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APPENDIX 1 CALCULATION AND ANALYTICAL PROCEDURES

The data collected while evaluating the performance of the catalyst was manipulated using a variety of procedures. The various definitions of the parameters used are given below, as are the details of the analytical procedures used to collect the necessary data. A detailed sample calculation is given in Appendix 2 while details of the procedures used and the results obtained while developing the kinetic model are given in Chapters 5 and 6 and Appendices 3 to 5.

A1.1 SYSTEM PRESSURE

The pressure drop across the reactor was negligible during normal operation. Never the less, both the reactor inlet and outlet pressures were measured. All pressures reported in this work were calculated from the average of these values, and expressed in kPa(a). The ambient pressure was considered constant and equal to 85 kPa.

A1.2 SYSTEM TEMPERATURE

The reaction and regeneration temperatures profiles in the pilot plant reactor were determined using six fixed thermocouples in the centre of the catalyst bed, while in the bench scale reactor the temperature profile was determined using a mobile thermocouple. In both cases compensation for the ambient temperature was done by the electronics of the temperature recorders. In all other cases the ambient temperature was considered constant and equal to 25°C.

A1.3 FLOW RATES

During the course of an experiment the mass of liquid and gaseous material entering and leaving the reactor system were recorded at regular time intervals. In the case of the water entering the system the volume change in a graduated feed pot was recorded and the mass flow rate calculated using

$$F_{W_{t_n,t_{n+1}}} = \frac{\left(V_{C_{t_n}} - V_{C_{t_{n+1}}}\right) \cdot D_W}{t_{n+1} - t_n} \qquad \text{A1-1}$$

where

$F_{W\,tn,tn+1}$ is the average water flow rate over the time interval, g·hr^{-1},
$V_{c\,tn}$ is the feed cylinder volume at the start of the time interval, ml,
$V_{C\,tn+1}$ is the feed cylinder volume at the end of the time interval, ml,
t_n is the time at the start of the interval, hr,
t_{n+1} is the time at the end of the interval, hr and
D_W is the density of the water which was fixed at 1 g·ml^{-1} in this study.

Using, where applicable the same notation as above, the mass flow rate of hydrocarbons entering the system was calculated using

$$F_{H_{t_n,t_{n+1}}} = \frac{M_{C_{t_n}} - M_{C_{t_{n+1}}}}{t_{n+1} - t_n} \qquad \text{A1-2}$$

where

$F_{H\,tn,tn+1}$ is the average hydrocarbon flow rate over the time interval, g·hr^{-1},
$M_{C\,tn}$ is the mass of the feed cylinder at the start of the interval, g and
$M_{C\,tn+1}$ is the mass of the feed cylinder at the end of the interval, g.

The mass flow rates of the products leaving the reactor were also calculated. In the case of the liquid products these were collected, weighed and the flow rate calculated using

$$F_{L_{t_n,t_{n+1}}} = \frac{M_{L_{t_n,t_{n+1}}}}{t_{n+1} - t_n} \qquad \text{A1-3}$$

where

$F_{L\ tn,tn+1}$ is the average flow rate of liquid products over the time interval, g·hr^{-1} and
$M_{L\ tn,tn+1}$ is the total mass of liquid collected over the time interval, g.

and in the case of the gaseous products the volume produced at ambient conditions was measured, using a wet gas flowmeter (WGFM), and using the ideal gas law the flow rate calculated with

$$F_{G_{t_n,t_{n+1}}} = \frac{\left(V_{t_{n+1}} - V_{t_n}\right) \cdot p \cdot Mo_{OUT}}{Z \cdot R \cdot T} \qquad \text{A1-4}$$

where

$F_{G\ tn,tn+1}$ is the average flow rate of gaseous products over the time interval, g·hr^{-1},
p is the ambient pressure, $p = 85$ kPa,
V_{tn} is the WGFM reading at the start of the time interval, l,
V_{tn+1} is the WGFM reading at the end of the time interval, l,
R is the universal gas constant, $R = 8.314$ kPa·l·K^{-1}·mol^{-1},
T is the ambient temperature, $T = 298$ K,
Mo_{out} is the average molar·mass of the product gas, g·mol^{-1} and
z is the compressibility factor, -.

Using gas chromatography the composition of the gaseous products was determined and the average molar mass calculated using

$$Mo_X = \sum Mo_{i,X} \cdot WF_{i,X} \qquad \text{A1-5}$$

where

$Mo_{i,x}$ is the molar mass of component i, g·gmol^{-1} and

$WF_{i,x}$ is the mass fraction of component i in the gas, -, with X=OUT for the gaseous products and X=IN for the hydrocarbon feed.

The average molecular mass calculated using the procedure given above was found for both the feed stream and gaseous product stream to be approximately 56 g·gmol^{-1} and was thus fixed at this value throughout the study. The compressibility factor was calculated using the generalized compressibility factor correlation of Pitzer as outlined by Smith and van Ness (1981:89) and found to be on average equal to 1 ± 0.02. It was therefore assumed to be equal to 1 in this study.

As the flow rates calculated in the manner outlined above represent the average flow rate over the time interval they may be considered to approximate the flow rate at the mid point of the time interval over which they were measured. This corresponding mid point time was calculated using

$$t_{n,n+1} = \frac{t_n + t_{n+1}}{2} \qquad \text{A1-6}$$

where

t_n is the time at the start of the time interval, hr,

t_{n+1} is the time at the end of the time interval, hr and

$t_{n,n+1}$ is the mid point of the time interval, hr.

In an attempt to eliminate the 'noise' inherent to a system of this nature, a two point moving average smoothing technique was used. This entails calculating the average of two successive flow rates in each case using

$$F_{X_{t_{n-1},t_n;t_n,t_{n+1}}} = \frac{F_{X_{t_{n-1},t_n}} + F_{X_{t_n,t_{n+1}}}}{2} \qquad \text{A1-7}$$

where

F_X is the average of two successive flow rates, g/hr with X equal to W, H, L or G depending on which stream is being examined.

The mid point of the time interval for which the average flow rate was calculated was in turn determined using

$$t_{n-1;n+1} = \frac{t_{n-1} + 2 \cdot t_n + t_{n+1}}{4} \qquad \text{A1-8}$$

which if the time interval between samples is held constant reduces to

$$t_{n-1;n+1} = t_n \qquad \text{A1-9}$$

Hence, in all subsequent calculations or when plotting flow rates vs time the average value of two successive flow rates ($F_{X\,tn-1,tn;tn,tn+1}$) was used together with the average time (t_n). For the sake of simplicity the time subscript of the parameters will not be shown while developing and discussing the remaining equations.

A1.4 MASS BALANCE

The average mass balance was calculated using the total mass of the feeds used, and products collected, over the entire on-line period with

$$MB = \frac{\left(\sum F_L + \sum F_G\right) \cdot 100}{\sum F_W + \sum F_H} \qquad \text{A1-10}$$

where

MB	is the average mass balance, mass %,
ΣF_L	is the total mass of liquid collected during the on-line period, g,
ΣF_G	is the total mass of gas produced during the on-line period, g,
ΣF_W	is the total mass of water used during the on-line period, g and
ΣF_H	is the total mass of hydrocarbons used during the on-line period, g.

Deviations in the mass balance from 100 % may be attributed to either errors in the flow readings, calibration of the WGFM or scale, or to actual losses. In the latter case two alternative exists. Either, the material was lost before the reactor, in which case the mass of material passing over the catalyst bed was equal to the mass of material leaving the reactor, or the material was lost after the reactor in which case the mass of feed passing over the catalyst was equal to the mass of material entering the reactor. The calculated liquid hourly space velocity of the hydrocarbons, the water to hydrocarbon ratio and the residence time would depend on where the mass loss occurred. In this study both values were calculated but only the average values reported. In all cases however, the results obtained were only included if the mass balance was 100 ± 5 %.

A1.5 LIQUID HOURLY SPACE VELOCITY (LHSV)

If the mass loss was assumed to have occurred after the reactor the average LHSV was calculated using

$$LHSV_{After} = \frac{\sum F_H \cdot \rho_C}{HR \cdot \rho_H \cdot W_C} \qquad \text{A1-11}$$

where

$LHSV_{After}$	is the LHSV of the hydrocarbons assuming that all mass loss occurred after the reactor, hr^{-1},
HR	is the total time on-line, hr,
ρ_C	is the bulk density of the catalyst, $g \cdot ml^{-1}$,
ρ_C	is 0.85 g/ml for Catalyst A and 0.65 $g \cdot ml^{-1}$ for Catalyst B,
ρ_H	is the liquid density of the butenes at 25°C of 0.59 $g \cdot ml^{-1}$ and
W_C	is the mass of catalyst, g.

If the mass loss was assumed to have occurred before the reactor and ignoring the small quantity of oil formed as a by-product, the average LHSV of the hydrocarbons was calculated using

$$LHSV_{Before} = \frac{\sum F_G \cdot \rho_C}{HR \cdot \rho_H \cdot W_C} \qquad \text{A1-12}$$

where

$LHSV_{Before}$	is the LHSV of the hydrocarbons assuming that all mass loss occurred before the reactor, hr^{-1}.

In all cases when LHSV are quoted they represent the average of these two values calculated using

$$\mathrm{LHSV} = \frac{\mathrm{LHSV}_{\mathrm{After}} + \mathrm{LHSV}_{\mathrm{Before}}}{2} \qquad \text{A1-13}$$

where

LHSV is the average liquid hourly space velocity of the hydrocarbons, hr^{-1}.

A1.6 WEIGHT HOURLY SPACE VELOCITY (WHSV)

If the mass loss was assumed to have occurred after the reactor the average butene WHSV was calculated using

$$\mathrm{WHSV}_{\mathrm{After}} = \frac{\mathrm{WF}_{C''_{4,IN}} \cdot \sum F_H}{W_C \cdot \mathrm{HR}} \qquad \text{A1-14}$$

where

$\mathrm{WHSV}_{\mathrm{After}}$ is the WHSV of the butenes assuming that all mass loss occurred after the reactor, hr^{-1} and

$\mathrm{WF}_{C4'',IN}$ is the mass fraction of the four isomers of butene in the feed, -.

If the mass loss was assumed to have occurred before the reactor and ignoring the small quantity of oil formed as a by-product, the average WHSV of the butenes was calculated using

$$WHSV_{Before} = \frac{WF_{C_{4,OUT}^{=}} \cdot \sum F_G}{W_C \cdot HR} \qquad \text{A1-15}$$

where

$WHSV_{Before}$ is the WHSV of the butenes assuming that all mass loss occurred before the reactor, hr^{-1} and

$WF_{C4'',OUT}$ is the mass fraction of the four isomers of butene in the product, -.

In all cases when WHSV are quoted they represent the average of the two values calculated using

$$WHSV = \frac{WHSV_{After} + WHSV_{Before}}{2} \qquad \text{A1-16}$$

where

WHSV is the average weight hourly space velocity of the butenes, hr^{-1}.

A1.7 RESIDENCE TIME (RT)

If the mass loss was assumed to have occurred after the reactor the average residence time was calculated using

$$RT_{After} = \frac{W_C \cdot p_R \cdot 3600}{\left(\frac{\sum F_L}{Mo_W} + \frac{\sum F_G}{Mo_{H,IN}} \right) \cdot R \cdot T_R \cdot \rho_C} \qquad \text{A1-17}$$

where

RT_{After}	is the RT of the reactants assuming that all mass loss occurred after the reactor, s,
p_R	is the reactor pressure, kPa(a),
3600	is a conversion factor from hr to s,
$Mo_{H,IN}$	is the average molar mass of the hydrocarbon feed, $Mo_{H,IN} = 56$ g·g mol^{-1},
Mo_W	is the molar mass of water, $Mo_W = 18$ g·g mol^{-1},
T_R	is the reactor temperature, K and
R	is the universal gas constant, R = 8314 kPa·cm^3·mol^{-1}·K^{-1}.

If the mass loss was assumed to have occurred before the reactor and ignoring the small quantity of oil formed as a by-product, the average RT of the reactants was calculated using

$$RT_{Before} = \frac{W_C \cdot p_R \cdot 3600}{\left(\frac{\sum F_L}{Mo_W} + \frac{\sum F_G}{Mo_{H,OUT}}\right) \cdot R \cdot T_R \cdot \rho_C} \qquad \text{A1-18}$$

where

RT_{Before}	is the RT of the reactants assuming that all mass loss occurred before the reactor, s and
$Mo_{H,OUT}$	is the average molar mass of the hydrocarbon feed, $Mo_{H,OUT} = 56$ g·gmol^{-1}.

In all cases when RT are quoted they represent the average of the two values calculated using

$$RT = \frac{RT_{After} + RT_{Before}}{2} \qquad \text{A1-19}$$

where

RT	is the average residence time of the reactants, s.

A1.8 WATER TO HYDROCARBON RATIO (W/H)

If the mass loss was assumed to have occurred after the reactor the average W/H ratio was calculated using

$$W/H_{After} = \frac{\sum F_W \cdot Mo_{H,IN}}{\sum F_H \cdot Mo_W} \qquad \text{A1-20}$$

where

W/H_{After} is the water to hydrocarbon ratio assuming that all mass was lost after the reactor, molar,

$Mo_{H,IN}$ is the average molar mass of the hydrocarbon feed, 56 $g{\cdot}gmol^{-1}$ and

Mo_W is the molar mass of water, 18 $g{\cdot}gmol^{-1}$.

If the mass loss was assumed to have occurred before the reactor and ignoring the small quantity of oil formed the average W/H ratio was calculated using

$$W/H_{Before} = \frac{\sum F_W \cdot Mo_{H,OUT}}{\sum F_G \cdot Mo_W} \qquad \text{A1-21}$$

where

W/H_{Before} is the water to hydrocarbon ratio assuming that all mass was lost before the reactor, molar and

$Mo_{H,OUT}$ is the average molar mass of the gaseous products, $Mo_{H,OUT} = 56\ g{\cdot}gmol^{-1}$.

In all cases when W/H ratios are quoted it is the average of the two values calculated using

$$W/H = \frac{W/H_{After} + W/H_{Before}}{2} \qquad \text{A1-22}$$

where

W/H is the average water to hydrocarbon ratio, molar.

A1.9 WATER TO BUTENE MOLE PERCENT (Mp)

If the mass loss occurred after the reactor the Mp was calculated using

$$Mp_{After} = \frac{\sum F_W \cdot Mo_{H,IN} \cdot 100}{\sum F_H \cdot WF_{C^{=}_{4,IN}} \cdot M_W + \sum F_W \cdot Mo_{H,IN}} \qquad \text{A1-23}$$

where

Mp_{After} is the water to butene mole percent assuming that all mass was lost after the reactor, mole percent.

If the mass loss was assumed to have occurred before the reactor and ignoring the small quantity of oil formed the average Mp was calculated using

$$Mp_{Before} = \frac{\sum F_L \cdot Mo_{H,OUT} \cdot 100}{\sum F_G \cdot WF_{C^{=}_{4,OUT}} \cdot M_W + \sum F_L \cdot Mo_{H,OUT}} \qquad \text{A1-24}$$

where

Mp_{Before} is the water to butene mole percent assuming that all mass loss occurred before the reactor, mole percent.

In all cases when Mp is quoted it is the average of the two values calculated using

$$Mp = \frac{Mp_{After} + Mp_{Before}}{2} \qquad \text{A1-25}$$

where

Mp is the average water to butenes, mole percent.

