Refinery Operations Planning

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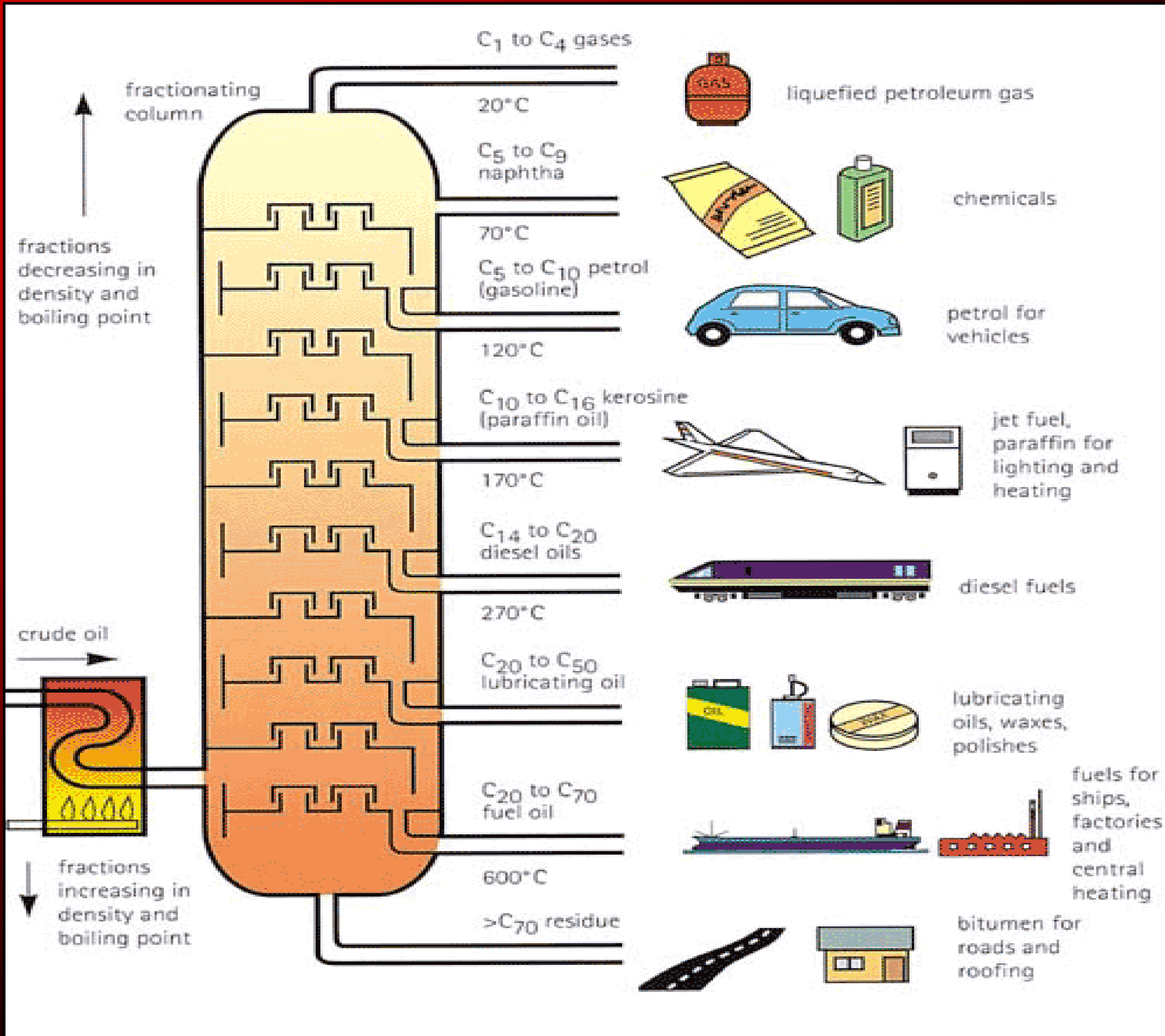
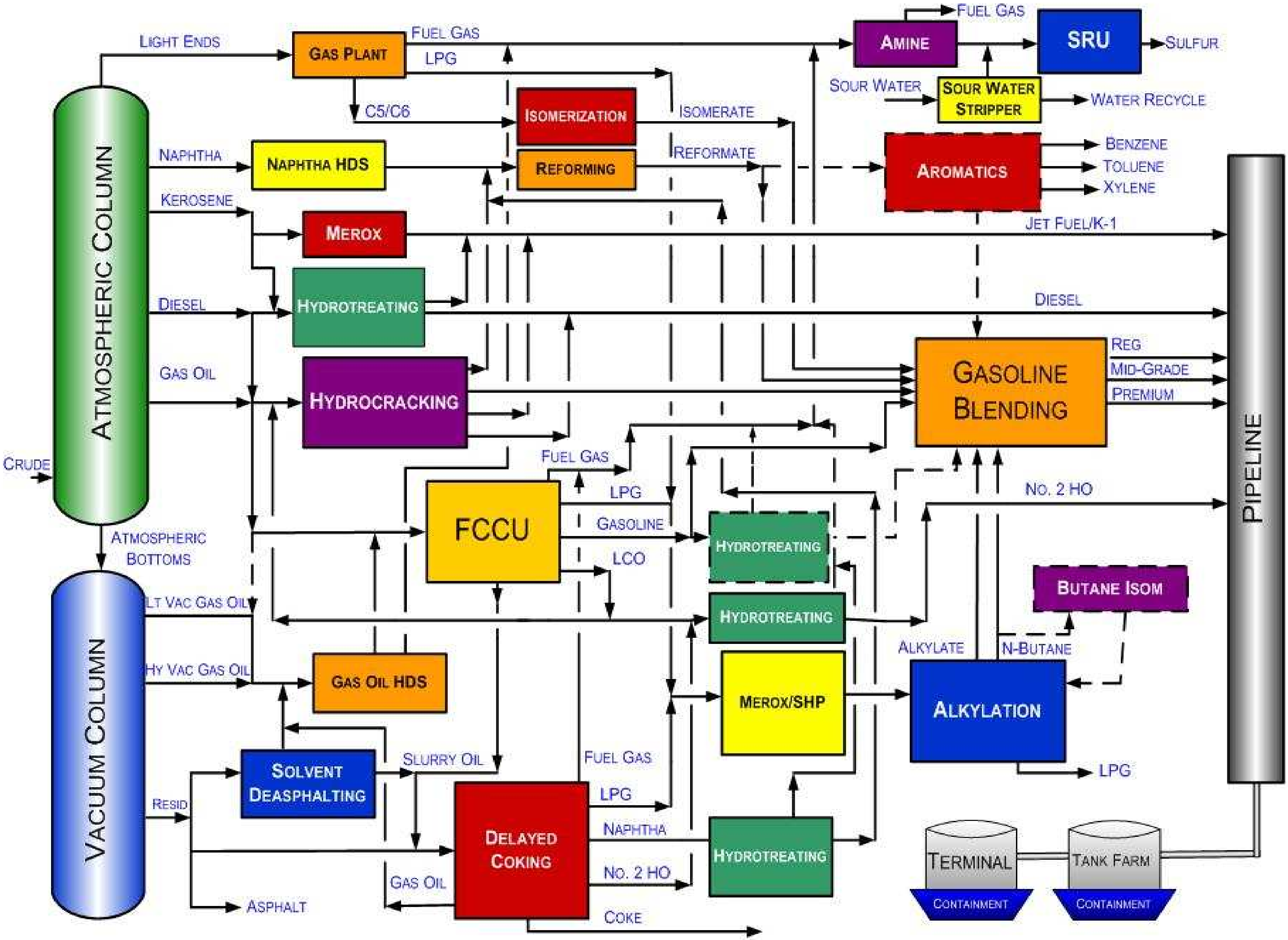
Refinery Operations Planning

- What is a refinery?
  - Takes crude oil and converts it into gasoline
  - Distills crude into light, medium, and heavy fractions
    - Lightest fractions – gasoline, liquid petroleum gas
    - Medium fractions – kerosene and diesel oil
    - Heavy fractions – gas oils and residuum

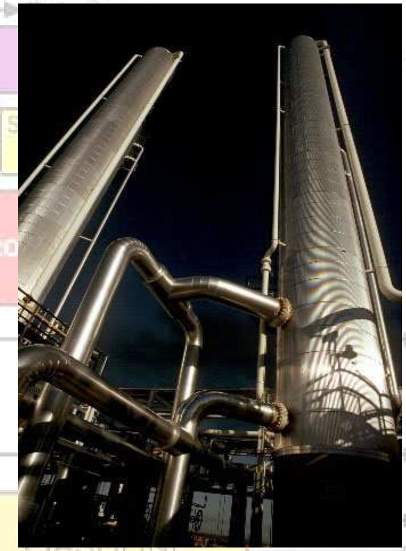


C_1 to C_4 gases
fractionating column
20°C
liquefied petroleum gas
C_5 to C_9 naphtha
chemicals
70°C
fractions decreasing in density and boiling point
C_5 to C_{10} petrol (gasoline)
petrol for vehicles
120°C
C_{10} to C_{16} kerosine (paraffin oil)
jet fuel, paraffin for lighting and heating
170°C
C_{14} to C_{20} diesel oils
diesel fuels
270°C
crude oil
C_{20} to C_{50} lubricating oil
lubricating oils, waxes, polishes
C_{20} to C_{70} fuel oil
fuels for ships, factories and central heating
600°C
fractions increasing in density and boiling point
>C_{70} residue
bitumen for roads and roofing



Light Ends
Gas Plant
Fuel Gas
LPG
C5/C6
Isomerization
Isomerate
Reformate
Amine
Fuel Gas
SRU
Sulfur
Sour Water
Sour Water Stripper
Water Recycle
Atmospheric Column
Naphtha
Naphtha HDS
Reforming
Aromatics
Benzene
Toluene
Xylene
Kerosene
Merox
Jet Fuel/K-1
Hydrotreating
Diesel
Diesel
Gas Oil
Hydrocracking
Gasoline Blending
Reg
Mid-Grade
Premium
Crude
Fuel Gas
LPG
FCCU
Gasoline
LCO
Hydrotreating
No. 2 HO
Pipeline
Atmospheric Bottoms
Vacuum Column
Lt Vac Gas Oil
Hydrotreating
Butane Isom
Hy Vac Gas Oil
Gas Oil HDS
Alkylate
N-Butane
Merox/SHP
Alkylation
Solvent Deasphalting
Slurry Oil
Fuel Gas
LPG
Resid
Delayed Coking
Naphtha
Hydrotreating
No. 2 HO
Gas Oil
Asphalt
Coke
Terminal
Tank Farm
Containment
Containment

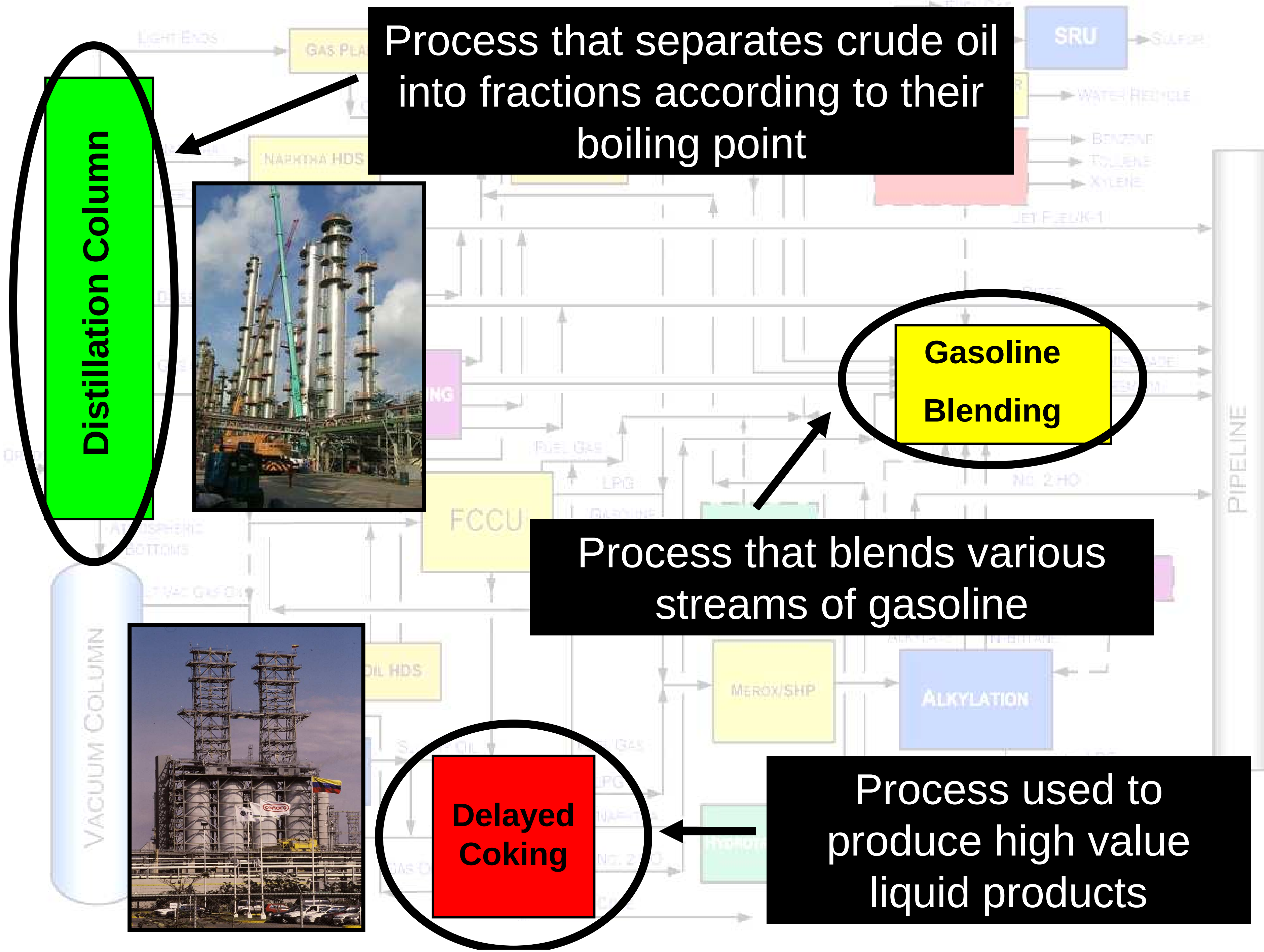
Reformer



Process used to increase the octane number of light crude fractions

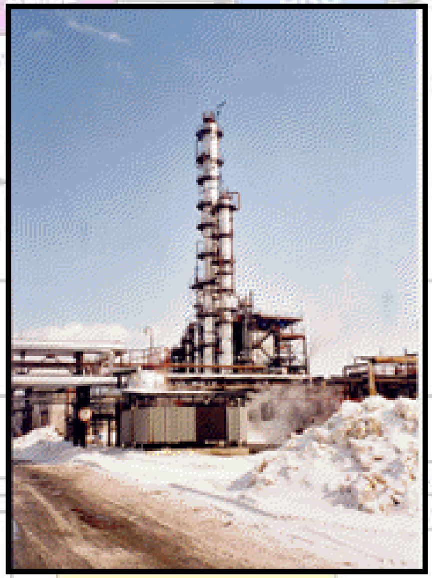
Hydrocracker

Process that is fed by heavier fractions to produce lighter fractions


Process that separates crude oil into fractions according to their boiling point
Distillation Column
Gasoline Blending
Process that blends various streams of gasoline
Delayed Coking
Process used to produce high value liquid products
SRU
NAPHTHA HDS
FCCU
PIPELINE
VACUUM COLUMN
MEROX/SHP
ALKYLATION

Isomerization

Process that converts normal, straight chain paraffins to iso-paraffins



Hydrotreating

Process that uses H_2 to break up sulfur, nitrogen compounds, and aromatics

Refinery Operations Planning

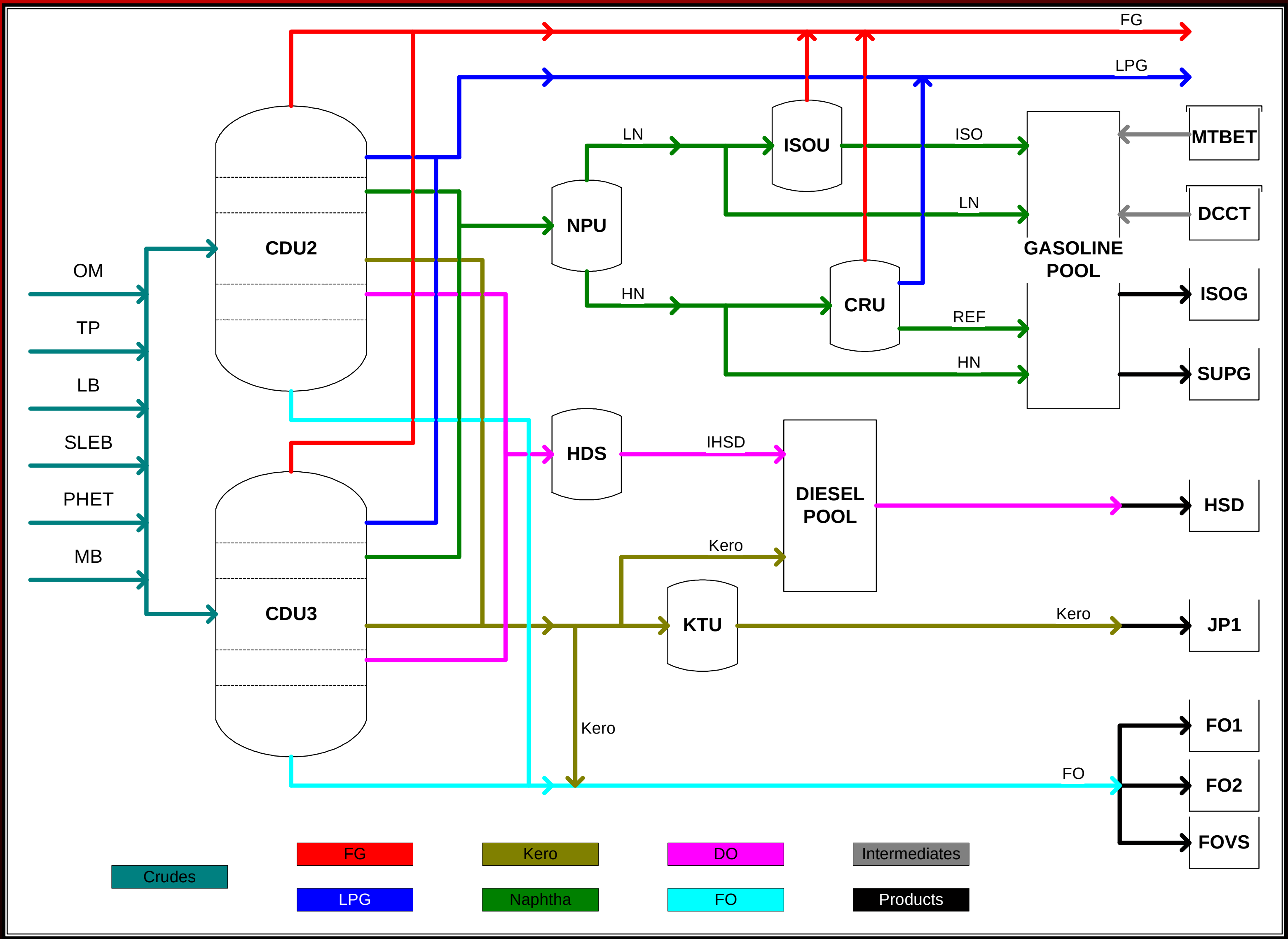
"Refining is a complex operation that depends upon the human skills of operators, engineers, and planners in combination with cutting edge technology to produce the products that meet the demands of an intensely competitive market."

