
  - Dubai vs Brent, FO vs HSD deciding factor

- **Secondary Units- BBU**
  - Suitable for VR having high Asphaltenes
  - Releases cutter stock for value added products
  - Seasonal and region specific demand
  - No import facility
  - Dubai vs Brent, FO vs HSD deciding factor

Input cost Optimization

Input Cost = f (Type of crude, Logistic cost, other inputs)

- **Crude Type**
  - LS Crude (Low S, High API, High Dist.)
    - Lower Operating cost
    - Higher FOB and logistic cost
  - HS Crude (High S, Medium API, Medium Dist.)
    - High Operating cost
    - Medium FOB and Lower Logistic cost
  - Hy. Crude (High / Low S, Low API, Low Dist.)
    - High Operating cost
    - High viscosity affecting PL capacity
    - High Acid no., Metal content
    - Cheaper crude
  - The capability of type of crude processing will depend on Refinery configuration
Refinery LP Model

Input
- Available Crude Basket
- Crude and Product Prices at refinery gate
- Product demand
- Shutdown Slate
- Change in product specs.

Model
- Crude Assays
- Process unit configuration
- Feed Blends
- Product Blends
- Product Specs

Objective: Profit Maximization

Output
- Crude Mix and Qty.
- Product pattern
- Sec Unit capacity utilisation
- Sec Units feed and Product Blends

Provision for 24 Multi-periods

Basics of Optimization

Optimization within Refinery

✓ Optimization among Refineries
### Refineries configuration

<table>
<thead>
<tr>
<th>Units</th>
<th>IOCL REFINERIES</th>
<th>ASSOCIATES REFINERIES</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>J</td>
<td>P</td>
</tr>
<tr>
<td>CAP, MMTPA</td>
<td>13.70</td>
<td>12.00</td>
</tr>
<tr>
<td>CDU</td>
<td>☑</td>
<td>☑</td>
</tr>
<tr>
<td>VDU</td>
<td>☑</td>
<td>☑</td>
</tr>
<tr>
<td>RFCC/FCC</td>
<td>☑</td>
<td>☑</td>
</tr>
<tr>
<td>HCU/OHCU</td>
<td>☑</td>
<td>☑</td>
</tr>
<tr>
<td>VBU</td>
<td>☑</td>
<td>☑</td>
</tr>
<tr>
<td>BBU</td>
<td>☑</td>
<td>☑</td>
</tr>
<tr>
<td>COKER</td>
<td>☑</td>
<td>☑</td>
</tr>
<tr>
<td>LOBS</td>
<td>☑</td>
<td>☑</td>
</tr>
<tr>
<td>PY/CHEMICAL</td>
<td>☑</td>
<td>☑</td>
</tr>
</tbody>
</table>

### Optimization Between Refineries

**Synergy among multi-refinery operation to maximize over all profit**

- Intermediate stream sharing
- Refinery configuration
- Planned shutdown schedule
- Capacity constraint in One refinery and availability in other Refinery

- **SRGO** (J- > P/M, BGR->G/B) : HS crude & prod. Optimization
- **Reformat** (J/B/D -> G) : Optimization between Naphtha & MS
- **PXN** ( M- > P ) : HS crude maximization
- **IFO** (J- > P ) : HS crude maximization
- **PNCP Feed** (J/M - > P) : Naphtha export minimization
Basics of Optimization

Optimization within Refinery

Optimization among Refineries

✓ Petroleum Supply Chain Optimization

Corporate Supply Chain

Domestic Crude

Imp. LS Crude

Imp. HS Crude

Crude Imports

Refining

International Trade
- Crude
- Products

Prod. Transfer

Mktg.

Prod. Imports / Exports

Domestic Demand

Imports / Exports

OMCs exchange

Up-Stream
(High Lead time)

Down-Stream

Support

Pipe Lines /

Support
Indian Refineries

- Operates 10 of India's 18 refineries
- Refining capacity: 60.2 MMTPA (1.2 mbpd) - largest in the country
- 41% refining share in the country

Total capacity in the country: 148.9 MMTPA (as of 1 Apr’09)

Infrastructure

- Crude
  - Vadinar / Mundra port (VLCC) for North-West Refineries
    - SMPL for Gujarat, Panipat & Mathura
    - Mundra for Panipat
  - Haldia Port for East coast Refineries
    - Lower Draft and port congestion
    - HBCPL for Barauni Refinery
    - Commissioning of Paradeep-Haldia crude pipeline

- Product
  - Demand growth in North West Sector
  - Euro-III products & ATF demand in Metro cities
  - Product movement from East to North-West
  - Limited export facility at Haldia port
  - Dahej / Kandla for Naphtha Export
  - No Import / Export facility for ATF and Bitumen
Complexity in Indian Oil Supply Chain

- 40 Crudes in basket from S. America to S.E.Asia
- 10 Refineries
- Large distribution network
  - 10 major products
  - 200 Depots (excluding LPG network)
  - 40 Terminals
  - 17 Pipelines
  - 4 Transportation modes
- One crude pipeline catering to 3 refineries
- Crude procurement 3 months in advance

Down stream Oil Industry: Overview

Integrated Supply Chain Management

SCOR model
Source: The Supply Chain Council

IOCL, BPCL, HPCL

Up-stream time Mgmt
M+4 Months

Down-stream time Mgmt.
Crude evaluation / purchase

- Line up crude term contract for 50-60% of requirement
- Spot / short term purchase for balance quantity
- Buy crude giving maximum Supply chain margin
- Based on landed crude price & domestic products pricing
- Crude purchase at Vadinar & Paradeep port
  - Synergy between already purchased crude
  - Crude matching with demand
  - Domestic market discounts
  - Products sale at domestic demand location price
  - Excess product for export based on economics
  - Variable operating cost (Fuel & Loss)
  - Emission norms consideration

Supply Chain Objectives

- Maximize Corporate Profits
  - Profit Refinery + Profit Mktg. = Profit Corporate?
- Optimize the following
  - Raw material
  - Operating cost of refinery
  - Products Logistics Cost ensuring minimal under recovery
  - Inventory cost
  - Synchronized & optimized business process operation
- Supply chain Visibility with their interdependency
- Quick response / Corrective actions to address internal / external contingencies
SCM: Integrated Approach

- Crude evaluation & Procurement?
- What crude to Feed?
- What & Where To Make?
- Corporate IP
- Distribution Planning?
- Demand Forecast?