Alternatively the average water to butenes mole percent may be calculated from the water to hydrocarbon ratio (W/H) using

$$Mp = \frac{(W/H) \cdot 100}{(W/H) + WF_{C^{=}_{4,IN}}} \qquad \text{A1-26}$$

A1.10 LOSS OF BUTENES (LB)

The loss of butenes is an expression to calculate the quantity of the feed converted to compounds which cannot be rearranged to isobutene by means of recycling. This includes all compounds lighter and heavier than the butenes and all paraffinic material formed and gives an indication of the extent of by-product formation. The loss of butenes was calculated using

$$LB = \frac{\left(WF_{C^{=}_{4,IN}} - WF_{C^{=}_{4,OUT}}\right) \cdot 100}{WF_{C^{=}_{4,IN}}} \qquad \text{A1-27}$$

where

LB	is the loss of butenes, mass %,
$WF_{C4'',IN}$	is the mass fraction of the four isomers of butene in the feed and
$WF_{C4'',OUT}$	is the mass fraction of the four isomers of butene in the product.

A1.11 TOTAL CONVERSION (CT)

The total conversion expresses the quantity of n-butenes, converted to isobutene, and all gaseous by-products. *Cis*-2- and *trans*-2-butene are not considered to be products in this case while the quantity of oil and carbon formed were neglected . It was further assumed, although not strictly speaking correct, that the isobutene entering the system leaves unaltered, i.e., that it is an inert. The Total Conversion was calculated using

$$CT = \frac{\left[\left(WF_{C_{4,IN}^{=}} - WF_{I-C_{4,IN}^{=}}\right) - \left(WF_{C_{4,OUT}^{=}} - WF_{I-C_{4,OUT}^{=}}\right)\right]\cdot 100}{WF_{C_{4,IN}^{=}} - WF_{I-C_{4,IN}^{=}}} \qquad \text{A1-28}$$

where

CT	is the total conversion of the n-butenes to isobutene and all other by-products, mass %,
$WF_{I-C4'',IN}$	is the mass fraction of isobutene in the feed gas and
$WF_{I-C4'',OUT}$	is the mass fraction of isobutene in the product gas.

A1.12 ISOBUTENE SELECTIVITY (SI)

The isobutene selectivity, determines the percentage of isobutene formed per quantity of n-butenes converted. This and all subsequent selectivities were calculated assuming, as was done in the case of the total conversion, that the isobutene entering the system was an inert. The isobutene selectivity was calculated using

$$SI = \frac{\left(WF_{I-C_{4,OUT}^{=}} - WF_{I-C_{4,IN}^{=}}\right) \cdot 100}{\left(WF_{C_{4,IN}^{=}} - WF_{I-C_{4,IN}^{=}}\right) - \left(WF_{C_{4,OUT}^{=}} - WF_{I-C_{4,OUT}^{=}}\right)} \qquad \text{A1-29}$$

where

SI is the isobutene selectivity, mass %.

A1.13 ISOBUTENE YIELD (YI)

The yield, determined by the product of the selectivity and the total conversion, is the quantity of isobutene formed per unit of n-butenes fed to the system and was calculated using

$$YI = \frac{CT \cdot SI}{100} \qquad \text{A1-30}$$

where

YI is the isobutene yield, mass %.

A1.14 CRACKING SELECTIVITY (SC)

The percentage lights that were formed per quantity of the four isomers of butene converted was calculated using

$$SC = \frac{\left(WF_{<C_{4,OUT}} - WF_{<C_{4,IN}}\right) \cdot 100}{\left(WF_{C_{4,IN}^{=}} - WF_{I-C_{4,IN}^{=}}\right) - \left(WF_{C_{4,OUT}^{=}} - WF_{I-C_{4,OUT}^{=}}\right)} \qquad \text{A1-31}$$

where

SC is the cracking selectivity, mass %,
$WF_{<C4,OUT}$ is the mass fraction of lights in the product gas, - and
$WF_{<C4,IN}$ is the mass fraction of lights in the feed gas, -.

A1.15 HYDROGEN TRANSFER SELECTIVITY (SH)

The percentage paraffins and dienes formed per quantity of the isomers of butene converted was calculated using

$$SH = \frac{\left[\left(WF_{C_{4,OUT}^{'}} + WF_{1,3-C_{4,OUT}^{''}}\right) - \left(WF_{C_{4,IN}^{'}} + WF_{1,3-C_{4,IN}^{''}}\right)\right]\cdot 100}{\left(WF_{C_{4,IN}^{'}} - WF_{I-C_{4,IN}^{'}}\right) - \left(WF_{C_{4,OUT}^{'}} - WF_{I-C_{4,OUT}^{'}}\right)} \qquad \text{A1-32}$$

where

SH is the hydrogen transfer selectivity, mass %,
$WF_{1,3-C4'''',OUT}$ is the mass fraction of dienes in the product gas,
$WF_{1,3-C4'''',IN}$ is the mass fraction of dienes in the feed gas,
$WF_{C4',OUT}$ is the mass fraction of n-butane + isobutane in the product gas and
$WF_{C4',IN}$ is the mass fraction of n-butane + isobutane in the feed gas.

A1.16 OLIGOMERISATION SELECTIVITY (SO)

The percentage heavies that are formed per quantity of butene converted was calculated using

$$SO = \frac{\left(WF_{>C_{4,OUT}} - WF_{>C_{4,IN}}\right)\cdot 100}{\left(WF_{C_{4,IN}^{'}} - WF_{I-C_{4,IN}^{'}}\right) - \left(WF_{C_{4,OUT}^{'}} - WF_{I-C_{4,OUT}^{'}}\right)} \qquad \text{A1-33}$$

where

SO is the oligomerisation selectivity, mass %,

$WF_{>C4,OUT}$ is the mass fraction of heavies in the product gas and

$WF_{>C4,IN}$ is the mass fraction of heavies in the feed gas.

A1.17 1-BUTENE CONVERSION (CB)

As an indication of how hard the catalyst was working the conversion of 1-butene was calculated. In this case *cis*-2- and *trans*-2- butene together with all other components were considered to be products. The 1-butene selectivity was calculated using

$$CB = \frac{\left(WF_{1-C^{\cdot}_{4,IN}} - WF_{1-C^{\cdot}_{4,OUT}}\right)\cdot 100}{WF_{1-C^{\cdot}_{4,IN}}} \qquad \text{A1-34}$$

where

CB is the 1-butene conversion, mass %,

$WF_{1-C4",OUT}$ is the mass fraction of 1-butene in the product gas and

$WF_{1-C4",IN}$ is the mass fraction of 1-butene in the feed gas.

A1.18 GAS CHROMATOGRAPHIC PROCEDURES

To quantify the effect of the operating conditions and the feed composition on the performance of the material the composition of the product and feed gas had to be determined. This was done using a Varian 3400 gas chromatograph whose responses from the flame ionization detector (FID) were monitored by an on-board integrator. The column used to separate the gases into the separate components was a porous layer open tubular (PLOT) capillary column. The column of fused silica was 50 m long with a inner diameter of 0.53 mm the inside wall of which was coated with Al_2O_3/KCl. The conditions used to operate the chromatograph and a typical result obtained are shown below and in Appendix 2.

TABLE A1.1 : GAS CHROMATOGRAPH OPERATING CONDITIONS

Parameter	Setting
Chromatograph	Varian 3400
Detector	Flame ionization detector
Attenuation	4
Range	10^{-10} amps/mV
Column	PLOT capillary column
Length	50 m
Internal diameter	0.53 mm
Outer diameter	0.70 mm
Column pre-pressure	5 psi(g) at 70°C
Stationary phase	Al_2O_3/KCl
Coating thickness	10 µm
N_2 flow rate, carrier	3 ml/min at STP
N_2 flow rate, make up	30 ml/min at STP
H_2 flow rate	30 ± 1 ml/min at STP
Air flow rate	300 ± 15 ml/min at STP
Split flow	300 ± 1 ml/min at STP
Sample volume	50 µl
Split ratio	100 to 1
Injector temperature	250°C
Detector temperature	250°C
Temperature program	5 min at 70°C 5°C/min to 175°C 4 min at 175°C
Analysis time	30 min

As the response of the detector varies for each component, the area percent measured are not directly proportional to the mass percent. Hence, the relative sensitivity of the detector for each of the compounds has to be determined. This can then be used to convert the area percent to mass percent. By dividing each area with the appropriate relative sensitivity to obtain the true area count and normalizing the results to obtain the mass percentage of each component. However, for an FID detector, the light hydrocarbons relative sensitivities are all approximately equal to one, as was determined by Deitz (1967:68). This is shown in Table A1.2. Hence, in this work the area percentages were assumed to be equal to the mass percentages.

TABLE A1.2 : RELATIVE DETECTOR SENSITIVITIES

Component	Relative Sensitivity
Methane	0.97
Ethane	0.97
Ethene	1.02
Propane	0.98
n-Butane	1.09
C_5^+	0.99

A typical G.C. trace obtained is shown in Figure A1-1. The residence time of the various components and hence the sequence of the peaks was determined using a variety of pure standards and data supplied with the column.

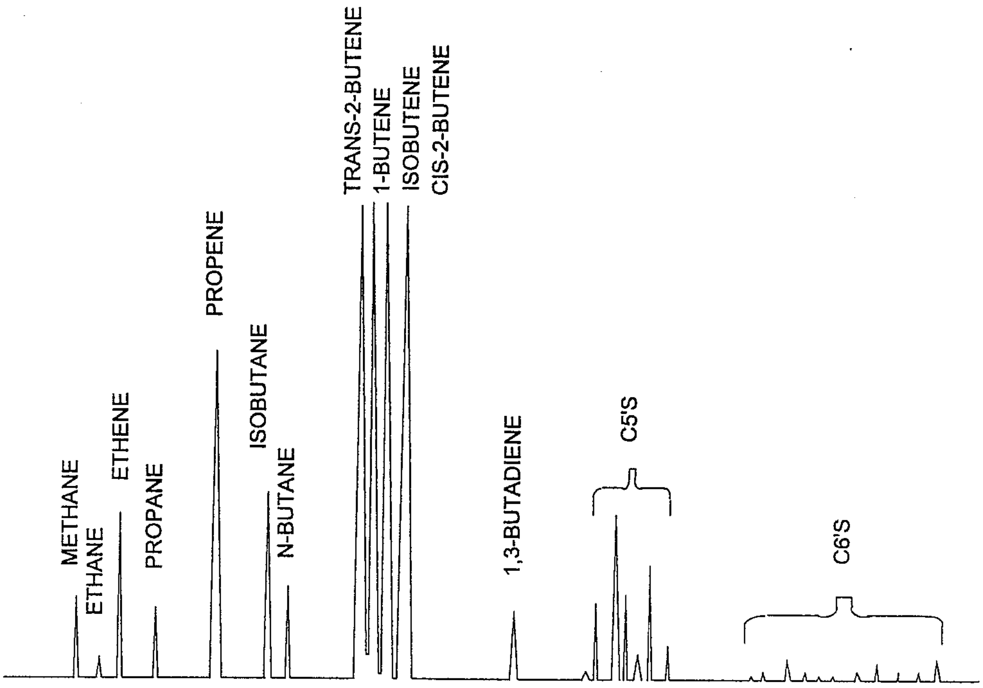

Figure A1.1 : Typical G.C. trace of the gaseous products

APPENDIX 2 SAMPLE CALCULATION

The data collected during the experiment were analysed using a variety of procedures. Given here are the average values of the raw data collected during a typical activity check performed using the second catalyst charge. Also given are the results of the various manipulations as outlined in Appendix 1. For additional details regarding the experimental operating procedure see Chapter 3.

A2.1 GENERAL RUN DATA

TABLE A2.1 : GENERAL RUN SUMMARY

Activity Check	Set point	Measured Out	Measured In	Average
Run Name	ISOM-178	ISOM-178	ISOM-178	ISOM-178
Feed	Feed A	Feed A	Feed A	Feed A
Temperature, °C	520	521.2	521.2	521
Pressure, kPa(a)	150	150.9	151.8	151
C4 Cut Flow, $g{\cdot}h^{-1}$	92.3	90.3	89.4	89.9
Butene Flow, $g{\cdot}h^{-1}$	78	76.4	75.6	76
Water Flow, $g{\cdot}h^{-1}$	59.3	57.2	56.9	57.1
Catalyst Mass, g	50	50	50	50
Ratio Water / Butene, molar	2.4	2.3	2.3	2.3
WHSV, Butene, h^{-1}	1.6	1.5	1.5	1.5
Total Run Time, h	15	15	15	15
LHSV, C4 Cut, h^{-1}	2	2	2	2
Ratio Water / C4 Cut, molar	2	2	2	2
Residence Time, s	1.27	1.27	1.28	1.28

TABLE A2.2 : AVERAGE MASS BALANCE DATA

Activity Check-44	Measured in	Measured out	Balance, %
Water, $g \cdot h^{-1}$	56.9	57.2	100.53
C4 Cut, $g \cdot h^{-1}$	89.4	90.3	101.01
Overall, $g \cdot h^{-1}$	146.3	147.5	100.82

A2.2 GASEOUS COMPONENTS

A2.2.1 HYDROCARBONS

The composition of the gaseous components were determined using gas chromatography. The feed and average product gas compositions are given.

TABLE A2.3 : FEED AND AVERAGE PRODUCT GAS COMPOSITION

Name	Feed	Product
Methane, mass %	0.00	0.10
Ethane, mass %	0.00	0.03
Ethene, mass %	0.00	0.14
Propane, mass %	1.03	1.24
Propene, mass %	1.60	3.10
Isobutane, mass %	1.51	1.73
n-Butane, mass %	10.25	10.49
trans-2-Butene, mass %	2.12	23.33
1-Butene, mass %	71.85	18.84
Isobutene, mass %	8.06	21.66
cis-2-Butene, mass %	2.50	17.82
1,3-Butadiene, mass %	0.03	0.05
C_5's, mass %	1.05	1.44
C_6's, mass %	0.00	0.03

TABLE A2.4 : GROUPED FEED AND PRODUCT COMPOSITIONS

Species	Feed	Product
trans-2-Butene. mass %	2.12	23.33
1-Butene, mass %	71.85	18.84
Isobutene, mass %	8.06	21.66
cis-2-Butene, mass %	2.50	17.83
Lights, < C_4, mass %	2.63	4.61
n-Butane + Isobutane, mass %	11.77	12.21
Heavies, >C_4, mass %	1.04	1.47
1,3 Butadiene, mass %	0.02	0.06
Total n-Butene+Isobutene, mass %	84.54	81.65
Total n-Butene, mass %	76.48	59.99

TABLE A2.5 : CATALYST PERFORMANCE

Parameter	Value
Loss of Butenes, mass %	3.42
Total Conversion, mass %	21.56
1-Butene Conversion, mass %	73.78
Isobutene Selectivity, mass %	82.45
Cracking Selectivity, mass %	11.98
Hydrogen Transfer Selectivity, mass %	2.95
Oligomerisation Selectivity, mass %	2.62

A2.2.2 OXYGENATES

Apart from hydrocarbons, Feed A also contained a variety of oxygenates amounting to 0.28 mass % as shown in Table A2.6. For details of the effect of the oxygenates on the performance of the catalyst, see Chapter 4.

TABLE A2.6 : FEED A OXYGENATE CONTENT

Oxygenate	Quantity
Acid, mass % as Acetic Acid	<0.01
Carbonyls, mass % as MEK	0.03
Alcohols, mass % as Ethanol	0.15
Esters, mass % as Ethyl Acetate	0.1

A2.3 : LIQUID PRODUCTS

A2.3.1 : OXYGENATES

The process water collected contained on average 1800 ppm acetone and 200 ppm butanone. For a detailed discussion as to the effects of the oxygenates on the performance of the catalyst, see Chapter 4.

A2.3.2 : HYDROCARBONS

Apart from the oxygenates, a small quantity of oil was also produced during the on-line period. By combining the water from a number of runs, sufficient oil could be collected for a G.C. analysis. Due to the negligible quantities of oil formed, the presence of the oil was ignored during the manipulation and interpretation of the experimental results.

