



EXAMPLE PURPOSE This example illustrates the simulation of a FCCU main fractionator with ProSimPlus.

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**CORRESPONDING PROSIMPLUS FILE** *PSPS\_EX\_EN-Fractionating-Column.pmp3* 

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## **1. PROCESS MODELING**

## 1.1. Process presentation

The distillation system consists of a main column coupled with a side stripper. This column is a stripping column with a partial condenser and a three-phase flash.

The input data of this problem is available in [SIM83].

## 1.2. <u>Process flowsheet</u>



## 1.3. Compounds

The fractionating column is fed by a hydrocarbon effluent coming from the cracking reactor, two products containing hydrocarbons and lights (gland oil, rich sponge oil), and steam.

The streams "Reactor effluent", "Gland oil" and "Rich sponge oil" are petroleum cuts mixtures defined by distillation curves and lights composition data. The pseudo-compounds are generated using their normal boiling point, molar weight and density (available in [SIM81]) and given below.

Compound	T <sub>b</sub> (°F)	Mw (g/mol)	Density
NBP-325(K)	126	75.95	0.7009
NBP-337(K)	147	81.98	0.70585
NBP-355(K)	179	91.34	0.71433
NBP-373(K)	212	202.27	0.72256
NBP-390(K)	243	111.23	0.73137
NBP-409(K)	276	121.62	0.74029
NBP-426(K)	307	131.49	0.74916
NBP-444(K)	340	139.56	0.77576
NBP-462(K)	372	149.12	0.80681
NBP-479(K)	402	155.84	0.84471
NBP-495(K)	432	162.68	0.88078
NBP-515(K)	468	177.16	0.8936
NBP-533(K)	499	190.45	0.90216
NBP-550(K)	531	203.4	0.92054
NBP-569(K)	564	216.46	0.93825
NBP-586(K)	596	229.09	0.95501
NBP-604(K)	627	240.57	0.98194
NBP-621(K)	659	255.59	0.99173
NBP-638(K)	688	268.61	1.0036
NBP-656(K)	721	285.17	1.01404
NBP-674(K)	754	301.9	1.02194
NBP-692(K)	786	319.42	1.02817
NBP-710(K)	818	337.01	1.03323
NBP-726(K)	848	355	1.03597
NBP-746(K)	883	377.44	1.03642
NBP-775(K)	935	406.2	1.04928
NBP-816(K)	1010	449.13	1.06699
NBP-859(K)	1086	493.56	1.08271
NBP-887(K)	1137	524.42	1.09248

The pseudo-compounds creation service is available in the thermodynamic calculator editor as illustrated below.

CALCULATOR         This window helps you to define the context of your thermodynamic calculator         FILE         Open       COMPOUNDS       MODEL       BINARIES       PARAMETERS         PACKAGE       I       WATER       7732-18-5       COMPOUNDS         Services       I       WATER       772-37-9       COMPOUNDE         Galculate       CABON MONOXIDE       630-08-0       Save as       FILE         Calculate       I       CABON MONOXIDE       630-08-0       Save as       FILE         Calculate       I       CABON MONOXIDE       630-08-0       Save as       File       Save as         Diagrams       Phythish       Permittene       74-82-8       EDT       Package         PROPIEINE       115-07-1       PROPIEINE       115-07-1       Package	-
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16 3-METHYL-1-BUTENE 563-45-1 🔮 Remove all the compounds	
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Comments 23 NBP-409K	
24 NBP-426(K) Temperature dependent pro	perties
25 NBP-444(K)	
Calculator type 26 NBP-462(K)	
Native 27 NBP-479(K)	
Show the expert mode 28 NBP-495(K) (1) Compare the compounds	
29 NBP-515(K)	
30 NBP-533(K) OKDER	
31 NEP-330(N) 32 NEP-300(N)	
32 NBP-586(K) OV Move this compound down	
34 NBP-604(K)	
35 NBP-621(K)	
36 NBP-638(K)	
37 NBP-656(K)	
38 NBP-674(K)	
39 NBP-692(K)	
40 NBP-710(k)	
41 NBP-726(K)	
42 ND-740[N 43 NB-775(K)	
44 NBP356(K)	
45 NBP-859IK)	
46 NBP-887(K)	
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In addition to pseudo-compounds, the compounds of the process are: water,  $H_2S$ ,  $N_2$ , CO,  $CO_2$ ,  $H_2$ , methane, ethylene, ethane, propylene, propane, isobutene, isobutane, n-butane, isopentane, 3-methyl-1-butene, n-pentane.