Integrated Planning Model

- Supply
- Distribution
- PORTS
- Depots
- Basic Transportation Structure
- R1
- R2
- R3
- Rn
### Integrated Planning (IP) Model

<table>
<thead>
<tr>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>- Crude Availability at Ports</td>
<td>- Refinery wise T'put &amp; Crude Alocation</td>
</tr>
<tr>
<td>- Location level Demand</td>
<td>- Crude requirement for future period</td>
</tr>
<tr>
<td>- Desired Inventory build up / depletion</td>
<td>- Refinery wise Product Pattern</td>
</tr>
<tr>
<td>- Committed Exports, Imports</td>
<td>- Detailed Distribution Plan</td>
</tr>
<tr>
<td>- Exchanges with OMCs</td>
<td>Product wise, mode wise</td>
</tr>
<tr>
<td>- Planned Shutdown schedule</td>
<td>- Purchases, Exchanges</td>
</tr>
<tr>
<td>- Changes in product specs.</td>
<td>- Gross Margin</td>
</tr>
<tr>
<td>- Crude Prices / Purchase Cost</td>
<td></td>
</tr>
<tr>
<td>- Product Prices</td>
<td></td>
</tr>
</tbody>
</table>

**Objective:** Profit Maximisation

**Provision of Multi-period planning**

### Model Sizes

<table>
<thead>
<tr>
<th>Models</th>
<th>Constraints (No of Rows)</th>
<th>Variables (No of Columns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Refinery Planning, RPMS</td>
<td>2500 - 5500</td>
<td>6000 - 14500</td>
</tr>
<tr>
<td>Distribution Planning, SAND</td>
<td>2500 - 5500</td>
<td>8500 - 19000</td>
</tr>
<tr>
<td>Integrated Planning</td>
<td>23000</td>
<td>63000</td>
</tr>
</tbody>
</table>
Benefits

- Optimizes the whole supply chain giving higher margins and increased profitability
- Crude selection and allocation which takes into account product demands, refinery capabilities and effect of crudes already procured
- Optimal refinery production planning considering crude assay, unit capacities, product specs and demand pattern
- Optimal distribution planning considering transportation costs, taxes and duties and transportation constraints

THANK YOU
Overview of Industrial Practices in Planning & Scheduling

-Dayanand Deshpande,
12 Jun 2009
Honeywell

Agenda

• Supply Chain Management & Structure of Advanced Planning Systems (APS)

• Planning
  – Demand Planning & Forecasting
  – Advanced Planning and Optimisation
  – Distribution Planning

• Scheduling
  – Production Scheduling
  – Distribution Scheduling (Rail/ Road/ Ship and Pipeline Scheduling)

• Implementation of APS – A case study

• Conclusions & Outlook
 SCM - Another Short-lived Management philosophy???

- "The task of integrating organisational units along a supply chain and coordinating material, information and financial flows in order to fulfil (ultimate) customer demands with the aim of improving competitiveness of a supply chain as a whole"

<table>
<thead>
<tr>
<th>Benefit Area</th>
<th>Sample Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reduction in Inventories</td>
<td>Specialty manufacturer reduced inventory $15M in first year</td>
</tr>
<tr>
<td>Improved Forecasting</td>
<td>• Adjustment in safety stock</td>
</tr>
<tr>
<td></td>
<td>• Statistics can reduce error 10%</td>
</tr>
<tr>
<td></td>
<td>• Collaboration can reduce error 30%</td>
</tr>
<tr>
<td>Lower Supply Chain Costs</td>
<td>• Reduction in premium freight costs</td>
</tr>
<tr>
<td></td>
<td>• Improved customer satisfaction</td>
</tr>
<tr>
<td></td>
<td>Loop scout contributed to refrigeration production increase valued at $1.7M/year at Honeywell Multi Products plant in Geismar, LA</td>
</tr>
<tr>
<td>Improved Efficiency / Capacity</td>
<td>Non Linear Control implementation for polymers manufacturer saved millions of dollars per year</td>
</tr>
<tr>
<td></td>
<td>• Reduce process variability</td>
</tr>
<tr>
<td></td>
<td>• Improved quality</td>
</tr>
<tr>
<td></td>
<td>• Increased throughput</td>
</tr>
<tr>
<td>Asset Utilization / Reliability</td>
<td>Loop scout contributed to refrigeration production increase valued at $1.7M/year at Honeywell Multi Products plant in Geismar, LA</td>
</tr>
<tr>
<td></td>
<td>• 3-8% Improvement</td>
</tr>
</tbody>
</table>

Supply Chain Management - Issues

- Variability in Feedstock availability, grades and prices
- Naphtha import/export decisions
- End-customer demand impacts RM selection and vice-versa
- Difficulty in matching production runs/sequencing to varying demand
- Real time production/yield data important
- Substitutions/variety
- Large SKUs
- Variability of product demand and prices
- Correlation with other product demand
- Huge complexity, cyclic business and vulnerable to uncertainties

Feedstock | Primary | Secondary
Decisions – Supply Chain Planning & Scheduling

**Time Horizon**

- **Long term Planning**
  - 5-10 years
  - (Plant/warehouse locn, LRP, modes of trnsprt, strategic alliances)

- **Mid term Planning**
  - Mon/yr
  - (Exchange Arrangement/Marketing Campaigns/Positioning Analysis)

- **Short term Planning**
  - Weeks/Mon
  - (Annual Plan/Monthly Plan)

**Scheduling**

- Days/weeks
- (Rail-Road schedule/pipeline schedule/production Schedule)

Long Term Plans set objectives, strategies and policies.
Near Term Constraints and conditions require course corrections.