Sources: http://www.exxon.mobil.com/UK-English/Operations/UK_OP_Ref_RefOp.asp and http://static.flickr.com/18/24007819_4d67ab2c0b.jpg

Refinery Operations Planning

- Planning groups in a refinery attempt to optimize the refinery's profits by purchasing specific amounts of different crudes
- Based on:
  - Projected market demands and prices
  - Unit capabilities
  - Planned turnarounds

Refinery Operations Planning

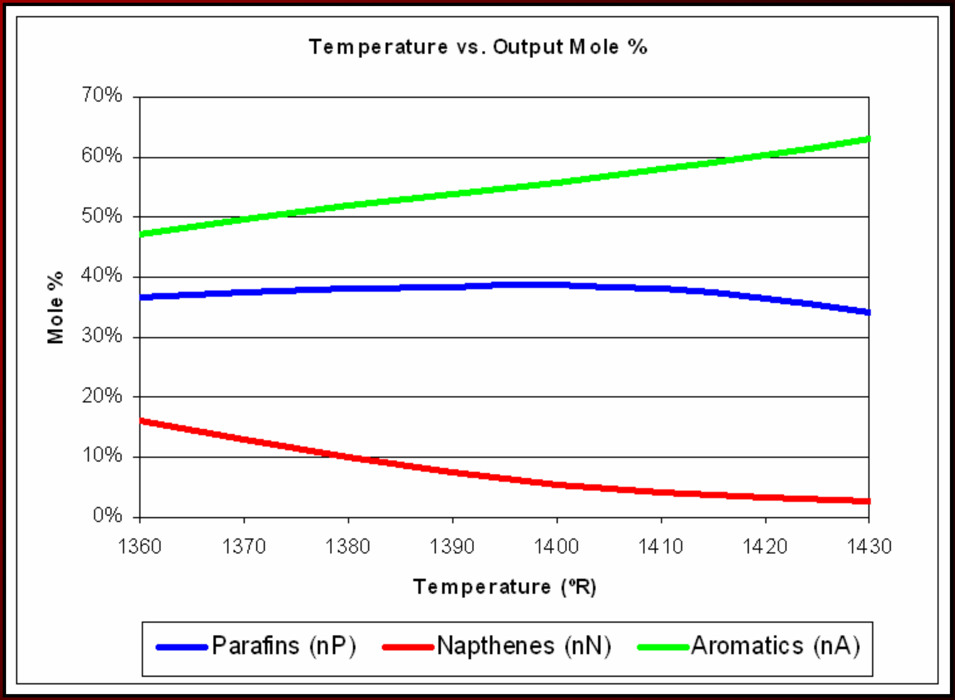


Refinery Operations Planning

- Planning Example
  - Winter
    - high fuel oil demand → more fuel (heating) oil produced
  - Summer
    - lower fuel oil demand → more gasoline produced

Refinery Operations Planning

- LP models use average operating conditions
- Graph shows that average operating conditions may not optimize particular unit (CRU)

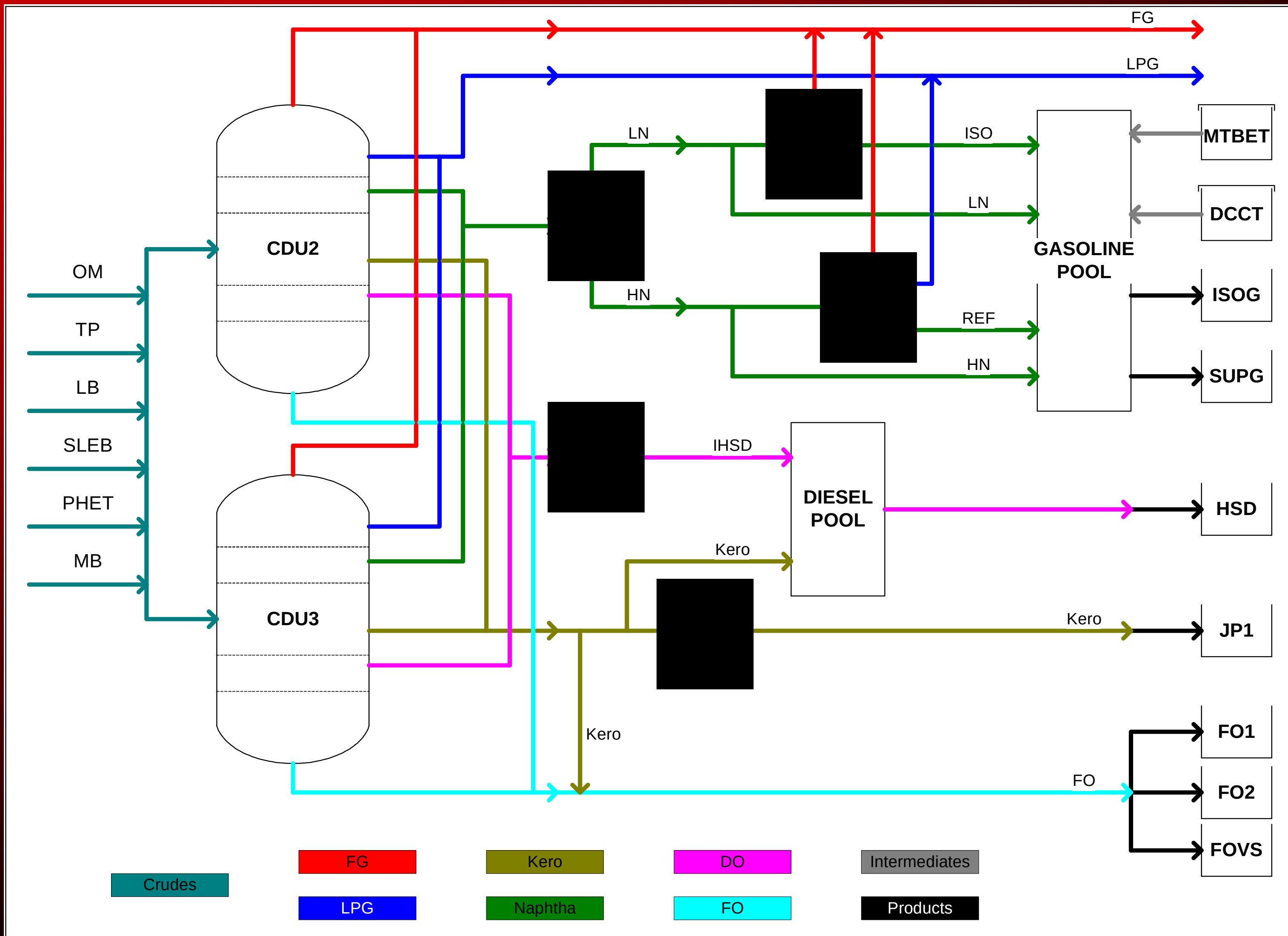


Current Models

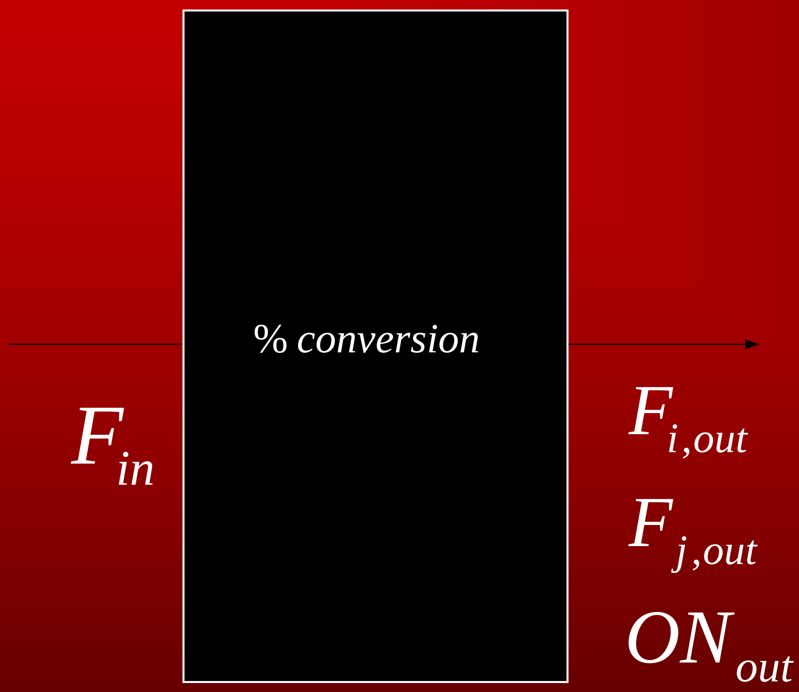
- Current models operate linearly (LP)
  - Black Box Theory

- PIMS (by Aspentech)
- RPMS (by Honeywell Hi-Spec Solutions)
- GRMPTS (by Haverly)

Black Box Theory



LP Planning

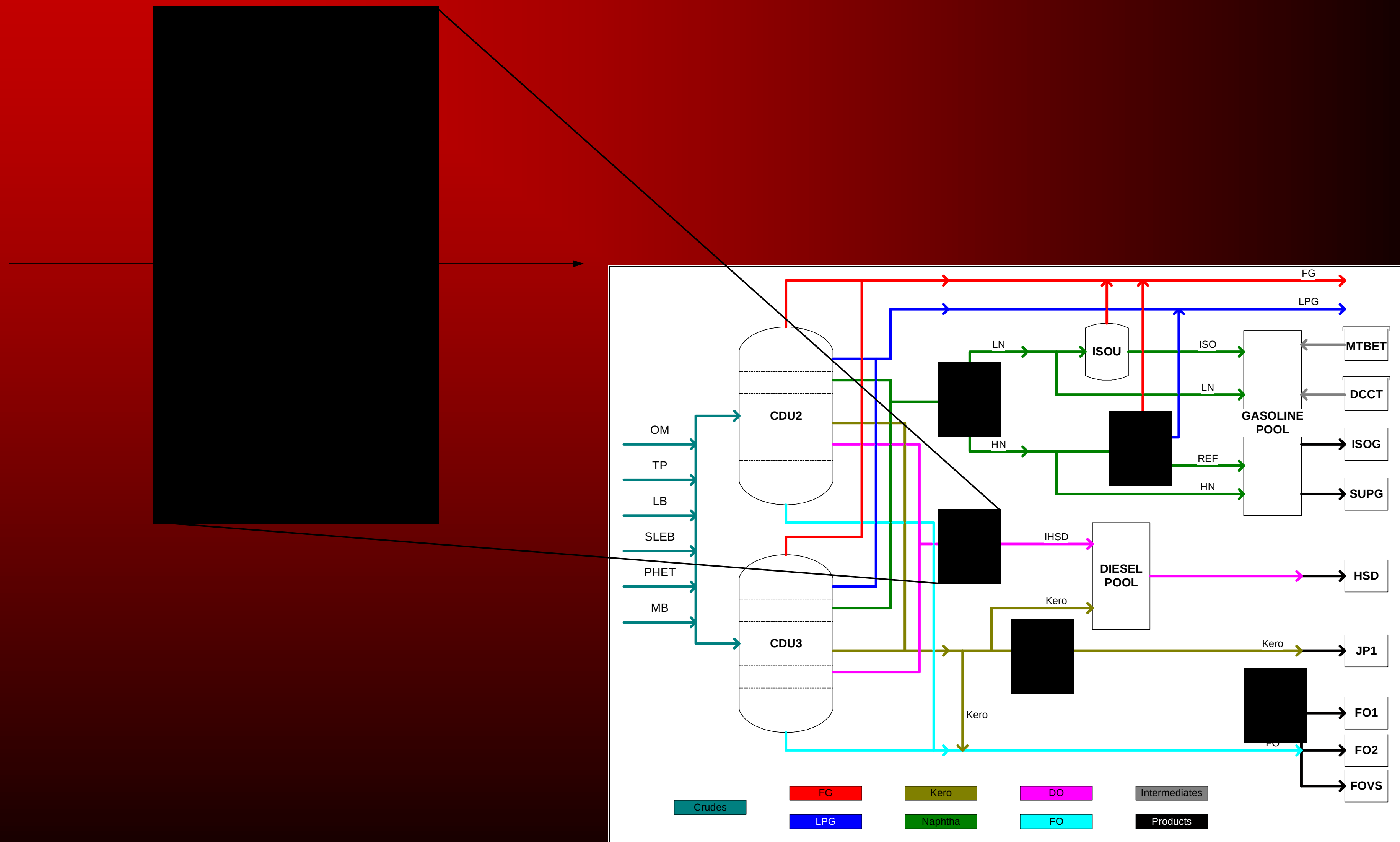


$$F_{i,out} = 0.75 \cdot F_{in}$$

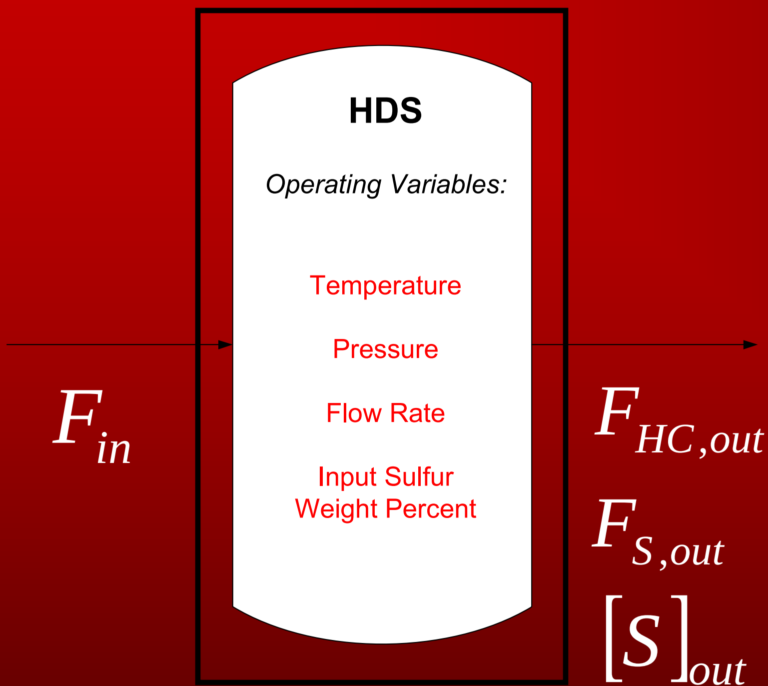
$$F_{j,out} = 0.25 \cdot F_{in}$$

$$ON_{out} = 98$$

Modeling Unit Operations



Modeling Unit Operations



$$F_{S,out} = f(T,P,F)$$

General Goal

- To effectively model a refinery's unit operations in the overall planning model.
- Bangchak refinery in Thailand is used as a case study.

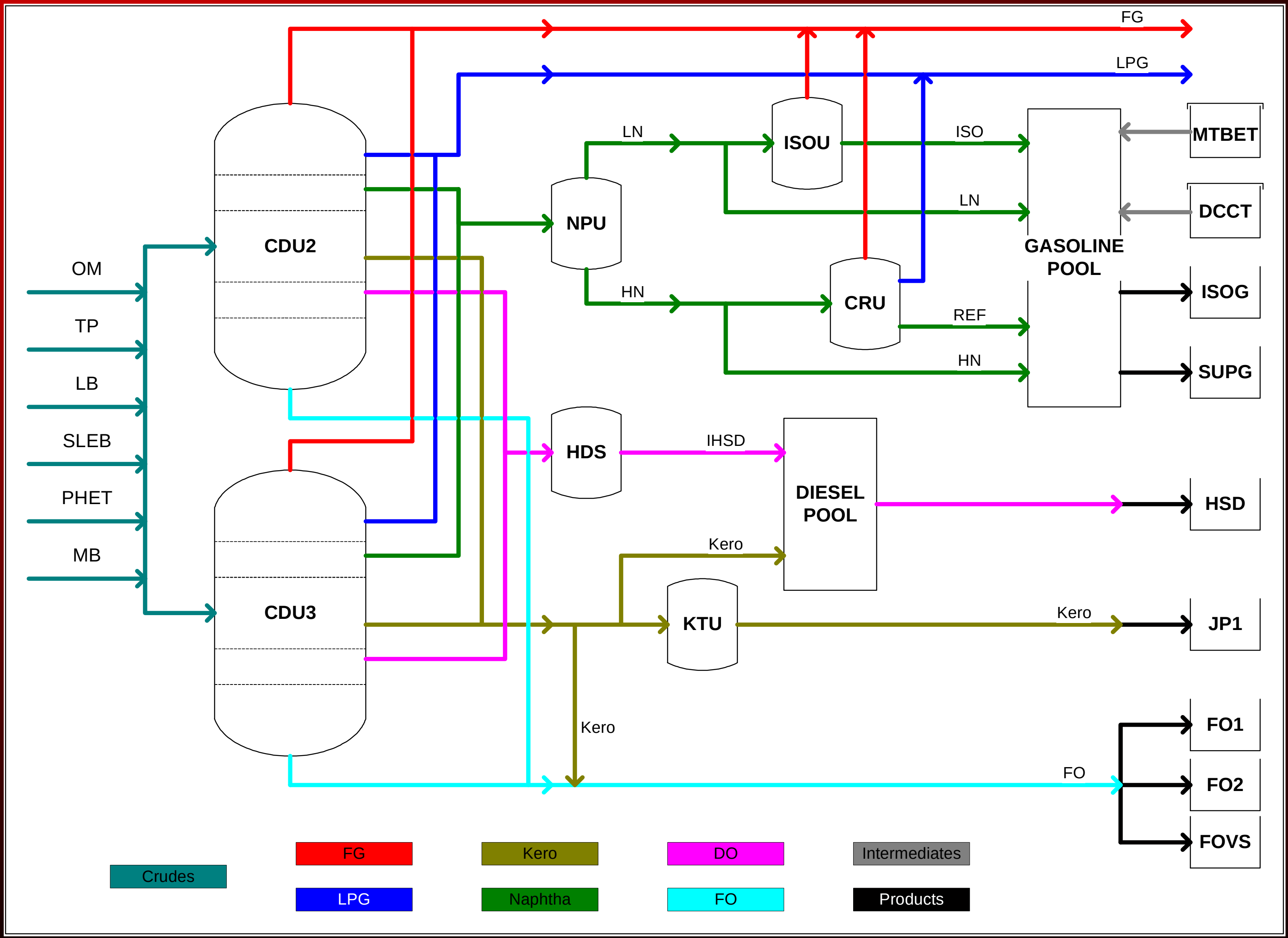
More Specific Goals

- Model Hydrotreaters
- Model Catalytic Reformers
- Model Isomerization
- Tie Unit Operations to GRM
  – Add Operating Costs
- Tie Unit Operations to blending
  – Calculate blending properties
- Integrate Fuel Gas system
- Create Hydrogen balance

Original LP Model

- LP model developed
  - Operates using Black Box theory
- Optimizes purchased crudes and additives
- Evaluates uncertainty and risk

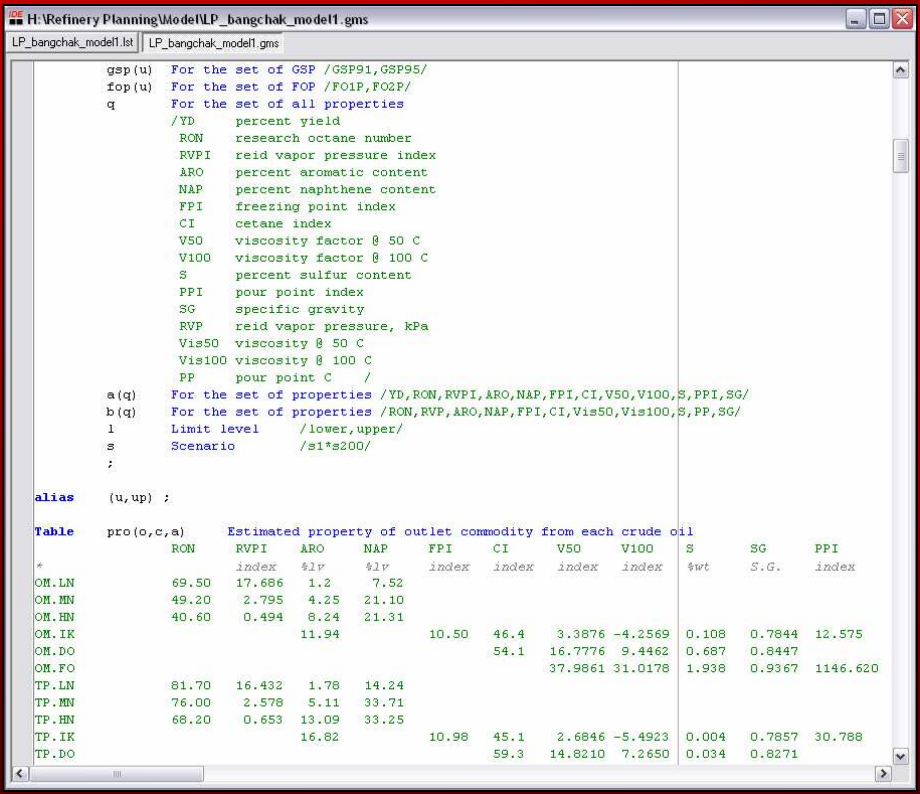
Bangchak Refinery



Bangchak Refinery

- Hydrotreating
  - NPU2
  - NPU3
  - HDS
  - KTU
- Catalytic Reforming
  - CRU2
  - CRU3
- Isomerization
  - ISOU

Bangchak Model



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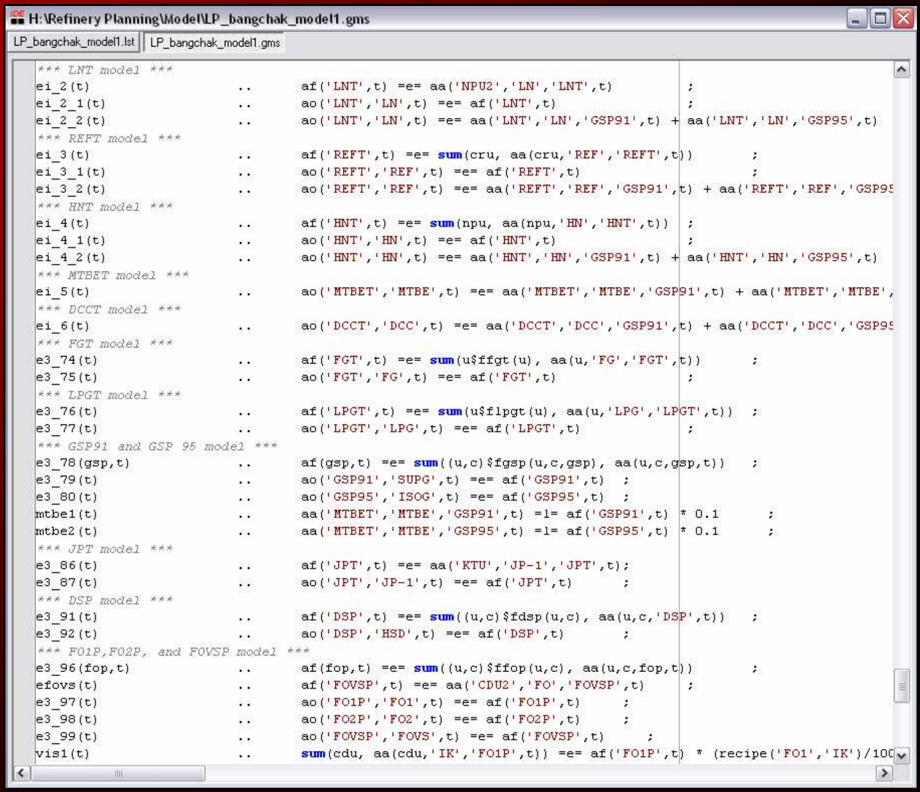
LP_bangchak_model1.lst | LP_bangchak_model1.gms

```
         gsp(u)  For the set of GSP /GSP91,GSP95/
         fop(u)  For the set of FOP /FO1P,FO2P/
         q       For the set of all properties
                 /YD     percent yield
                  RON    research octane number
                  RVPI   reid vapor pressure index
                  ARO    percent aromatic content
                  NAP    percent naphthene content
                  FPI    freezing point index
                  CI     cetane index
                  V50    viscosity factor @ 50 C
                  V100   viscosity factor @ 100 C
                  S      percent sulfur content
                  PPI    pour point index
                  SG     specific gravity
                  RVP    reid vapor pressure, kPa
                  Vis50  viscosity @ 50 C
                  Vis100 viscosity @ 100 C
                  PP     pour point C    /
         a(q)    For the set of properties /YD,RON,RVPI,ARO,NAP,FPI,CI,V50,V100,S,PPI,SG/
         b(q)    For the set of properties /RON,RVP,ARO,NAP,FPI,CI,Vis50,Vis100,S,PP,SG/
         l       Limit level     /lower,upper/
         s       Scenario        /s1*s200/
         ;

alias    (u,up) ;

Table    pro(o,c,a)     Estimated property of outlet commodity from each crude oil
                 RON     RVPI    ARO     NAP     FPI     CI      V50     V100    S       SG      PPI
*                        index   %lv     %lv     index   index   index   index   %wt     S.G.    index
OM.LN            69.50   17.686   1.2     7.52
OM.MN            49.20    2.795   4.25   21.10
OM.HN            40.60    0.494   8.24   21.31
OM.IK                            11.94           10.50   46.4     3.3876 -4.2569 0.108   0.7844  12.575
OM.DO                                                    54.1    16.7776  9.4462 0.687   0.8447
OM.FO                                                            37.9861 31.0178 1.938   0.9367  1146.620
TP.LN            81.70   16.432   1.78   14.24
TP.MN            76.00    2.578   5.11   33.71
TP.HN            68.20    0.653  13.09   33.25
TP.IK                            16.82           10.98   45.1     2.6846 -5.4923 0.004   0.7857  30.788
TP.DO                                                    59.3    14.8210  7.2650 0.034   0.8271
```