TABLE A2.7 : OIL COMPOSITION

C No.	normal paraffins	iso-paraffins	branch paraffins	olefins	alkyl-benzenes	indanes + tetralines	di - aromatic	diphenyl + naphthene	tri - aromatics	Unknown
C4	1.45	0.09	0.00	6.24	0.00	0.00	0.00	0.00	0.00	0.00
C5	0.23	0.02	0.02	1.11	0.00	0.00	0.00	0.00	0.00	0.00
C6	0.03	0.11	0.35	1.32	0.24	0.00	0.00	0.00	0.00	0.00
C7	4.16	5.78	0.94	4.64	1.61	0.00	0.00	0.00	0.00	0.00
C8	0.28	1.53	0.78	7.61	9.29	0.00	0.00	0.00	0.00	0.00
C9	0.10	0.72	0.28	3.21	9.85	0.19	0.00	0.00	0.00	0.00
C10	0.06	0.93	0.51	0.85	5.60	1.10	0.37	0.00	0.00	1.11
C11	0.04	0.39	0.37	0.62	1.72	1.29	1.54	0.00	0.00	0.49
C12	0.07	0.87	0.21	1.37	2.24	2.16	1.07	0.00	0.00	0.20
C13	0.05	1.46	0.21	0.26	0.03	0.65	0.89	0.14	0.00	0.33
C14	0.06	0.54	0.00	0.16	0.39	0.12	0.33	0.15	0.03	0.15
C15	0.08	0.15	0.26	0.17	0.02	0.05	0.28	0.25	0.20	0.13
C16	0.03	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.14
C17	0.07	0.10	0.00	0.00	0.06	0.00	0.00	0.00	0.00	0.16
C18	0.07	0.26	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.32
C19	0.08	0.03	0.00	0.00	0.15	0.16	0.00	0.00	0.00	0.65
C20	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C21	0.08	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C22	0.04	0.28	0.00	0.00	0.26	0.00	0.00	0.00	0.00	0.00
C23	0.08	0.09	0.00	0.00	0.31	0.00	0.00	0.00	0.00	0.00
C24	0.06	0.14	0.00	0.00	0.27	0.00	0.00	0.00	0.00	0.00
C25	0.02	0.12	0.00	0.00	0.22	0.00	0.00	0.00	0.00	0.00
C26	0.03	0.10	0.00	0.00	0.09	0.00	0.00	0.00	0.00	0.00
C27	0.00	0.09	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	7.22	14.25	3.93	27.56	32.38	5.72	4.48	0.54	0.23	3.68

APPENDIX 3. DERIVATION OF THE KINETIC EQUATIONS

Shown here are the details of the derivation when generating the various kinetic relationships considered in Chapter 6. Although, derivations were previously developed (Aris, 1965), it is was repeated here as it was needed for the derivation of the rate equations for all of the other cases considered.

A3.1 REACTION STEPS

The following steps are involved in the transformation of n-butene (n) to isobutene (i), via the mono-molecular mechanism over a single catalytic site.

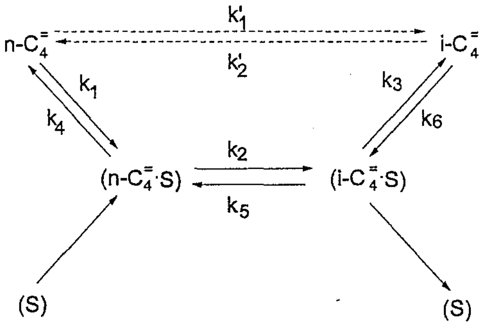

Figure A3.1 : n-Butene isomerisation reaction steps

where

(S)	represents a vacant surface site, -,
n-C4	represents a molecule of n-butene in the gas phase, -,
i-C4	represents a molecule of isobutene in the gas phase, -,
(n-$C_4^=$·S)	represents a molecule of n-butene on the surface of the catalyst, -,
(i-$C_4^=$·S)	represents a molecule of isobutene on the surface of the catalyst, -,
k_i	are the frequency factors for Case 2 to Case 8, i=1 to 6, mol·kg^{-1}·s^{-1}·kPa^{-1} and
k'_j	are the frequency factors for Case 1, j=1 or 2, mol·kg^{-1}·s^{-1}·kPa^{-1}.

By assuming one, two or all three of the reaction steps to be equal, but not equal to zero or irreversible, a total of eight cases present themselves. These, with the bracketed values representing the number of rate limiting steps assumed, are :

Case 1 : Bulk reaction of the n-butene to the isobutene (1)
Case 2 : Adsorption of the n-butene (1)
Case 3 : Surface reaction of the n-butene to the isobutene (1)
Case 4 : Desorption of the isobutene (1)
Case 5 : Surface reaction of the n-butene to the isobutene plus desorption of the isobutene(2)
Case 6 : Adsorption of the n-butene and desorption of the isobutene (2)
Case 7 : Adsorption of the n-butene plus surface reaction of the n-butene to the isobutene (2)
Case 8 : Adsorption of the n-butene, surface reaction of the n-butene to the isobutene plus desorption of the isobutene (3)

A3.2 DERIVATION OF RATE EQUATION

As may be seen from Figure A3.1, three distinct reaction steps during the transformation of the n-butenes to isobutene may be identified, i.e., adsorption of the n-butene, surface reaction of the n-butene to isobutene and desorption of the isobutene.

Using the same nomenclature as before, the n-butene chemisorption step may be written using

$$\text{n-}C_4^{=} + (S) \underset{k_4}{\overset{k_1}{\rightleftharpoons}} (\text{n-}C_4^{=} \cdot S) \tag{A3-1}$$

Assuming both the forward and reverse reaction to be first order and using a mass action law, the overall rate of adsorption of the n-butene may be written as :

$$r_a = k_1 \cdot P_{n-C_4^=} \cdot (S) - k_4 \cdot (n\text{-}C_4^= \cdot S) \qquad \text{A3-2}$$

where

r_a is the overall rate of adsorption, mol·s^{-1}·kg^{-1},

The surface chemical reaction step in turn is :

$$(n\text{-}C_4^= \cdot S) \underset{k_5}{\overset{k_2}{\rightleftarrows}} (i\text{-}C_4^= \cdot S) \qquad \text{A3-3}$$

If both reactions are assumed to be first order, the net rate of the transformation of n-butene to isobutene, i.e., the surface reaction may be expressed as

$$r_s = k_2 \cdot (n\text{-}C_4^= \cdot S) - k_5 \cdot (i\text{-}C_4^= \cdot S) \qquad \text{A3-4}$$

where

r_s is the overall surface reaction rate, mol·s^{-1}·kg^{-1} and

Finally, the desorption of the isobutene, i.e., the desorption step may be written, with the same nomenclature as before, using

$$(i\text{-}C_4^= \cdot S) \underset{k_6}{\overset{k_3}{\rightleftarrows}} P_{i-C_4^=} + (S) \qquad \text{A3-5}$$

Assuming both the desorption and the adsorption of the isobutene to be first order and using a mass action law, the overall rate of desorption of the isobutene may be written as

$$r_d = k_3 \cdot (i\text{-}C_4^{=} \cdot S) - k_6 \cdot P_{i\text{-}C_4^{=}} \cdot (S) \qquad \text{A3-6}$$

where

r_d is the overall rate of desorption, $mol \cdot s^{-1} \cdot kg^{-1}$,

To complete the description of the reaction, a balance over the active sites is required. This may be expressed using,

$$(S)_t = (S) + (i\text{-}C_4^{=} \cdot S) + (n\text{-}C_4^{=} \cdot S) \qquad \text{A3-7}$$

where

$(S)_t$ is the total number of active sites, -.

Together with the appropriate assumption, by manipulating Equations A3-2, A3- 4, A3-6 and 7, the kinetic expressions describing each of the eight cases may be derived. Details of this procedure for Case 8, are given below.

A3.3 CASE 8 : DERIVATION

For Case 8, all of the reaction rates are assumed to be equal but not equal to zero so that

$$r = -r_n = r_a = r_s = r_d = +r_i \qquad \text{A3-8}$$

Rearranging Equation 6 in terms of ($i\text{-}C_4^{=} \cdot S$) we get

$$(i\text{-}C_4^{=} \cdot S) = \frac{r}{k_3} + \frac{k_6}{k_3} \cdot P_{i\text{-}C_4^{=}} \cdot (S) \qquad \text{A3-9}$$

Similarly, rearranging Equation A3-2 in terms of $(n\text{-}C_4^{=}\cdot S)$ we get

$$(n\text{-}C_4^{=}\cdot S) = -\frac{r}{k_4} + \frac{k_1}{k_4}\cdot P_{n\text{-}C_4^{=}}\cdot(S) \qquad \text{A3-10}$$

Substituting Equation A3-9 and Equation A3-10 into Equation A3-4 we get

$$r = -\frac{k_2}{k_4}\cdot r + \frac{k_2\cdot k_1}{k_4}\cdot P_{n\text{-}C_4^{=}}\cdot(S) - \frac{k_5}{k_3}\cdot r - \frac{k_5\cdot k_6}{k_3}\cdot P_{i\text{-}C_4^{=}}\cdot(S) \qquad \text{A3-11}$$

Rearranging Equation A3-11 in terms of C_S we obtain

$$(S) = \frac{\dfrac{k_2}{k_4} + \dfrac{k_5}{k_3} + 1}{\dfrac{k_2\cdot k_1}{k_4}\cdot P_{n\text{-}C_4^{=}} - \dfrac{k_5\cdot k_6}{k_3}\cdot P_{i\text{-}C_4^{=}}}\cdot r \qquad \text{A3-12}$$

Substituting Equation A3-9, Equation A3-10 into Equation A3-7 and rearranging, we obtain

$$(S)_t = (S)\cdot\left(1 + \frac{k_1}{k_4}\cdot P_{n\text{-}C_4^{=}} + \frac{k_6}{k_3}\cdot P_{i\text{-}C_4^{=}}\right) + r\cdot\left(\frac{1}{k_3} - \frac{1}{k_4}\right) \qquad \text{A3-13}$$

Combining Equation A3-12 and Equation A3-13 and rearranging in terms of r we obtain

$$r = \frac{(S)_t\cdot\left(\dfrac{k_2\cdot k_1}{k_4}\cdot P_{n\text{-}C_4^{=}} - \dfrac{k_5\cdot k_6}{k_3}\cdot P_{i\text{-}C_4^{=}}\right)}{\left(\dfrac{k_2}{k_4} + \dfrac{k_5}{k_3} + 1\right)\cdot\left(1 + \dfrac{k_1}{k_4}\cdot P_{n\text{-}C_4^{=}} + \dfrac{k_6}{k_3}\cdot P_{i\text{-}C_4^{=}}\right) + \left(\dfrac{1}{k_3} - \dfrac{1}{k_4}\right)\cdot\left(\dfrac{k_2\cdot k_1}{k_4}\cdot P_{n\text{-}C_4^{=}} - \dfrac{k_5\cdot k_6}{k_3}\cdot P_{i\text{-}C_4^{=}}\right)} \qquad \text{A3-14}$$

After multiplying both the top and bottom line of Equation A3-14 by $k_4/\{k_2\cdot k_1\}$ and rearranging we get

$$r=\frac{(S)_t\cdot\left(P_{n\text{-}c_4^=}-\frac{k_4\cdot k_5\cdot k_6}{k_1\cdot k_2\cdot k_3}\cdot P_{i\text{-}c_4^=}\right)}{\left(\frac{1}{k_1}+\frac{k_5\cdot k_4}{k_1\cdot k_2\cdot k_3}+\frac{k_4}{k_1\cdot k_2}\right)+\left(\frac{k_5}{k_2\cdot k_3}+\frac{1}{k_2}+\frac{1}{k_3}\right)\cdot P_{n\text{-}c_4^=}+\left(\frac{k_6}{k_1\cdot k_3}+\frac{k_4\cdot k_6}{k_1\cdot k_2\cdot k_3}+\frac{k_5\cdot k_6}{k_1\cdot k_2\cdot k_3}\right)\cdot P_{i\text{-}c_4^=}} \qquad \text{A3-15}$$

Using the equilibrium relationships $K_a = k_1 / k_2$, $K_s = k_2 / k_5$ and $K_d = k_3 / k_6$ together with $K = \{k_1 \cdot k_2 \cdot k_3\} / \{k_4 \cdot k_5 \cdot k_6\}$, Equation A3-16 may further be rearranged to obtain

$$r=\frac{(S)_t\cdot\left(P_{n\text{-}c_4^=}-\frac{P_{i\text{-}c_4^=}}{K}\right)}{\left(\frac{1}{k_1}+\frac{1}{k_6\cdot K}+\frac{1}{k_2\cdot K_a}\right)+\left(\frac{1+K_s}{K\cdot k_6}+\frac{1}{k_2\cdot K_a}\right)\cdot K_a\cdot P_{n\text{-}c_4^=}+\left(\frac{1}{k_2\cdot K_a}+\frac{1+K_s}{k_1\cdot K_s}\right)\cdot\frac{P_{i\text{-}c_4^=}}{K_d}} \qquad \text{A3-16}$$

As sufficient data is available, a total of 392 data points, it will be possible to evaluate the effect of temperature on each of the reaction steps, i.e., a multi-step modelling approach can be used. The temperature dependency of the individual k_i values with i = 1 to 6, may be approximated via the Arrhenius equation using

$$k_i = k_i^1 \cdot \exp\left(\frac{-k_i^2}{R\cdot T}\right) \qquad \text{A3-17}$$

where

k_i are the frequency factors for Case 2 to Case 8 with i=1 to 6 and with $k_i = k'_j$ with j = 1 or 2, for Case 1, $mol\cdot kg^{-1}\cdot s^{-1}\cdot kPa^{-1}$,
k_i^1 is the pre-exponential factor, traditionally represented by k_i^o, $mol\cdot kg^{-1}\cdot s^{-1}\cdot kPa^{-1}$ and
k_i^2 is the activation energy, traditionally represented by E, $cal\cdot mol^{-1}$.

Hence, a total of 12 variables will simultaneously have to be evaluated. The procedure used is discussed in detail in Chapter 6 and Appendices 4 and 5.

A3.4 LISTING OF KINETIC EXPRESSIONS DEVELOPED

Using the procedure as outlined above, the kinetic expressions describing each of the eight cases considered, were derived. The final kinetic equation together with the nature and number (bracketed) of the rate limiting step(s) are shown below for each case.