**Structure of Advanced Planning Systems**

- **Procure**
- **Produce**
- **Distribute**
- **Sell**

- **Long-Term**
  - Strategic Planning

- **Mid-Term**
  - Master Planning
  - Demand Planning
  - Purchasing and MRP
  - Production Planning
  - Distribution Planning
  - Production Scheduling
  - Tx Planning & Scheduling
  - Demand Fulfillment & ATP

(source: Supply chain Management and Advanced Planning Hartmut Stattler & Kilger)
Demand Planning

- Starting point of supply chain planning
- Three stages of Demand Planning
  - Statistical Forecasting
  - Judgemental (user) inputs
  - Collaboration
- Enablers – Advanced Forecasting Techniques
  - Moving Average
  - Exponential Smoothing
  - Holt and Winters
  - Box-Jenkins
  - Dynamic Regression
  - Discrete Distributions
  - Poisson & Negative Binomial

Demand Forecasting Process

1. Gather sales history
2. Clean data
   - Fix product/name changes
   - Fix non-optimal shipment history
3. Prioritize customers
   - Identify ABC criteria
   - Consolidate Tier C customers
4. Pass onto Statistical Forecasting

Procure
Produce
Distribute
Sell
Strategic Planning
Master Planning
Demand Planning
Demand Fulfillment & ATP
Distribution Planning
Transport Planning & Scheduling
Production Planning
Production Scheduling
Purchasing and MRP
Forecasting Views

View all data from all sources – plan, forecast, sales reps, actual, financial.

Scroll through any number of years.

Collaborative Forecasting

Statistics as a start
Entered by Sales Rep
Sales Mgr auto accepted
HQ revised
Consensus determined
Master Planning and Optimisation – Why Now?

- Shareholders demand higher profits
- Customers/Competitors force service improvements
- M&A’s yield more complex supply chains
  - More plants, distribution locations, and products
- eBusiness requires accurate, automated collaboration
- Enablers:
  - Better data (ERP, SCP)
  - Improved supply chain models
  - Improved LP solvers – ILOG/ xpress
  - Faster CPU’s

Supply Chain Optimiser

- Determines most profitable customer and product mix
- Considers customer demands and margins, production capacity, and production/distribution costs

**Inputs**
- Customer Demand
- Production Capability
- Prices and Costs
- Production & Distribution Costs

**Outputs**
- Optimized Sales Plan
- Optimized Production Plan
Typical Uses of SCO

- Optimize & balance the supply-demands
- Evaluate customer trade-offs
- Examine equipment capacity changes
- Identify profit opportunities

Distribution Planning - Highlights

- Use of LP and MIP for optimising the profitability (Max sales – dist. Cost)
- Multiplant, multiwarehouse problem
- Construct a distribution network directly on a map
- Manipulating the Map Interface
Distribution Planning

- Multi-Period Capabilities
- "what if" analysis
- Solution Reporting
- Capabilities
- Customized Reports

Distribution Replenishment Planning

- Predicts material needs at plants, supply points and vendor managed inventory locations
- Generates replenishment schedules to meet unsatisfied material demands
- Adjusts replenishment plans as supplies and demands vary
- Considers lead times, lot sizes, production schedules, policies & constraints

Demo
Production Scheduling

- Wide range of processes
  - Continuous, semi-continuous, batch...
  - MTO – MTS – mixed mode
- Supports decision support & what-if analysis
  - Tied to financial model
- Includes embedded optimization algorithms
- Open architecture for unique optimization plug-ins

Distribution Planning and Scheduling

- Distribution Planning
  - Road/Rail Scheduling
  - Pipeline Scheduling
  - Ship Scheduling
Rail Road Scheduling

Provides a single screen for Inventory Visibility

Highlights

Complex Technical Integration
(Includes interfaces from diverse sources)

- ERP for Shipped Sales and Open Orders
- Inventory
- In-transit and Stock Transfers
- Inputs from Demand Planning Solution
- Inputs from Monthly Distribution Plan (integration with SAND)
- Inputs from customized GUIs
System for Fleet Scheduling & Optimization

- Fleet management
- LNG and other refined products
- Contract management
- Update Schedule and Annual Delivery Program (ADP)
- Replenishment
- Operational Decision Support and Re-planning of Operations

The Fleet Scheduling Problem

- Assign cargoes to ships
- Decide optimal visiting sequences for each ship
- A complex combinatorial problem
  - 3 vessels and 5 cargoes ⇒ 243 alternatives
  - 10 vessels and 20 cargoes ⇒ 100,000,000,000,000,000,000 alternatives
- Constraints:
  - Capacity
  - Time windows (multiple)
  - Compatibility
  - Etc...
- Rescheduling often needed
Main Components (1)

- Electronic charts
- Information of ships, cargoes, ports etc
- Automatic calculation of distances
- Graphical user interface
- Ship positions reports by satellite
- Optimization tool for fleet scheduling
- Calculation for manual planning
- Automatic update of ETA

Main Components (2)