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LP_bangchak_model1.lst | LP_bangchak_model1.gms

```
*** LNT model ***
ei_2(t)             ..    af('LNT',t) =e= aa('NPU2','LN','LNT',t)          ;
ei_2_1(t)           ..    ao('LNT','LN',t) =e= af('LNT',t)                 ;
ei_2_2(t)           ..    ao('LNT','LN',t) =e= aa('LNT','LN','GSP91',t) + aa('LNT','LN','GSP95',t)
*** REFT model ***
ei_3(t)             ..    af('REFT',t) =e= sum(cru, aa(cru,'REF','REFT',t))      ;
ei_3_1(t)           ..    ao('REFT','REF',t) =e= af('REFT',t)                    ;
ei_3_2(t)           ..    ao('REFT','REF',t) =e= aa('REFT','REF','GSP91',t) + aa('REFT','REF','GSP95
*** HNT model ***
ei_4(t)             ..    af('HNT',t) =e= sum(npu, aa(npu,'HN','HNT',t))  ;
ei_4_1(t)           ..    ao('HNT','HN',t) =e= af('HNT',t)                 ;
ei_4_2(t)           ..    ao('HNT','HN',t) =e= aa('HNT','HN','GSP91',t) + aa('HNT','HN','GSP95',t)
*** MTBET model ***
ei_5(t)             ..    ao('MTBET','MTBE',t) =e= aa('MTBET','MTBE','GSP91',t) + aa('MTBET','MTBE',
*** DCCT model ***
ei_6(t)             ..    ao('DCCT','DCC',t) =e= aa('DCCT','DCC','GSP91',t) + aa('DCCT','DCC','GSP95
*** FGT model ***
e3_74(t)            ..    af('FGT',t) =e= sum(u$ffgt(u), aa(u,'FG','FGT',t))     ;
e3_75(t)            ..    ao('FGT','FG',t) =e= af('FGT',t)                 ;
*** LPGT model ***
e3_76(t)            ..    af('LPGT',t) =e= sum(u$flpgt(u), aa(u,'LPG','LPGT',t))  ;
e3_77(t)            ..    ao('LPGT','LPG',t) =e= af('LPGT',t)              ;
*** GSP91 and GSP 95 model ***
e3_78(gsp,t)        ..    af(gsp,t) =e= sum((u,c)$fgsp(u,c,gsp), aa(u,c,gsp,t))   ;
e3_79(t)            ..    ao('GSP91','SUPG',t) =e= af('GSP91',t)  ;
e3_80(t)            ..    ao('GSP95','ISOG',t) =e= af('GSP95',t)  ;
mtbe1(t)            ..    aa('MTBET','MTBE','GSP91',t) =l= af('GSP91',t) * 0.1      ;
mtbe2(t)            ..    aa('MTBET','MTBE','GSP95',t) =l= af('GSP95',t) * 0.1      ;
*** JPT model ***
e3_86(t)            ..    af('JPT',t) =e= aa('KTU','JP-1','JPT',t);
e3_87(t)            ..    ao('JPT','JP-1',t) =e= af('JPT',t)      ;
*** DSP model ***
e3_91(t)            ..    af('DSP',t) =e= sum((u,c)$fdsp(u,c), aa(u,c,'DSP',t))   ;
e3_92(t)            ..    ao('DSP','HSD',t) =e= af('DSP',t)       ;
*** FO1P,FO2P, and FOVSP model ***
e3_96(fop,t)        ..    af(fop,t) =e= sum((u,c)$ffop(u,c), aa(u,c,fop,t))      ;
efovs(t)            ..    af('FOVSP',t) =e= aa('CDU2','FO','FOVSP',t)      ;
e3_97(t)            ..    ao('FO1P','FO1',t) =e= af('FO1P',t)     ;
e3_98(t)            ..    ao('FO2P','FO2',t) =e= af('FO2P',t)     ;
e3_99(t)            ..    ao('FOVSP','FOVS',t) =e= af('FOVSP',t)     ;
vis1(t)             ..    sum(cdu, aa(cdu,'IK','FO1P',t)) =e= af('FO1P',t) * (recipe('FO1','IK')/10C
```

Hydrotreating

- The purpose of hydrotreating is to remove undesired impurities from the stream
  - Sulfur
  - Nitrogen
  - Basic Nitrogen
  - Aromatics

Hydrotreating Reactions

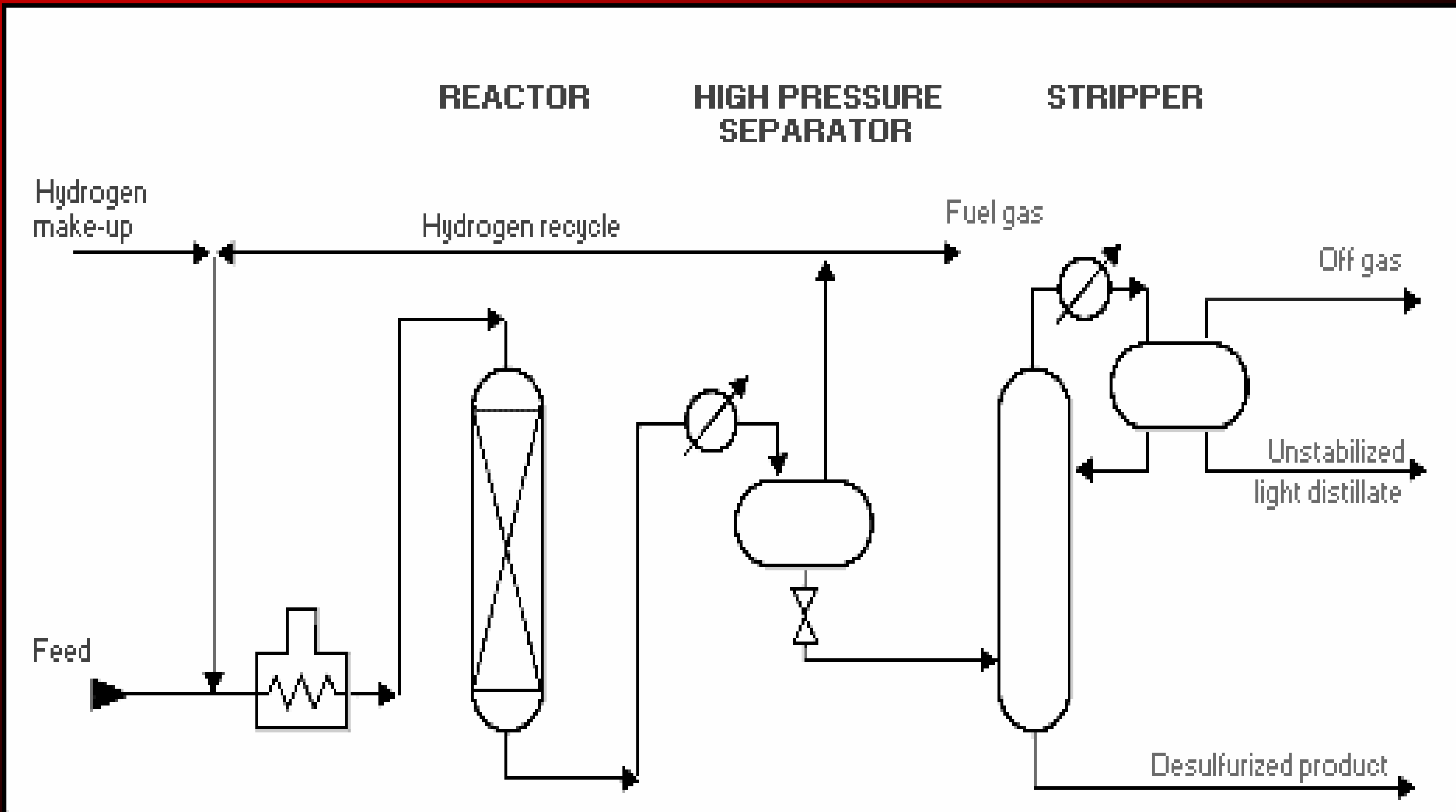
1. Desulfurization:
   - a. Mercaptans: $RSH + H_2 \rightarrow RH + H_2S$
   - b. Sulfides: $R_2S + 2H_2 \rightarrow 2RH + H_2S$
   - c. Disulfides: $(RS)_2 + 3H_2 \rightarrow 2RH + 2H_2S$
   - d. Thiophenes:

$+ 4H_2 \rightarrow C_4H_{10} + H_2S$

2. Denitrogenation:
   - a. Pyrrole: $C_4H_4NH + 4H_2 \rightarrow C_4H_{10} + NH_3$
   - b. Pyridine: $C_5H_5N + 5H_2 \rightarrow C_5H_{12} + NH_3$
3. Deoxidation:
   - a. Phenol: $C_6H_5OH + H_2 \rightarrow C_6H_6 + H_2O$
   - b. Peroxides: $C_7H_{13}OOH + 3H_2 \rightarrow C_7H_{16} + 2H_2O$
4. Dehalogenation:
   Chlorides: $RCl + H_2 \rightarrow RH + HCl$
5. Hydrogenation:
   Pentane: $C_5H_{10} + H_2 \rightarrow C_5H_{12}$
6. Hydrocracking:
   $C_{10}H_{22} \rightarrow C_4H_8 + C_6H_{14}$

- Most common non-hydrocarbon by-products:
  - H_2S
  - NH_3

Hydrotreating PFD



Hydrotreating Model

- Langmuir-Hinshelwood kinetic rate law

- Main operating variables
  - Temperature (600-800℃)
  - Pressure (100-3000 psig)
  - H_2/HC ratio (2000 ft^3/bbl)
  - Space Velocity (1.5-9.0)
    - Based on Flow Rate and Volume

Langmuir-Hinshelwood

$$r = -k \cdot \left[\frac{C_S \cdot C_{H_2}^{0.45}}{\left(1 + K_{H_2S} \cdot C_{H_2S}\right)^2} \right]$$

$$k = A \cdot e^{-\frac{E}{R \cdot T}}$$

$$K_{H_2S} = 41769.84 \cdot e^{\frac{2761}{R \cdot T}}$$

Where, k = rate constant

K_{H_2S} = adsorption equilibrium constant

A = Arrhenius constant

E = activation energy

HDS Inputs

- Variables
  - Temperature
  - Pressure
  - Flow Rate
- Data
  - Sulfur weight percent*
  - H_2/HC ratio (2000 ft^3/bbl)
  - Sizing constant (1.8E8)

*Sulfur weight percent is set as a constant due to small effect on percent conversion and specifying too many variables in the overall model causes non-convergence

Excel Model

Microsoft Excel - hydrotreater.HDS.xls

M14 =L14/0.000001

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1																	
2	**Pr (psi)**	**775**															
3	**Pr (kPa)**	**5341.9643**			**k0**												
4	**T (deg F)**	**680**			**4.27E+09**												
5	**T (deg C)**	**360**															
6	**T (K)**	**633**								% conversion		s	**0.466756**				
7	**R (kcal/molK)**	**0.001986**			132000												
8	**R(J/molK)**	**8.3145**															
9	**Flow Oil (bbl/day)**	**8430**															
10	**H2 / HC ft3/bbl**	**2000**			0.08988	g/L											
11	**mol/hr**	**8.85E+05**															
12	**SG Oil**	**0.89**															
13	**MW Oil**	**200**			16.35								ppm				131.9
14	**Flow Oil (g/hr)**	**49701324**										0.00046	**463.6245**				127.5
15	**Flow Oil (mol/hr)**	**248506.62**															118.9
16	**LHSV**	**2.66**															94.07
17	**Flow Hydrogen (mol/hr)**	**8.85E+05**			ΔW (kg)		5.50E+05										
18	**TOTAL FLOW (mol/hr)**	**1133101.6**															
19	**Cto (mol/m3)**	**1014.9885**															
20	**Cto (mol/cm3)**	**0.001015**															
21					W (kg)		4.99E+07										
22		**Sulfur**	**0.005**								**http://www.eia.doe.gov/oiaf/servicerpt/ulsd/pdf/chapter5.pdf**						
23		**Nitrogen**			W(lb)		1.10E+08										
24	X_	**Basic Nitrogen**									**http://www.eia.doe.gov/oiaf/servicerpt/ulsd/chapter3.html**						
25		**Aromatic**															
26		**Sulfur**	**1242.533**								**http://www.kbcat.com/pdfs/tech/tp_010.pdf**						
27		**Nitrogen**	**0**		**ks**	**kn**	**kbn**	**kar**			http://www.ask.com/web?q=hydrotreater+model+kinetic&qsrc=0&o=33						
28	F_	**Basic Nitro**	**0**		**5.47E-02**						http://www.eng.uwo.ca/people/aray/Naveen%20Hydrocracking.pdf						
29		**Aromatic**	**0**		**Kh2s**												
30					**70581.8099**					g/cm3				mol/cm3			
31			W		rs	rn	rbn	rar		cs	cn	cbn	car	ch	ch2s		Fs
32			0		-2.9373E-05	0.00E+00	0.00E+00	0.00E+00		2.23E-04	0.00E+00	0.00E+00	0.00E+00	7.92E-04	0.00E+00		1.24E+03
33	HIDDEN	1	550000		-2.8932E-05	0.00E+00	0.00E+00	0.00E+00		2.20E-04	0.00E+00	0.00E+00	0.00E+00	7.92E-04	1.45E-08		1.23E+03
34		2	1100000		-2.8499E-05	0.00E+00	0.00E+00	0.00E+00		2.17E-04	0.00E+00	0.00E+00	0.00E+00	7.92E-04	2.87E-08		1.21E+03
35		3	1650000		-2.8074E-05	0.00E+00	0.00E+00	0.00E+00		2.14E-04	0.00E+00	0.00E+00	0.00E+00	7.92E-04	4.28E-08		1.19E+03
36		4	2200000		-2.7657E-05	0.00E+00	0.00E+00	0.00E+00		2.11E-04	0.00E+00	0.00E+00	0.00E+00	7.92E-04	5.66E-08		1.18E+03
37		5	2750000		-2.7248E-05	0.00E+00	0.00E+00	0.00E+00		2.09E-04	0.00E+00	0.00E+00	0.00E+00	7.92E-04	7.02E-08		1.16E+03
38		6	3300000		-2.6847E-05	0.00E+00	0.00E+00	0.00E+00		2.06E-04	0.00E+00	0.00E+00	0.00E+00	7.92E-04	8.36E-08		1.15E+03
39		7	3850000		-2.6452E-05	0.00E+00	0.00E+00	0.00E+00		2.03E-04	0.00E+00	0.00E+00	0.00E+00	7.92E-04	9.69E-08		1.13E+03
40		8	4400000		-2.6065E-05	0.00E+00	0.00E+00	0.00E+00		2.01E-04	0.00E+00	0.00E+00	0.00E+00	7.92E-04	1.10E-07		1.12E+03
41		9	4950000		-2.5685E-05	0.00E+00	0.00E+00	0.00E+00		1.98E-04	0.00E+00	0.00E+00	0.00E+00	7.92E-04	1.23E-07		1.11E+03
42		10	5500000		-2.5312E-05	0.00E+00	0.00E+00	0.00E+00		1.96E-04	0.00E+00	0.00E+00	0.00E+00	7.92E-04	1.35E-07		1.09E+03

Sheet1 / Sheet2 / Sheet3

Ready

GAMS Model

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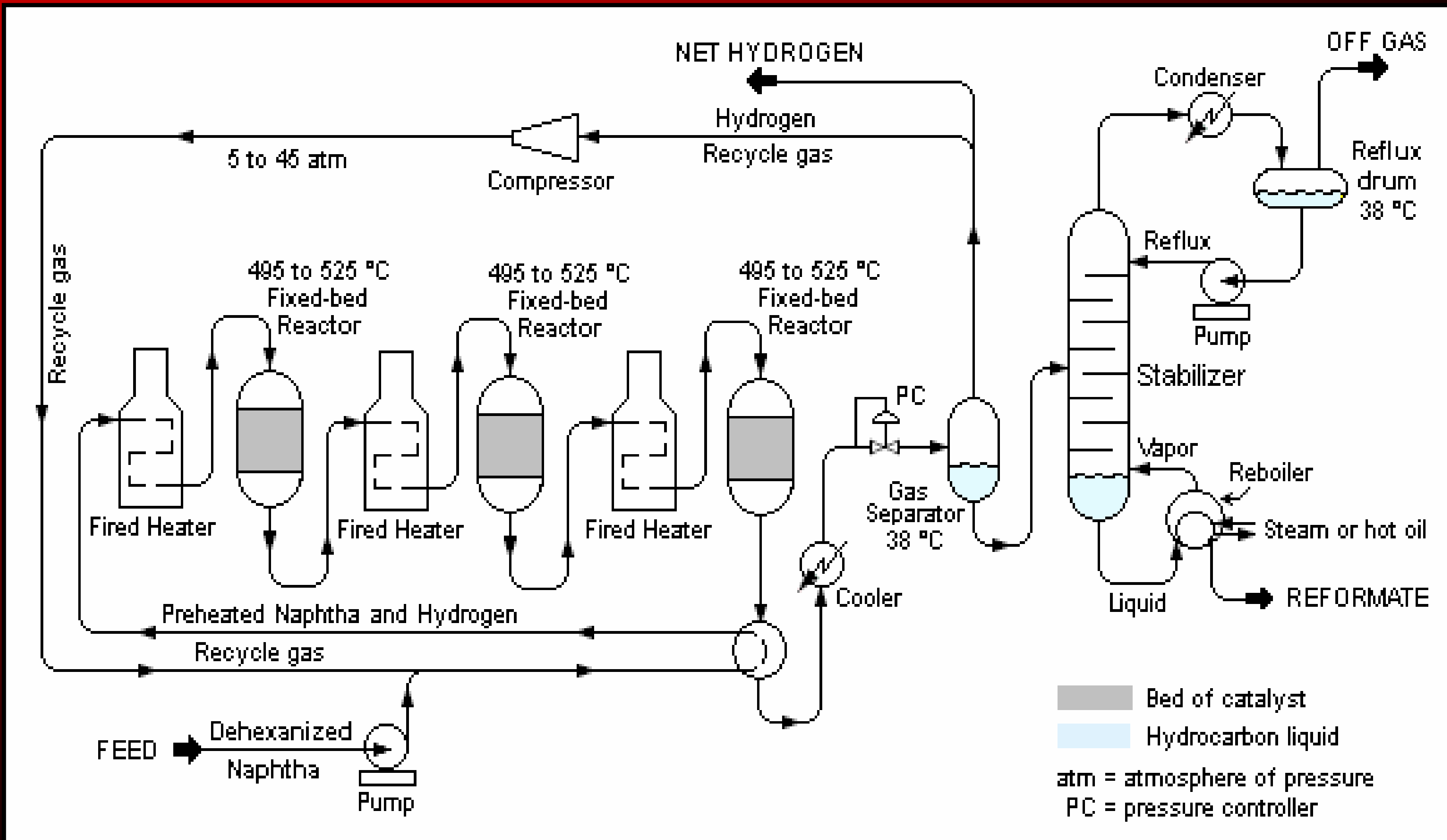
newHDS.gms

```
for(s3 = 1 to card(s) ,
     Xc(s) = 0 + 1$(ord(s) = s3);
     OFlow = sum(s, Xc(s)*scenarios(s,'f'));

P2 = 101.325*P1/14.7 ;
T2 = (T1-32)/1.8 ;
T3 = T2+273 ;
HFlow = OFlow*H2HC*28.3*0.08988/(2.02*24) ;
OFlow1 = OFlow*158987*sg/24 ;
OFlow2 = OFlow1/mw ;
Flow = HFlow+OFlow2 ;
Ct0 = P2*1000/(R*T3) ;
Ct0b = Ct0/1000000 ;
SFlow = OFlow2*perc ;
ks = k0*exp(-E/(R*T3)) ;
Kh2s = 41769.84*exp(2761/(R*T3)) ;
delx = x/(card(y)-1) ;

fs('0') = SFlow ;
fh('0') = HFlow ;
cs('0') = Ct0b*SFlow*mw/Flow ;
ch('0') = Ct0b*HFlow/Flow ;
ch2s('0') = 0 ;

rate('0') = -ks*60*cs('0')*ch('0')**0.45/(1+Kh2s*ch2s('0'))**2 ;

fs('1') = fs('0')+rate('0')*delx ;
fh('1') = fh('0')+rate('0')*delx ;
cs('1') = Ct0b*fs('1')*mw/Flow ;
ch('1') = Ct0b*fh('1')/Flow ;
ch2s('1') = ch('0')-ch('1') ;

rate('1') = -ks*60*cs('1')*ch('1')**0.45/(1+Kh2s*ch2s('1'))**2 ;

fs('2') = fs('1')+rate('1')*delx ;
fh('2') = fh('1')+rate('1')*delx ;
```

Catalytic Reforming

- Process used to increase the octane number of light crude fractions
- Converts low-octane naptha into high-octane aromatics
- High octane product is useful for creating premium gasolines
- Hydrogen is the by-product

Catalytic Reforming Process Flow Diagram



Catalytic Reforming Unit Operating Conditions

- Low pressures (30- 40atm)
- High Temperatures (900- 950 ºF)
- Feedstock
  - Heavy naphtha from hydrotreating unit
- Catalyst
  - Platinum bi-function catalyst on Alumina support
- Continuous process
  - Catalyst is removed, replaced, and regenerated continuously and online

Catalytic Reforming Model

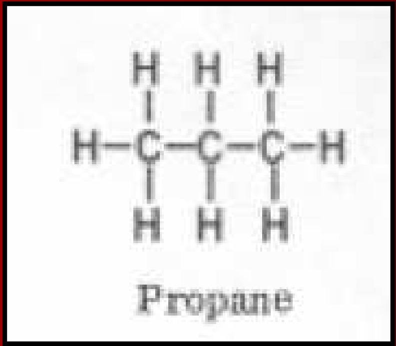
- Model Purpose
  - Predict the output of system through simplified inputs
  - Optimal Operating Parameters = Maximum Yield and Profit
- Model Method
  - Differential equations with changeable input parameters
- Model Challenges
  - Complicated components (pseudo)
  - Extreme operating conditions
  - Complicated reactions

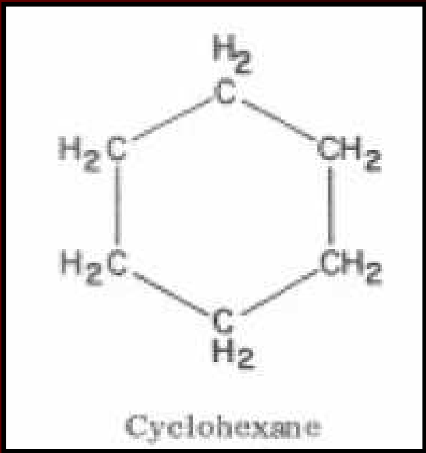
Catalytic Reforming Model

- Input Parameters
  - Temperature
  - Pressure
  - Volumetric Flowrates
  - Component Composition (Mole %)
    - Napthenes
    - Paraffins
    - Aromatics
- Output Parameters
  - Reformate
  - Hydrogen
  - Liquefied Petroleum Gas