Case 1 : Bulk reaction of n-butene to isobutene (1)

$$r = \left(k_1' \cdot P_{n-C_4^=} - k_2' \, P_{i-C_4^=}\right) \qquad \text{A3-19}$$

Case 2 : Adsorption of n-butene (1)

$$r = \frac{(S)_t \cdot \left(P_{n-C_4^=} - \dfrac{P_{i-C_4^=}}{K} \right)}{\left(\dfrac{1}{k_1}\right) + \left(\dfrac{K_s + 1}{k_1 \cdot K_s}\right) \cdot \dfrac{P_{i-C_4^=}}{K_d}} \qquad \text{A3-20}$$

Case 3 : Surface reaction of n-butene to isobutene (1)

$$r = \frac{(S)_t \cdot \left(P_{n-C_4^=} - \dfrac{P_{i-C_4^=}}{K} \right)}{\left(\dfrac{1}{k_2 \cdot K_a}\right) + \left(\dfrac{1}{k_2 \cdot K_a}\right) \cdot K_a \cdot P_{n-C_4^=} + \left(\dfrac{1}{k_2 \cdot K_a}\right) \cdot \dfrac{P_{i-C_4^=}}{K_d}} \qquad \text{A3-21}$$

Case 4 : Desorption of the isobutene (1)

$$r = \frac{(S)_t \cdot \left(P_{n-C_4^{=}} - \dfrac{P_{i-C_4^{=}}}{K} \right)}{\left(\dfrac{1}{k_6 \cdot K} \right) + \left(\dfrac{1 + K_s}{k_6 \cdot K} \right) \cdot K_a \cdot P_{n-C_4^{=}}} \qquad \text{A3-22}$$

Case 5 : Surface reaction of n-butene to isobutene plus desorption of isobutene (2)

$$r = \frac{(S)_t \cdot \left(P_{n-C_4^{=}} - \dfrac{P_{i-C_4^{=}}}{K} \right)}{\left(\dfrac{1}{k_6 \cdot K} + \dfrac{1}{k_2 \cdot K_a} \right) + \left(\dfrac{1 + K_s}{k_6 \cdot K} + \dfrac{1}{k_2 \cdot K_a} \right) \cdot K_a \cdot P_{n-C_4^{=}} + \left(\dfrac{1}{k_2 \cdot K_a} \right) \cdot \dfrac{P_{i-C_4^{=}}}{K_d}} \qquad \text{A3-23}$$

Case 6 : Adsorption of n-butene plus desorption of isobutene (2)

$$r = \frac{(S)_t \cdot \left(P_{n-C_4^{=}} - \dfrac{P_{i-C_4^{=}}}{K} \right)}{\left(\dfrac{1}{k_1} + \dfrac{1}{k_6 \cdot K} \right) + \left(\dfrac{1}{k_6 \cdot K} + \dfrac{1}{k_3 K_a} \right) \cdot K_a \cdot P_{n-C_4^{=}} + \left(\dfrac{1}{k_1 \cdot K_s} + \dfrac{1}{k_1} \right) \cdot \dfrac{P_{i-C_4^{=}}}{K_d}} \qquad \text{A3-24}$$

Case 7 : Adsorption of n-butene plus surface reaction of n-butene to isobutene (2)

$$r = \frac{(S)_t \cdot \left(P_{n-C_4^{=}} - \dfrac{P_{i-C_4^{=}}}{K} \right)}{\left(\dfrac{1}{k_1} + \dfrac{1}{k_2 \cdot K_a} \right) + \left(\dfrac{1}{k_2 \cdot K_a} \right) \cdot K_a \cdot P_{n-C_4^{=}} + \left(\dfrac{1}{k_2 \cdot K_a} + \dfrac{K_s + 1}{k_1 \cdot K_s} \right) \cdot \dfrac{P_{i-C_4^{=}}}{K_d}} \qquad \text{A3-25}$$

Case 8 : Adsorption of n-butene plus surface reaction of n-butene to isobutene plus desorption of isobutene (3)

$$r = \frac{(S)_t \cdot \left(P_{n-C_4^=} - \frac{P_{i-C_4^=}}{K} \right)}{\left(\frac{1}{k_1} + \frac{1}{k_6 \cdot K} + \frac{1}{k_2 \cdot K_a} \right) + \left(\frac{1 + K_s}{k_6 \cdot K} + \frac{1}{k_2 \cdot K_a} \right) \cdot K_a \cdot P_{n-C_4^=} + \left(\frac{1}{k_2 \cdot K_a} + \frac{K_s + 1}{k_1 \cdot K_s} \right) \cdot \frac{P_{i-C_4^=}}{K_d}} \tag{A3-26}$$

APPENDIX 4. KINETIC MODEL REQUIREMENTS

In Chapter 5, the results from an investigation as to the models required to predict the performance of the pilot plant and the bench scale reactor systems were discussed. Given here, in Appendix 4, are the details of the various calculation procedures used in support of the discussion presented in Chapter 5.

A4.1 OPERATING PARAMETERS

The deviation from ideal plug flow in the pilot plant and the bench scale reactor systems, when operated at the base case conditions were determined for both. The relevant operating parameters are summarised in Table A4.1 below. (See also Chapter 3, Section 3.5 and Appendix 2).

TABLE A4.1 : OPERATING CONDITIONS AND PHYSICAL DATA

Reactor	Pilot Plant	Bench Scale	
Temperature, K	793	793	793
Pressure, kPa(a)	150	150	150
1-Butene Flow, $kg{\cdot}s^{-1}$	25.6e-6	3.77e-6	6.67e-6
H_2O Flow, $kg{\cdot}s^{-1}$	16.5e-6	2.42e-6	4.29e-6
Catalyst Mass, kg	50.0e-3	7.35e-3	13.0e-3
Catalyst Density, $kg{\cdot}m^{-3}$	650	650	650
Tube Diameter, m	25.4e-3	13.1e-3	13.1e-3
Particle Diameter, m	1.5e-3	1.5e-3	1.5e-3
Cross Sectional Area, m^2	506.7e-6	134.8e-6	134.8e-6
Bed Height, m	151.8e-3	83.8e-3	148.4e-3
Mass Velocity, $kg{\cdot}m^{-2}{\cdot}s^{-1}$	83.1e-3	45.9e-3	81.3e-3
Linear Velocity, $m{\cdot}s^{-1}$	119.2e-3	65.8e-3	116.5e-3
Residence Time, s	1.27	1.27	1.27

A4.2 REACTOR MODEL

The two-dimensional form of the mass conservation equation of a pseudo-homogeneous fixed bed reactor model was presented by Smith (1981:555) and may be written for component i, in the differential form, using

$$\frac{\partial}{\partial r}\left(r \cdot (D_e)_r \cdot \frac{\partial C_i}{\partial r} \right) + r \cdot \frac{\partial}{\partial z}\left(- u \cdot C_i + (D_e)_L \cdot \frac{\partial C_i}{\partial z} \right) - r_i \cdot \rho_B \cdot r = 0 \qquad \text{A4-1}$$

with boundary conditions of

$$\frac{\partial C_i}{\partial z} = 0 \quad \text{at } z = L \qquad \text{A4-2}$$

$$C_i = C_{i,in} \quad \text{at } z = 0 \text{ for all } r \qquad \text{A4-3}$$

$$\frac{\partial C_i}{\partial r} = 0 \quad \text{at } r = R_0 \text{ for all } z \qquad \text{A4-4}$$

$$\frac{\partial C_i}{\partial r} = 0 \quad \text{at } r = 0 \text{ for all } z \qquad \text{A4-5}$$

The analogous expression to Equation A4-1 for energy, i.e., a two-dimensional energy conservation equation, as adapted from (Smith, 1988:563) is

$$\frac{\partial}{\partial r}\left((\lambda_e)_r + r \cdot (\lambda_e)_r \cdot \frac{\partial T}{\partial r} \right) + r \cdot \frac{\partial}{\partial z}\left(- u \cdot \rho_g \cdot C_p + (\lambda_e)_L \cdot \frac{\partial T}{\partial z} \right) - r_p \cdot \rho_B \cdot r \cdot (\Delta H_r) = 0 \qquad \text{A4-6}$$

with boundary conditions of

$$\frac{\partial T}{\partial z} = 0 \quad \text{at } z = L \qquad \text{A4-7}$$

$$T = T_{in} \quad \text{at } z = 0 \text{ for all } r \tag{A4-8}$$

$$\frac{\partial T}{\partial r} = \frac{\alpha_w}{(\lambda_{er})_r} . (T - T_w) \quad \text{at } r = R_o \text{ for all } z \tag{A4-9}$$

$$\frac{\partial T}{\partial r} = 0 \quad \text{at } r = 0 \text{ for all } z \tag{A4-10}$$

where

r	is the radius of the element, m,
R_o	is the bed outer radius, m,
$(D_e)_r$	is the effective diffusivity in the radial direction, $m^2 \cdot s^{-1}$,
$(D_e)_L$	is the effective diffusivity in the axial direction, $m^2 \cdot s^{-1,}$
$C_{i,in}$	is the inlet concentration of component i, $mole \cdot m^{-3}$,
C_i	is the concentration of component i, $mole \cdot m^{-3}$,
u	is the superficial velocity in the axial direction, $m \cdot s^{-1}$,
ρ_B	is the density of the catalyst in the bed, $kg \cdot m^{-3}$,
z	is the height of the element, m,
r_i	is the global rate of disappearance of component i, $mol \cdot s^{-1} \cdot kg^{-1}$,
$(\lambda_e)_r$	is the effective radial thermal conductivity coefficient, $W \cdot m^{-1} \cdot K^{-1}$,
$(\lambda_e)_L$	is the effective axial thermal conductivity coefficient, $W \cdot m^{-1} \cdot K^{-1}$,
α_w	is the heat transfer coefficient at the reactor wall, $W \cdot m^{-2} K^{-1}$,
ρ_g	is the density of the gas, $kg \cdot m^{-3}$,
C_p	is the gas heat capacity, $J \cdot kg^{-1} \cdot K^{-1}$,
ΔH_r	is the heat of reaction, $J \cdot mole^{-1}$,
T	is the temperature, K,
T_{in}	is the inlet temperature, K and
T_w	is the wall temperature, K.

For isothermal operation with concentration gradients only in the axial direction and with the transport mechanism operating in this direction being the overall flow itself, if deviations from ideal plug flow due to radial and axial heat and mass transfer effects are not significant and if the linear velocity does not vary with height, then a one-dimensional model may be used. In this case Equation A4-2 may be neglected and Equation A4-1 simplified (Foment and Bischoff, 1990:403) to :

$$-u\cdot\frac{\partial C_i}{\partial Z}=r_i\cdot\rho_B \qquad \text{A4-11}$$

with boundary conditions

$$C_i=C_{i,in} \quad \text{at } z=0 \qquad \text{A4-12}$$

$$\frac{\partial C_i}{\partial z}=0 \quad \text{at } z=L \qquad \text{A4-13}$$

where

C_i is concentration of reactant i, mole·m^{-3},
u is the superficial velocity in the axial direction, m·s^{-1},
ρ_B is the density of the catalyst in the bed, kg·m^{-3},
z is the height of the element, m,
r_i is the global rate of disappearance of component i, mol·s^{-1}·kg^{-1} and
L is the total bed height, m.

A4.3 SIGNIFICANCE OF RADIAL DEVIATIONS FROM IDEAL PLUG FLOW

Mears (1971:130) proposed that deviations from ideal plug flow due to heat transport limitations is less than 5 %, if the left hand side (LHS) of Equation A14-4 is less than 0.4, that is

$$\frac{(-\Delta H_r)\cdot r_p\cdot\rho_B\cdot d_t^2\cdot E}{4\cdot\lambda_{er}\cdot R\cdot T_W^2}\cdot\left[1+8\cdot\left(\frac{\lambda_{er}}{\alpha_W\cdot d_p}\right)\cdot\left(\frac{d_p}{d_t}\right)\right]<0.4 \qquad \text{A4-14}$$

where

ΔH_r is the heat of reaction, $J \cdot kmol^{-1}$,
r_p is the reaction rate, $kmol \cdot m_{cat}^{-1} \cdot s^{-1}$,
ρ_B is the bulk density of the catalyst, $kg \cdot m^{-3}$,
d_t is the reactor tube diameter, m,
E is the activation energy, $J \cdot kmol^{-1}$,
λ_{er} is the effective radial thermal conductivity, $W \cdot m^{-1} \cdot K^{-1}$,
R is the universal gas constant, $kmol \cdot kPa(a) \cdot m^{-3} \cdot K^{-1}$,
T_W is the wall temperature, K and
α_w is the heat transfer coefficient at the reactor wall, $W \cdot m^{-2} \cdot K^{-1}$.

The procedures and the necessary equations used to calculate the various parameters listed above are given below. A summary of the final and intermediate results are given in Table A4.5

A4.3.1 HEAT OF REACTION, ΔH_r

The heats of the double bond and skeletal isomerisation reactions were calculated from the heats of formation (Stull, 1969:314). Using the thermodynamic equilibrium ratios of the various butenes at 520°C as given in Chapter 2, Section 2.3.6, (Kilpatrick et al., 1946:559), the effective reaction heat was calculated to be $\Delta H_r = -8.58e6\ J \cdot kmol^{-1}$.

A4.3.2 ACTIVATION ENERGY, E

The butene skeletal isomerisation activation energy has been measured in a number of studies (See Section 2.3.8 for details). The conservative value of 8.4e6 $J \cdot kmole^{-1}$ as recorded by Choudhary and Doraiswamy (1975:228), was used in these investigations.

A4.3.3 EFFECTIVE RADIAL THERMAL CONDUCTIVITY, λ_{er}

The radial flux by effective thermal conduction may be considered to consist of two contributions, the first dynamic, i.e., depending on the flow conditions and the second static depending on the solid (Froment and Bischoff, 1979:452) so that

$$\lambda_{er} = \lambda_{er}^{o} + \lambda_{er}^{t} \qquad \text{A4-15}$$

where

λ_{er}^{o} is the static contribution to the effective thermal conductivity, $W \cdot m^{-1} \cdot K^{-1}$ and

λ_{er}^{t} is the dynamic contribution to the effective thermal conductivity, $W \cdot m^{-1} \cdot K^{-1}$.

A4.3.4 EFFECTIVE RADIAL THERMAL CONDUCTIVITY - STATIC, λ_{er}^{o}

The static contribution, λ_{er}^{o} to the effective radial thermal conductivity was calculated using (Froment and Bischoff, 1979:454)

$$\frac{\lambda_{er}^{o}}{\lambda_{ge}} = \varepsilon \cdot \left(1 + \beta \cdot \frac{d_p \cdot \alpha_{rv}}{\lambda_{ge}} \right) + \frac{\beta \cdot (1 - \varepsilon)}{\dfrac{1}{\dfrac{1}{\Phi} + \dfrac{\alpha_{rs} \cdot d_p}{\lambda_{ge}}} + \dfrac{2}{3} \cdot \dfrac{\lambda_{ge}}{\lambda_{se}}} \qquad \text{A4-16}$$

where

λ_{ge} is the effective thermal conductivity of the fluid, $J \cdot m^{-1} \cdot s^{-1} \cdot K^{-1}$,

λ_{se} is the effective thermal conductivity of the solid, $J \cdot m^{-1} \cdot s^{-1} \cdot K^{-1}$,

ε is the void fraction, -,

α_{rv} is the void radiation heat transfer coefficient, $J \cdot m^{-2} \cdot s^{-1} \cdot K^{-1}$,

α_{rs} is the solid radiation heat transfer coefficient, $J \cdot m^{-2} \cdot s^{-1} \cdot K^{-1}$, ß is a coefficient that depends on the particular geometry and packing density, comprised between 0.9 and 1.0 (Froment and Bischoff, 1990:455). In this study ß was assumed to be equal to 0.95 and

Φ is a packing specific constant, -(Froment and Bischoff, 1990:455).

A4.3.5 FLUID EFFECTIVE THERMAL CONDUCTIVITY, λ_{ge}

The ideal gas thermal conductivity of water and n-butene were calculated (Reid 1987:514) using

$$\lambda_{gi} = A_i + B_i \cdot T + C_i \cdot T^2 + D_i \cdot T^3 \qquad \text{A4-17}$$

where

A_i to D_i are constants specific for component i in the ideal gas thermal conductivity equation, -,

T is the temperature, K and

λ_{gi} is the thermal conductivity of component i, $W \cdot m^{-1} \cdot K^{-1}$.

The effective thermal conductivity of the fluid phase was calculated using

$$\lambda_{ge} = \sum_{i=1}^{N} y_i \cdot \lambda_{gi} \qquad \text{A4-18}$$

where

y_i is the mole fraction of component i, - and

λ_{gi} is the thermal conductivity of component i, $W \cdot m^{-1} \cdot K^{-1}$.

Using the data shown in Table A4.2 below, the effective thermal conductivity of the fluid at 793 K was calculated. The calculated thermal conductivity of water at 793 K (0.067 $W \cdot m^{-1} K^{-1}$) compares well with the value of 0.059 $W \cdot m^{-1} \cdot K^{-1}$ reported by Holman (1976:505).