Optimise

Maintain Data

Visualise
Conclusions & Outlook

- APS Solutions deliver tangible/ intangible benefits
- Challenges remain in terms of
  - Integration among different modules
  - Change Management
- Technologies such as RFID, SOA would be helpful in APS going forward
Mathematical Programming for Scheduling of Process Operations

Dr. Munawar Abdul Shaik

B.E. (Hons.) Chemical, BITS Pilani, 1997
M.E. (Chemical), BITS Pilani, 2000
Ph.D. (Chemical Engg.) IIT Bombay, 2005
Post-Doctoral Fellow, Chemical Engg., Princeton University, 2005-2007

Assistant Professor
Department of Chemical Engineering

Basic Definitions & Applications

**Scheduling:** Efficient management of resources over a set of units to perform a group of activities in an optimal fashion

**Planning:** What? Where? How much?

**Scheduling:** How?

**Applications:**
- **Operations Research Community:**
  - Flowshops & Jobshops
  - Scheduling of Personnel, Vehicles etc.
- **Chemical Engineering:**
  - **Batch plants:** Food, Pharmaceuticals, Paper products & Specialty Chemicals
  - **Continuous/Semi-continuous:** Petrochemical & Refinery operations
Chemical engineers have made significant contributions in *Operations Scheduling* in the past two decades

- Shah, Pantelides et al → Imperial College, London
- Grossmann et al → CMU
- Floudas et al → Princeton Univ.
- Karimi et al → NUS
- Reklaitis, Pekny et al → Purdue
- Pinto et al → RPI
- Ierapetritou et al → Rutgers Univ.

Supply Chain of an Enterprise

**Challenges:**
- Different time scales
- Consistent Decisions
- Infrequent Revision
- Large-size Problems

Vertical Integration in an Enterprise is Desirable
Planning and Scheduling

Multi-site Production Planning:

- Period 1, Period 2, ..., Period T
- Site 1, Site 2, ..., Site N
- Time Horizon is longer

Medium-term & Short-term Scheduling:

- Period t, Site n
- Relatively Short Time Horizons

Typical Time Horizons:
- Planning: 3 months to 1 year
- Medium-term: week or month
- Short-term: hour or day

Problem Statement

Given:
- Set of products along with their demands and due dates
- Set of manufacturing locations
- Process flow sheet at each plant
- Equipment and storage capacities
- Batch processing time for each product in all stages
- Transition times (sequence dependent)
- Production, transportation, inventory or earliness, and tardiness costs

For Planning determine:
- Order allocation across plants
- Amounts of products to be produced
- Length of short-term horizon

For Scheduling determine:
- Optimal sequencing at each plant
- Start and finish times of different tasks on each unit
- Optimal inventory levels
- Optimal dispatch schedule
Classification of Scheduling Problems

- **Batch Plants**
  - Continuous/Semi-continuous
  - Mixed production lines

- **Serial units**
  - Parallel lines
  - Hybrid flowshops

- **Discrete time**
  - Continuous-time formulation

- **Medium-term Scheduling**
  - Short-term scheduling
  - Cyclic scheduling
  - Robust scheduling
  - Reactive scheduling

- **Slot-based**
  - Global-event based
  - Unit-specific-event based
  - Precedence based

---

Classification of Scheduling Problems

- **Max Profit**
- **Min Make Span**
- **Min Tardiness/Earliness**

- **Multi-product plants (job shops)**
- **Multi-purpose plants (flow shops)**

- **Without Resources**
  - With Resources (Utilities)

- **Unlimited Storage**
  - No Storage / Zero-wait
  - Finite-Intermediate Storage

- **Dedicated Storage**
  - Flexible Storage
Classification of Scheduling Problems

Multi-product plants (flow shop)

Multi-purpose plants (job shop)

Process Representation

- State-Task Network (STN)
- Resource-Task Network (RTN)
- Recipe diagrams

STN Representation:

Gantt Chart Schedule:
Different Time Representations

- **Discrete Time Representation**
  - Time intervals of equal length common to all units

- **Continuous Time Representation I**
  - Slot based
  - Both start and end times of tasks have to be at an event
  - 5 slots or 6 events
  - Time intervals of unequal and unknown length common to all units

- **Continuous Time Representation II**
  - Global event based
  - Only the start times of tasks have to be at an event
  - 4 events

- **Continuous Time Representation III**
  - Unit Specific event based
  - Only 2 events

Scheduling Characteristics

- **Performance criteria**
  - Profit maximization
  - Make-span minimization
  - Mean-flow time minimization
  - Average tardiness minimization

- **Transfer policies**
  - UIS (Unlimited Intermediate Storage)
  - NIS (No Intermediate Storage)
  - FIS (Finite Intermediate Storage)
  - ZW (Zero-Wait Policy)
  - MIS (Mixed Intermediate Storage)
Mathematical Model

Max Profit or Min Makespan

s.t. Allocation constraints
     Material balance constraints
     Capacity constraints
     Storage constraints
     Duration constraints
     Sequence constraints
     Demand constraints
     Due date constraint
     Time horizon constraints

Mixed-Integer Linear/Nonlinear Optimization Problem

Solution of the Scheduling Model

➢ Broadly Two approaches for solution:
   → Deterministic Methods
   → Stochastic Methods

Commercial Software:

Modeling Languages
- GAMS
- ILOG OPL Studio
- MOSEL from XPRESSMP
- AMPL, LINGO etc.