Catalytic Reforming Components

- Paraffins
  - Straight chain hydrocarbons
  - Highest H:C ratio



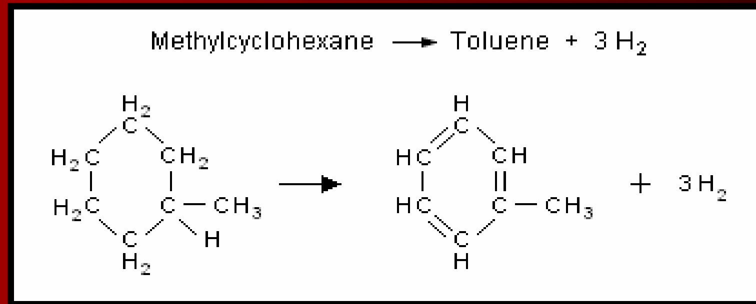


- Napthenes
  - Cyclic hydrocarbons
  - Medium H:C ratio

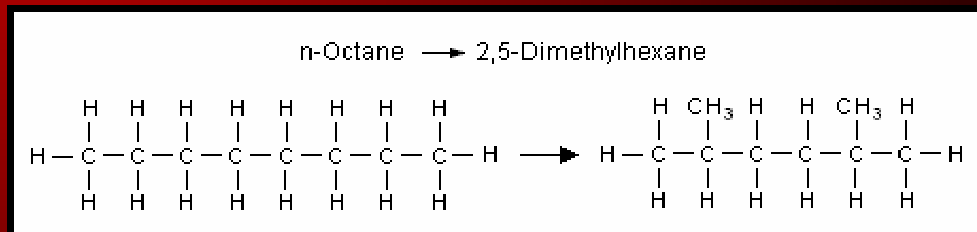
- Aromatics
  - Cyclic hydrocarbons
  - Lowest H:C ratio

Catalytic Reforming Reactions

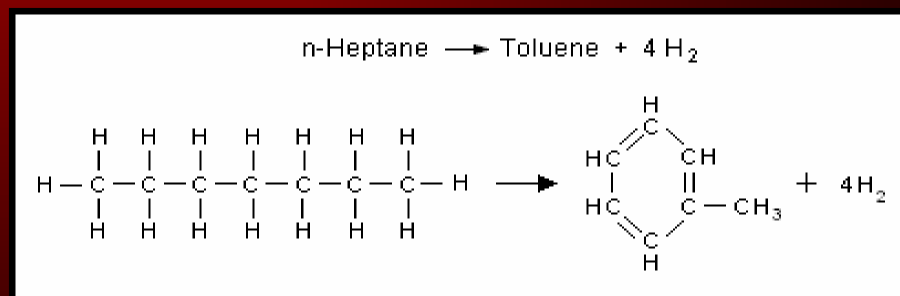
- Dehydrogenation



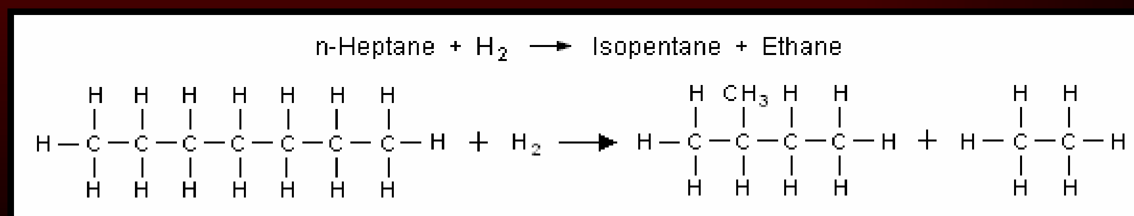
- Isomerization



- Aromatization



- Hydrocracking



Catalytic Reforming Model

- Simplified Reactions and Equations from Smith (1959)
- Modeled Reactions
  - Dehydrogenation, Cyclization, Aromatization, and Hydrocracking

$$(1) Napthenes \longleftrightarrow aromatics + 3 * H_2$$

$$(2) Paraffins \longleftrightarrow napthenes + H_2$$

$$(3) Hydrocracking\_of\_paraffins$$

$$(4) Hydrocracking\_of\_napthenes$$

Catalytic Reforming Stoichiometry

$$(1) C_nH_{2n} \longleftrightarrow C_nH_{2n-6} + 3H_2$$

$$(2) C_nH_{2n+2} \longleftrightarrow C_nH_{2n} + H_2$$

$$(3) C_nH_{2n+2} + \left(\frac{n-3}{3}\right)H_2 \longrightarrow \frac{n}{15}C_1 + \frac{n}{15}C_2 + \frac{n}{15}C_3 + \frac{n}{15}C_4 + \frac{n}{15}C_5$$

$$(4) C_nH_{2n} + \frac{n}{3}H_2 \longrightarrow \frac{n}{15}C_1 + \frac{n}{15}C_2 + \frac{n}{15}C_3 + \frac{n}{15}C_4 + \frac{n}{15}C_5$$

Where n is the number of carbon atoms.

Catalytic Reforming Empirical Kinetic Model

$$\hat{k}_{P1} = \exp\left(23.21 - \frac{34750}{T}\right), [=] \frac{moles}{(hr)(lb\_cat.)(atm)}$$

$$K_{P1} = \frac{P_A * P_H^3}{P_N} = \exp\left(46.15 - \frac{46045}{T}\right), [=] atm^3$$

$$\hat{k}_{P2} = \exp\left(35.98 - \frac{59600}{T}\right), [=] \frac{moles}{(hr)(lb\_cat.)(atm)^2}$$

$$K_{P2} = \frac{P_P}{P_N * P_H} = \exp\left(\frac{8000}{T} - 7.12\right), [=] atm^{-1}$$

$$\hat{k}_{P3} = \hat{k}_{P4} = \exp\left(42.97 - \frac{62300}{T}\right), [=] \frac{moles}{(hr)(lb\_cat.)}$$

Catalytic Reforming Rate Law Model

$$-\hat{r}_1 = \hat{k}_{P1}\left(P_N - \frac{P_A * P_H{}^3}{K_{P1}} \right) [=] \frac{moles\_napthene\_converted\_to\_aromatics}{(hr)(lb\_cat.)}$$

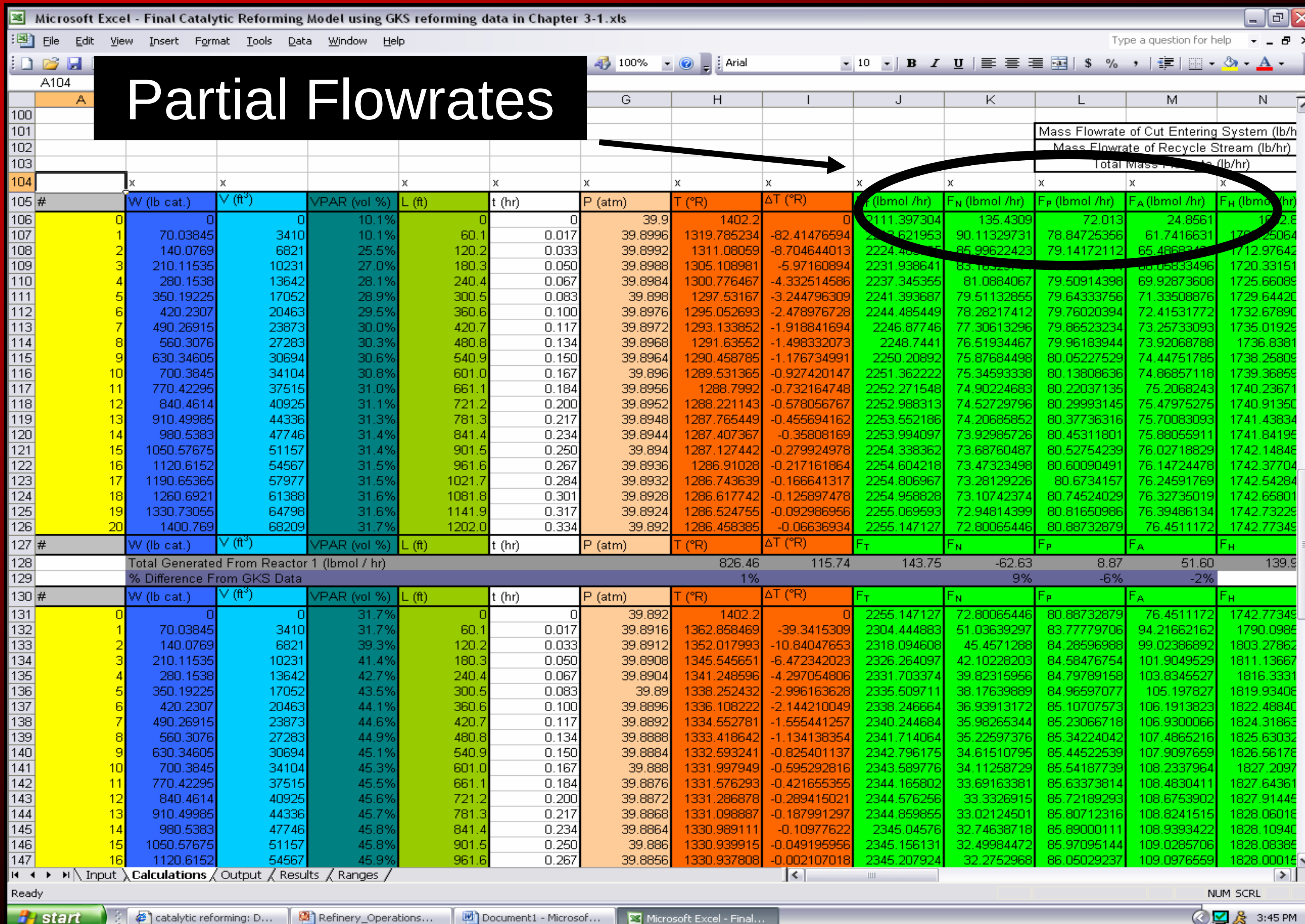
$$-\hat{r}_2 = \hat{k}_{P2}\left(P_N * P_H - \frac{P_P}{K_{P2}} \right) [=] \frac{moles\_napthene\_converted\_to\_paraffins}{(hr)(lb\_cat.)}$$

$$-\hat{r}_3 = \hat{k}_{P3}\left(\frac{P_P}{P} \right) [=] \frac{moles\_paraffins\_converted\_by\_hydrocracking}{(hr)(lb\_cat.)}$$

$$-\hat{r}_4 = \hat{k}_{P4}\left(\frac{P_N}{P} \right) [=] \frac{moles\_napthenes\_converted\_by\_hydrocracking}{(hr)(lb\_cat.)}$$

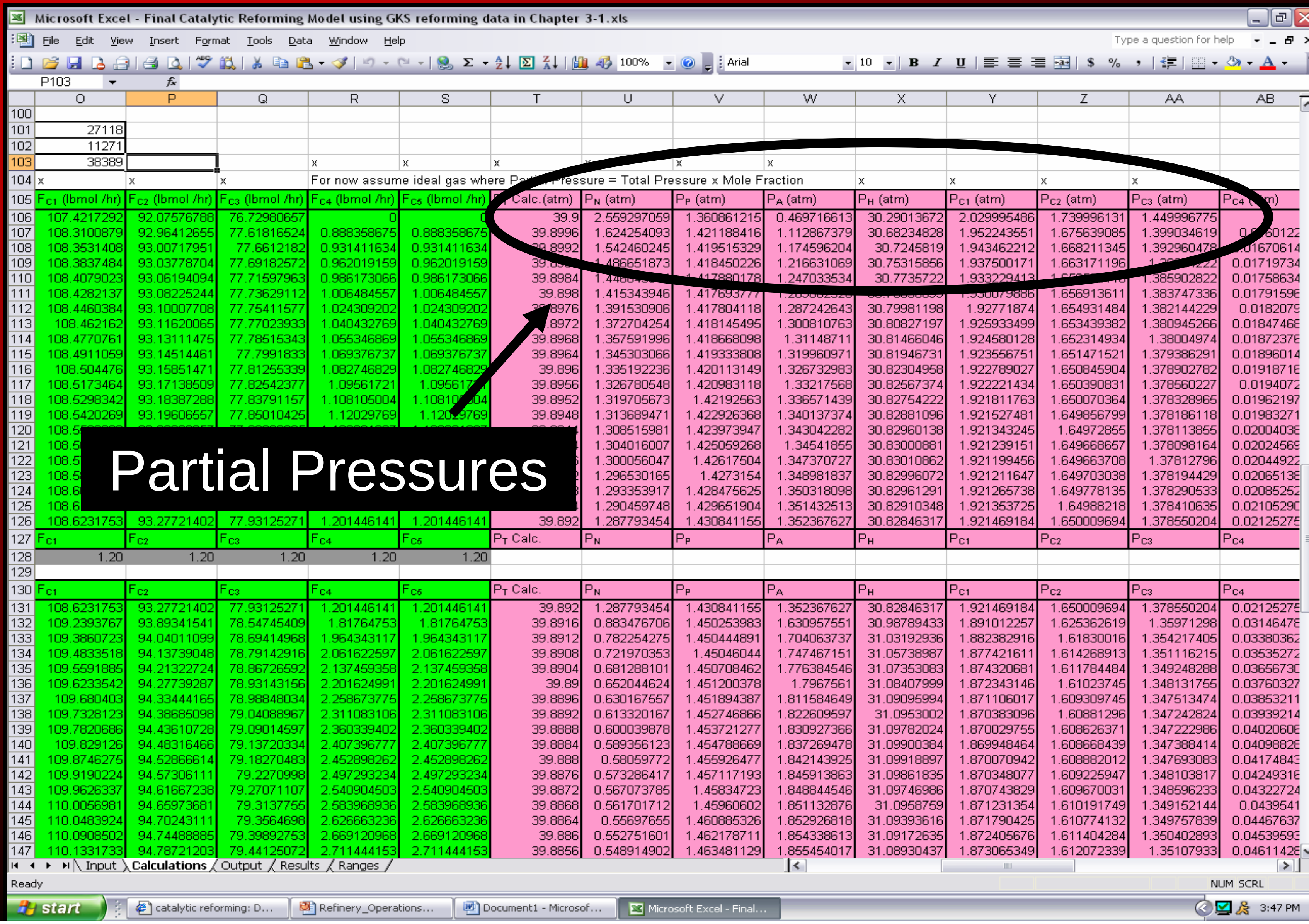
Excel Model

Partial Flowrates



	A	B	C	D	E	F	G	H	I	J	K	L	M	N
104		x	x		x	x	x	x	x	x	x	x	x	x
105	#	W (lb cat.)	V (ft^3)	VPAR (vol %)	L (ft)	t (hr)	P (atm)	T (°R)	ΔT (°R)	F_T (lbmol /hr)	F_N (lbmol /hr)	F_P (lbmol /hr)	F_A (lbmol /hr)	F_H (lbmol /hr)
106	0	0	0	10.1%	0	0	39.9	1402.2	0	2111.397304	135.4309	72.013	24.8561	[illegible]
107	1	70.03845	3410	10.1%	60.1	0.017	39.8996	1319.785234	-82.41476594	[illegible]	90.11329731	78.84725356	61.7416631	[illegible]
108	2	140.0769	6821	25.5%	120.2	0.033	39.8992	1311.08059	-8.704644013	[illegible]	85.99622423	79.14172112	[illegible]	1712.97642
109	3	210.11535	10231	27.0%	180.3	0.050	39.8988	1305.108981	-5.97160894	2231.938641	[illegible]	[illegible]	[illegible]	1720.33151
110	4	280.1538	13642	28.1%	240.4	0.067	39.8984	1300.776467	-4.332514586	2237.345355	81.0884067	79.50914398	69.92873608	1725.66089
111	5	350.19225	17052	28.9%	300.5	0.083	39.898	1297.53167	-3.244796309	2241.393687	79.51132855	79.64333756	71.33508876	1729.64420
112	6	420.2307	20463	29.5%	360.6	0.100	39.8976	1295.052693	-2.478976728	2244.485449	78.28217412	79.76020394	72.41531772	1732.67890
113	7	490.26915	23873	30.0%	420.7	0.117	39.8972	1293.133852	-1.918841694	2246.87746	77.30613296	79.86523234	73.25733093	1735.01929
114	8	560.3076	27283	30.3%	480.8	0.134	39.8968	1291.63552	-1.498332073	2248.7441	76.51934467	79.96183944	73.92068788	1736.8381
115	9	630.34605	30694	30.6%	540.9	0.150	39.8964	1290.458785	-1.176734991	2250.20892	75.87684498	80.05227529	74.44751785	1738.25809
116	10	700.3845	34104	30.8%	601.0	0.167	39.896	1289.531365	-0.927420147	2251.362222	75.34593338	80.13808636	74.86857118	1739.36859
117	11	770.42295	37515	31.0%	661.1	0.184	39.8956	1288.7992	-0.732164748	2252.271548	74.90224683	80.22037135	75.2068243	1740.23671
118	12	840.4614	40925	31.1%	721.2	0.200	39.8952	1288.221143	-0.578056767	2252.988313	74.52729796	80.29993145	75.47975275	1740.91350
119	13	910.49985	44336	31.3%	781.3	0.217	39.8948	1287.765449	-0.455694162	2253.552186	74.20685852	80.37736316	75.70083093	1741.43834
120	14	980.5383	47746	31.4%	841.4	0.234	39.8944	1287.407367	-0.35808169	2253.994097	73.92985726	80.45311801	75.88055911	1741.84195
121	15	1050.57675	51157	31.4%	901.5	0.250	39.894	1287.127442	-0.279924978	2254.338362	73.68760487	80.52754239	76.02718829	1742.14848
122	16	1120.6152	54567	31.5%	961.6	0.267	39.8936	1286.91028	-0.217161864	2254.604218	73.47323498	80.60090491	76.14724478	1742.37704
123	17	1190.65365	57977	31.5%	1021.7	0.284	39.8932	1286.743639	-0.166641317	2254.806967	73.28129226	80.6734157	76.24591769	1742.54284
124	18	1260.6921	61388	31.6%	1081.8	0.301	39.8928	1286.617742	-0.125897478	2254.958828	73.10742374	80.74524029	76.32735019	1742.65801
125	19	1330.73055	64798	31.6%	1141.9	0.317	39.8924	1286.524755	-0.092986956	2255.069593	72.94814399	80.81650986	76.39486134	1742.73229
126	20	1400.769	68209	31.7%	1202.0	0.334	39.892	1286.458385	-0.06636934	2255.147127	72.80065446	80.88732879	76.4511172	1742.77349
127	#	W (lb cat.)	V (ft^3)	VPAR (vol %)	L (ft)	t (hr)	P (atm)	T (°R)	ΔT (°R)	F_T	F_N	F_P	F_A	F_H
128		Total Generated From Reactor 1 (lbmol / hr)						826.46	115.74	143.75	-62.63	8.87	51.60	139.9
129		% Difference From GKS Data						1%			9%	-6%	-2%	
130	#	W (lb cat.)	V (ft^3)	VPAR (vol %)	L (ft)	t (hr)	P (atm)	T (°R)	ΔT (°R)	F_T	F_N	F_P	F_A	F_H
131	0	0	0	31.7%	0	0	39.892	1402.2	0	2255.147127	72.80065446	80.88732879	76.4511172	1742.77349
132	1	70.03845	3410	31.7%	60.1	0.017	39.8916	1362.858469	-39.3415309	2304.444883	51.03639297	83.77779706	94.21662162	1790.0985
133	2	140.0769	6821	39.3%	120.2	0.033	39.8912	1352.017993	-10.84047653	2318.094608	45.4571288	84.28596988	99.02386892	1803.27862
134	3	210.11535	10231	41.4%	180.3	0.050	39.8908	1345.545651	-6.472342023	2326.264097	42.10228203	84.58476754	101.9049529	1811.13667
135	4	280.1538	13642	42.7%	240.4	0.067	39.8904	1341.248596	-4.297054806	2331.703374	39.82315956	84.79789158	103.8345527	1816.3331
136	5	350.19225	17052	43.5%	300.5	0.083	39.89	1338.252432	-2.996163628	2335.509711	38.17639889	84.96597077	105.197827	1819.93408
137	6	420.2307	20463	44.1%	360.6	0.100	39.8896	1336.108222	-2.144210049	2338.246664	36.93913172	85.10707573	106.1913823	1822.48840
138	7	490.26915	23873	44.6%	420.7	0.117	39.8892	1334.552781	-1.555441257	2340.244684	35.98265344	85.23066718	106.9300066	1824.31863
139	8	560.3076	27283	44.9%	480.8	0.134	39.8888	1333.418642	-1.134138354	2341.714064	35.22597376	85.34224042	107.4865216	1825.63032
140	9	630.34605	30694	45.1%	540.9	0.150	39.8884	1332.593241	-0.825401137	2342.796175	34.61510795	85.44522539	107.9097659	1826.56178
141	10	700.3845	34104	45.3%	601.0	0.167	39.888	1331.997949	-0.595292816	2343.589776	34.11258729	85.54187739	108.2337964	1827.2097
142	11	770.42295	37515	45.5%	661.1	0.184	39.8876	1331.576293	-0.421655355	2344.165802	33.69163381	85.63373814	108.4830411	1827.64361
143	12	840.4614	40925	45.6%	721.2	0.200	39.8872	1331.286878	-0.289415021	2344.576256	33.3326915	85.72189293	108.6753902	1827.91445
144	13	910.49985	44336	45.7%	781.3	0.217	39.8868	1331.098887	-0.187991297	2344.859855	33.02124501	85.80712316	108.8241515	1828.06018
145	14	980.5383	47746	45.8%	841.4	0.234	39.8864	1330.989111	-0.10977622	2345.04576	32.74638718	85.89000111	108.9393422	1828.10940
146	15	1050.57675	51157	45.8%	901.5	0.250	39.886	1330.939915	-0.049195956	2345.156131	32.49984472	85.97095144	109.0285706	1828.08385
147	16	1120.6152	54567	45.9%	961.6	0.267	39.8856	1330.937808	-0.002107018	2345.207924	32.2752968	86.05029237	109.0976559	1828.00015