TABLE A4.2 : IDEAL GAS EQUATION THERMAL CONDUCTIVITY COEFFICIENTS

Species	A	B	C	D	λ_{gi}@793K $W{\cdot}m^{-1}{\cdot}K^{-1}$	y_i, -
1-Butene	-10.5e-3	57.7e-6	101.8e-9	-42.7e-12	0.078	0.33
Water	7.3e-3	-10.1e-6	180.1e-9	-91.0e-12	0.067	0.67

A4.3.6 SOLID EFFECTIVE THERMAL CONDUCTIVITY, λ_{se}

The effective thermal conductivity of a porous solid is a function of the volume fraction of the void phase and the thermal conductivities of the bulk fluid and solid phases. The effective thermal conductivity of the particle may be calculated (Woodside, and Messmer, 1961:1688) using

$$\lambda_{se} = \lambda_s \cdot \left(\frac{\lambda_{ge}}{\lambda_s} \right)^{1-\epsilon_s} \qquad \text{A4-19}$$

where

λ_g is the thermal conductivity of the fluid phase, $W{\cdot}m^{-1}{\cdot}K^{-1}$,

λ_s is the thermal conductivity of the solid, $W{\cdot}m^{-1}{\cdot}K^{-1}$,

λ_{se} is the effective thermal conductivity of the catalyst, $W{\cdot}m^{-1}{\cdot}K^{-1}$ and

ϵ_s is the solid void fraction, -.

In this study, the solids voidage fraction was calculated, using an average particle volume of 14.2e-9 m^3 (d_p = 2.0e-3 m), average particle mass of 5.0e-6 kg, bulk density of 650 $kg{\cdot}m^{-3}$, bed voidage of 0.465, and the average pore volume, measured for the 700°C calcined and steamed catalyst, of 0.52e-3 $m^3{\cdot}kg^{-1}_{cat}$ to be ϵ_s =0.68. The thermal conductivity of sintered alumina, was found to be 0.8 $W{\cdot}m^{-1}{\cdot}K^{-1}$ (Lide, 1996:12-179) with that of the fluid having previously been calculated to be λ_{ge} = 0.07 $W{\cdot}m^{-1}{\cdot}K^{-1}$ giving an effective solid thermal conductivity of the catalyst of λ_{se} = 0.37 $W{\cdot}m^{-1}{\cdot}K^{-1}$. This value falls well within the accepted limits of between 0.173 $J{\cdot}s^{-1}{\cdot}m^{-1}{\cdot}K^{-1}$ and 0.692 $J{\cdot}s^{-1}{\cdot}m^{-1}{\cdot}K^{-1}$ as reported by Smith (1988:477).

A4.3.7 BED VOID FRACTION, ϵ

The effective fractional voidage of a packed bed of 1/16" spheres (d_p = 1.58e-3 m) was reported to be ϵ = 0.41 (Coulson et al., 1980:127). Alternatively, the void fraction in packed bed of spheres was also correlated as a function of the particle and tube diameter by Haughey and Beveridge (1969:130) to be

$$\epsilon = 0.38 + 0.073 \cdot \left[1 + \frac{([d_t / d_p] - 2)^2}{[d_t / d_p]^2} \right] \qquad \text{A4-20}$$

where

ϵ is the effective bed voidage, -,
d_p is the average particle diameter, m and
d_t is the diameter of the tube, m.

At an average particle diameter of 1.5e-3 m the effective bed voidage for the pilot plant (d_t = 2.54e-2 m) was calculated to be ϵ = 0.51 and for the bench scale reactor system (d_t = 13.1e-3 m) to be ϵ = 0.50. During all subsequent calculations the average bed voidage of ϵ = 0.46 was used.

A4.3.8 VOID RADIATION HEAT TRANSFER COEFFICIENT, α_{rv}

The void radiation heat transfer coefficient α_{rv} may be calculated Froment and Bischoff (1990:454) using

$$\alpha_{rv} = \frac{0.227e\text{-}3}{1 + \frac{\varepsilon}{2 \cdot (1 - \varepsilon)} \cdot \frac{(1 - p)}{p}} \cdot \left[\frac{T}{100} \right]^3 \qquad \text{A4-21}$$

where

α_{rv} is the void radiation heat transfer coefficient, $J \cdot m^{-2} \cdot s^{-1} \cdot K^{-1}$,

T is the temperature, K and

p is the emissivity of the solid, -.

The emissivity of strongly oxidised alumina was found to be between 0.2 and 0.3 at temperatures of between 55°C and 550°C (Lide, 1996:10-261), which together with the average bed voidage ($\epsilon = 0.46$) gives a void radiation heat transfer coefficient of $\alpha_{rv} = 0.05\ J \cdot m^{-2} \cdot s^{-1} \cdot K^{-1}$ at a temperature of 793 K.

A4.3.9 SOLID RADIATION HEAT TRANSFER COEFFICIENT, α_{rs}

The solids radiation heat transfer coefficient α_{rs} may be calculated using the same nomenclature as before (Froment and Bischoff, 1990:455), with

$$\alpha_{rs} = \frac{0.227e-3 \cdot p}{(2-p)} \cdot \left[\frac{T}{100}\right]^3 \qquad \text{A4-22}$$

The radiation coefficient of the solid, at a temperature of 793 K and using an average emissivity of 0.25, was calculated to be $\alpha_{rs} = 0.02\ J \cdot m^{-2} \cdot s^{-1} \cdot K^{-1}$.

A4.3.10 DENSITY FACTOR, ϕ

The density factor ϕ may be calculated for the bed voidage fraction of between $\epsilon = 0.260$ and $\epsilon = 0.476$, (Kunii and Smith, 1960) as reported by Froment and Bischoff (1990:455)

$$\phi = \phi_2 + (\phi_1 - \phi_2)\frac{\varepsilon - 0.260}{0.476 - 0.260} \qquad \text{A4-23}$$

The values of ϕ_1 and ϕ_2 may be obtained from the ratio of the effective solid thermal conductivity (λ_{se} = 0.37 J·m^{-1}·K^{-1}) and the effective fluid thermal conductivity (λ_g = 0.07 J·m^{-1}·K^{-1}). For this study the appropriate values were taken from Froment and Bischoff (1990:455), for $\lambda_{se}/\lambda_{ge}$ = 5.3 to be ϕ_1 = 0.2 and ϕ_2 = 0.1 respectively to give ϕ = 0.195.

A4.3.11 EFFECTIVE RADIAL THERMAL CONDUCTIVITY - DYNAMIC, λ_{er}^t

The dynamic contribution (λ_{er}^t) may be calculated using (Froment and Bischoff, 1979:456)

$$\frac{\lambda_{er}^t}{\lambda_{ge}} = \psi \cdot \frac{C_{pe} \cdot \mu_e}{\lambda_{ge}} \cdot \frac{d_p \cdot G}{\mu_e} \qquad \text{A4-24}$$

and

$$\psi = \frac{0.14}{1 + 46 \cdot \left(\frac{d_p}{d_t} \right)^2} \qquad \text{A4-25}$$

where

C_p is the fluid heat capacity, J·kg^{-1}·K^{-1},
μ is the fluid dynamic viscosity, kg·m^{-1}·s^{-1},
λ is the fluids thermal conductivity, kW·m^{-1}·K^{-1} and
G is the superficial mass velocity, kg·m^{-2}·s^{-1}.

A4.3.12 FLUID EFFECTIVE HEAT CAPACITY, c_{pe}

The ideal gas thermal conductivity of water and n-butene were calculated (Coulson et al., 1983:765) using

$$C_{pi} = A_i + B_i \cdot T + C_i \cdot T^2 + D_i \cdot T^3 \qquad \text{A4-26}$$

where

A_i to D_i are constants in the ideal gas heat capacity equation for component i, -,

T is the temperature, K and

C_{Pi} is the heat capacity of component i, J·mol^{-1}·K^{-1}.

The effective heat capacity of the fluid phase (C_{pe}) was in turn calculated using

$$C_{pe} = \sum_{i=1}^{N} y_i \cdot C_{pi} \qquad \text{A4-27}$$

where

y_i is the mole fraction of component i, - and

C_{Pi} is the heat capacity of component i, J·mol^{-1}·K^{-1}.

Using the data shown in Table A4.3 below, together with the appropriate mole fractions, molar masses and average feed molecular mass of 30.6 kg·kmol^{-1}, the effective heat capacity of the fluid was calculated to be C_{pe} = 2730 J·kg^{-1}·K^{-1}.

TABLE A4.3 : IDEAL GAS EQUATION HEAT CAPACITY COEFFICIENTS

Species	A	B	C	D	C_{pe}@793K J·mole^{-1}·K^{-1}	y_i, -
1-Butene	-3.0	353.2e-3	-198.2e-6	44.6e-9	174.7	0.33
Water	32.2	1.9e-3	10.6e-6	-3.6e-9	38.6	0.67

The calculated ideal gas heat capacity for water at 793 K of 38.6 J·mol^{-1}·K^{-1} compares well with the value of 38.7 J·mol^{-1}·K^{-1} as reported by Holman (1976:505).

A4.3.13 FLUID VISCOSITY CORRELATION

According to Chung et al. (1986 and 1984) as reported by Reid at al. (1987:397), the viscosity of a gas may be calculated using

$$\mu_i = 40.785 \cdot \frac{F_{ci} \cdot (M_i \cdot T)^{0.5}}{V_{ci}^{2/3} \cdot \Omega_v} \qquad \text{A4-28}$$

where

μ_i	is the viscosity of component i, cP,
M_i	is the molecular weight of component i, g·mol^{-1},
T	is the temperature, K,
V_{ci}	is the critical volume of component i, cm^3·mol^{-1},
Ω_v	is the viscosity collision integral, - and
F_{ci}	is a molecular shape and polarity correction factor, -.

The viscosity collision integral may in turn be calculated using

$$\Omega_v = 1.16145 \cdot \left(\frac{T}{T_{ci}}\right)^{-0.14874} + 0.52487 \cdot \exp\left(-0.77320 \cdot \frac{T}{T_{ci}}\right) + 2.16178 \cdot \exp\left(-2.43787 \cdot \frac{T}{T_{ci}}\right) \qquad \text{A4-29}$$

The molecular shape and polarity correction factor may be calculated using

$$F_{ci} = 1 - 0.2756 \cdot \omega_i + 0.059035 \cdot \eta_{ri}^4 + \kappa_i \qquad \text{A4-30}$$

And the dipole moment may be calculated using

$$\eta_{ri} = 131.3 \cdot \frac{\eta_i}{(V_{ci} \cdot T_{ci})^{0.5}} \qquad \text{A4-31}$$

where

T_{ci} is the critical temperature of component i, K,

ω_i is the acentric factor for component i, -,

κ_i is a special correction factor for highly polar substances, -,

η_{ri} is a dimensionless dipole moment for component i, - and

η_i is the dipole moment for component i, debyes.

The appropriate values of the various constants for both water and 1-butene at 793K are shown in Table A4.4 below. The calculated viscosity of water at 793 K of 282.4 μP compares well with the value of 278.6 μP as reported by Holman (1976:505).

TABLE A4.4 : VISCOSITY EQUATION PARAMETERS

Species	M_i, $g{\cdot}mol^{-1}$	T_{ci}, K	V_{ci}, $cm^3{\cdot}mol^{-1}$	ω_i, -	η_i, -	κ_i, -	F_{ci}, -	Ω_{vi}, -	μ_i, cP
1-Butene	56	419.6	240.0	0.05	0.3	0.000	0.962	1.11	192.8
Water	18	647.3	57.1	0.344	1.8	0.076	1.12	1.29	282.4

A4.3.14 VISCOSITY OF GAS MIXTURES

An interpolative procedure to calculate the viscosity of a mixture of gases at low pressure was presented by Wilke (1950:517) using

$$\mu_m = \sum_{i=1}^{n} \frac{y_i \cdot \mu_i}{\sum\limits_{j=1}^{n} y_j \cdot \phi_{ij}} \qquad \text{A4-32}$$

where

$$\phi_{ij} = \frac{[1 + (\mu_i/\mu_j)^{0.5} \cdot (M_j/M_i)^{0.25}]^2}{[8 \cdot (1 + M_i/M_j)]^{0.5}} \qquad \text{A4-33}$$

ϕ_{ji} is in turn found by interchanging subscripts or by

$$\phi_{ji} = \frac{\mu_j}{\mu_i} \cdot \frac{M_i}{M_j} \cdot \phi_{ij} \qquad \text{A4-34}$$

where

ϕ_{ij} is a interaction factor for component i and j, -,
M_x is the molar weight of the specific component, x=i or j, $g{\cdot}mol^{-1}$,
y_x is the mole fraction of the specific component, x = i or j, -,
μ_x is the viscosity of the specific component, x=i or j, cP and
μ_m is the effective viscosity of the mixture, cP.

Using this procedure, the effective viscosity of the mixture was calculated to be 270.2 cP.

A4.3.15 WALL HEAT TRANSFER COEFFICIENT, α_W

The heat transfer coefficient at the reactor wall may be calculated (Froment and Bischoff, 1979:452), using

$$\alpha_W \cdot (T_R - T_W) = -\lambda_{er}\left(\frac{\partial T}{\partial r}\right)_W \qquad \text{A4-35}$$

where

T_R is the temperature at the centre of the reactor, K and
T_W is the temperature at the wall of the reactor, K.

The differential term $(\partial T/\partial r)_W$ representing the change in temperature with the radius at the wall. This may be determined using a two-dimensional reactor model. Alternatively the wall heat transfer coefficient, $\alpha_{w,}$ may also be calculated using (Beek, 1962:303) as reported by Smith (1988:572) using

$$Nu = 0.203 \cdot Re^{0.33} \cdot Pr^{0.33} + 0.22 \cdot Re^{0.8} \cdot Pr^{0.4} \qquad \text{A4-36}$$

Using the same nomenclature as before, the Nusselt Number, Nu, may be calculated (Holman, 1976:xvii) using

$$Nu = \frac{\alpha_W \cdot d_p}{\lambda_{ge}} \qquad \text{A4-37}$$

The corresponding Prandtl number (Pr) may be calculated (Holman, 1976:xvii) using

$$Pr = \frac{C_p \cdot \mu_m}{\lambda_{ge}} \qquad \text{A4-38}$$

and the modified Reynolds number may be calculated (Holman , 1976:xvii) using

$$Re = \frac{d_p \cdot G}{\mu_m} \qquad \text{A4-39}$$

Using the criterion as proposed by Mears (1971:545) together with the various procedures outlined above, the importance of the deviation from ideal plug flow due to heat transport limitations were calculated. The necessary data and results are given in Table A4.5.

It can be concluded from the results shown in Table A4-5 that radial heat transport effects are not significant enough to require the use of a two-dimensional reactor model. Furthermore, as mass transport effects are usually negligible in comparison to heat transport effects (Mears, 1971:545), this suggests that deviation from ideal plug flow due to mass transport effects may also be considered negligible.