Solvers
- LP/MILP → CPLEX
- MINLP → SBB, DICOPT, BARON
- NLP → SNOPT, MINOS, CONOPT
- DAEs → MINOPT
Short-Term Scheduling: Batch Plants

Shaik & Floudas (2008)

- Unit-Specific Event-based Continuous-time formulation for Short-Term Scheduling of Batch Plants without Resources (such as utilities)
- The work is extension of STN model of Ierapetritou & Floudas (1998)
- Improved Sequencing Constraints (for handling sequence-dependent changeovers)
- Alternate approach for handling dedicated finite-intermediate storage without the need for considering storage as a separate task
- Additional tightening constraint
- Limitation: Does not allow tasks to take place over multiple events

Short-Term Scheduling Model

Nomenclature

Sets
- $I$: tasks
- $I_r$: tasks related to resource $r$
- $R$: resources
- $R^e$: equipment resources
- $R^m$: material resources
- $RFIS$: material resources with finite dedicated storage
- $N$: event points within the time horizon

Parameters
- $H$: scheduling horizon
- $P_r$: price of resource $r$
- $D_r$: demand for resource $r$
- $\tau^e$: sequence independent clean up time
- $\tau^{ed}_{i,i'}$: sequence-dependent clean up time required between tasks $i$ and $i'$
- $E^{min}_r$: lower bound on the availability of resource $r$
- $E^{max}_r$: upper bound on the availability of resource $r$
- $\mu^e_r$, $\mu^m_r$: proportion of equipment resource produced, consumed in task $i$, $\mu^e_r \geq 0$, $\mu^m_r \leq 0$
- $\rho^e_r$, $\rho^m_r$: proportion of material resource produced, consumed in task $i$, $\rho^e_r \geq 0$, $\rho^m_r \leq 0$
Short-Term Scheduling Model

Nomenclature

Binary variables

\( w(i,n) \) Assign the beginning of task \( i \) at event \( n \)

Positive variables

\( b(i,n) \) Amount of material processed by task \( i \) in event \( n \)

\( E_0(r) \) initial amount of resource \( r \) available or required from external sources

\( E(r,n) \) excess amount of resource \( r \) available at event \( n \)

\( T^a(i,n) \) time at which task \( i \) starts at event \( n \)

Capacity Constraints

\[ w(i,n)B^i_{\text{min}} \leq b(i,n) \leq w(i,n)B^i_{\text{max}} \quad \forall i \in I, n \in N \] (1)

\[ E^r_{\text{min}} \leq E(r,n) \leq E^r_{\text{max}} \quad \forall r \in R, n \in N \] (2)

Excess Resource Balances

The amount of a resource \( r \) produced or consumed by task \( i \) is represented as:

\[ \mu_i w(i,n) + \rho_i b(i,n) \]

\[ E(r,n) = E(r,n-1) + \sum_{i \in I} \left( \mu_i^r w(i,n-1) + \rho_i^r b(i,n-1) \right) + \sum_{i \in I} \left( \mu_i^r w(i,n) + \rho_i^r b(i,n) \right) \quad \forall r \in R, n \in N, n > 1 \] (3a)

\[ E(r,n) = E_0(r) + \sum_{i \in I} \left( \mu_i^r w(i,n) + \rho_i^r b(i,n) \right) \quad \forall r \in R, n \in N, n = 1 \] (3b)

Analysis for Material Resources: (Reduces to the material balances in STN)

Analysis for Equipment Resources: (keeps track of the status of a unit)

A separate task is assumed for each task suitable in multiple equipment resources

Analysis for Material Resources: (Reduces to the material balances in STN)
Short-Term Scheduling Model

Sequencing Constraints

(i) Same task in the same unit

\[ T'(i, n+1) \geq T'(i, n) + \alpha_i w(i, n) + \beta_i b(i, n) \quad \forall i \in I, n \in N, n < N \]  

(ii) Different tasks in the same unit:

(a) No changeovers or cleanup times:

\[ T'(i, n+1) \geq T'(i', n) + \alpha_{i'} w(i', n) + \beta_{i'} b(i', n) \quad \forall r \in R', i, i' \in I, n \in N, n < N \]  

(b) Sequence-independent cleanup times:

\[ T'(i, n+1) \geq T'(i', n) + \alpha_{i'} w(i', n) + \beta_{i'} b(i', n) + \tau_{i'} w(i', n) \quad \forall r \in R', i, i' \in I, i \neq i', n \in N, n < N \]  

(c) Sequence-dependent changeovers:

\[ T'(i, n) \geq T'(i', n') + \alpha_{i'} w(i', n') + \beta_{i'} b(i', n') + \tau_{i'} w(i', n) - H(1 - w(i', n')) - H \sum_{i \neq i'} \sum_{n < N} w(i', n) \]

\[ \forall r \in R', i, i' \in I, i \neq i', n < N, n' < N \]  

(iii) Different tasks in different units:

\[ T'(i, n+1) \geq T'(i', n) + \alpha_{i'} w(i', n) + \beta_{i'} b(i', n) - H(1 - w(i', n)) \]

\[ \forall r \in R', i, i' \in I, i \neq i', n \in N, n < N \]  

Time Bounding Constraints

\[ T'(i, n) \leq H \quad \forall i \in I, n \in N \]  

\[ T'(i, N) + \alpha_i w(i, N) + \beta_i b(i, N) \leq H \quad \forall i \in I \]  

Tightening Constraint

\[ \sum_{i \in I} \sum_{n \in N} (\alpha_i w(i, n) + \beta_i b(i, n)) \leq H \quad \forall r \in R' \]  

The tightening constraint provides a better LP relaxation.
Objective Function

Maximization of Profit

\[
\text{Max Profit} = \sum_{r \in R} P \left( E(r, N) + \sum_{i \in I} \left( \mu_r^p w(i, N) + \rho_r^p b(i, N) \right) \right) \tag{9}
\]

Minimization of Makespan (MS)