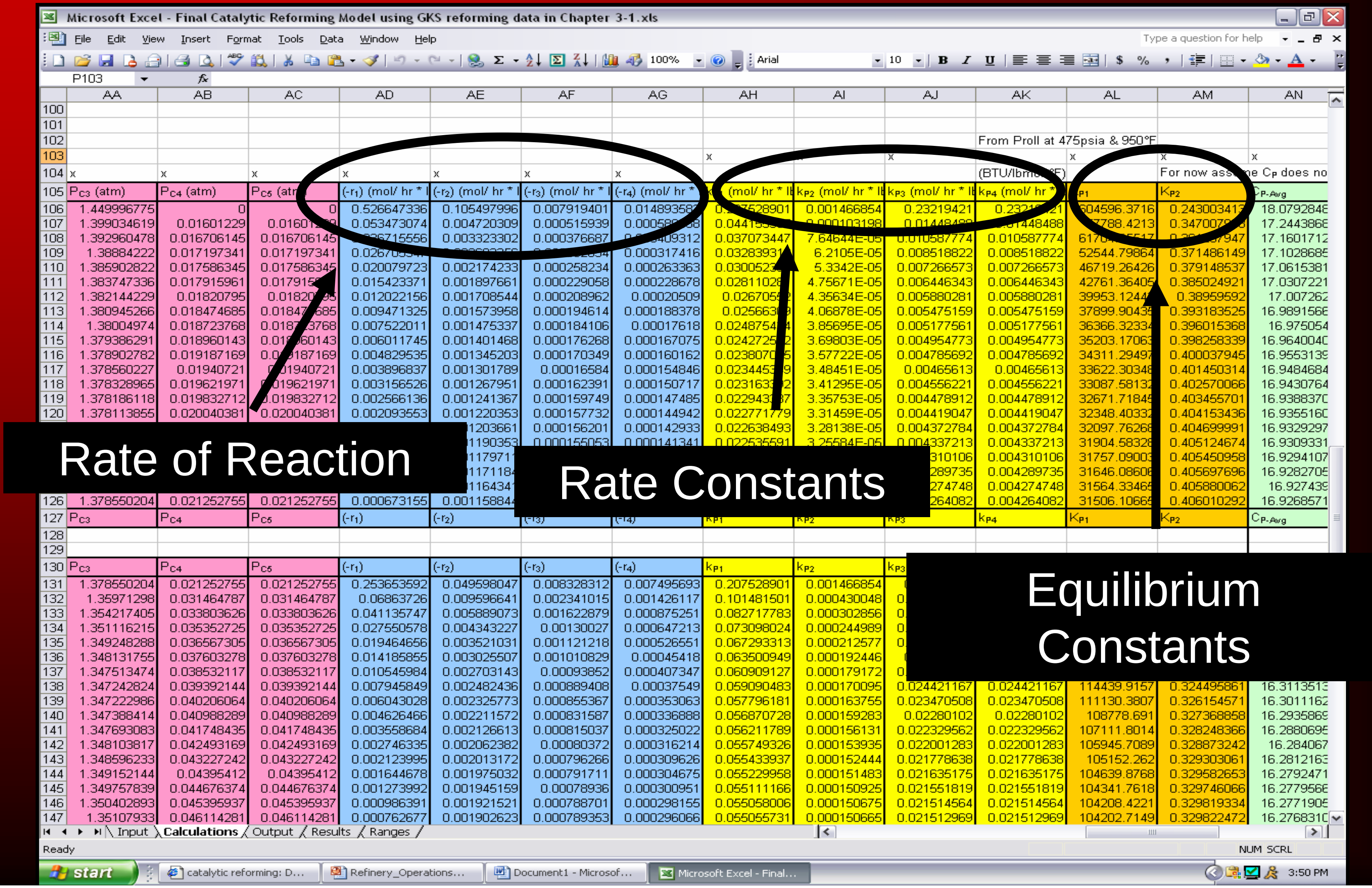
Excel Model



	O	P	Q	R	S	T	U
100							
101	27118						
102	11271						
103	38389			x	x	x	x
104	x	x	x	For now assume ideal gas where [illegible] Pressure = Total Pressure x Mole Fraction			
105	F_{C1} (lbmol /hr)	F_{C2} (lbmol /hr)	F_{C3} (lbmol /hr)	F_{C4} (lbmol /hr)	F_{C5} (lbmol /hr)	[illegible] Calc. (atm)	P_N (atm)
106	107.4217292	92.07576788	76.72980657	0	0	39.9	2.559297059
107	108.3100879	92.96412655	77.61816524	0.888358675	0.888358675	39.8996	1.624254093
108	108.3531408	93.00717951	77.6612182	0.931411634	0.931411634	[illegible]	1.542460245
109	108.3837484	93.03778704	77.69182572	0.962019159	0.962019159	[illegible]	1.486651873
110	108.4079023	93.06194094	77.71597963	0.986173066	0.986173066	39.8984	[illegible]
111	108.4282137	93.08225244	77.73629112	1.006484557	1.006484557	39.898	1.415343946
112	108.4460384	93.10007708	77.75411577	1.024309202	1.024309202	[illegible]	1.391530906
113	108.462162	93.11620065	77.77023933	1.040432769	1.040432769	[illegible]	1.372704254
114	108.4770761	93.13111475	77.78515343	1.055346869	1.055346869	39.8968	1.357591996
115	108.4911059	93.14514461	77.7991833	1.069376737	1.069376737	39.8964	1.345303066
116	108.504476	93.15851471	77.81255339	1.082746829	1.082746829	39.896	1.335192236
117	108.5173464	93.17138509	77.82542377	1.09561721	[illegible]	39.8956	1.326780548
118	108.5298342	93.18387288	77.83791157	1.108105004	[illegible]	39.8952	1.319705673
119	108.5420269	93.19606557	77.85010425	1.12029769	[illegible]	39.8948	1.313689471
120	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.308515981
121	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.304016007
122	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.300056047
123	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.296530165
124	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.293353917
125	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.290459748
126	108.6231753	93.27721402	77.93125271	1.201446141	1.201446141	39.892	1.287793454
127	F_{C1}	F_{C2}	F_{C3}	F_{C4}	F_{C5}	P_T Calc.	P_N
128	1.20	1.20	1.20	1.20	1.20		
129							
130	F_{C1}	F_{C2}	F_{C3}	F_{C4}	F_{C5}	P_T Calc.	P_N
131	108.6231753	93.27721402	77.93125271	1.201446141	1.201446141	39.892	1.287793454
132	109.2393767	93.89341541	78.54745409	1.81764753	1.81764753	39.8916	0.883476706
133	109.3860723	94.04011099	78.69414968	1.964343117	1.964343117	39.8912	0.782254275
134	109.4833518	94.13739048	78.79142916	2.061622597	2.061622597	39.8908	0.721970353
135	109.5591885	94.21322724	78.86726592	2.137459358	2.137459358	39.8904	0.681288101
136	109.6233542	94.27739287	78.93143156	2.201624991	2.201624991	39.89	0.652044624
137	109.680403	94.33444165	78.98848034	2.258673775	2.258673775	39.8896	0.630167557
138	109.7328123	94.38685098	79.04088967	2.311083106	2.311083106	39.8892	0.613320167
139	109.7820686	94.43610728	79.09014597	2.360339402	2.360339402	39.8888	0.600039878
140	109.829126	94.48316466	79.13720334	2.407396777	2.407396777	39.8884	0.589356123
141	109.8746275	94.52866614	79.18270483	2.452898262	2.452898262	39.888	0.58059772
142	109.9190224	94.57306111	79.2270998	2.497293234	2.497293234	39.8876	0.573286417
143	109.9626337	94.61667238	79.27071107	2.540904503	2.540904503	39.8872	0.567073785
144	110.0056981	94.65973681	79.3137755	2.583968936	2.583968936	39.8868	0.561701712
145	110.0483924	94.70243111	79.3564698	2.626663236	2.626663236	39.8864	0.55697655
146	110.0908502	94.74488885	79.39892753	2.669120968	2.669120968	39.886	0.552751601
147	110.1331733	94.78721203	79.44125072	2.711444153	2.711444153	39.8856	0.548914902

	V	W	X	Y	Z	AA	AB
100							
101							
102							
103	x	x					
104			x	x	x	x	
105	P_P (atm)	P_A (atm)	P_H (atm)	P_{C1} (atm)	P_{C2} (atm)	P_{C3} (atm)	P_{C4} [illegible]
106	1.360861215	0.469716613	30.29013672	2.029995486	1.739996131	1.449996775	
107	1.421188416	1.112867379	30.68234828	1.952243551	1.675639085	1.399034619	[illegible]
108	1.419515329	1.174596204	30.7245819	1.943462212	1.668211345	1.392960478	[illegible]
109	1.418450226	1.216631069	30.75315856	1.937500171	1.663171196	[illegible]	0.01719734
110	1.417880178	1.247033534	30.7735722	1.933229413	[illegible]	1.385902822	0.01758634
111	1.417693777	[illegible]	[illegible]	[illegible]	1.656913611	1.383747336	0.01791596
112	1.417804118	1.287242643	30.79981198	1.92771874	1.654931484	1.382144229	0.0182079
113	1.418145495	1.300810763	30.80827197	1.925933499	1.653439382	1.380945266	0.01847468
114	1.418668098	1.31148711	30.81466046	1.924580128	1.652314934	1.38004974	0.01872376
115	1.419333808	1.319960971	30.81946731	1.923556751	1.651471521	1.379386291	0.01896014
116	1.420113149	1.326732983	30.82304958	1.922789027	1.650845904	1.378902782	0.01918716
117	1.420983118	1.33217568	30.82567374	1.922221434	1.650390831	1.378560227	0.0194072
118	1.42192563	1.336571439	30.82754222	1.921811763	1.650070364	1.378328965	0.01962197
119	1.422926368	1.340137374	30.82881096	1.921527481	1.649856799	1.378186118	0.01983271
120	1.423973947	1.343042282	30.82960138	1.921343245	1.64972855	1.378113855	0.02004038
121	1.425059268	1.34541855	30.83000881	1.921239151	1.649668657	1.378098164	0.02024569
122	1.42617504	1.347370727	30.83010862	1.921199456	1.649663708	1.37812796	0.02044922
123	1.4273154	1.348981837	30.82996072	1.921211647	1.649703038	1.378194429	0.02065138
124	1.428475625	1.350318098	30.82961291	1.921265738	1.649778135	1.378290533	0.02085252
125	1.429651904	1.351432513	30.82910348	1.921353725	1.64988218	1.378410635	0.02105290
126	1.430841155	1.352367627	30.82846317	1.921469184	1.650009694	1.378550204	0.02125275
127	P_P	P_A	P_H	P_{C1}	P_{C2}	P_{C3}	P_{C4}
128							
129							
130	P_P	P_A	P_H	P_{C1}	P_{C2}	P_{C3}	P_{C4}
131	1.430841155	1.352367627	30.82846317	1.921469184	1.650009694	1.378550204	0.02125275
132	1.450253983	1.630957551	30.98789433	1.891012257	1.625362619	1.35971298	0.03146478
133	1.450444891	1.704063737	31.03192936	1.882382916	1.61830016	1.354217405	0.03380362
134	1.45046044	1.747467151	31.05738987	1.877421611	1.614268913	1.351116215	0.03535272
135	1.450708462	1.776384546	31.07353083	1.874320681	1.611784484	1.349248288	0.03656730
136	1.451200378	1.7967561	31.08407999	1.872343146	1.61023745	1.348131755	0.03760327
137	1.451894387	1.811584649	31.09095994	1.871106017	1.609309745	1.347513474	0.03853211
138	1.452746866	1.822609597	31.0953002	1.870383096	1.60881296	1.347242824	0.03939214
139	1.453721277	1.830927366	31.09782024	1.870029755	1.608626371	1.347222986	0.04020606
140	1.454788669	1.837269478	31.09900384	1.869948464	1.608668439	1.347388414	0.04098828
141	1.455926477	1.842143925	31.09918897	1.870070942	1.608882012	1.347693083	0.04174843
142	1.457117193	1.845913863	31.09861835	1.870348077	1.609225947	1.348103817	0.04249316
143	1.45834723	1.848844546	31.09746986	1.870743829	1.609670031	1.348596233	0.04322724
144	1.45960602	1.851132876	31.0958759	1.871231354	1.610191749	1.349152144	0.0439541
145	1.460885326	1.852926818	31.09393616	1.871790425	1.610774132	1.349757839	0.04467637
146	1.462178711	1.854338613	31.09172635	1.872405676	1.611404284	1.350402893	0.04539593
147	1.463481129	1.855454017	31.08930437	1.873065349	1.612072339	1.35107933	0.04611428

Excel Model


Microsoft Excel - Final Catalytic Reforming Model using GKS reforming data in Chapter 3-1.xls
Rate of Reaction
Rate Constants
Equilibrium Constants

GAMS Model

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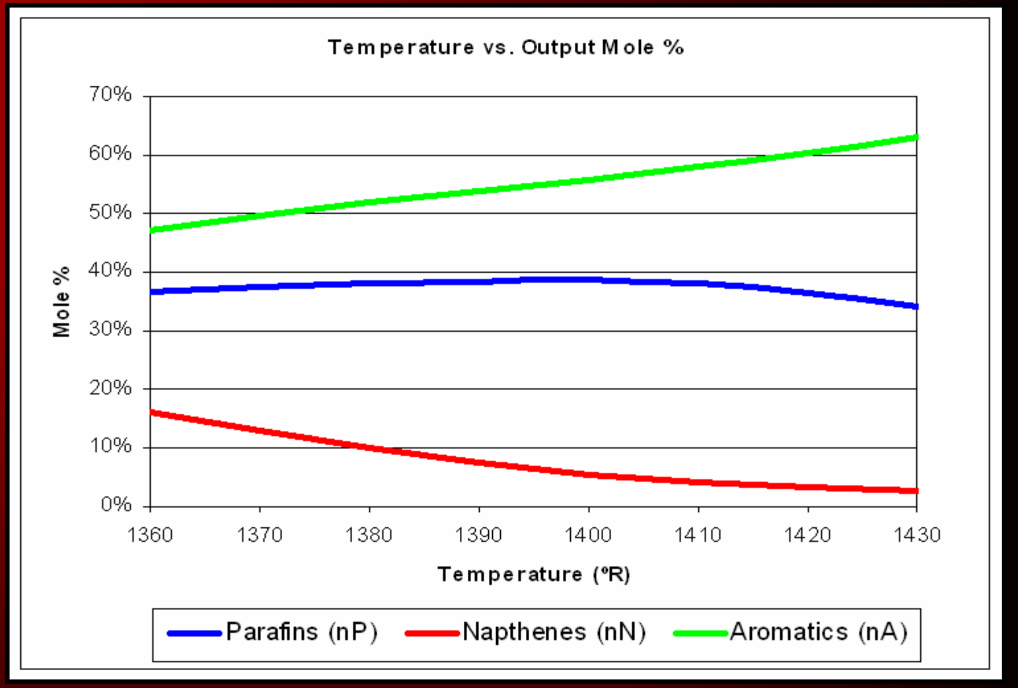
CRU2-1.gms

```
Set        y / 0*65 /
           s / 1*10 /
           v / t, p, f / ;

Scalar
           feed flow rate of cut entering (lbmol.hr)      / 232.3 /
           r1temp rankine  / 1402.2 /
           r2temp          / 1402.2 /
           r3temp
           r1pres atm      / 39.9 /
           r2pres          / 39.892 /
           r3pres

           par parafin     / 0.31 /
           nap napthene    / 0.583 /
           aro aromatics   / 0.107 /
           api gravity     / 54.3 /
           cp btu.lbF      / 0.731 /

           H2feed ratio    / 6.90 /
           hydmol hyd mol in recycyle      / 0.853 /
           meth_prop meth.prop     / 1.4 /
           eth_prop eth.prop       / 1.2 /
           recycle_mw
           recycle_cp btu.lbF      / 1.628 /

           recycle_hyd lbmol.hr
           recycle_meth
           recycle_eth
           recycle_prop

           r1diam ft       / 8.5 /
           r2diam ft       / 8.5 /
           r3diam ft       / 8.5 /

           r1vel ft.hr     / 3600 /
           r2vel ft.hr     / 3600 /
           r3vel ft.hr     / 3600 /

           drop pres drop per reactor      / 0.4 /

           r1cat_feed weight cat per flow (lb.lbmol.hr)    / 6.03 /
           r2cat_feed weight cat per flow (lb.lbmol.hr)    / 6.03 /
           r3cat_feed weight cat per flow (lb.lbmol.hr)    / 9.9 /

           r1cat mass (lb)
           r2cat
           r3cat
```

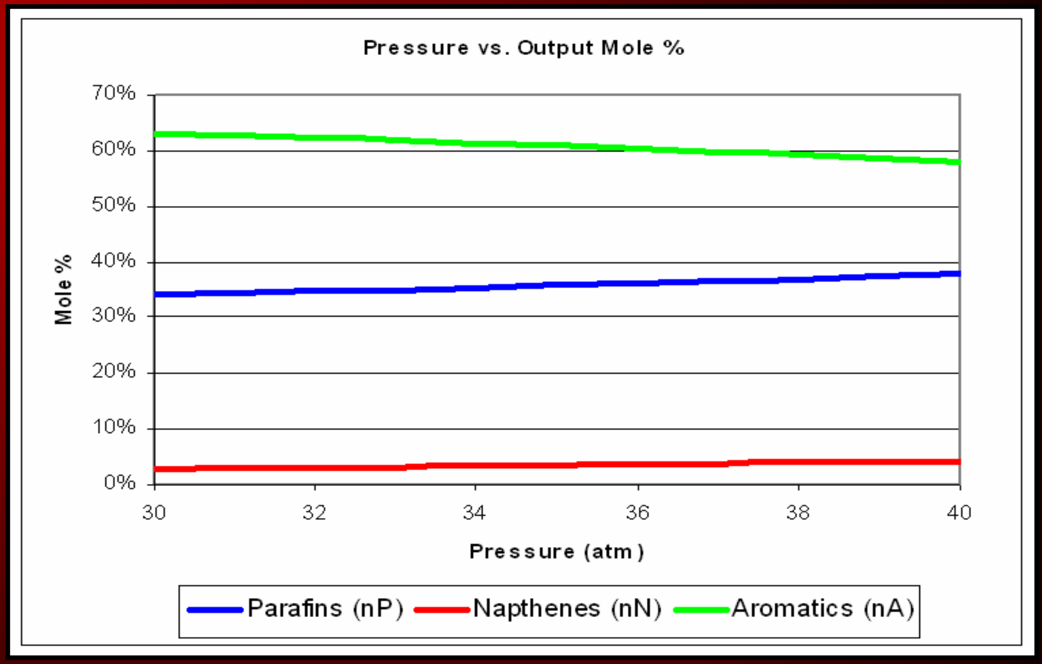
Catalytic Reforming Model Results

- Increased Temperature Dependence
  - Endothermic reactions
  - Increase rate constant
  - Increase equilibrium constant
  - Increase concentration of aromatics



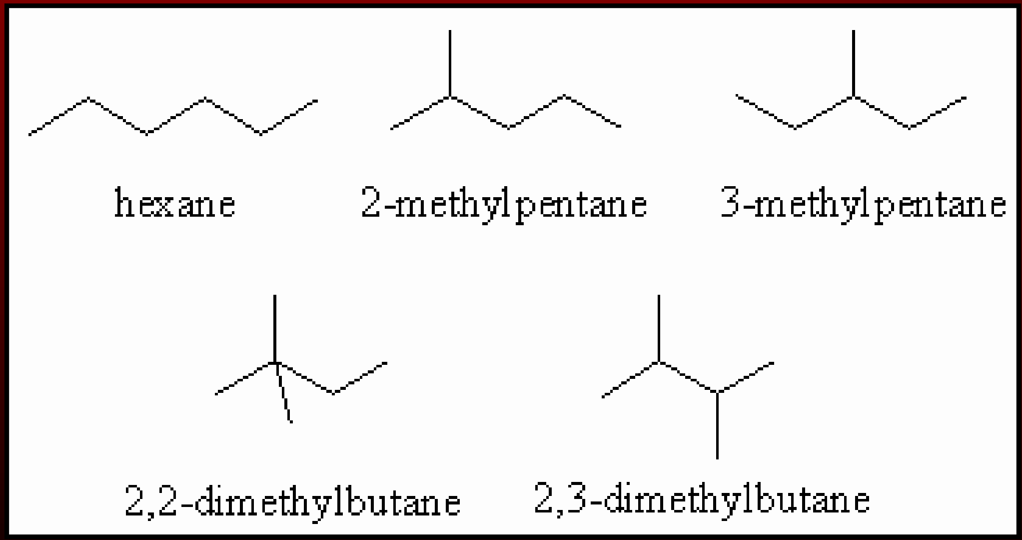
Catalytic Reforming Model Results

- Decreased Pressure Dependence
  - Increase overall reaction rate for hydrocracking
  - Increases concentration of aromatics



Isomerization

- Gas-phase catalyzed reaction
- Transforms a molecule into a different isomer
- Transforms straight chained isomers into branched isomers
- Increases octane rating of gasoline



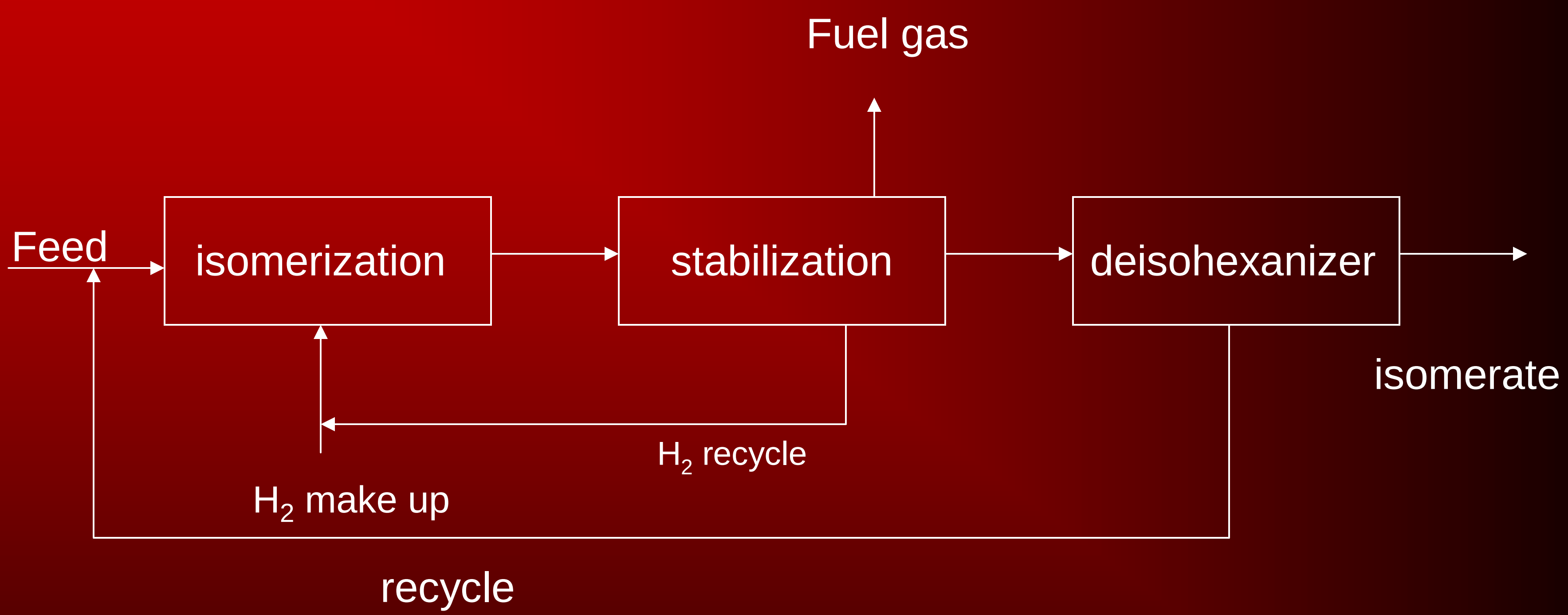
Isomerization Unit

- 2 types of catalysts most commonly used
  - Platinum/chlorinated alumina
  - Platinum/zeolite