## 1.4. Thermodynamic model

The studied process deals with mixtures of water and hydrocarbons. Thus, the Peng-Robinson (PR) equation of state with the "Water-Hydrocarbons" option has been chosen. The liquid molar volume calculation uses the "Ideal mixture" model.

## 1.5. Operating conditions

## 1.5.1. Feeds

The feed properties are given in the following table.

	Partial molar flowrates (lbmol/h)		Partial mass flowrates (lb/h)			
	<b>Reactor effluent</b>	Gland Oil	<b>Rich Sponge oil</b>	Steam 2	Steam 3	Steam 6
WATER	571.7455	0.0000	0.0000	1000	1000	2350
HYDROGEN SULFIDE	119.1349	0.0000	11.3847	0	0	0
NITROGEN	71.7524	0.0000	1.4636	0	0	0
CARBON MONOXIDE	6.0690	0.0000	0.0000	0	0	0
CARBON DIOXIDE	13.6333	0.0000	0.0000	0	0	0
HYDROGEN	292.6588	0.0000	0.4961	0	0	0
METHANE	257.4331	0.0000	4.5504	0	0	0
ETHYLENE	42.0617	0.0000	2.2814	0	0	0
ETHANE	77.3196	0.0000	17.8257	0	0	0
PROPYLENE	312.5401	0.0000	10.3375	0	0	0
PROPANE	140.0775	0.0000	7.6878	0	0	0
ISOBUTENE	351.9283	0.0000	12.0307	0	0	0
ISOBUTANE	125.4043	0.0000	4.4733	0	0	0
n-BUTANE	47.1750	0.0000	3.0109	0	0	0
ISOPENTANE	178.5146	0.0000	12.5574	0	0	0
3-METHYL-1-BUTENE	226.4206	0.0000	9.9953	0	0	0
n-PENTANE	30.9767	0.0000	2.7720	0	0	0
NBP-325(K)	75.1235	0.0000	0.0000	0	0	0
NBP-337(K)	194.3412	0.0000	0.0000	0	0	0
NBP-355(K)	173.5292	0.0000	0.0000	0	0	0
NBP-373(K)	146.1561	0.0000	0.0000	0	0	0
NBP-390(K)	137.3204	0.0000	0.0000	0	0	0
NBP-409(K)	116.2538	0.0000	0.0000	0	0	0
NBP-426(K)	109.4752	0.0000	0.0000	0	0	0
NBP-444(K)	106.5823	0.5961	5.8067	0	0	0
NBP-462(K)	108.2828	1.0388	10.1191	0	0	0
NBP-479(K)	124.8481	1.3964	13.6025	0	0	0
NBP-495(K)	71.3718	2.7966	27.2421	0	0	0
NBP-515(K)	53.5058	4.6527	45.3226	0	0	0
NBP-533(K)	59.2491	4.9738	48.4505	0	0	0
NBP-550(K)	61.0015	4.1917	40.8319	0	0	0
NBP-569(K)	63.8801	3.5796	34.8694	0	0	0
NBP-586(K)	79.0126	3.4629	33.7326	0	0	0
NBP-604(K)	165.7175	3.0199	29.4173	0	0	0
NBP-621(K)	167.1575	2.0422	19.8933	0	0	0
NBP-638(K)	129.4807	0.3775	3.6773	0	0	0
NBP-656(K)	60.4776	0.0000	0.0000	0	0	0
NBP-674(K)	35.9724	0.0000	0.0000	0	0	0
NBP-692(K)	22.9229	0.0000	0.0000	0	0	0
NBP-710(K)	15.8420	0.0000	0.0000	0	0	0
NBP-726(K)	8.1898	0.0000	0.0000	0	0	0
NBP-746(K)	2.1190	0.0000	0.0000	0	0	0
NBP-775(K)	3.9871	0.0000	0.0000	0	0	0
NBP-816(K)	2.8048	0.0000	0.0000	0	0	0
NBP-859(K)	2.0608	0.0000	0.0000	0	0	0
NBP-887(K)	0.5742	0.0000	0.0000	0	0	0
Temperature (°F)	927.939	200.000	118.710	314.946	312.160	312.160
Pressure (psig)	15.000	13.846	205.000	15.000	13.462	13.000