Demand Constraints

\[
E(r, N) + \sum_{i \in I} (\mu_r^p w(i, N) + \rho_r^p b(i, N)) \geq D_r \quad \forall r \in R^S \tag{10}
\]

Time Bounding Constraints

\[
T'(i, N) + \alpha_r w(i, N) + \beta_r b(i, N) \leq MS \quad \forall i \in I \tag{11}
\]

Modified Tightening Constraint

\[
\sum_{i \in I} (\alpha_r w(i, n) + \beta_r b(i, n)) \leq MS \quad \forall r \in R'^i \tag{12}
\]

This is the model for Unlimited Intermediate storage (UIS)

Benchmark Examples

Example 1

Sundaramoorthy & Karimi (2005), and Shaik, Janak, Floudas (2006)

- Problem involves 5 units, 3 processing tasks, and 4 states (1 feed, 2 int, 1 product)
- Variable batch sizes and processing times
- Finite intermediate storage (FIS) for intermediates S2 and S3
- Consider two objective functions:
  - Maximization of Profit for 3 cases of different time horizons:
    - Case 1a: H=8 hr
    - Case 1b: H=12 hr
    - Case 1c: H=16 hr
  - Minimization of Makespan for 2 cases of different demands:
    - Case 1a: D_4 = 2000 mu
    - Case 1b: D_4 = 4000 mu
Benchmark Examples

Example 2

- Problem involves 4 units, 8 processing tasks, 9 states (3 feed, 4 int, 2 product)
- Variable batch sizes and processing times
- Finite intermediate storage (FIS) for intermediates S4, S5, S6 and S7
- Consider two objective functions:
  - Maximization of Profit for 3 cases of different time horizons:
    - Case 2a: H=8 hr
    - Case 2b: H=12 hr
  - Minimization of Makespan for the following demands:
    - $D_3 = 200 \text{ mu}$
    - $D_9 = 200 \text{ mu}$

Example 3

- Problem involves 6 units, 11 processing tasks, 13 states (4 feed, 7 int, 2 product)
- Variable batch sizes and processing times
- Finite intermediate storage (FIS) for all intermediates S3 – S7, S9 and S10
- Consider two objective functions:
  - Maximization of Profit for 2 cases of different time horizons:
    - Case 3a: H=8 hr
    - Case 3b: H=12 hr
  - Minimization of Makespan for 2 cases of different demands:
    - Case 3a: $D_{12} = 100 \text{ mu}$, $D_{13} = 200 \text{ mu}$
    - Case 3b: $D_{12} = D_{13} = 250 \text{ mu}$
# Benchmark Examples

Data of coefficients of processing times of tasks, limits on batch sizes of units

<table>
<thead>
<tr>
<th>Task</th>
<th>Unit</th>
<th>$\alpha_{ij}$</th>
<th>$\beta_{ij}$</th>
<th>$\beta_{ij}^{\min}$ (mu)</th>
<th>$\beta_{ij}^{\max}$ (mu)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Task1 ($i=1$)</td>
<td>Unit1</td>
<td>1.333</td>
<td>0.01333</td>
<td>---</td>
<td>100</td>
</tr>
<tr>
<td>Task2 ($i=2$)</td>
<td>Unit2</td>
<td>1.333</td>
<td>0.01333</td>
<td>---</td>
<td>150</td>
</tr>
<tr>
<td>Task3 ($i=3$)</td>
<td>Unit3</td>
<td>1.000</td>
<td>0.00500</td>
<td>---</td>
<td>200</td>
</tr>
<tr>
<td>($i=4$)</td>
<td>Unit4</td>
<td>0.667</td>
<td>0.00445</td>
<td>---</td>
<td>150</td>
</tr>
<tr>
<td>($i=5$)</td>
<td>Unit5</td>
<td>0.667</td>
<td>0.00445</td>
<td>---</td>
<td>150</td>
</tr>
</tbody>
</table>

Example 1

Data of storage capacities, initial stock levels and prices of various resources

<table>
<thead>
<tr>
<th>Storage capacity (mu)</th>
<th>Initial stock (mu)</th>
<th>Price ($/mu$)</th>
<th>Storage capacity (mu)</th>
<th>Initial stock (mu)</th>
<th>Price ($/mu$)</th>
<th>Storage capacity (mu)</th>
<th>Initial stock (mu)</th>
<th>Price ($/mu$)</th>
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<tbody>
<tr>
<td>Resource</td>
<td></td>
<td></td>
<td>S1</td>
<td>UL AA</td>
<td>0</td>
<td>UL AA</td>
<td>0</td>
<td>UL AA</td>
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<tr>
<td>S2</td>
<td>200</td>
<td>0</td>
<td>UL AA</td>
<td>0</td>
<td>UL AA</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S3</td>
<td>250</td>
<td>0</td>
<td>UL AA</td>
<td>0</td>
<td>100</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S4</td>
<td>UL</td>
<td>0</td>
<td>5</td>
<td>100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S5</td>
<td>--</td>
<td>--</td>
<td>200</td>
<td>0</td>
<td>300</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S6</td>
<td>--</td>
<td>--</td>
<td>150</td>
<td>0</td>
<td>150</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S7</td>
<td>--</td>
<td>--</td>
<td>200</td>
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<td>150</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>S8</td>
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<td>--</td>
<td>UL</td>
<td>0</td>
<td>10</td>
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<td></td>
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<tr>
<td>S9</td>
<td>--</td>
<td>--</td>
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<td>0</td>
<td>150</td>
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<tr>
<td>S11</td>
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<td>150</td>
<td>0</td>
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</tr>
<tr>
<td>S12</td>
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<td>UL</td>
<td>0</td>
<td>5</td>
<td></td>
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</tr>
<tr>
<td>S13</td>
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<td>--</td>
<td>UL</td>
<td>0</td>
<td>5</td>
<td></td>
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</tr>
</tbody>
</table>