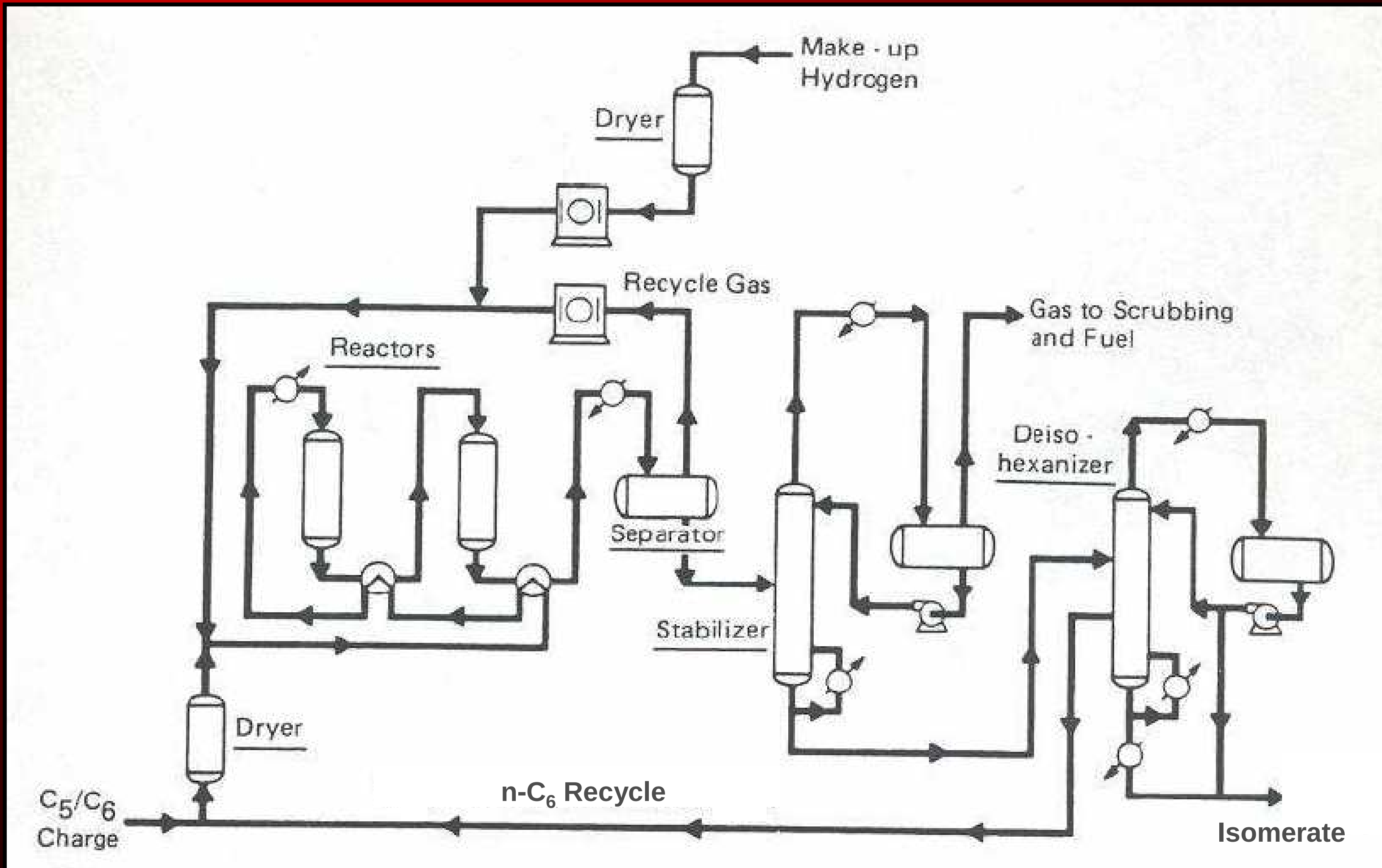
Isomerization Unit

- Feeds
  - Butanes
  - Pentanes
  - Hexanes
  - Small amounts Benzene
  - Make-up Hydrogen
- Products
  - Branched alkanes

Isomerization Unit



Isomerization



Isomerization Model

- Goal
  - To create a model that determines the products of the isomerization unit
- Model inputs
  - Temperature (range depends on catalyst used)
  - Mass flow rate
  - H_2/HC ratio (typical values 0.1-4)
  - Feed stream concentrations
- Model outputs
  - Product weight percents

Isomerization Model

- Modeling
  - Determine feed partial pressures
  - N-Butane kinetic model
  - N-Pentane kinetic model
  - N-Hexane kinetic model

Isomerization – Partial Pressures

- Antoine Equation
  - $\log_{10}P_o = A - B/(T+C)$
  - T = temperature in °C
  - P_o = vapor pressure in mmHg
- Partial Pressure
  - Used to determine mole fraction each component

Isomerization – N-Butane Model

- Bursian (1972)

- $$r_{nC4} = -K_1 \frac{P_{nC4}}{P_{H2}} + K_2 \frac{P_{iC4}}{P_{H2}}$$

- $$K = Ae^{\frac{-E}{RT}}$$

N-Butane	E (J/mol)	A
K1	58615.2	3973362
K2	66988.8	25296143

Isomerization - N-Pentane Model

- Aleksandrov (1976)

- $$K_{eq} = e^{\frac{1861}{TR} - \frac{1.299}{R}}$$

n-pentane	E (kcal/mol)	E (J/mol)	A
K1	10.1	42.2887	4023.872
K2	119.5	500.3465	7331.974

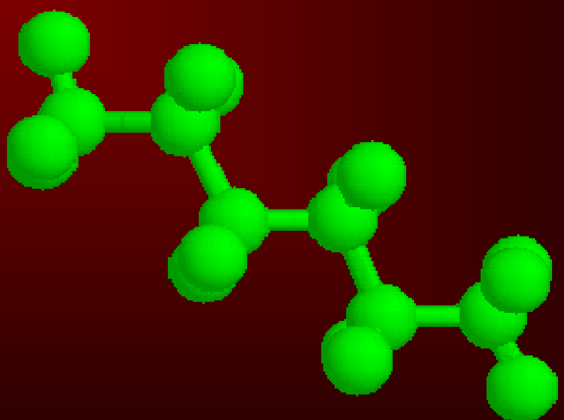
- $$r_{nC5} = -[K_2 (\frac{C_{nC5}}{H_2})^{0.125} - 0.0000197t][K_{eq} C_{nC5} - (K_{eq} + 1) C_{iC5}]$$

Isomerization - N-Hexane Model

- Cheng-Lie (1991)

- $$\frac{dC_i}{dt} = -\left(\sum_{j=1}^{5} K_{j,i}\right) \cdot C_i + \sum_{j=1}^{5} K_{i,j} C_j$$

n-Hexane	1
3-MP	2
2-MP	3
2,3-DMB	4
2,2-DMB	5



Isomerization Model

- Rate equations solved using finite integration
- Output - concentrations of various isomers in product stream

Isomerization Model - Excel

Microsoft Excel - Isomerization Unit Shobe-1

Row	A	B	C	D	E	F	G	H	I
1		**Inputs**					Mass (g)	4800000	Mass(kg)
2		Inlet Mass Flow Rate (g/s)	16000				Pressure (atm)	28.06504807	
3		Temperature (K)	400	Temperature (	126.85		Volume (L)	71745.35082	
4		H2/HC	2.4				R (atm L)/(mol	0.0820575	
5		dt (sec)	15	dt(hr)	0.004166667		Time (mins)	5	
6							Time (sec)	300	15
7					x	x		x	x
8		**Feed Components**	**wt%[1]**	**MW**	**moles**	**mole fraction**	**Concentration**	**Psat (atm)**	**Partial Pressure (at**
9		**i-C4**	0	58.08	0.000	0.000	0	31.348	0
10	x	**C4**	0.4	58.08	330.579	0.005	0.004607665	23.350	0.125827934
11	x	**Isopentane**	19.6	72.15	13039.501	0.213	0.181746983	12.018	2.554591178
12	x	**n-pentane**	28.5	72.15	18960.499	0.309	0.264274949	10.308	3.185992459
13	x	**cyclopentane**	1.4	70.13	958.220	0.016	0.013355854	7.375	0.115192343
14	x	**dimethyl-2,2-butane**	0.9	86.18	501.276	0.008	0.006986883	6.898	0.056362551
15		**2,3-dimethylbutane**	2.2	86.18	1225.342	0.020	0.017079048	5.762	0.1151016
16		**2-methyl pentane**	13.1	86.18	7296.356	0.119	0.101697969	5.568	0.662283794
17		**3-methyl pentane**	10.2	86.18	5681.133	0.093	0.079184678	5.160	0.477879903
18	x	**n-c6**	18.6	86.18	10359.712	0.169	0.14439559	4.582	0.773811908
19	x	**methylcyclopentane**	2.8	84.16	1596.958	0.026	0.022258699	4.179	0.108795343
20	x	**cyclohexane**	0.4	84.16	228.137	0.004	0.003179814	3.332	0.012391276
21	x	**benzene**	1.9	78.11	1167.584	0.019	0.016274005	3.478	0.066195614
22		**Sum**	**100**		**61345.298**	**1.000**	**0.855042137**	**123.358**	**8.254425904**
23		**Hydrogen**			43302.563		0.603559156		19.81062217
24									
25									
26									
27			1	Conversion Processes Table 6.5					
28									

Row	J	K	L	M	N	O	P	Q	R	S
1	4800		Octane	81.69696	After Iso					
2				71.6364	Before Iso					
7	**Product Values**							**Conversions**		
8	**Concentration**	**Mole Fracti**	**Moles**	**Mass (g)**	**Wt%**	**Volume F**	**Butanes**	**Pentanes**	**Hexanes**	
9	0.073247324	0.00260991	192.4373	11176.76	0.233	5.618822	0.58	0.59	0.59	
10	0.05258061	0.00187353	138.1412	8023.24	0.167	4.033473				
11	0.181746983		13039.5	940800	19.603	432.0191				
12	0.264274949		18960.5	1368000	28.504	628.191				
13				67200	1.400	30.85851				
14	0.006826403		489.7627	42207.75	0.879	17.65111				
15	0.020985851		1505.637	129755.8	2.704	54.26336				
16	0.113493286		8142.616	701730.6	14.621	293.4609				
17	0.064397186		4620.199	398168.7	8.296	166.5126		41.20951181		
18	0.143540368		10298.35	887512.2	18.492	371.154				
19				134400	2.800	56.20554				
20				19200	0.400	8.029363				
21				91200	1.900	38.13947				
22				**4799375**		2106.137				
23										
26							4.7788E-09	-4.7788E-09		1.316

Row	A	B	C	D	E	F	G	H	I	J
29			**Concentrations**							
30	Time (hr)	Time (sec)	**i-C4**	**C4**	**Isopentane**	**n-pentane**	**dimethyl-2,2-b**	**2,3-dimethylbu**	**2-methyl pentane**	**3-methyl pentane**
31	0	0	0	0.125827934	0.181746983	0.264274949	0.006986883	0.017079048	0.101697969	0.079184678
32	0.004167	15	0.008393682	0.117434253	0.181746983	0.264274949	0.006978773	0.01727654	0.102531303	0.078200708
33	0.008333	30	0.015939985	0.109887949	0.181746983	0.264274949	0.006970671	0.017473837	0.103333586	0.077247861
34	0.0125	45	0.022724457	0.103103477	0.181746983	0.264274949	0.006962579	0.017670934	0.104105852	0.07632511
35	0.016667	60	0.028824008	0.097003926	0.181746983	0.264274949	0.006954495	0.017867823	0.1048491	0.075431464
36	0.020833	75	0.034307783	0.091520151	0.181746983	0.264274949	0.006946421	0.018064501	0.105564295	0.074565964
37	0.025	90	0.039237948	0.086589986	0.181746983	0.264274949	0.006938356	0.01826096	0.106252371	0.073727681
38	0.029167	105	0.043670392	0.082157542	0.181746983	0.264274949	0.0069303	0.018457195	0.106914231	0.07291572
39	0.033333	120	0.047655362	0.078172573	0.181746983	0.264274949	0.006922253	0.018653203	0.107550748	0.072129211
40	0.0375	135	0.051238032	0.074589903	0.181746983	0.264274949	0.006914216	0.018848977	0.108162766	0.071367317
41	0.041667	150	0.054459016	0.071368918	0.181746983	0.264274949	0.006906187	0.019044512	0.108751101	0.070629227
42	0.045833	165	0.057354828	0.068473106	0.181746983	0.264274949	0.006898168	0.019239805	0.109316543	0.069914157
43	0.05	180	0.059958295	0.065869639	0.181746983	0.264274949	0.006890157	0.019434851	0.109859855	0.069221347
44	0.054167	195	0.062298932	0.063529002	0.181746983	0.264274949	0.006882156	0.019629646	0.110381774	0.068550066
45	0.058333	210	0.064403271	0.061424663	0.181746983	0.264274949	0.006874164	0.019824185	0.110883015	0.067899604
46	0.0625	225	0.066295168	0.059532766	0.181746983	0.264274949	0.006866181	0.020018465	0.111364267	0.067269276

Row	K
30	**n-c6**
31	0.14439559
32	0.14435261
33	0.14430966
34	0.14426673
35	0.14422382
36	0.14418094
37	0.14413809
38	0.14409525
39	0.14405244
40	0.14400966
41	0.14396689
42	0.14392415
43	0.14388143
44	0.14383872
45	0.14379604
46	0.14375338

Row	M	N	O	P	Q	R	S
29		**Change in Concentra**					
30	Time (sec)	**i-C4**	**C4**	**Isopentane**	**n-pentane**	**dimethyl-2,2**	**2,3-di**
31	0	0.00839368	-0.00839	1.99117E-11	-1.99117E-11	-8.111E-06	0.000
32	15	0.0075463	-0.00755	1.99117E-11	-1.99117E-11	-8.102E-06	0.000
33	30	0.00678447	-0.00678	1.99117E-11	-1.99117E-11	-8.092E-06	0.000
34	45	0.00609955	-0.0061	1.99117E-11	-1.99117E-11	-8.083E-06	0.00
35	60	0.00548378	-0.00548	1.99117E-11	-1.99117E-11	-8.074E-06	0.000
36	75	0.00493016	-0.00493	1.99117E-11	-1.99117E-11	-8.065E-06	0.000
37	90	0.00443244	-0.00443	1.99117E-11	-1.99117E-11	-8.056E-06	0.000
38	105	0.00398497	-0.00398	1.99117E-11	-1.99117E-11	-8.047E-06	0.000
39	120	0.00358267	-0.00358	1.99117E-11	-1.99117E-11	-8.038E-06	0.000
40	135	0.00322098	-0.00322	1.99117E-11	-1.99117E-11	-8.029E-06	0.000
41	150	0.00289581	-0.0029	1.99117E-11	-1.99117E-11	-8.019E-06	0.000
42	165	0.00260347	-0.0026	1.99117E-11	-1.99117E-11	-8.01E-06	0.000
43	180	0.00234064	-0.00234	1.99117E-11	-1.99117E-11	-8.001E-06	0.000
44	195	0.00210434	-0.0021	1.99117E-11	-1.99117E-11	-7.992E-06	0.000
45	210	0.0018919	-0.00189	1.99117E-11	-1.99117E-11	-7.983E-06	0.00
46	225	0.0017009	-0.0017	1.99117E-11	-1.99117E-11	-7.974E-06	0.000

Isomerization Model - GAMS

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iso_unit.gms

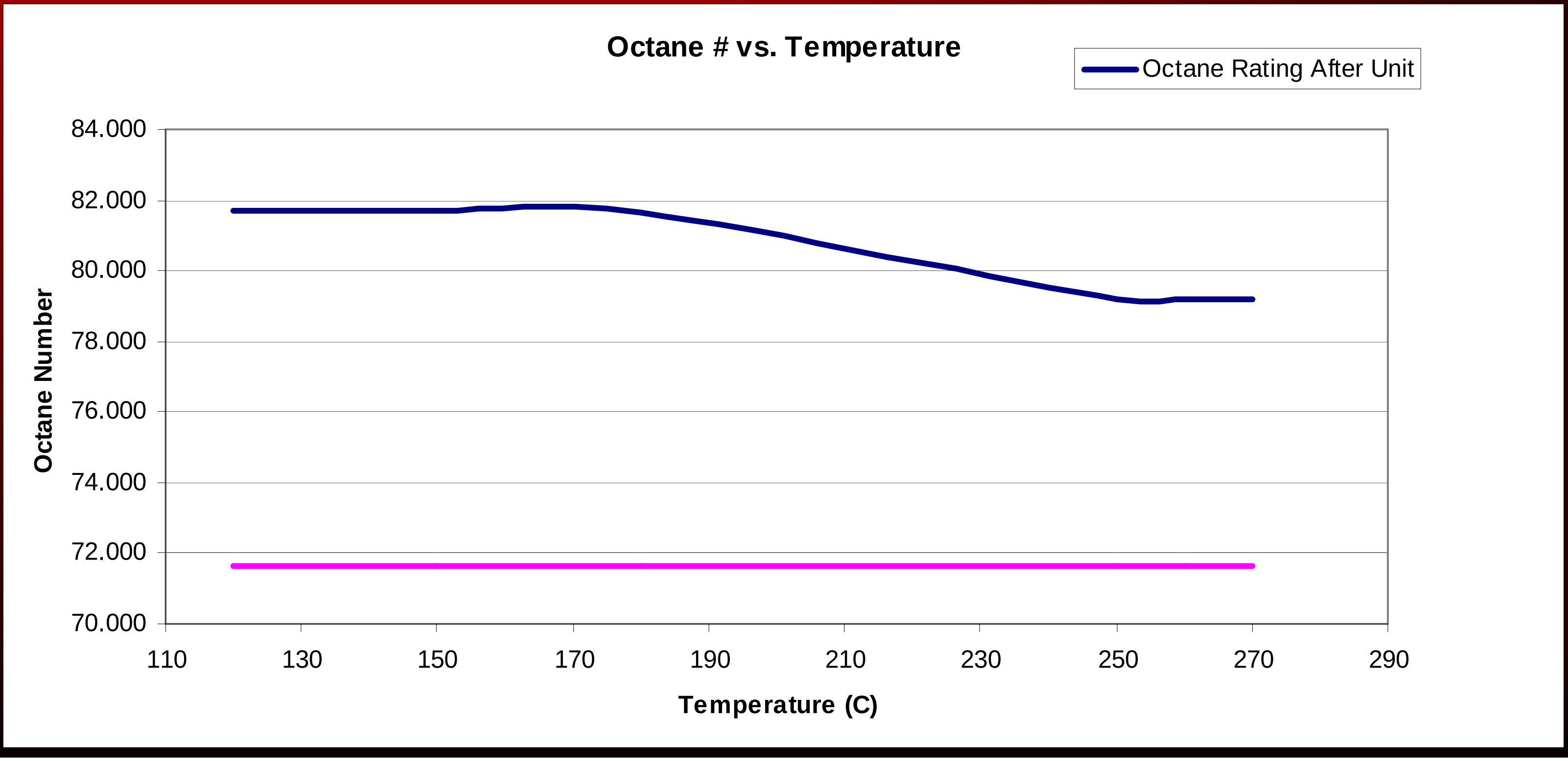
```
*Euler Step 20

conciC4('20')=conciC4('19')+rate_iC4('19')*step;
concC4('20')=concC4('19')+rate_C4('19')*step;
conciC5('20')=conciC5('19')+rate_C5('19')*step/3600;
concC5('20')=concC5('19')+rate_C5('19')*step/3600;
conc22DB('20')=conc22DB('19')+rate_22DB('19')*step;
conc23DB('20')=conc23DB('19')+rate_23DB('19')*step;
conc2MP('20')=conc2MP('19')+rate_2MP('19')*step;
conc3MP('20')=conc3MP('19')+rate_3MP('19')*step;
concC6('20')=concC6('19')+rate_C6('19')*step;
rate_C4('20')=-butK1*concC4('20')/Phyd+butK2*conciC4('20')/Phyd;
rate_iC4('20')=-rate_C4('20');
rate_C5('20')=-(pentK2*(concC5('20')/concHyd)**0.125-0.0000197*step/3600)*(pentKeq*concC5('20')-(pentKeq+1)*conciC5('20'));
rate_iC5('20')=-rate_C5('20');
rate_22DB('20')=hexK_C6_22DB*concC6('20')+hexK_3MP_22DB*conc3MP('20')+hexK_2MP_22DB*conc2MP('20')+hexK_23DMB_22DB*conc23DB('20')+hexK_22DMB_22DB*conc22DB(
rate_23DB('20')=hexK_C6_23DB*concC6('20')+hexK_3MP_23DB*conc3MP('20')+hexK_2MP_23DB*conc2MP('20')+hexK_23DMB_23DB*conc23DB('20')+hexK_22DMB_23DB*conc22DB(
rate_2MP('20')=hexK_C6_2MP*concC6('20')+hexK_3MP_2MP*conc3MP('20')+hexK_2MP_2MP*conc2MP('20')+hexK_23DMB_2MP*conc23DB('20')+hexK_22DMB_2MP*conc22DB('20')-
rate_3MP('20')=hexK_C6_3MP*concC6('20')+hexK_3MP_3MP*conc3MP('20')+hexK_2MP_3MP*conc2MP('20')+hexK_23DMB_3MP*conc23DB('20')+hexK_22DMB_3MP*conc22DB('20')-
rate_C6('20')=hexK_C6_C6*concC6('20')+hexK_3MP_C6*conc3MP('20')+hexK_2MP_C6*conc2MP('20')+hexK_23DMB_C6*conc23DB('20')+hexK_22DMB_C6*conc22DB('20')-concC6

molefracfinaliC4=conciC4('20')/Pressure;
molefracfinalC4=concC4('20')/Pressure;
molef_iC4=(mole('C4')+mole('iC4'))*molefracfinaliC4/(molefracfinaliC4+molefracfinalC4);
molef_C4=(mole('C4')+mole('iC4'))*molefracfinalC4/(molefracfinaliC4+molefracfinalC4);
molef_iC5=conciC5('20')*volume;
molef_C5=concC5('20')*volume;
molef_22DB=conc22DB('20')*volume;
molef_23DB=conc23DB('20')*volume;
molef_2MP=conc2MP('20')*volume;
molef_3MP=conc3MP('20')*volume;
molef_C6 =concC6('20')*volume;
massfiC4= molef_iC4*MW('iC4');
massfC4= molef_C4*MW('C4');
```