### 1.5.2. Main column

#### 1.5.2.1.Parameters

- Characteristics:
  - Stripper with partial condenser
  - Number of theoretical stages: 15
  - o Operating mode specifications: condenser duty to be withdraw
  - o Condenser duty to be withdraw: 0 Btu/h
  - Liquid distillate flowrate: 0 lbmol/h
  - Pressure profile: 10 psig at the condenser, 10 psig at stage 2 and 15 psig at the bottom
- Feeds:
  - Stream 1 at stage 14 (Reactor effluent)
  - Stream 4 at stage 12 (Gland oil)
  - Stream 3 at stage 11 (Steam 3)
  - Stream 5 at stage 7 (Rich sponge oil)
  - Stream 11 at stage 7 (Side stripper head stream)
- Sidestreams:
  - Stream 12 at stage 8 (Side stripper feed stream)
  - Stream 14 at stage 9 (Sponge oil)
  - Stream 15 at stage 11 (Heavy cycle)
- Pumparound 1:
  - From stage 4 to stage 2 (liquid phase)
  - Flowrate calculated for a duty of -1 MBtu/h
  - Temperature difference: -100 °F
- Pumparound 2:
  - From stage 11 to stage 10 (liquid phase)
  - Flowrate calculated for a duty of -10 MBtu/h
  - Temperature difference: -100 °F

- Pumparound 3:
  - From stage 15 to stage 13 (liquid phase)
  - Flowrate calculated for a duty of -10 MBtu/h
  - Temperature difference: -75 °F

#### 1.5.2.2.Objectives

- Flowrate (volume standard liquid) at stage 12: 150 bbl/h

Adjusted variable: duty at pumparound 1

- Flowrate (volume standard liquid) of the liquid sidestream 14: 215 bbl/h
   Adjusted variable: sidestream flowrate 14
- Flowrate (volume standard liquid) of the liquid sidestream 15: 433.33 bbl/h
   Adjusted variable: sidestream flowrate 15
- Bottom liquid product flowrate: 46.83 bbl/h (volume standard liquid)

Adjusted variable: duty at pumparound 3

#### 1.5.2.3. Initialization

- Liquid sidestream flowrate at stage 8: 400 lbmol/h (this flowrate is adjusted by a specification on the side stripper)
- Liquid sidestream flowrate at stage 9: 300 lbmol/h (this flowrate is adjusted by a specification)
- Liquid sidestream flowrate at stage 11: 500 lbmol/h (this flowrate is adjusted by a specification)
- Pumparound 1 reboiler duty: -1 MBtu/h (cooling)
- Pumparounds 2 and 3 reboiler duty: -10 MBtu/h (cooling)

### 1.5.3. Side-stripper

### 1.5.3.1.Parameters

- Characteristics:
  - o Absorber
  - Number of theoretical stages: 2
  - Pressure: 13 psig

#### 1.5.3.2.Objectives

- Bottom liquid product flowrate: 230 bbl/h in volume standard liquid

Adjusted variable: feed flowrate (Stream 12)

#### 1.5.4. General 3-phase flash

#### 1.5.4.1.Parameters

- Characteristics:
  - Temperature: 100 °F
  - Pressure: 5 psig

#### 1.5.5. Numerical parameters

The default numerical parameters are used for all the unit operations expected for the main column: the maximum damping factor has been set to 0.3 and the maximum number of iterations to 100.

## 2. RESULTS

## 2.1. Mass and energy balances

This document only presents the most relevant stream results. In ProSimPlus, mass and energy balances are provided for every stream. Results are also available at the unit operation level (result tab in the configuration window).