UL – Unlimited storage capacity
AA – Available as and when required

Sundaramoorthy & Karimi (2005), and Shaik, Janak, Floudas (2006)
### Other models used in Comparative Study

**STN:**


**RTN:**


**Recipe Diagrams:**

### Abbreviation used

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Used Models</th>
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<tbody>
<tr>
<td>I&amp;F</td>
<td>STN</td>
</tr>
<tr>
<td>L&amp;F</td>
<td>STN</td>
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<tr>
<td>FIS</td>
<td>STN</td>
</tr>
<tr>
<td>CBMN</td>
<td>RTN</td>
</tr>
<tr>
<td>S&amp;F</td>
<td>RTN</td>
</tr>
<tr>
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### Computational Results (UIS)

**Example 1: Maximization of Profit**

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*a* Suboptimal solution. Relative Gap: 1.24%
### Computational Results (UIS)

#### Example 2

**Maximization of Profit**

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* Suboptimal solution; Relative Gap: 1.59 %, 2.58%*/

**Limitation:** Does not allow tasks to occur over multiple events (motivation for the Unified Model)

---

### Computational Results (UIS)

#### Example 3

**Maximization of Profit**

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* Suboptimal solution
Scheduling of Refinery Operations

Dr. Munawar Abdul Shaik
Assistant Professor
Department of Chemical Engineering

A Typical Oil Refinery

- Crude-oil refining into useful petroleum products:
  - LPG, gasoline, diesel fuel, kerosene, heating oil, ...
- 3 parts:
  - Crude-oil unloading and blending
  - Fractionation and reaction processes
  - Product blending and shipping

(Mendez et al., 2006)
• Scheduling horizon \([0, H]\)
• 4 types of resources:
  - Crude-oil marine vessels
  - Storage tanks
  - Charging tanks
  - Crude Distillation Units (CDUs)
• 3 types of operations:
  - Unloading: Vessel unloading to storage tanks
  - Transfer: Transfer from storage tanks to charging tanks
  - Distillation: Distillation of charging tanks

Crude-oil Scheduling problem

• Given
  - Refinery configuration
  - Logistics constraints
  - Initial tanks inventory and composition
  - Vessels arrival time, inventory level and composition
  - Distillation specifications and demands (planning decisions)
• Determine
  - Required operations
  - Timing decisions
  - Transfer volumes
• Minimize
  - Cost of distilled crude-oil mixtures

(Mendez et al., 2006)
Crude-oil Scheduling problem: Example

- **Common logistics constraints:**
  - Only one docking station available for vessel unloadings
  - No simultaneous inlet and outlet operations on tanks
  - Crude distillation units can only be charged by one tank
  - Continuous distillation

(Mendez et al., 2006)
Consider Integration of Planning and Scheduling for an M-stage Hybrid Flowshop Plant

Multi-level Decomposition of the Overall Problem of Integration of Planning and Scheduling


Proposed Multi-level Structure for Lube-oil scheduling

- **Level-1**: Planning over a multi-period horizon: Order Redistribution
- **Level-2**: Detailed scheduling in each period: Meeting Production Targets
- **Level-3**: Operator level inventory scheduling: ISTR (Individual Tank Assignments)

Embedding proactive/contingency measures
Multi-level Structure for Lube-oil scheduling

Abstractions

- Level-1
  - Traditional timeslot usage
  - Assumed slopping losses
  - Abstracted inventory

- Level-2
  - Modified timeslot definition for slopping (Abstraction of total available compatible tank volumes)

- Level-3
  - ISTR (tank assignments)

Increasing model granularity

Level-2: Extensions to Large problems

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Level-3: Tank assignments

Suppose: Tanks each 50 m³ capacity

Level-3: ISTR algorithm

- Sub-profile generation
- Non-overlapping zones
- Reuse of tanks
Reactive scheduling between first two levels

Level-1
1000 hr 900 hr 800 hr

Level-2
$T_s = 724.4$ hr

Nominal schedule for first period

Receding horizon for intrusion

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<td>0</td>
</tr>
<tr>
<td>99.9</td>
<td>899.66</td>
<td>0</td>
</tr>
<tr>
<td>100</td>
<td>900</td>
<td>0.795</td>
</tr>
<tr>
<td>101</td>
<td>900</td>
<td>12.98</td>
</tr>
</tbody>
</table>

Local disturbances are attenuated locally

Cyclic Scheduling Problem

Multistage Multiproduct Continuous Plant
(Pinto & Grossmann, 1994)
Mathematical Formulation

Time slot representation

stage 1
stage 2
stage M

Transition
processing

time

MINLP model for Cyclic Scheduling

Maximize

Profit = \sum_{i} p_i \frac{W_{Pi}}{T_c} - \sum_{i} \sum_{m} C_{inv} m_i \frac{L_{im}}{T_c} - \sum_{i} \sum_{j} \sum_{k} \sum_{m} C_{tr}_{ij} \frac{Z_{ijkm}}{T_c}

- \frac{1}{2} \sum_{i} \sum_{k} C_{inv} f_{ij} \alpha_{iM} R_{pM} \left(1 - \frac{T_{ppM}}{T_c}\right) T_{ppM}

subject to

\sum_{k} y_{ikm} = 1 \quad \forall i \quad \forall m \quad (2a)

\sum_{i} y_{ikm} = 1 \quad \forall k \quad \forall m \quad (2b)

\sum_{j} z_{ijkm} = y_{ikm} \quad \forall j \quad \forall k \quad \forall m \quad (3a)