TABLE A4.5 : SIGNIFICANCE OF RADIAL DEVIATIONS FROM IDEAL PLUG FLOW

Reactor	Pilot Plant	Bench Scale	
$\| -\Delta H_r \|$, $J \cdot kmol^{-1}$	8.58e6	8.58e6	8.58e6
r_b, $kmol \cdot kg^{-1}_{cat} \cdot s^{-1}$ (maximum)	2.16e-6	2.16e-6	2.16e-6
ρ_B, $kg \cdot m^{-3}$	650	650	650
d_t, m	25.4e-3	13.1e-3	13.1e-3
d_p, m	1.5e-3	1.5e-3	1.5e-3
E, $J \cdot kmol^{-1}$	89.4e6	89.4e6	89.4e6
λ_{er}, $J \cdot s^{-1} \cdot m^{-1} \cdot K^{-1}$	0.13	0.09	0.1
T_w, K	793	793	793
R, $J \cdot kmol^{-1} \cdot K^{-1}$	8314	8314	8314
α_w, $J \cdot s^{-1} \cdot m^{-1} . K^{-1}$	48.4	32.8	47.7
{Tube to Particle Diameter Ratio, -} > 10	12.7	6.6	6.6
$\{(\|-\Delta H_r\| \cdot r_p \cdot \rho_B \cdot d_t^2 \cdot E)/(4 \cdot \lambda_{er} \cdot R \cdot T_W^2))(1+8 \cdot \lambda_{er}/(\alpha_w \cdot d_t))\}<0.4$	0.48	0.24	0.19
Deviation, %	6.0	3.0	2.4

A4.3.16 RADIAL TEMPERATURE PROFILE

The need for a two-dimensional model to account for radial heat transport effects can also be examined by calculating the radial temperature profile. Assuming that the diffusivities are not sensitive to r or to z, that the velocity is not a function of z and neglecting axial dispersion of mass and energy, the mass conservation expression (Equation A4-1) may

be written in terms of conversion (Smith, 1988:582) as

$$\frac{\partial x}{\partial z} - \frac{d_p}{Pe_r} \cdot \left(\frac{1}{r} \cdot \frac{\partial x}{\partial r} + \frac{\partial^2 x}{\partial r^2} \right) - \frac{r_p \cdot \rho_B}{(G/\bar{M}) \cdot y_o} = 0 \qquad \text{A4-40}$$

Similarly, making the same kind of assumptions as for the mass balance, the two-dimensional energy conservation Equation (A4-6) may be rearranged to (Smith, 1988:582) give

$$- G \cdot C_{pe} \cdot \frac{\partial T}{\partial z} + (\lambda_e)_r \cdot \left(\frac{1}{r} \cdot \frac{\partial T}{\partial r} + \frac{\partial T}{\partial r^2} \right) - r_p \cdot \rho_B \cdot \Delta H_r = 0 \qquad \text{A4-41}$$

where

x	is the fractional conversion, -,
z	is the increment height, m,
d_p	is the particle diameter, m,
Pe_r	is the radial Peclet number for mass transfer, -,
r	is the radius of the element, m,
r_p	is the reaction rate, $mole \cdot kg^{-1} \cdot s^{-1}$,
ρ_B	is the catalyst bed bulk density, $kg \cdot m^{-3}$,
G	is the mass velocity, $kg \cdot m^{-2} \cdot s^{-1}$,
C_{pe}	is the effective gas heat capacity, $J \cdot kg^{-1} \cdot K^{-1}$,
T	is the temperature, K,
$(\lambda_e)_r$	is the effective radial thermal conductivity, $W \cdot m^{-1} \cdot K^{-1}$ and
ΔH_r	is the heat of reaction, $J \cdot mole^{-1}$.

Using an explicit method based on writing the differential equation in difference form, both the temperature and conversion as a function of both the axial and the radial position may be calculated (Smith, 1988:584). As may be seen from Figures A4-1, when operating the reactor at the base case conditions, the radial temperature profile as predicted by the two-dimensional homogeneous model, is always less than 1°C higher than the wall temperature of 520°C. A similar deviation was observed in the axial temperature profile at the centre of the reactor, from direct measurement (See Section 5.4.2). Hence, the temperature may be approximated by the jacket temperature at all points inside the reactor and solving the enthalpy balance is not required.

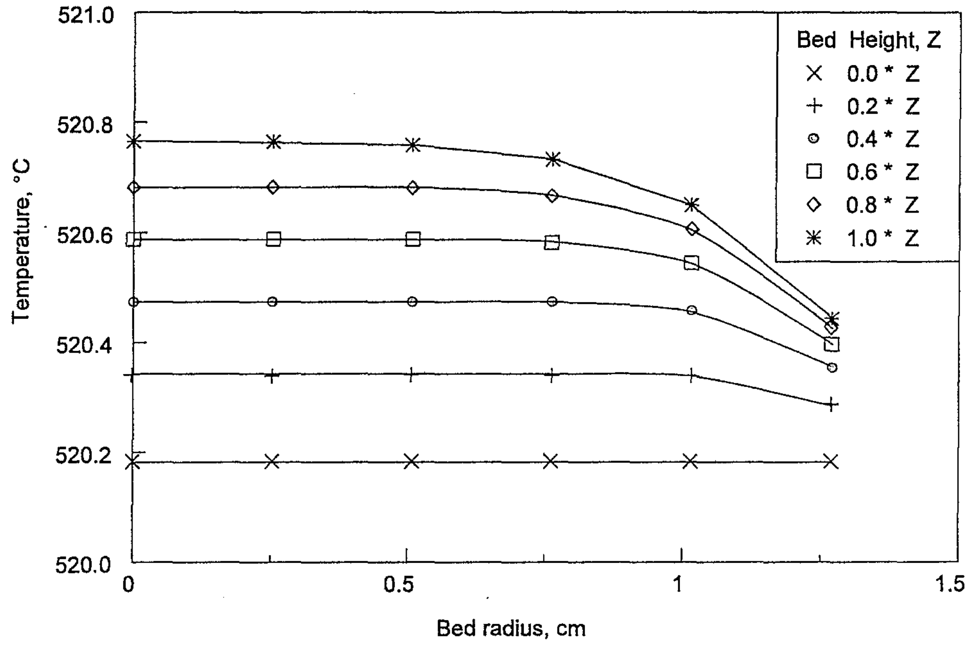

Figure A4.1 : Radial temperature profile vs bed height

A4.4 SIGNIFICANCE OF AXIAL DEVIATION FROM IDEAL PLUG FLOW

The flow in a packed bed may also deviate from ideal plug flow due to axial mixing. When the reaction rate has a maximum value at some intermediate position due to a hot spot for example, axial dispersion may only be neglected according to Froment and Bischoff (1990:448) when

$$(Pe_L)_m = \frac{d_p \cdot u_s}{(D_e)_L} >>> \max\left|\frac{\partial X}{\partial(z/d_p)}\right| \qquad \text{A4-42}$$

and

$$(Pe_L)_h = \frac{C_{pe} \cdot d_p \cdot u_s \cdot \rho_{ge}}{\lambda_{eL}} >>> \max\left|\frac{\partial T}{\partial(z/d_p)}\right| \qquad \text{A4-43}$$

The differential terms ($|\partial X/\partial z|$) and ($|\partial T/\partial z|$) may be approximated from a solution of a basic one-dimensional pseudo-homogeneous model. Alternatively, when the rate changes uniformly with increasing bed height, such as when the bed is operated isothermally in the axial direction, then the point at which the importance of axial mixing has to be determined is at the bed inlet. In this case axial dispersion may be considered to be negligible Froment and Bischoff (1990:448) if

$$(Pe_L)_m = \frac{d_p \cdot u_s}{(D_e)_L} >>> \frac{r_b \cdot \rho_B \cdot d_p}{u_s \cdot C_o} \qquad \text{A4-44}$$

and

$$(Pe_L)_h = \frac{d_p \cdot u_s \cdot C_{pe} \cdot \rho_{ge}}{\lambda_{eL}} >>> \frac{(-\Delta H) \cdot r_b \cdot \rho_b \cdot d_p}{(T_o - T_w) \cdot u_s \cdot \rho_{ge} \cdot C_{pe}} \qquad \text{A4-45}$$

where

$(Pe_L)_m$	is Peclet number for mass transfer in the axial direction, -,
u_s	is the fluid superficial velocity, $m \cdot s^{-1}$,
ρ_{ge}	is the effective density of the gas, $kg \cdot m^{-2}$,
$(D_e)_L$	is the dispersion coefficient in the axial direction, $m^2 \cdot s^{-1}$,
X	is the fractional conversion, -,
$(Pe_L)_h$	is the Peclet number in the axial direction for heat transfer, -,
C_{pe}	is the effective heat capacity of the gas, $J \cdot kg^{-1} \cdot K^{-1}$,
λ_{eL}	is the effective axial thermal conductivity, $W \cdot m^{-1} \cdot K^{-1}$,
T_W	is the temperature at the wall, K and
T_o	is the inlet temperature, K.

A4.4.1 PECLET NUMBER FOR AXIAL MASS TRANSPORT

The experimental data of McHenry and Wilhelm (1957) for gases as reported by Smith (1988:558) suggests that for Reynolds numbers above about 10, the Peclet number for mass transport in the axial direction$(Pe_L)_m$ may be assumed to be equal to 2. Alternatively, Froment and Bischoff (1990:447) presented additional data suggesting that the Peclet number, based on the particle diameter, may be considered to lie between 1 and 2 for Reynolds numbers from 0.015 to 1000. In this work the effective diffusivity $(D_e)_L$ was calculated from basic principles, as discussed previously, and the Peclet number evaluated directly. The results obtained using both the calculated and average Peclet number are shown in Table A4-6 below.

A4.4.2 PECLET NUMBER FOR AXIAL HEAT TRANSPORT

A set of relations to calculate the effective axial thermal conductivity (λ_{eL}) could not be found, as little information is available (Froment and Bischoff, 1990:447). During this study, the effective axial thermal conductivity (λ_{eL}) was assumed to be equal to the effective radial thermal conductivity (λ_{er}) when calculating the Peclet number for axial heat transport $((Pe_L)_h)$. As may be seen from Table A4-6, the respective criteria, to check for significant axial deviations from ideal plug flow due to heat and / or mass transfer effects, indicate that these are not significant enough to justify the use of a two-dimensional reactor model.

A4.5 SIGNIFICANCE OF VARIATIONS IN THE LINEAR VELOCITY

The two-dimensional reactor model may further be simplified if the linear velocity is independent of the axial position in the catalyst bed. The linear velocity may be effected by a volume expansion / contraction during reaction as well as temperature and / or pressure gradients.

A4.6 SIGNIFICANCE OF THE PRESSURE DROP

Using the Ergun equation (Ergun, 1952), the pressure drop across the pilot plant reactor may be calculated with

TABLE A4.6 : SIGNIFICANCE OF AXIAL DEVIATIONS FROM IDEAL PLUG FLOW

Reactor	Pilot	Bench scale	
Particle Diameter, m	1.5e-3	1.5e-3	1.5e-3
Superficial Velocity, $m\cdot s^{-1}$	1.19e-1	6.58e-2	1.16e-1
Global Reaction Rate, $kmol\cdot kg^{-1}_{cat}\cdot s^{-1}$	2.16e-6	2.16e-6	2.16e-6
Bed Density, $kg\cdot m^{-3}$	650	650	650
1-Butene Feed Concentration, $kmol\cdot m^{-3}$	7.58e-3	7.58e-3	7.58e-3
Heat of Reaction, $J\cdot kmole^{-1}$	-8.58e6	-8.58e6	-8.58e-6
Wall Temperature, (As calculated), K	794	794	794
Central Temperature, K	793	793	793
Effective Gas Density, $kg\cdot m^{-3}$	9.36e-1	9.36e-1	9.36e-1
Effective Gas Heat Capacity, $J\cdot kmol^{-1}\cdot K^{-1}$	83.9e3	83.9e3	83.9e3
Effective Thermal Conductivity, $W\cdot m^{-1}\cdot K^{-1}$	1.17e-1	9.36e-2	1.06e-1
Average Peclet Number, $(Pe_L)_m$	2	2	2
Average Diffusivity $(De)_L$	8.94e-5	4.94e-5	8.73e-5
Calculated Diffusivity	5.09e-5	5.09e-5	5.09e-5
Check for Deviation from Ideal Plug Flow Due to Axial Mass Transfer Effects			
Calculated Peclet Number, $(Pe_L)_m$	3.51	1.94	3.43
$\{(r_b\cdot\rho_B\cdot d_p)/(u_s\cdot C_o)\} < (Pe_L)_m$	2.33e-3	4.22e-3	2.38e-3
Check for Deviation from Ideal Plug Flow Due to Axial Heat Transfer Effects			
Calculated Peclet Number, $(Pe_L)_h$	3.90	2.70	4.23
$\{(\lvert-\Delta H\rvert\cdot r_b\cdot\rho_b\cdot d_p) / ((T_o - T_w)\cdot u_s\cdot\rho_{ge}\cdot C_{pe})\} < (Pe_L)_h$	1.93e-3	3.49e-3	1.9e-3

$$\frac{-\Delta P}{l} = k_1\cdot\frac{(1-\varepsilon)^2\cdot\mu_g\cdot u_g}{\varepsilon^3\cdot d_p^2} + k_2\cdot\frac{(1-\varepsilon)\cdot\rho_g\cdot u_g^2}{\varepsilon^3\cdot d_p} \qquad \text{A4-46}$$

where

ΔP is the pressure drop, Pa,

l is the total catalyst bed height, m,

ε is the bed fractional voidage, -,
μ_g is the viscosity of the gas, $Pa \cdot s^{-1}$,
k_1 is the Carman-Kozeny constant for viscous losses, - and
k_2 is the Burke-Plummer constant for kinetic losses, -.

The values of the constants k_1 and k_2 should of cause be determined separately. However, as a fist approximation, the values measured for flow through ring packing, i.e., $k_1 = 150$ and $k_2 = 1.75$ will be used. (Ergun, 1952:89) The fractional voidage for packed columns of sphere with an average diameter of d_p = 1.5e-3 m was in turn calculated to be $\epsilon = 0.465$.

A4.7 SIGNIFICANCE OF THE ADIABATIC TEMPERATURE POTENTIAL

Typically, adiabatically operated reactor are not isothermal, i.e., the temperature at the inlet differs from that at the outlet of the catalyst bed. During an exothermic reaction the heat generated has to be removed via the effluent stream. Hence, in the absence of losses the overall adiabatic temperature rise, at equilibrium conversion, may be calculated (Westerterp et al., 1993:267) using

$$\Delta T_{ad} = \frac{(-\Delta H_r)_A \cdot C_{A_o} \cdot \zeta_A}{\rho_{ge} \cdot C_{pe}} \tag{A4-47}$$

where

C_{Ao} is the inlet concentration of reactant A, $mol \cdot m^{-3}$,
ζ_A is the fractional conversion of component A at equilibrium, -,
ρ_{ge} is the effective density of the reaction mixture, $kg \cdot m^{-3}$,
C_{pe} is the effective heat capacity of the reaction mixture, $J \cdot kg^{-1} \cdot K^{-1}$ and
ΔT_{ad} is the potential adiabatic temperature rise, -.

At the base case conditions, see Chapter 3, Section 3.5, the adiabatic temperature rise was calculated to be 9.1 K (See also Section 2.3.5). Alternatively, also in the absence of losses, the temperature may be calculated as a function of the catalyst bed height (Froment and Bischoff, 1990:403) using

$$\frac{\partial T}{\partial z} = \frac{(-\Delta H_r)\cdot r_p \cdot \rho_B}{u \cdot \rho_{ge} \cdot C_{pe}} \qquad \text{A4-48}$$

where

u is the superficial gas velocity, $m \cdot s^{-1}$,
ρ_{ge} is the effective density of the gas, $kg \cdot m^{-3}$ and
C_{Pe} is the effective heat capacity of the gas, $J.kg \cdot K^{-1}$.

A4.8 SIGNIFICANCE OF INTER- AND INTRA- PARTICLE RESISTANCES

To development the intrinsic kinetic equation it has to be confirmed that both heat and mass transfer resistances are negligible, i.e., that the temperature and the partial pressure of the reactants and products in the bulk of the fluid are equal to those on the surface and at the centre of the catalyst particle. Details of the procedures used to quantify the inter- and intra-particular heat and mass transfer resistances are presented here. A summary of the final and intermediate results are shown in Table 4.7.

A4.8.1 SIGNIFICANCE OF INTER-PARTICLE HEAT TRANSFER

For vapour phase systems, the greater part of the resistance to heat transfer is often in the boundary layer or film around the catalyst particle, rather than within, as the thermal conductivity of the solid is larger than that of the gas. In the case of a highly exothermic reaction the particle temperature can become considerably higher than the bulk stream temperature. A criterion for detecting the onset of a heat transport limitation was developed by Mears (1971:128) using the perturbation approach. The heat transfer resistance of the film is assumed to be lumped at the surface. If the observed rate is to deviate by less than 5 %, the criterion requires (Mears, 1971:543) that

$$\frac{-\Delta H\cdot r_p\cdot \rho_B\cdot d_p\cdot E}{2\cdot h\cdot R\cdot T^2} < 0.15 \qquad \text{A4-49}$$

where

h is the gas to particle heat transfer coefficient, $W\cdot m^{-2}\cdot K^{-1}$.