#### Inlet streams:

Streams		1	2	3	4	5	6
From		Reactor effluent	Steam 2	Steam 3	Gland oil	Rich sponge oil	Steam 6
То		Main column	Main column	Main column	Main column	Main column	Side Stripper
Total flow	lbmol/h	5162.1	55.5	55.5	32.1	413.8	130.4
Mole fractions							
WATER		0.11076	1	1	0	0	1
HYDROGEN SULFIDE		0.02308	0	0	0	0.02751	0
NITROGEN		0.01390	0	0	0	0.00354	0
CARBON MONOXIDE		0.00118	0	0	0	0.00000	0
CARBON DIOXIDE		0.00264	0	0	0	0.00000	0
HYDROGEN		0.05669	0	0	0	0.00120	0
METHANE		0.04987	0	0	0	0.01100	0
ETHYLENE		0.00815	0	0	0	0.00551	0
ETHANE		0.01498	0	0	0	0.04307	0
PROPYLENE		0.06055	0	0	0	0.02498	0
PROPANE		0.02714	0	0	0	0.01858	0
ISOBUTENE		0.06818	0	0	0	0.02907	0
ISOBUTANE		0.02429	0	0	0	0.01081	0
n-BUTANE		0.00914	0	0	0	0.00728	0
ISOPENTANE		0.03458	0	0	0	0.03034	0
3-METHYL-1-BUTENE		0.04386	0	0	0	0.02415	0
n-PENTANE		0.00600	0	0	0	0.00670	0
NBP-325(K)		0.01455	0	0	0	0	0
NBP-337(K)		0.03765	0	0	0	0	0
NBP-355(K)		0.03362	0	0	0	0	0
NBP-373(K)		0.02831	0	0	0	0	0
NBP-390(K)		0.02660	0	0	0	0	0
NBP-409(K)		0.02252	0	0	0	0	0
NBP-426(K)		0.02121	0	0	0	0	0
NBP-444(K)		0.02065	0	0	0.01855	0.01403	0
NBP-462(K)		0.02098	0	0	0.03233	0.02445	0
NBP-479(K)		0.02419	0	0	0.04346	0.03287	0
NBP-495(K)		0.01383	0	0	0.08705	0.06583	0
NBP-515(K)		0.01037	0	0	0.14482	0.10952	0
NBP-533(K)		0.01148	0	0	0.15481	0.11708	0
NBP-550(K)		0.01182	0	0	0.13047	0.09867	0
NBP-569(K)		0.01237	0	0	0.11142	0.08426	0
NBP-586(K)		0.01531	0	0	0.10778	0.08151	0
NBP-604(K)		0.03210	0	0	0.09400	0.07109	0
NBP-621(K)		0.03238	0	0	0.06356	0.04807	0
NBP-638(K)		0.02508	0	0	0.01175	0.00889	0
NBP-656(K)		0.01172	0	0	0	0	0
NBP-674(K)		0.00697	0	0	0	0	0
NBP-692(K)		0.00444	0	0	0	0	0
NBP-710(K)		0.00307	0	0	0	0	0
NBP-726(K)		0.00159	0	0	0	0	0
NBP-746(K)		0.00041	0	0	0	0	0
NBP-775(K)		0.00077	0	0	0	0	0
NBP-816(K)		0.00054	0	0	0	0	0
NBP-859(K)		0.00040	0	0	0	0	0
NBP-887(K)		0.00011	0	0	0	0	0
Physical state		Vapor	Vapor	Vapor	Liquid	Liquid	Vapor
Temperature	°F	927.9	314.9	312.2	200.0	118.7	312.2
Pressure	psig	15.0	15.0	13.5	13.8	205.0	13.0
Molar weight	g/mol	98.7	18.0	18.0	200.8	163.5	18.0