\sum_{i} z_{ijkm} = y_{jk-1m} \quad \forall i \quad \forall k \quad \forall m \quad (3b)
MINLP model for Cyclic Scheduling

\[ T_{sp_{ikm}} - U_{i_{km}}^{r} V_{ikm} \leq 0 \quad \forall i \quad \forall k \quad \forall m \quad (4a) \]

\[ T_{ep_{ikm}} - U_{i_{km}}^{r} V_{ikm} \leq 0 \quad \forall i \quad \forall k \quad \forall m \quad (4b) \]

\[ T_{pp_{ikm}} - U_{i_{km}}^{r} V_{ikm} \leq 0 \quad \forall i \quad \forall k \quad \forall m \quad (4c) \]

\[ T_{pp_{ikm}} = T_{ep_{ikm}} - T_{sp_{ikm}} \quad \forall i \quad \forall k \quad \forall m \quad (4d) \]

\[ \sum_{i} T_{sp} \ i_{jm} = \sum_{i} \sum_{j} \tau_{jm} z_{ijm} \quad \forall m \quad (5a) \]

\[ \sum_{i} T_{sp} \ (i_{k+1})_{jm} = \sum_{i} T_{ep} \ i_{km} + \sum_{i} \sum_{j} \tau_{jm} z_{ijm} \quad \forall k < NK \quad \forall m \quad (5b) \]

\[ T_{c} \geq \sum_{k} \left( \sum_{i} T_{pp} \ i_{km} + \sum_{i} \sum_{j} \tau_{jm} z_{ijm} \right) \quad (5c) \]

Inventory Breakpoints

- Stage \( m \)
  - \( T_{pp_{ikm}} \)
  - \( T_{sp_{ikm}} \)
  - \( T_{ep_{ikm}} \)

- Stage \( m+1 \)
  - \( T_{pp_{i(k+1)m}} \)
  - \( T_{sp_{i(k+1)m}} \)
  - \( T_{ep_{i(k+1)m}} \)
Inventory Breakpoints

\[ I_{1,m} = I_{0,m} + \alpha_{im} R_{pm} \min \left\{ \sum \limits_{k} T_{sp,ikm} + \sum \limits_{k} T_{pp,ikm} \right\} \]
\[ I_{2,m} = I_{1,m} + (\alpha_{im} R_{pm} - R_{p,(m+1)}) \max \left\{ 0, \sum \limits_{k} T_{ep,ikm} - \sum \limits_{k} T_{sp,ikm} \right\} \]
\[ I_{3,m} = I_{2,m} - R_{p,(m+1)} \min \left\{ \sum \limits_{k} T_{pp,ikm} + \sum \limits_{k} T_{ep,ikm} - \sum \limits_{k} T_{sp,ikm} \right\} \]

\[ 0 \leq I_{1,m} \leq I_{m} \]
\[ 0 \leq I_{2,m} \leq I_{m} \]
\[ 0 \leq I_{3,m} \leq I_{m} \]

\[ I_{3,m} = I_{0,m} \quad \forall i \quad \forall m \quad (6) \]

\[ W_{pm} = \alpha_{SM} R_{p,M} z_{ikm} \sum \limits_{k} T_{pp,ikm} \quad \forall i \quad (7a) \]

\[ W_{pm} \geq D_{c} T_{c} \quad \forall i \quad (7b) \]

Mathematical model

Variables:

\[ y_{ikm} \in \{0,1\} \]
\[ 0 \leq z_{ikm} \leq 1 \]
\[ T_{sp,ikm}, T_{ep,ikm}, T_{pp,ikm}, W_{p,m}, T_{c}, I_{m}, I_{0,m}, I_{1,m}, I_{2,m}, I_{3,m} \geq 0 \]

Most of the Scheduling problems in Chemical Engineering result in MILP/MINLP models with large number of binary and continuous variables.
3P2S Scheduling Problem

Product sale price ($/ton) demand (kg/h)

<table>
<thead>
<tr>
<th>Product</th>
<th>sale price ($/ton)</th>
<th>demand (kg/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>150</td>
<td>50</td>
</tr>
<tr>
<td>B</td>
<td>400</td>
<td>100</td>
</tr>
<tr>
<td>C</td>
<td>650</td>
<td>250</td>
</tr>
</tbody>
</table>

3P2S Problem data

<table>
<thead>
<tr>
<th>stage 1</th>
<th>stage 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>product</td>
<td>processing rate (kg/h)</td>
</tr>
<tr>
<td>---------</td>
<td>------------------------</td>
</tr>
<tr>
<td>A</td>
<td>800</td>
</tr>
<tr>
<td>B</td>
<td>1200</td>
</tr>
<tr>
<td>C</td>
<td>1000</td>
</tr>
</tbody>
</table>

Transition times (sequence dependent)

<table>
<thead>
<tr>
<th>product</th>
<th>stage 1</th>
<th>stage 2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
<td>B</td>
</tr>
<tr>
<td>---------</td>
<td>---------</td>
<td>---------</td>
</tr>
<tr>
<td>A</td>
<td>-</td>
<td>10</td>
</tr>
<tr>
<td>B</td>
<td>3</td>
<td>-</td>
</tr>
<tr>
<td>C</td>
<td>8</td>
<td>3</td>
</tr>
</tbody>
</table>
3P2S Solution

stage 1

stage 2

Inv (ton)

Profit = $442.53 / hr
Cycle time = 94.05 hr
Variables = 146 (18 bin)
Constraints = 162
CPU time = 12.43 sec

<table>
<thead>
<tr>
<th>Product</th>
<th>demand (kg/hr)</th>
<th>production (kg/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>B</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>C</td>
<td>250</td>
<td>758</td>
</tr>
</tbody>
</table>