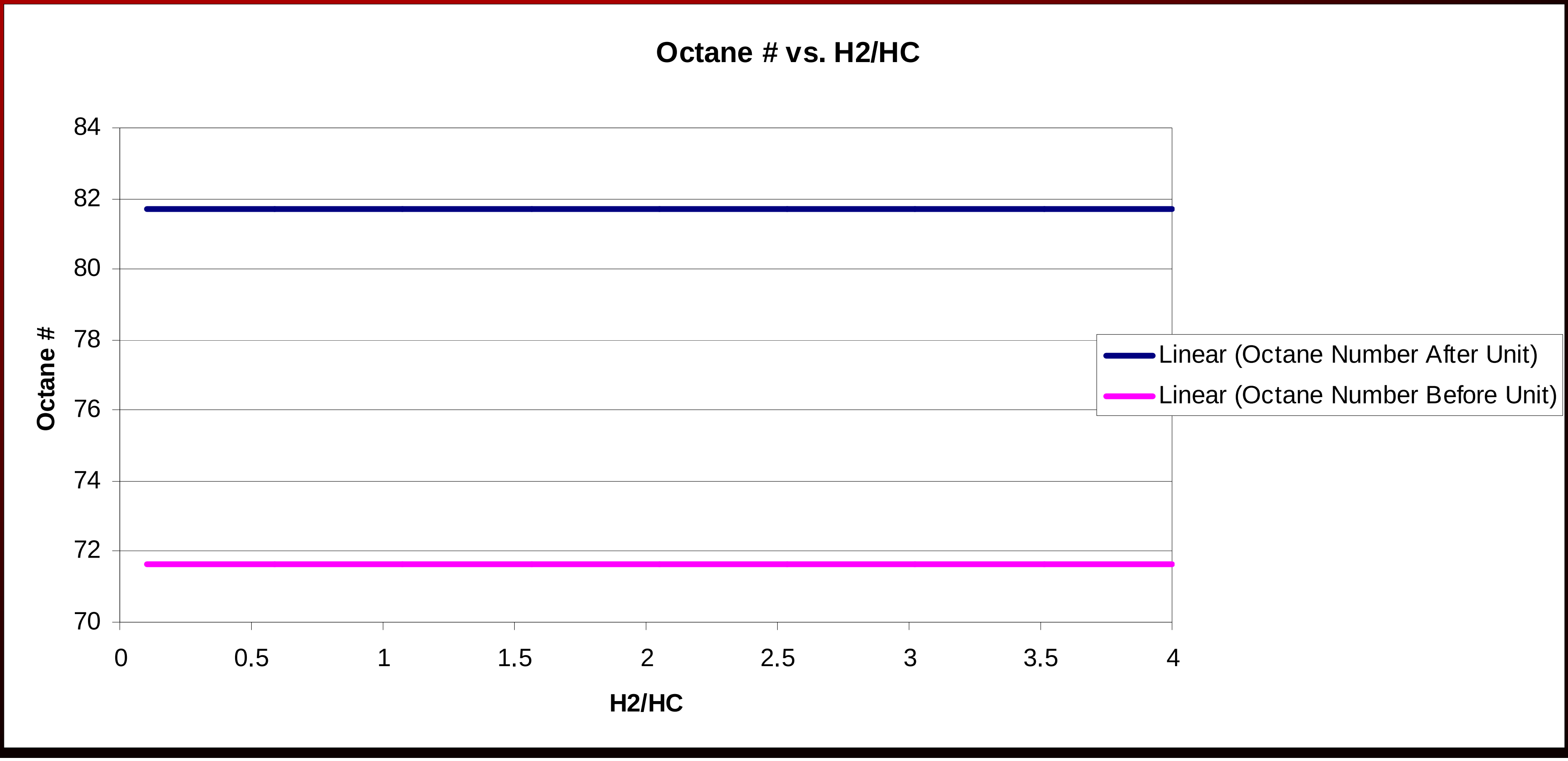
Isomerization Model Results

- Temperature Increase
  – Pt/Chlorinated Alumina 120-180℃
  – Pt/Zeolite 250-270℃

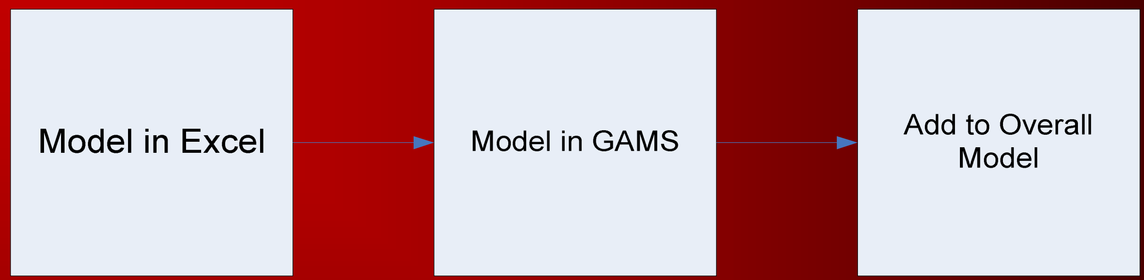


Isomerization Model Results

- H_2/HC Ratio increase
  - Range 0.1-4



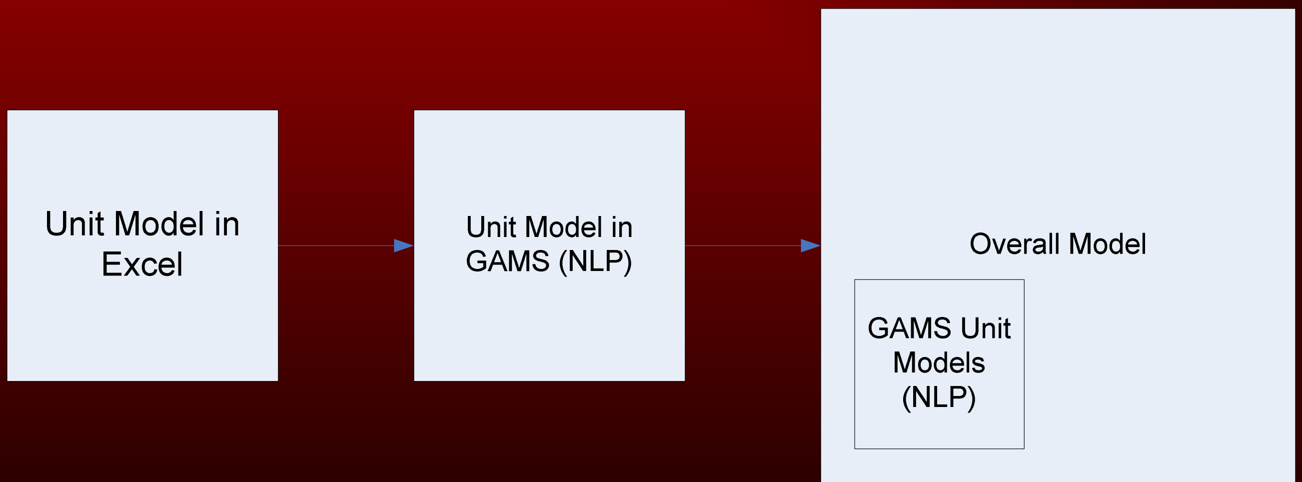
Modeling Unit Operations



- Excel
  - Excel is not used for overall model due to the problem being too complex for Excel's Solver
- CPLEX
  - CPLEX is a MIP mathematical optimization program
- GAMS
  - User interface for CPLEX

Option #1 (NLP)

- Model each unit in Excel
- Transfer to GAMS (NLP)
- Add NLP directly into GAMS model



Option #1 (NLP)

- Problems
  - Non-linearities in overall model create difficulty to determine global optimum
  - Added one unit (HDS)
    - Overall model converged
    - GRM changed (because operating costs were added)
    - Recommendations remained the same
  - Added second unit (NPU2)
    - Overall model did not converge
- Did Not Use

Linearization of a Non-Linear Problem

- For example, a CSTR has the following equations:

$$X = \frac{V \cdot (-r_A)}{F_{A0}} \qquad -r_A = k \cdot C_A^{0.5} \cdot C_B^2 \qquad k = k_0 \cdot e^{-\frac{E}{R \cdot T}}$$

- X can be shown as a function of the input variables:

$$X = f(T, C_{A0}, C_{B0})$$

Linearization of a Non-Linear Problem

- To linearize, discretize the input variables
  - Where Z is a binary variable

$$X = \sum_{(T, C_{A0}, C_{B0})} Z(T, C_{A0}, C_{B0}) \cdot f(T, C_{A0}, C_{B0})$$

$$\sum_{(T, C_{A0}, C_{B0})} Z(T, C_{A0}, C_{B0}) = 1$$

T =	C_{A0} =	C_{B0} =
500 F	0.92 mol/L	0.50 mol/L
600 F	0.94 mol/L	0.55 mol/L
700 F	0.96 mol/L	0.60 mol/L
800 F	0.98 mol/L	0.65 mol/L
900 F	1.00 mol/L	0.70 mol/L

$$X = \frac{V \cdot (-r_A)}{F_{A0}} \qquad -r_A = k \cdot C_A^{0.5} \cdot C_B^2 \qquad k = k_0 \cdot e^{-\frac{E}{R \cdot T}}$$

Non-Linearities in Unit Operations

- CSTR

$$X = \frac{V \cdot (-r_A)}{F_{A0}} \qquad -r_A = k \cdot C_A^{0.5} \cdot C_B^{2} \qquad k = k_0 \cdot e^{-\frac{E}{R \cdot T}}$$

- Catalytic Reformer

$$\hat{k}_{P2} = \exp\left(35.98 - \frac{59600}{T}\right)$$

$$K_{P2} = \frac{P_P}{P_N * P_H} \qquad K_{P1} = \frac{P_A * P_H^3}{P_N}$$

$$\hat{k}_{P3} = \hat{k}_{P4} = \exp\left(42.97 - \frac{62300}{T}\right)$$

$$\hat{k}_{P1} = \exp\left(23.21 - \frac{34750}{T}\right)$$

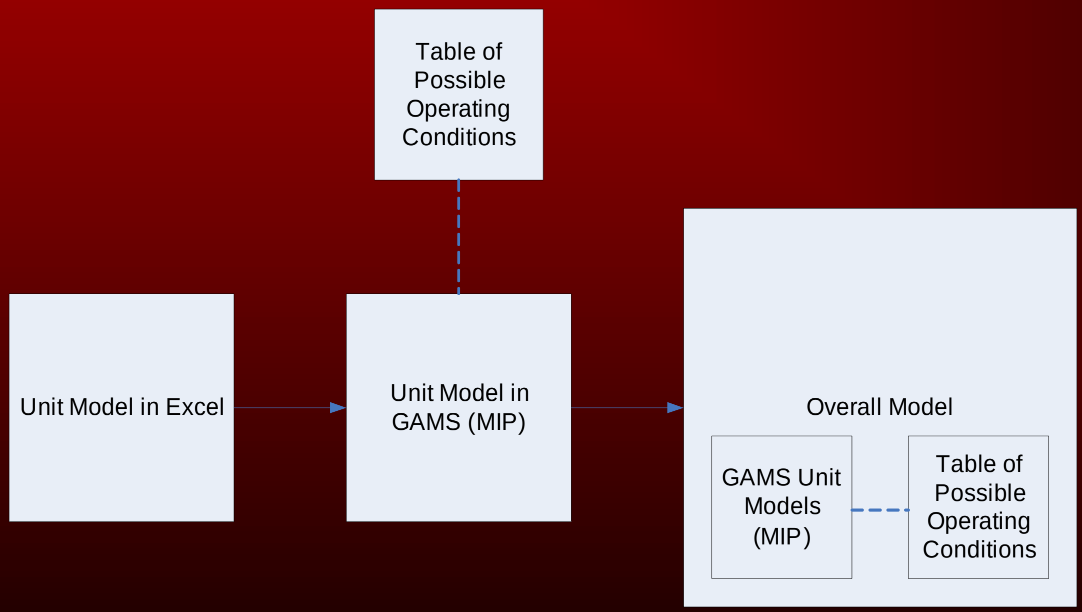
$$-\hat{r}_1 = \hat{k}_{P1}\left(P_N - \frac{P_A * P_H^3}{K_{P1}}\right)$$

$$-\hat{r}_2 = \hat{k}_{P2}\left(P_N * P_H - \frac{P_P}{K_{P2}}\right)$$

$$-\hat{r}_3 = \hat{k}_{P3}\left(\frac{P_P}{P}\right) \qquad -\hat{r}_4 = \hat{k}_{P4}\left(\frac{P_N}{P}\right)$$

Option #2 (MIP)

- Take Excel model
- Write MIP utilizing table of possible variables
- Add MIP directly into GAMS model



Option #2 (MIP)

- Did not attempt to use
  - Overall model would theoretically work
  - Model would become extremely long
  - Would require more memory and resources
  - Less user friendly than option #3

Option #3 (MIP Brute Force)

- Take Excel model
- Model MIP in GAMS
- Have MIP write to an overall table
- Utilize binary variables in overall model to select variables based on the table and constraints

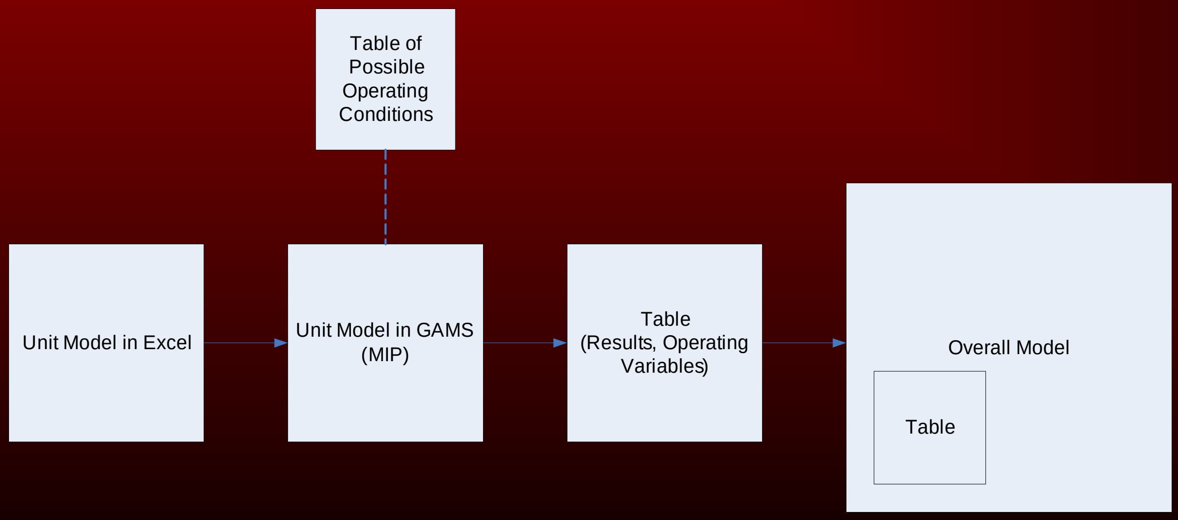


Table Generation

$$X = \sum_{(T, C_{A0}, C_{B0})} Z(T, C_{A0}, C_{B0}) \cdot X(T, C_{A0}, C_{B0})$$

		C_{B0} =				
T =	C_{A0} =	0.50 mol/L	0.55 mol/L	0.60 mol/L	0.65 mol/L	0.70 mol/L
500 F	0.92 mol/L	0.74	0.22	0.75	0.54	0.93
500 F	0.94 mol/L	0.10	0.39	0.79	0.32	0.38
500 F	0.96 mol/L	0.72	0.70	0.06	0.28	0.22
500 F	0.98 mol/L	0.54	0.57	0.53	0.24	0.22
500 F	1.00 mol/L	0.91	0.41	0.80	0.66	0.97
600 F	0.92 mol/L	0.33	0.12	0.09	0.77	0.08
600 F	0.94 mol/L	0.04	0.70	0.78	0.79	0.58
600 F	0.96 mol/L	0.48	1.00	0.00	0.52	0.24
600 F	0.98 mol/L	0.86	0.40	0.85	0.10	0.27
600 F	1.00 mol/L	0.15	0.42	0.91	0.72	0.59
700 F	0.92 mol/L	0.00	0.62	0.69	0.29	0.85
700 F	0.94 mol/L	0.73	0.78	0.47	0.93	0.55
700 F	0.96 mol/L	0.83	0.45	0.46	0.54	0.64
700 F	0.98 mol/L	0.94	0.43	0.69	0.25	0.88
700 F	1.00 mol/L	0.25	0.01	0.61	0.26	0.07
800 F	0.92 mol/L	0.25	0.64	0.55	0.40	0.68
800 F	0.94 mol/L	0.37	0.87	0.14	0.31	0.96
800 F	0.96 mol/L	0.52	0.58	0.37	0.61	0.71
800 F	0.98 mol/L	0.46	0.20	0.17	0.99	0.37
800 F	1.00 mol/L	0.04	0.82	0.81	0.81	0.86
900 F	0.92 mol/L	0.83	0.39	0.50	0.57	0.10
900 F	0.94 mol/L	0.27	0.52	0.35	0.81	0.96
900 F	0.96 mol/L	0.71	0.09	0.63	0.45	0.03
900 F	0.98 mol/L	0.61	0.47	0.30	0.29	0.09
900 F	1.00 mol/L	0.30	0.35	0.52	0.84	0.02

Option #3 (MIP Brute Force)

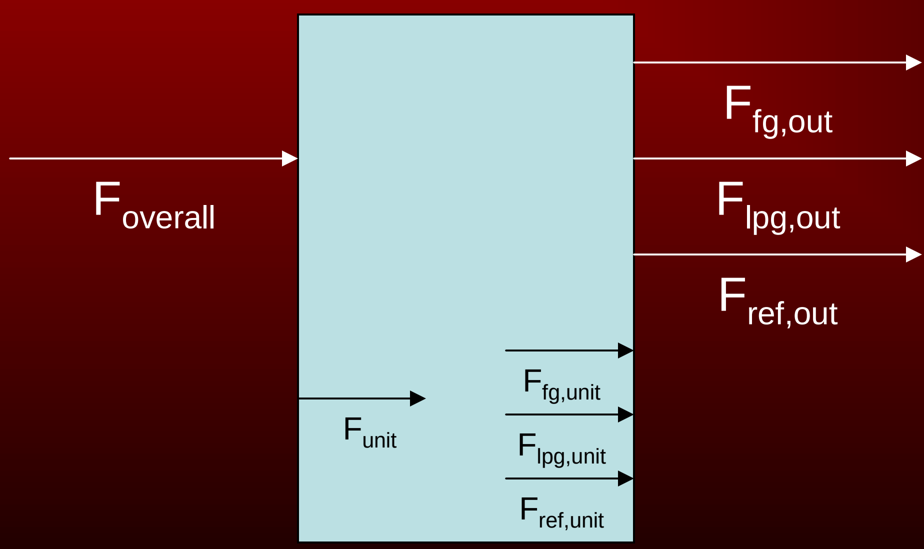
- Currently being used
  - Offers ease of use for the overall model
  - Drawback - more files are required to run the model
    - 26 tables utilized

Specific Modeling Issues

- “Best Choice” scenario
- Mass Balance
- Blending
- Additions

“Best Choice” Scenario

- Unit operations flow rates chosen by which scenario is nearest to the actual flow rate
- Allows for degrees of freedom in crude purchasing



"Best Choice" Scenario

$$F_{overall} - F_{unit} \leq d \qquad F_{unit} - F_{overall} \leq d$$

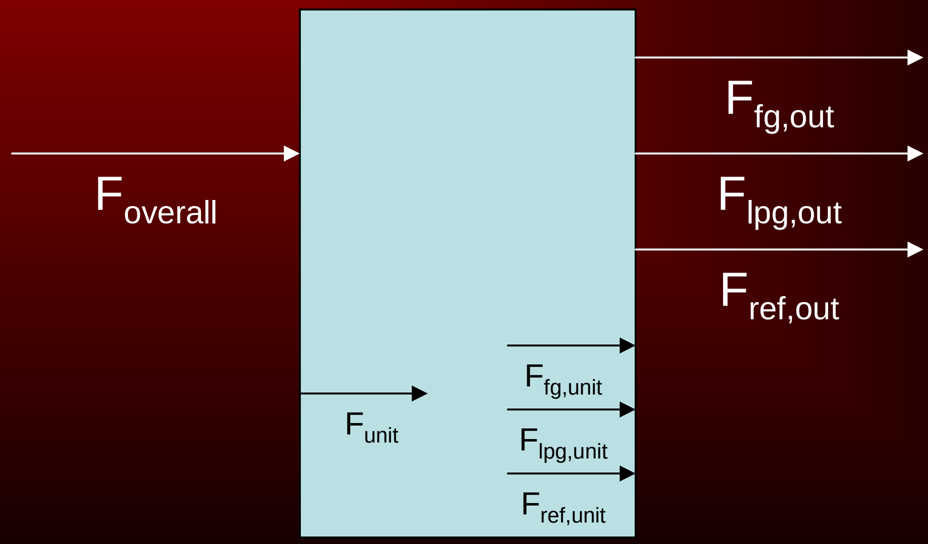
F =
15000 m^3/d
16000 m^3/d
17000 m^3/d
18000 m^3/d
19000 m^3/d

$$d = \frac{F2 - F1}{2} \; e.g. = \frac{16000 - 15000}{2} = 500$$

- F = flow rates
- d = difference between discretized unit flow rates

Mass Balance (CRU2, CRU3, ISOU)

- Solving the mass balance (2 options)
  - $F_{overall} = F_{out}$
    - Requires a non-linear equation ($Z*F_{overall}$)
    - Linearization possible, but requires massive amounts of memory (takes the program a long time to run)



Linearization of $Z*F_{overall}$

$$\Gamma(a,b,c) - x \cdot Z(a,b,c) \leq 0$$

$$\Gamma(a,b,c) \geq 0$$

$$\left(F_{overall} - \Gamma(a,b,c)\right) - x \cdot \left(1 - Z(a,b,c)\right) \leq 0$$

$$F_{overall} - \Gamma(a,b,c) \geq 0$$

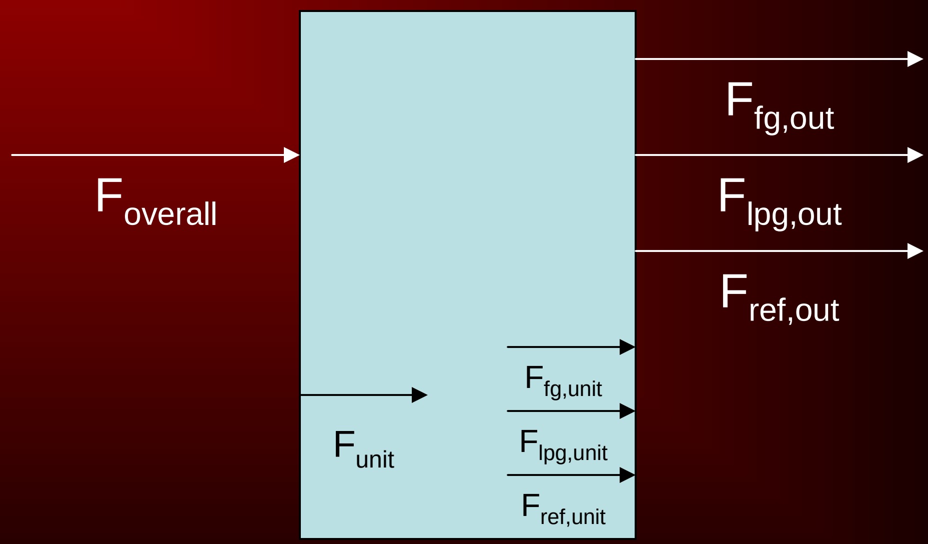
$$x = 1 \cdot 10^{10}$$

$$where \sum_{(a,b,c)} \Gamma(a,b,c) = \sum_{(a,b,c)} Z(a,b,c) \cdot F_{overall}$$