#### Outlet streams:

Streams		8	9	10	13	14	15	16
From		Flash	Flash	Flash	Side Stripper	Main column	Main column	Main column
То		Water	Wet gas	Unstabilized gasoline	Light cycle oil	Sponge oil plus gland oil	Heavy cycle oil	Decant plus slurry
Total flow	lbmol/h	690.3	2404.5	1397.4	380.4	330.1	593.5	53.2
Mole fractions								
WATER		1	0.04827	0.00128	0.00962	0.00126	0.00128	0.00380
HYDROGEN SULFIDE		0	0.05239	0.00310	3E-07	0.00024	0.00022	0.00008
NITROGEN		0	0.03039	0.00007	1E-09	0.00003	0.00003	0.00001
CARBON MONOXIDE		0	0.00252	0.00001	1E-10	0.00000	0.00000	0.00000
CARBON DIOXIDE		0	0.00558	0.00014	6E-09	0.00002	0.00002	0.00000
HYDROGEN		0	0.12177	0.00017	4E-09	0.00012	0.00014	0.00003
METHANE		0	0.10845	0.00074	2E-08	0.00019	0.00020	0.00005
ETHYLENE		0	0.01816	0.00044	2E-08	0.00005	0.00005	0.00002
ETHANE		0	0.03872	0.00138	8E-08	0.00012	0.00011	0.00003
PROPYLENE		0	0.12642	0.01305	1E-06	0.00075	0.00066	0.00024
PROPANE		0	0.05735	0.00684	7E-07	0.00035	0.00031	0.00011
ISOBUTENE		0	0.12673	0.04158	0.00001	0.00135	0.00113	0.00046
ISOBUTANE		0	0.04629	0.01302	0.00000	0.00045	0.00038	0.00015
n-BUTANE		0	0.01690	0.00671	0.00000	0.00020	0.00016	0.00007
ISOPENTANE		0	0.05097	0.04839	0.00002	0.00107	0.00085	0.00038
3-METHYL-1-BUTENE		0	0.06815	0.05117	0.00002	0.00126	0.00101	0.00045
n-PENTANE		0	0.00819	0.00995	0.00000	0.00020	0.00016	0.00007
NBP-325(K)		0	0.01374	0.02972	0.00002	0.00069	0.00053	0.00026
NBP-337(K)		0	0.02799	0.08970	0.00010	0.00208	0.00155	0.00076
NBP-355(K)		0	0.01601	0.09527	0.00019	0.00237	0.00169	0.00084
NBP-373(K)		0	0.00776	0.08976	0.00035	0.00258	0.00177	0.00089
NBP-390(K)		0	0.00404	0.08948	0.00067	0.00314	0.00205	0.00104
NBP-409(K)		0	0.00172	0.07809	0.00121	0.00354	0.00220	0.00111
NBP-426(K)		0	0.00081	0.07410	0.00230	0.00446	0.00261	0.00132
NBP-444(K)		0	0.00039	0.07561	0.00539	0.00652	0.00351	0.00176
NBP-462(K)		0	0.00019	0.07621	0.01515	0.01098	0.00500	0.00249
NBP-479(K)		0	0.00009	0.07379	0.05928	0.02688	0.00822	0.00400
NBP-495(K)		0	0.00002	0.02616	0.11948	0.04522	0.00720	0.00316
NDP-515(K)		0	6E-07	0.00561	0.17547	0.07827	0.00955	0.00555
		0	4L-08	0.00042	0.17800	0.10421	0.01032	0.00300
NBP-560(K)		0	3E-11	0.00003 2E-06	0.13880	0.11202	0.02030	0.00743
NBP-586(K)		0	JE-11 1E-12	2E-00	0.10032	0.12312	0.07589	0.01142
NBP-604(K)		0	5E-14	2E-08	0.07043	0.16755	0.18966	0.06571
NBP-621(K)		0	0	1E-09	0.03487	0 11351	0 22404	0 10138
NBP-638(K)		0	0	0	0.00926	0.05050	0.18043	0.11759
NBP-656(K)		0	0	0	0.00116	0.01275	0.08609	0.08890
NBP-674(K)		0	0	0	0.00023	0.00416	0.05030	0.08741
NBP-692(K)		0	0	0	0.00005	0.00141	0.02962	0.09134
NBP-710(K)		0	0	0	0.00001	0.00048	0.01732	0.10143
NBP-726(K)		0	0	0	1E-06	0.00011	0.00681	0.07726
NBP-746(K)		0	0	0	7E-08	0.00001	0.00106	0.02794
NBP-775(K)		0	0	0	6E-09	2E-06	0.00064	0.06775
NBP-816(K)		0	0	0	0	5E-08	0.00005	0.05210
NBP-859(K)		0	0	0	0	8E-10	3E-06	0.03867
NBP-887(K)		0	0	0	0	0	2E-07	0.01078
Physical state		Liquid	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	°F	100.0	100.0	100.0	414.2	489.8	563.5	656.1
Pressure	psig	5.0	5.0	5.0	13.0	12.7	13.5	15.0
Molar weight	g/mol	18.0	42.4	116.4	194.0	215.0	251.8	315.1