A4.8.2 SIGNIFICANCE OF INTER-PARTICLE MASS TRANSFER

If the rate of mass transfer across the external stagnant film surrounding the catalyst particle is comparable to the surface reaction rate, then the supply of reactant to the catalyst particle as well as the reaction rate contribute to the observed global rate. During kinetic investigations the intrinsic kinetics, the rate in the absence of transport resistances are sought, the validity of the assumption that the bulk and surface concentrations are equal, i.e., that the rate of reactant supply to the catalyst via diffusion across the stagnant film exceeds of the rate of reactant consumption via chemical reaction, has to be confirmed.

Using a mass action law the rate of n-butene consumption may be represented by

$$r_{n-C4''} = k_1\cdot\left(p_{n-C4''} - \frac{p_{i-C4''}}{K}\right) \qquad \text{A4-50}$$

where

$p_{n-C4''}$ is the n-butene partial pressure in the fluid, kPa(a),
$p_{1-C4''}$ is the isobutene partial pressure in the fluid, kPa(a),
k_1 is the reaction rate constant, $moles\cdot kg_{cat}^{-1}\cdot s^{-1}\cdot kPa(a)^{-1}$ and
K is the thermodynamic equilibrium constant, -.

$r_{n\text{-}C4''}$ is the rate of n-butene consumption, moles·kg_{cat}^{-1}·s^{-1}

The rate of n-butene consumption will be maximised when no isobutene is present. Hence, for purposes of calculating the contribution of film diffusion resistance to the global observed reaction rate, the maximum possible reaction rate will be used. The maximum possible rate of n-butene consumption may be calculated using

$$r_{n-C4''} = k_1 \cdot p_{n-C4''} \qquad \text{A4-51}$$

Starting from the bulk reaction rate, the reaction rate at the adjacent surface may be approximated using a Taylor expansion (Kreyszig, 1979:694) to give

$$r^{s}_{n-C4''} = r^{b}_{n-C4''} - k_1 \cdot (p^{b}_{n-C4''} - p^{s}_{n-C4''}) \qquad \text{A4-52}$$

where

$r^{s}_{n\text{-}C4''}$ is the surface n-butene consumption rate, moles·kg^{-1}_{cat}·s^{-1},
$p^{s}_{n\text{-}C4''}$ is the surface n-butene partial pressure, kPa(a),
$r^{b}_{n\text{-}C4''}$ is the bulk n-butene consumption rate, moles·kg^{-1}_{cat}·s^{-1} and
$p^{b}_{n\text{-}C4''}$ is the bulk n-butene partial pressure, kPa(a).

From which, after rearranging, the ratio of the surface and bulk reaction rates may be calculated using

$$\frac{r^{s}_{n-C4''}}{r^{b}_{n-C4''}} = 1 - \frac{p^{b}_{n-C4''} - p^{s}_{n-C4''}}{p^{b}_{n-C4''}} \qquad \text{A4-53}$$

Next, from a mass balance around the spherical catalyst particle, while simultaneously correcting the units of the surface reaction rate, we get

$$\frac{r^s_{n-C4''}\cdot\rho_B\cdot\pi\cdot d_p^3}{6\cdot(1-\epsilon)} = \frac{(k_g)_{n-C4''}\cdot(p^b_{n-C4''} - p^s_{n-C4''})\cdot\pi\cdot d_p^2}{R\cdot T\cdot\rho_g} \qquad \text{A4-54}$$

where

ρ_B	is the bulk density of the catalyst, kg·m^{-3},
d_p	is the particle diameter, m,
ϵ	is the bed voidage fraction, -,
$(k_g)_{n-C4''}$	is the mass transfer coefficient for n-butene, moles·m^{-2}·s^{-1},
R	is the universal gas constant, kmol·kPa(a)·m^{-3}·K^{-1},
T	is the bulk temperature, K and
ρ_g	is the fluid density, kg·m^{-3}.

Rearranging Equation A4-54 in terms of the partial pressure gradient, $(p^b_{n-C4''} - p^s_{n-C4''})$ and substituting into Equation A4-53 and rearranging, the ratio of the surface reaction rate to the bulk reaction rate may be calculated using

$$\frac{r^s_{n-C4''}}{r^b_{n-C4''}} = \frac{1}{1+\dfrac{r^b_{n-C4''}\cdot\rho_B\cdot R\cdot T\cdot\rho_g}{6\cdot(k_g)_{n-C4''}\cdot(1-\epsilon)\cdot p^b_{n-C4''}}} \qquad \text{A4-55}$$

Thus for the surface reaction rate not to deviate from the bulk reaction rate by more than 5 %, the right hand side of Equation A4-55 must be greater than or equal to 0.95. The procedure for calculating the mass transfer coefficient, $(k_g)_{n-C4''}$ and heat transfer coefficient, h, is presented below.

A4.8.2.1 MASS TRANSFER COEFFICIENT

The average transport coefficient between the bulk stream and particle surface can be correlated in terms of dimensionless groups which characterise the flow conditions such as the Sherwood and Schmidt numbers to calculate j-factors. The mass transfer coefficient, $(k_g)_{n\text{-}C4''}$ may be calculated via j_D factors.(Smith, 1988:394) using

$$j_D = \left(\frac{(k_g)_{n\text{-}C4''}\cdot\rho_f}{G}\right)\cdot\left(\frac{a_m}{a_t}\right)\cdot\left(\frac{\mu_f}{\rho_f\cdot D_{jm}}\right)^{2/3} \qquad \text{A4-56}$$

where

$(k_g)_{n\text{-}C4''}$	is the mass transfer coefficient, $mol\cdot m^{-2}\cdot s^{-1}$,
G	is the superficial mass velocity, $kg\cdot m^{-2}\cdot s^{-1}$,
μ_f	is the fluid dynamic viscosity, $kg\cdot m^{-1}\cdot s^{-1}$,
ρ_f	is the density of the fluid, $kg\cdot m^{-3}$,
D_{jm}	is the effective binary diffusivity coefficient, $m^2\cdot s^{-1}$,
a_m	is the external area available for mass transfer, m^2 and
a_t	is the total particle external area, m^2.

In this study the loss of effective mass transfer area due to particle to particle contact was not considered to be significant, i.e., a_m was assumed equal to a_t. The j_D factor may also be calculated as a function of the Reynolds number. For Reynolds numbers less than 190, and in a bed of spheres with a voidage of $\epsilon = 0.37$, j_D is well represented (Froment and Bischoff, 1990:128) by

$$j_D = 1.66\cdot\left(\frac{d_p\cdot G}{\mu_f}\right)^{-0.51} \qquad \text{A4-57}$$

Alternatively, for Reynolds numbers greater than 10, the available experimental data is well represented (Smith, 1988:395) by

$$j_D = \frac{0.458}{\epsilon}\cdot\left(\frac{d_p\cdot G}{\mu_f}\right)^{-0.407} \qquad \text{A4-58}$$

where

ε is the bed voidage fraction, -,

d_p is the diameter of the particle, m,

G is the superficial mass velocity, $kg \cdot m^{-2} \cdot s^{-1}$ and

μ_f is the dynamic viscosity. $kg \cdot m^{-1} \cdot s^{-1}$.

The procedure to calculate the effective binary diffusivity factor, D_{jm}, of component j in the mixture m, is discussed below.

A4.8.2.2 HEAT TRANSFER COEFFICIENT

Heat transfer between a fluid and particle surface in a packed bed occurs by the same molecular and convection process as mass transfer. For the heat transfer j-factor, j_H, the equation analogous to Equation A4-56 (Smith, 1988:395) is

$$j_H = \frac{h}{C_{pe} \cdot G} \cdot \left(\frac{a_m}{a_t} \right) \cdot \left(\frac{C_{pe} \cdot \mu_f}{\lambda_g} \right)^{2/3} \qquad \text{A4-59}$$

where

h is the heat transfer coefficient, $W \cdot m^{-2} \cdot K^{-1}$,

C_{pe} is the effective fluid heat capacity, $J \cdot kg^{-1} \cdot K^{-1}$,

G is the superficial mass velocity, $kg \cdot m^{-2} \cdot s^{-1}$,

μ_f is the dynamic viscosity. $kg \cdot m^{-1} \cdot s^{-1}$ and

λ_g is the effective gas thermal conductivity, $W \cdot m^{-1} \cdot K^{-1}$.

To minimise j_H, i.e., to ensure a conservative answer, heat transfer due to radiation will be neglected. Hence, Equation A4-59 and A4-56 are interchangeable, i.e., $j_H = j_D$ (Smith, 1988:395) and hence, the heat transfer coefficient (h) may be calculated.

A4.8.2.3 EFFECTIVE DIFFUSIVITY

The effective diffusivity coefficient in a binary mixture may be calculated (Reid et al., 1987 :583) using

$$D_{jk} = \frac{3}{16} \cdot \frac{(4 \cdot \pi \cdot k \cdot [T^{b} / M_{jk}])^{1/2}}{n \cdot \pi \cdot \sigma_{jk}^{2} \cdot \Omega_{D}} \cdot f_{D} \qquad \text{A4-60}$$

where

D_{jk}	is the diffusion coefficient of component j in k, $cm^{2} \cdot s^{-1}$,
M_i	is the molecular weight of the components, $g \cdot mol^{-1}$, i=j or k,
n	is the molar density of the mixture, $mol \cdot m^{-3}$,
k	is the Boltzman constant, k = 1.3805e-23 $J \cdot K^{-1}$,
T^{b}	is the bulk temperature, K,
σ_{jk}	is a characteristic length, Å,
Ω_D	is the diffusion collision integral, - and
f_D	is a correction factor.

The term M_{jk} may in turn be calculated using

$$M_{jk} = \frac{2}{(1/M_{j}) + (1/M_{k})} \qquad \text{A4-61}$$

If the molecular weights are of a similar order of magnitude, f_D lies between 1.0 and 1.02 regardless of the composition or intermolecular forces. Only if the molecular masses are very unequal and the light component is present in trace amounts, the value of f_D will vary between 1.0 and 1.1. In this study the correction factor f_D was set equal to unity. Using the ideal gas law to calculate n, Equation A4-60 may be rearranged to give

$$D_{jk} = \frac{0.00266 \cdot (T^{b})^{3/2}}{P_{T} \cdot M_{jk}^{1/2} \cdot \sigma_{jk}^{2} \cdot \Omega_{D}} \qquad \text{A4-62}$$

where

P_T is the total pressure, bar(a).

The interactions of the characteristic length parameters, designated by σ_{jk}, may in turn be calculated using

$$\sigma_{jk} = (\sigma_j \cdot \sigma_k)^{1/2} \qquad \text{A4-63}$$

and the characteristic length for each component, σ_i, where i stands for component j or k, may be calculated using

$$\sigma_i = \left(\frac{1.585 \cdot V_{b_i}}{1 + 1.3 \cdot \delta_i^2} \right)^{1/3} \qquad \text{A4-64}$$

where

V_{bi} is the liquid molar volume of component i at the normal boiling point, $cm^3 \cdot mol^{-1}$ and

δ_i is the characteristic length parameter for component i, where i= A or B, Å.

The diffusion collision integral may in turn be calculated for non-polar gases (Neufield et al., 1972:1100) using

$$\Omega_D = \frac{1.06036}{\left(\frac{k \cdot T}{\epsilon_{jk}} \right)^{0.15610}} + \frac{0.19300}{\exp\left(\frac{0.47635 \cdot k \cdot T}{\epsilon_{jk}} \right)} + \frac{1.03587}{\exp\left(\frac{1.52996 \cdot k \cdot T}{\epsilon_{jk}} \right)} + \frac{1.76474}{\exp\left(\frac{3.89411 \cdot k \cdot T}{\epsilon_{jk}} \right)} \qquad \text{A4-65}$$

However, as both water and to a lesser extent 1-butene are polar, the collision integral Ω_D calculated using the relationship proposed by (Neufield et al., 1972:1100) has to be corrected as proposed by Brokaw (1969:240) using

$$\Omega_D^P = \Omega_D + \frac{0.19 \cdot \delta_{jk}^2}{\left(\frac{k.T}{\epsilon_{jk}}\right)} \qquad \text{A4-66}$$

where

$\Omega^P{}_D$ is the collision integral for a polar mixture, -.

The ratio of the factor ϵ_{jk} / k, may in turn be calculated using

$$\frac{\epsilon_{jk}}{k} = \left(\frac{\epsilon_j}{k} \cdot \frac{\epsilon_k}{k}\right)^{1/2} \qquad \text{A4-67}$$

and the ratio of ϵ_i/k, where the subscript i refers to either component j or k, using

$$\frac{\epsilon_i}{k} = 1.18 \cdot (1 + 1.3 \cdot \delta_i^2) \cdot T_{b_i} \qquad \text{A4-68}$$

The polar parameter δ_i, where i refers to component j or k, may in turn be calculated using

$$\delta_i = \frac{1940 \cdot \mu_{p_i}^2}{V_{b_i} \cdot T_{b_i}} \qquad \text{A4-69}$$

where

μ_{pi} is the dipole moment of component i, debyes,
V_{bi} is the liquid molar volume at the normal boiling point of component i, $cm^3 \cdot mol^{-1}$ and
T_{bi} is the normal boiling point of component i at 1 atm, K.

The interaction of the dipole moments of the components in the binary gas mixture may in turn be calculated using

$$\delta_{jk} = (\delta_j \cdot \delta_k)^{1/2} \qquad \text{A4-70}$$

However, in this and most practical problems, more than two components are present. Thus, as the flux of the given component may be driven not only by its own concentration gradient but also by those of all other species present, an effective binary diffusivity for species j, diffusing through a mixture has to be calculated. This may be done for a general chemical reaction (Froment and Bischoff, 1990:131) using

$$\frac{1}{D_{jm}} = \frac{1}{1 + \Lambda_j \cdot y_j} \cdot \sum_{k \neq j}^{N} \cdot \frac{1}{D_{jk}} \cdot \left(y_k + y_j \cdot \frac{\zeta_k}{|\zeta_j|} \right) \qquad \text{A4-71}$$

where

D_{jm} is the effective binary diffusion coefficient of component j in a multi-component mixture m, $m^2 \cdot s^{-1}$,

y_j is the mole fraction of component j in the mixture, -,

D_{ik} is the effective diffusivity of component j in component k, $m^2 \cdot s^{-1}$ and

ζ_j is the stoichiometric coefficient of component j, with the convention that ζ is positive for products and negative for reactants, -.

The interaction of the stoichiometric coefficient on component j, Λ_j, which for equimolar counter diffusion, $\Lambda_j = 0$, may in turn be calculated using

$$\Lambda_j = \frac{r + s + \cdots - a - b - \cdots}{j} \qquad \text{A4-72}$$

where

r, s, · are the stoichiometric coefficients of the products, - and a, b, · are the stoichiometric coefficients of the reactants, -.

The significance of inter-particle heat and mass transfer were quantified using the above procedure and the results reported in Table A4-7. It may be seen from Table A4-7 that both inter-particle heat and mass transfer resistance were not significant. Hence, heterogeneous models to describe inter-particle heat and mass transfer phenomena were not required.