Mass Balance (CRU2, CRU3, ISOU)

- Successful solution
  - Advantage - requires far less memory
  - Disadvantage - mass is not completely balanced
    - Model not based on mass flow rates
    - Volumetric balances are inexact
    - If large amount of flow rate scenarios used, the error is minimized
      - Large amounts of scenarios does not slow down model

$$F_{reformate,out} = F_{reformate,unit}$$



Blending Model

$$F_a \cdot ON_a + F_b \cdot ON_b + F_c \cdot ON_c \geq F_{tot} \cdot ON_x$$

$$x = ISOG, SUPG$$

$$ON_{SUPG} = 91$$

$$ON_{ISOG} = 95$$

- ON_a dependant on Z, therefore Z*F appears again
  - Linearization used (only 3 required this time)

Linearization of Z*$F_{overall}$

$$\Gamma(a,b,c) - x \cdot Z(a,b,c) \leq 0$$

$$\Gamma(a,b,c) \geq 0$$

$$\left(F_{overall} - \Gamma(a,b,c)\right) - x \cdot \left(1 - Z(a,b,c)\right) \leq 0$$

$$F_{overall} - \Gamma(a,b,c) \geq 0$$

$$x = 1 \cdot 10^{10}$$

$$where \sum_{(a,b,c)} \Gamma(a,b,c) = \sum_{(a,b,c)} Z(a,b,c) \cdot F_{overall}$$

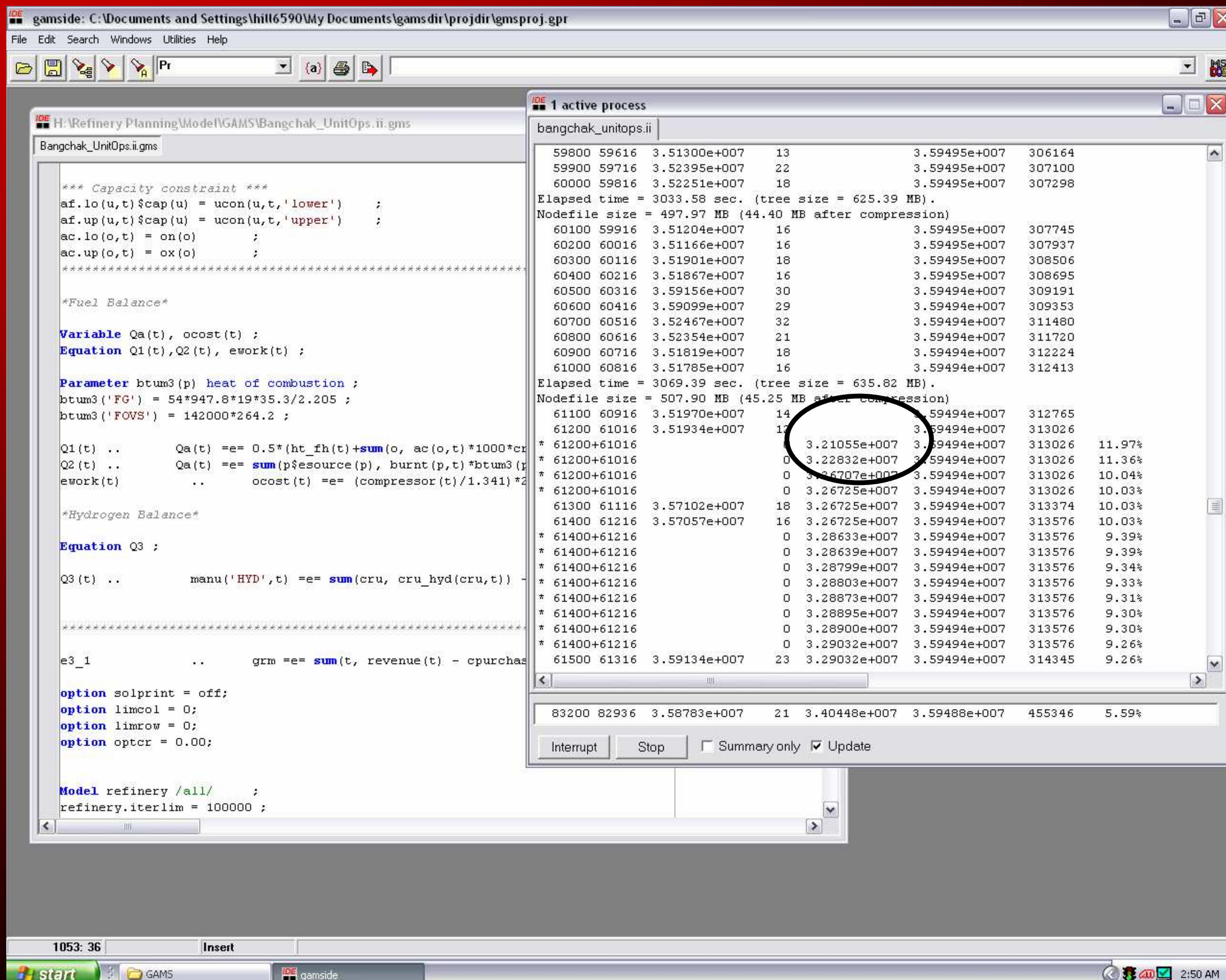
Additions

- Revised Fuel Balance
  - Fuel Gas and Fuel Oil burned
- Added Operating Costs associated with compression
- Added Hydrogen Balance

Results

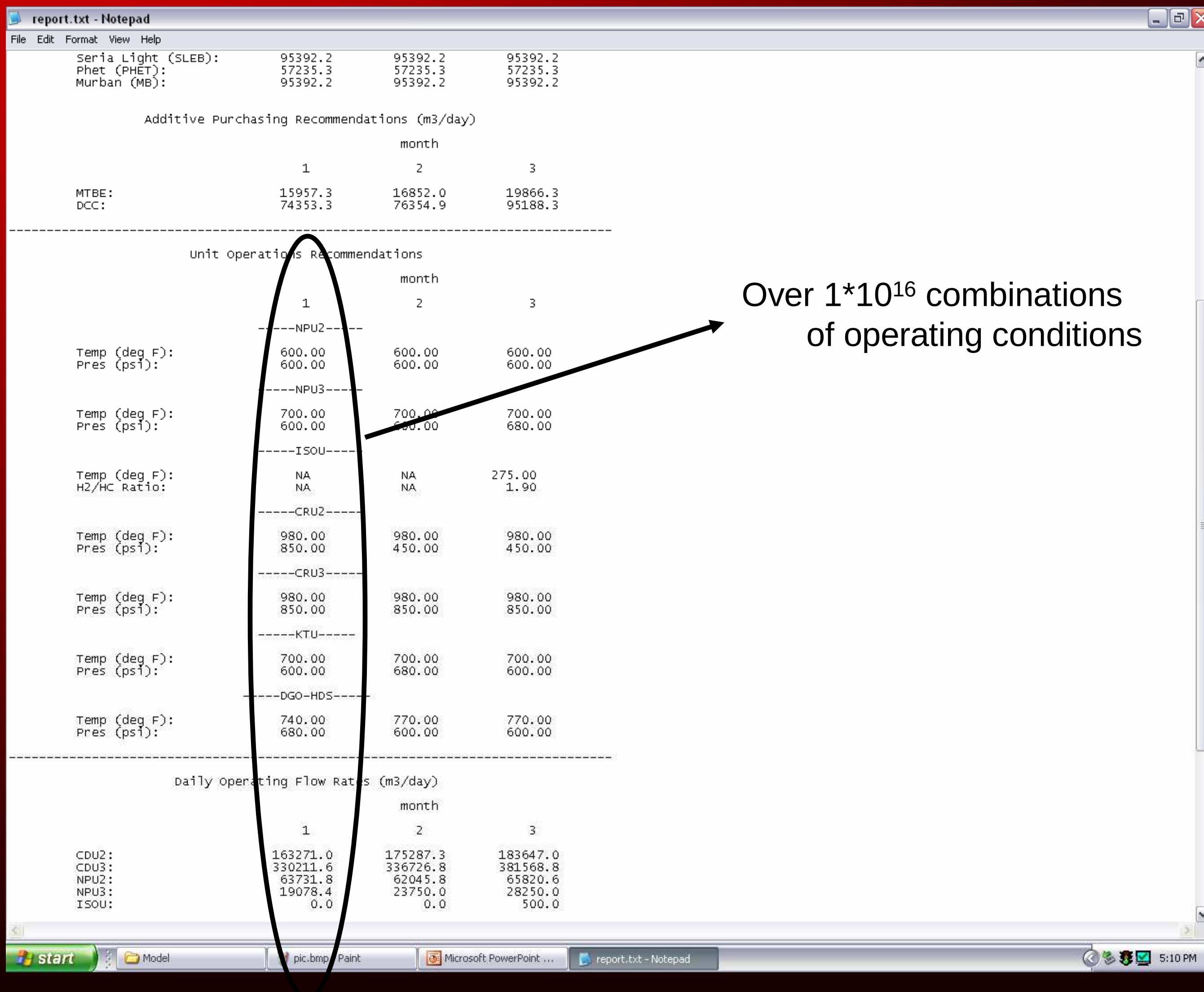
- Executed using CPLEX
  - Approximately 50 minutes to reach integer solution
  - Approximately 2 hours to reach optimal solution

It Works!



gamside: C:\Documents and Settings\hill6590\My Documents\gamsdir\projdir\gmsproj.gpr
File Edit Search Windows Utilities Help
H:\Refinery Planning\Model\GAMS\Bangchak_UnitOps.ii.gms
Bangchak_UnitOps.ii.gms
*** Capacity constraint ***
af.lo(u,t)$cap(u) = ucon(u,t,'lower') ;
af.up(u,t)$cap(u) = ucon(u,t,'upper') ;
ac.lo(o,t) = on(o) ;
ac.up(o,t) = ox(o) ;
Fuel Balance
Variable Qa(t), ocost(t) ;
Equation Q1(t),Q2(t), ework(t) ;
Parameter btum3(p) heat of combustion ;
btum3('FG') = 54*947.8*19*35.3/2.205 ;
btum3('FOVS') = 142000*264.2 ;
Hydrogen Balance
Equation Q3 ;
option solprint = off;
option limcol = 0;
option limrow = 0;
option optcr = 0.00;
Model refinery /all/ ;
refinery.iterlim = 100000 ;
1 active process
bangchak_unitops.ii
Elapsed time = 3033.58 sec. (tree size = 625.39 MB).
Nodefile size = 497.97 MB (44.40 MB after compression)
Elapsed time = 3069.39 sec. (tree size = 635.82 MB).
* 61200+61016 0 3.21055e+007 3.59494e+007 313026 11.97%
* 61200+61016 0 3.22832e+007 3.59494e+007 313026 11.36%
61300 61116 3.57102e+007 18 3.26725e+007 3.59494e+007 313374 10.03%
61400 61216 3.57057e+007 16 3.26725e+007 3.59494e+007 313576 10.03%
61500 61316 3.59134e+007 23 3.29032e+007 3.59494e+007 314345 9.26%
83200 82936 3.58783e+007 21 3.40448e+007 3.59488e+007 455346 5.59%
Interrupt
Stop
Summary only
Update
1053: 36
Insert
start
GAMS
gamside
2:50 AM

Results


report.txt - Notepad

File Edit Format View Help

Seria Light (SLEB):	95392.2	95392.2	95392.2
Phet (PHET):	57235.3	57235.3	57235.3
Murban (MB):	95392.2	95392.2	95392.2

Additive Purchasing Recommendations (m3/day)

	month		
	1	2	3
MTBE:	15957.3	16852.0	19866.3
DCC:	74353.3	76354.9	95188.3

Unit Operations Recommendations

	month		
	1	2	3
----NPU2----			
Temp (deg F):	600.00	600.00	600.00
Pres (psi):	600.00	600.00	600.00
----NPU3----			
Temp (deg F):	700.00	700.00	700.00
Pres (psi):	600.00	[illegible]	680.00
-----ISOU----			
Temp (deg F):	NA	NA	275.00
H2/HC Ratio:	NA	NA	1.90
-----CRU2-----			
Temp (deg F):	980.00	980.00	980.00
Pres (psi):	850.00	450.00	450.00
-----CRU3-----			
Temp (deg F):	980.00	980.00	980.00
Pres (psi):	850.00	850.00	850.00
-----KTU-----			
Temp (deg F):	700.00	700.00	700.00
Pres (psi):	600.00	680.00	600.00
-----DGO-HDS-----			
Temp (deg F):	740.00	770.00	770.00
Pres (psi):	680.00	600.00	600.00

Daily Operating Flow Rates (m3/day)

	month		
	1	2	3
CDU2:	163271.0	175287.3	183647.0
CDU3:	330211.6	336726.8	381568.8
NPU2:	63731.8	62045.8	65820.6
NPU3:	19078.4	23750.0	28250.0
ISOU:	0.0	0.0	500.0

Over $1*10^{16}$ combinations of operating conditions

Planning

- Currently planning is optimized and then unit operations are optimized
- Planning is highly dependent on unit operations
  - e.g. turnarounds, unit capacities

Results

- GRM has increased
  - Optimizing unit operations is more efficient

	GRM
Model without Unit Operations	$16,492,336.72
Model with Unit Operations	$34,130,901.06

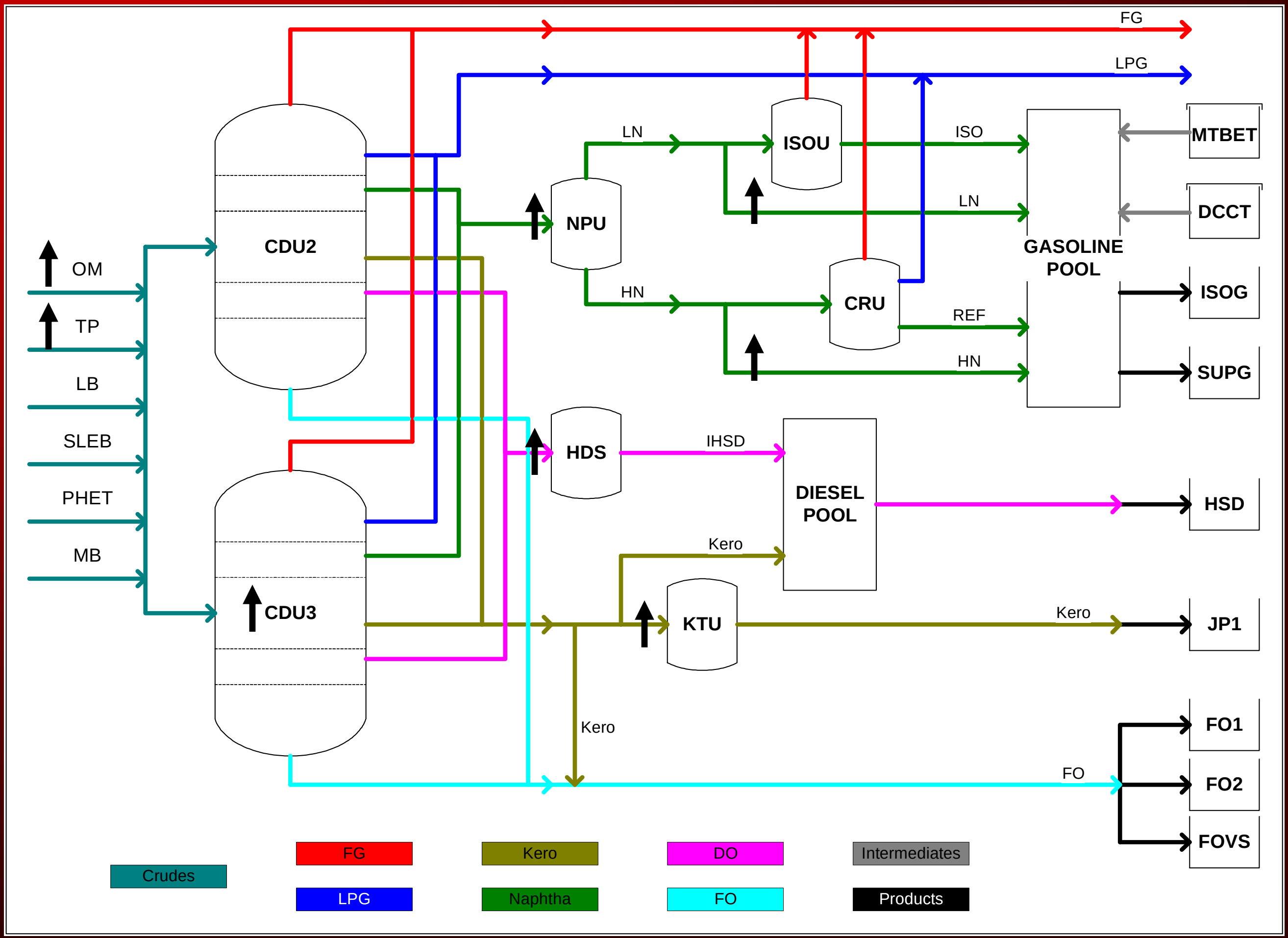
Results

- Purchased crudes and intermediates

Model without Unit Operations			
	1	2	3
Oman (OM):	167734.3	167339.3	165082.6
Tapis (TP):	13427.7	14317	19397.5
Labuan (LB):	0	0	0
Seria Light (SLEB):	95392.2	95392.2	95392.2
Phet (PHET):	57235.3	57235.3	57235.3
Murban (MB):	95392.2	95392.2	95392.2
MTBE:	13662	13700.7	13921.7
DCC:	68088	68301.8	69523.2

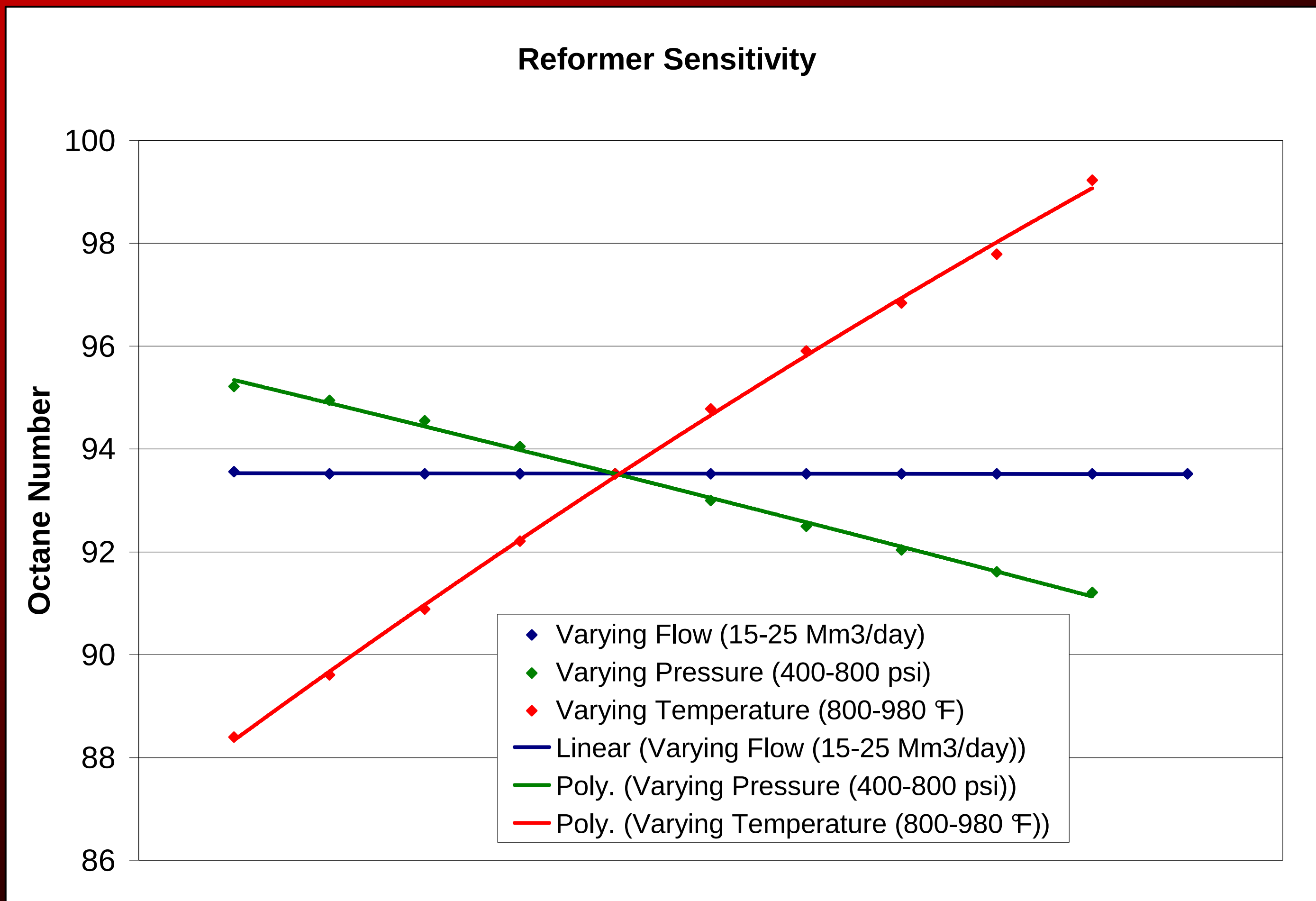
Model with Unit Operations			
	1	2	3
Oman (OM):	244486.2	262303.1	267899.8
Tapis (TP):	32853.3	41126.2	47392.2
Labuan (LB):	0	0	9041.4
Seria Light (SLEB):	95392.2	95392.2	95392.2
Phet (PHET):	57235.3	57235.3	57235.3
Murban (MB):	95392.2	95392.2	95392.2
MTBE:	18266	19392.8	20404.2
DCC:	87059.5	91153.7	93941.2

Results



FG
LPG
CDU2
CDU3
OM
TP
LB
SLEB
PHET
MB
LN
HN
NPU
ISOU
CRU
ISO
LN
REF
HN
GASOLINE POOL
MTBET
DCCT
ISOG
SUPG
HDS
IHSD
DIESEL POOL
Kero
KTU
Kero
HSD
JP1
Kero
FO
FO1
FO2
FOVS
Crudes
FG
LPG
Kero
Naphtha
DO
FO
Intermediates
Products

Discussion



Reformer Sensitivity
Octane Number
100
98
96
94
92
90
88
86
Varying Flow (15-25 Mm3/day)
Varying Pressure (400-800 psi)
Varying Temperature (800-980 °F)
Linear (Varying Flow (15-25 Mm3/day))
Poly. (Varying Pressure (400-800 psi))
Poly. (Varying Temperature (800-980 °F))

Discussion

- Optimizing unit operations adds another dimension to optimize refinery processing

- Can provide more thorough insight for decision making

Acknowledgments

- Dr. Miguel Bagajewicz
- DuyQuang Nguyen
- Mike Mills

- Sunoco Refinery (Tulsa, OK)
  - John Paris

Please, No Questions!

….Just Kidding