## 2.2. Process Performances

With ProSimPlus, it is possible to generate the TBP/ASTM curves of material streams. To do so, two ways are available:

- Select the option to plot the TBP/ASTM curves of all the material streams of the process during the next simulation in the tab "Flowsheet" as shown in the following figure:

File Edit Configuration	Flowsheet Tools Simulation Windows Help	
	Add an Equipment	E 📓 🗖 🔾 🖛 T 123
J 🔨 🛏 🛶 🖓 🛛 2	Connect	
Library Tree view Properti	Reconnect streams	[ 🔁 🔕 < > View name: Ma
🌣 Feed / Outlet	TBP/ASTM curves	Select all the material streams
× Absorbers	Update stream links	Deselect all the material streams
× 2-phase distillation	Clear all stream links	
🗧 Strippers	Initialize tear streams with the last simulation results	
	Hide the information streams	
🔆 3-phase distillation	Number streams automatically	
Liquid-liquid extraction	Update flowsheet tags value	

- Tick the "Calculate the TBP/ASTM curves for this stream" box in the configuration window of the material stream which TBP/ASTM curves have to be plotted during the next simulation as illustrated below:

Copy     Paste      Initialized stream      Iowrates and fractions     Temperature and Pressure      Flowrate specification     Partial mass flowrates									
Copy     Paste Initialized stream Iowrates and fractions Flowrate specification Partial mass flowrates									
Initialized stream       lowrates and fractions       Temperature and Pressure       Flowrate specification       Partial mass flowrates									
Interpretation         Temperature and Pressure           Flowrate specification         Partial mass flowrates	Initialized stream								
Flowrate specification Partial mass flowrates	Flowrates and fractions Temperature and Pressure								
Partial mass lowraids	Eleverate encoification								
Partial mass flowrates									
Unit Ib/h 👻									
# Components Mass flow rates									
1 WATER 0									
2 PROPANE 0									
3 ISOBUTANE 0									
4 n-BUTANE 0									
5 NBP-276(K) 0									
6 NBP-304(K) 0									
7 NBP-318(K) 0									
8 NBP-333(K) 0	*								
Humidity Not specified	-								

To reach this option the "Initialized stream" box has to be ticked and then unticked once the "Calculate the TBP/ASTM curves for this stream" box has been ticked.

The following figure shows on a same graph the TBP at 760 mmHg curve of the mixture of the feeds (excepted the water vapor streams) entering the main column and the ones of the obtained cuts:



## 2.3. Column profiles

Profiles can be accessed after the simulation in each column configuration window, in the "Profiles" tab. Double clicking on the profile will generate the corresponding graph. It is important to note that, in ProSimPlus, the first stage corresponds to the top stage and the last stage to the bottom stage (respectively the condenser and the reboiler in the case of a distillation column).

Stripper (\$COLD)								
Name: Main column								
Desc:								
Identification Parameters Scripts Report Streams Profiles Notes Advanced parameters								
name Description								
Main column - Temperature profile Temperature profile in the column								
Main column - Pressure profile Pressure profile in the column								
Main column - Liquid mole-fractions Liquid mole-fractions profile in the column								
Main column - Vapor mole-fractions Vapor mole-fractions profile in the column								
Main column - Liquid mass-fractions Liquid mass-fractions profile in the column								
Main column - Vapor mass-fractions Vapor mass-fractions profile in the column								
Main column - Enthalpies Enthalpies profile in the column								
Main column - Molar flowrates Molar flowrates profile in the column								
Main column - Mass flowrates Mass flowrates profile in the column								
Main column - Volume flowrates Volume flowrates profile in the column								
Plot Values								
ок	Cancel							

#### Main column:







Side stripper:





## REFERENCES

- [SIM83] Simulation Sciences Inc., SimSci Manual, Revision 1 (1983)
- [SIM81] Simulation Sciences Inc., Troubleshooting the FCCU main fractionators on the timesharing terminal, SimSci Process Technical Bulletin #23 (1981)