TABLE A4.7 : SIGNIFICANCE OF INTER-PARTICLE RESISTANCES

Reactor	Pilot	Bench scale	
Particle Diameter, m	1.5e-3	1.5e-3	1.5e-3
Global Reaction Rate, $\mathrm{kmol \cdot kg^{-1}_{cat} \cdot s^{-1}}$	2.16e-6	2.16e-6	2.16e-6
Bed Density, $\mathrm{kg \cdot m^{-3}}$	650	650	650
Heat of Reaction, $\mathrm{J \cdot kmole^{-1}}$	-8.58e6	-8.58e6	-8.58e-6
Activation Energy, $\mathrm{J \cdot kmole^{-1}}$	8.94e7	8.94e7	8.94e7
Bulk Temperature, K	793	793	793
Effective Gas Density, $\mathrm{kg \cdot m^{-3}}$	9.36e-1	9.36e-1	9.36e-1
Effective Gas Heat Capacity, $\mathrm{J \cdot kmol^{-1} \cdot K^{-1}}$	83.9e3	83.9e3	83.9e3
Effective Thermal Conductivity, $\mathrm{W \cdot m^{-1} \cdot K^{-1}}$	0.071	0.071	0.071
Effective Bed Voidage, -	0.46	0.46	0.46
Superficial Mass Velocity, $\mathrm{kg \cdot m^{-2} \cdot s^{-1}}$	8.31e-2	4.59e-2	8.13e-2
Bulk n-Butene Partial Pressure, kPa	50	50	50
Film mass Transfer Coefficient, $\mathrm{kg \cdot m^{-2} \cdot s^{-1}}$	2.11e-3	1.51e-3	2.12e-3
Effective Diffusion Coefficient, $\mathrm{m^2 \cdot s^{-1}}$	5.09e-5	5.09e-5	5.09e-5
Film Heat Transfer Coefficient, $\mathrm{W \cdot m^{-2} \cdot s^{-1}}$	121.4	86.7	121.5
Gas Constant, $\mathrm{kPa \cdot m^3 \cdot kmole^{-1} \cdot K^{-1}}$	8.314	8.314	8.314
Check for Inter-Particle Mass Transfer Limitations			
$1/(1+(r^b_{n-C4} \cdot \rho_B \cdot d_p \cdot R \cdot T \cdot \rho_g)/(6 \cdot (k_g)_{n-C4} \cdot (1-\epsilon) \cdot p^b_{n-c4}))>0.95$	0.96	0.95	0.96
Check for Inter-Particle Heat Transfer Limitations			
$\{(\lvert -\Delta H \rvert \cdot r_b \cdot \rho_b \cdot d_p \cdot E) / (2 \cdot h \cdot R \cdot T^2)\} < 0.15$	1.27e-3	1.78e-3	1.27e-3

A4.8.3 SIGNIFICANCE OF INTRA-PARTICLE HEAT TRANSFER

Heat transfer through the film around the catalyst particle will become limiting before heat transfer through the catalyst particle itself becomes limiting. As it has been confirmed that film heat transfer can be ignored, it is to be expected that intra-particle heat transfer will also not be limiting. A criterion proposed by Mears (1971:128) was used. Inter-particle heat transfer resistance will become limiting before intra-particle heat transfer resistance becomes limiting providing :

$$\frac{h \cdot d_p}{\lambda_{se}} < 10 \qquad \text{A4-73}$$

where

d_p is the particle diameter, m,

h is the film heat transfer coefficient, $W \cdot m^{-2} \cdot s^{-1}$ and

λ_{se} is the effective thermal conductivity of the solid, $W \cdot m^{-1} \cdot K^{-1}$.

An alternatively criterion to determine wether intra-particle heat transfer is limiting, that is valid wether diffusional limitations in the particle exist or not (Mears, 1971:542) is

$$\frac{|\Delta H| \cdot r_p \cdot d_p^2 \cdot E \cdot \rho_B}{4 \cdot \lambda_{se} \cdot T^2 \cdot R} < 1 \qquad \text{A4-74}$$

A4.8.4 SIGNIFICANCE OF INTRA-PARTICLE MASS TRANSFER

The presence of intra-particle diffusional resistance to mass transfer can be quantified by the relationship between the effectiveness factor and the Thiele modulus (Froment and Bischoff, 1990:159). In this study, when calculating the reaction rate inside the pore, the worst case, i.e., the maximum rate of n-butene consumption will be used. Hence, the n-butene skeletal isomerisation reaction will be considered to be first order and irreversible while checking whether resistance to intra-particle mass transfer is significant.

For any shape of catalyst particle and first order irreversible kinetics the Thiele modulus may be calculated Aris (1957) as reported by Froment and Bischoff (1990:160) using

$$\phi = \frac{V}{S} \cdot \left(\frac{k_1 \cdot \rho_s}{D^P_{jm}} \right)^{1/2} \qquad \text{A4-75}$$

where

k_1 is the reaction rate constant, $m^3_f \cdot kg^{-1}_{cat} \cdot s^{-1}$,
ρ_s is the density of the solid. $kg \cdot m^{-3}$,
V is the volume of the catalyst particle, m^3,
S is the surface area of the catalyst particle, m^2 and
D^P_{jm} is the effective binary diffusivity of component j in a multi-component mixture in the pore of the catalyst, $m^2 \cdot s^{-1}$.

The effectiveness factor may in turn be defined (Zeldowich, 1939), as reported by Froment and Bischoff, 1990:158) using

$$\eta = \frac{r_A^p}{r_A^b} \qquad \text{A4-76}$$

where

r_A^p is the reaction rate if slowed by diffusion in the pore, $moles \cdot kg^{-1}_{cat} \cdot s^{-1}$,
r_A^b is the reaction rate if not slowed by diffusion, $moles \cdot kg^{-1}_{cat} \cdot s^{-1}$ and
η is the effectiveness factor, -.

Hence, for the observed rate not to differ from the intrinsic rate, i.e., the rate in the absence of pore diffusion by more than 5 %, the effectiveness factor must be in excess of 0.95. The actual reaction rate that would be observed in the presence of pore diffusion limitations, for first order irreversible kinetics, would be

$$(r_A)_{obs} = \eta \cdot r_A \cdot C_A^b \qquad \text{A4-77}$$

where

$(r_A)_{obs}$ is the observed reaction rate, kmol·kg$^{-1}_{cat}$·s^{-1},
r^b_A is the reaction rate in the absence of transport limitations, kmol·kg$^{-1}_{cat}$·s^{-1} and
C^b_A is the bulk reactant concentration, kmol·m^{-3}.

Alternatively, the effectiveness factor may also be calculated from diffusion considerations, for a first order irreversible reaction (Froment and Bischoff, 1990:158) using

$$\eta = \frac{r_A^p}{r_A^b} = \frac{\tanh \phi}{\phi} \qquad \text{A4-78}$$

where

ϕ is the Thiele modulus as defined previously, -.

Based on the Weisz-Prater criterion (Weisz and Prater, 1954), (Froment and Bischoff, 1990:167) showed that by suitable manipulation of the above Equations, pore diffusion limitations are not significant if

$$\frac{(r_A \cdot \rho_s)_{obs} \cdot L^2}{D_{jm}^P \cdot C_A^b} \ll 1 \qquad \text{A4-79}$$

where

r_A is the observed rate of reaction of component A, kmol·kg$^{-1}_{cat}$·s^{-1},

ρ_s is the density of the solid, kg·m^{-3},

D^P_{jm} is the effective binary diffusivity of component j in a multi-component mixture in the pore of the catalyst particle, m^2·s^{-1} and

L is the volume (V) to surface area (S) ratio of the catalyst particle, which for spherical particle, reduces to $d_P/6$, m.

For a large ideal cylindrical pore, Ficks law for a binary system may be used to calculate the mass flux N_j defined as moles of j diffusing per unit pore cross sectional area and unit time. In this case, the effective binary fluid molecular diffusivity, as used in bulk transport phenomena, D_{jm}, may be used. However, in actual catalyst, the pore structure is far from ideal and again using Ficks law, the mass flux has to be expressed in terms of moles of j diffusing per unit pellet surface area and unit time. The effective binary diffusivity coefficient D_{jm} can not be used in this case and has to be modified to account for the actual open area and the tortuosity of the pores. The actual open area, according to Dupuit's law (Froment and Bischoff, 1990:145) is equivalent to the internal void fraction ϵ_s, usually with values of between 0.3 and 0.8. For the catalyst under review the solid void fraction was calculated to be $\epsilon_s = 0.68$. The diffusion path, due to the tortuous nature of the pores is also longer than the measurable pellet thickness. This tortuosity factor should have a value of approximately $3^{0.5}$ for loose random pore structures but measured values of 1.5 up to 10 have been reported while Satterfield (1970) states that many common catalyst materials have a tortuosity factor of 3 to 4. During this study, the tortuosity factor, in the absence of actual data was assumed to be $\tau = 3.5$. Hence, the bulk effective binary diffusivity coefficient, D_{jm}, may be adjusted for the conditions in a catalyst pore (Froment and Bischoff, 1990:146) using

$$D^P_{jm} = \frac{\epsilon_s}{\tau} \cdot D_{jm} \qquad \text{A4-80}$$

where

ϵ_s is the particle internal void fraction, - and

τ is the tortuosity factor, -.

As may be seen from Table A4-8, intra-particle heat and mass transfer limitations are not significant enough to warrant the use of a heterogeneous model to describe these.

TABLE A4.8 : SIGNIFICANCE OF INTRA-PARTICLE RESISTANCES

Reactor	Pilot	Bench scale	
Particle Diameter, m	1.5e-3	1.5e-3	1.5e-3
Global Reaction Rate, $kmol\cdot kg^{-1}_{cat}\cdot s^{-1}$	2.16e-6	2.16e-6	2.16e-6
Bed Density, $kg\cdot m^{-3}$	650	650	650
Heat of Reaction, $J\cdot kmole^{-1}$	-8.58e6	-8.58e6	-8.58e-6
Activation Energy, $J\cdot kmole^{-1}$	8.94e7	8.94e7	8.94e7
Bulk Temperature, K	793	793	793
Solid Density, $kg\cdot m^{-3}$	3731	3731	3731
Solid Thermal Conductivity, $W\cdot m^{-1}\cdot K^{-1}$	0.37	0.37	0.37
Solid Voidage, -	0.68	0.68	0.68
Bulk n-Butene Concentration, $kmole\cdot m^{-3}$	7.58e-3	7.58e-3	7.58e-3
Bulk Diffusion Coefficient, $m^2\cdot s^{-1}$	5.09e-5	5.09e-5	5.09e-5
Pore Diffusion Coefficient, $m^2\cdot s^{-1}$	9.89e-6	9.89e-6	9.89e-6
Film Heat Transfer Coefficient, $W\cdot m^{-2}\cdot S^{-1}$	121.4	86.7	121.5
Gas Constant, $J\cdot kmole^{-1}\cdot K^{-1}$	8314	8314	8314
Reaction Rate Constant, $m^3_f\cdot kg^{-1}\cdot s^{-1}$	2.85e-4	2.85e-4	2.85e-4
Thiele Modulus, -	8.2e-2	8.2e-2	8.2e-2
Check for Intra-Particle Mass Transfer Limitations			
$\{\tanh((d_p/6)(k_1\cdot\rho_s/D^p_{jm}))/(d_p/6)\cdot(k_1\cdot\rho_s/D^p_{jm})\} > 0.95$	0.998	0.998	0.998
$\{((r_p\cdot\rho_s)_{obs}\cdot(d_p/6)^2)/(D^p_{jm}\cdot C_A{}^b)\} < 1$	6.7e-3	6.7e-3	6.7e-3
Check for Intra-Particle Heat Transfer Limitations			
$\{(\lvert-\Delta H\rvert\cdot r_b\cdot\rho_b\cdot d_p{}^2\cdot E\cdot\rho_B) / (4\cdot\lambda_{se}\cdot R\cdot T^2)\} < 1$	3.11e-4	3.11e-4	3.11e-4
$\{(d_p\cdot h) / (\lambda_{se})\} < 10$	0.49	0.35	0.49

APPENDIX 5 - PROGRAM CODES AND DATA FILES

Given below is an algorithm of the calculation procedure used to model the kinetics of the isomerisation reaction, as are the actual FORTRAN source code and the input files. The FORTRAN code developed during this study is based on that originally set up by Keyser (1995). The listing of the Levenberg-Marquardt routine used is not given, as this is a commercially available program.

A5.1 PROGRAM ALGORITHM

Program : ISOMT.FOR

```
10    Open performance output file (File 1)
20    Open performance data file (File 2)
30    Open coefficient output file (File 3)
40    Open coefficient data file (File 4)
50    Call Input sub routine (INP)
60    Define counters, MDOEL, IXJAC, NSIG, EPS, DELTA, MAXFEN, IOPT
70    Set negative k and E values returned by the Levenberg-Marquardt routine equal to 1e-3, K1(1), K1(2), K1(3), K1(4), K1(5), K1(6), K1(7), K1(8), K1(9), K1(10), K1(11), K1(12)
80    Set counter equal to zero, SOM, SSQQ
90    Increment experiment counter, MDOEL
100   Assign experiment specific linear velocity, U(1)
110   Assign experiment specific inlet concentration variable, CTOT
120   Assign experiment specific total bed height variable, Z
130   Reset molar mass variable, GEMMOL
140   Reset bed increment counter to zero, JJ
150   Calculate increment inlet concentration for each component, CIN1(J,1,1)
160   Calculate average molecular weight at the increment inlet, GEMMOL
170   Calculate increment inlet mass flow rate, G
```

```
180 For each component, secure the increment inlet concentrations, C(J,1,1)
190 Increment bed increment counter, JJ
200 Calculate catalyst bed penetration depth, ZL
210 For each component, J, set the increment outlet concentration equal to the increment inlet concentration, C(J,JJ+1,1)
220 Set iteration counter equal to zero, ITEL
230 Increment iteration counter, ITEL
240 If ITEL greater than 500, Go to Line Number 390
250 For each component calculate partial pressures at the increment outlet, PNC4, PIC4, PBP, PH2O
260 For each reaction calculate the rate coefficients, XK1, XK2, XK3, XK4, XK5, XK6, XK7, XK8, XK9, XK10, XK11, XK12
270 Using the appropriate rate equation (Case 1 to 8), calculate the n-butene skeletal isomerisation rate, RSI
280 Using the by-product rate equation calculate the rate of by-product formation, RBP
290 For each component, J, calculate the reaction rate, R1(J)
300 Reset counters to zero, SOMC, GEMMOL
310 For each component, J, calculate the increment outlet concentrations using the calculated component reaction rates, R1(J), linear velocity and temperature, CNEW(J)
320 For each component, check the validity of the calculated concentration
330 Calculate the total increment outlet concentration, SOMC
340 Calculate increment outlet average molecular weight, GEMMOL
350 For each component, J, compare the previous increment outlet concentrations, C(J,JJ+1,1), with the calculated increment outlet concentrations, CNEW(J). If for any component the difference is greater than 1e-6, Go to Line Number 370
360 Go to Line Number 400
370 For each component, J, set the increment outlet concentrations, C(J,JJ+1,1), equal to the calculated increment outlet concentrations, CNEW(J)
380 Go to Line Number 230
390 Notify that convergence over the increment was not achieved
```

400 Calculate the difference between the actual, CTOT, and calculated, SOMC, increment outlet concentration, DS. If the difference is greater than 0.01, Notify that the concentration did not remain constant

410 Calculate the total mass flow rate at the increment outlet, GX

420 Calculate the difference between the actual, G, and calculated, GX, increment outlet mass flow rate, DX. If the difference is greater than 0.01, Notify that the mass flow rate is not constant

430 If the total distance into the catalyst bed, ZL, is less then the total bed height, Z, Go to Line Number 190

440 For each component, J, calculate the final increment outlet mole fraction, MOLOUT(J,1,I)

450 For each component, J, calculate the final increment outlet partial pressure, DUM1, DUM2, DUM3, DUM4

460 For n-butene, isobutene, and if included the by-products, calculate the fractional error between the actual and calculated final increment outlet partial pressures, F1, F2 and if included F3

470 Calculate the total experiment, I, specific error, F(I)

480 Summate the total sum of the experiment specific errors, SOM

490 Summate the sum of the squares of the experiment specific errors, SSQQ

500 If required, INK=1, write actual and calculated reactor outlet partial pressures to File 1

510 For each experiment, Notify the completion of the simulation loop

520 If the end of the experiment data file has not been reached, Go to Line Number 90

530 Calculate the difference between the previous and latest total sum of squares of the experiment specific errors. If the convergence criteria for the Marquard routine are not satisfied, adjust as needed the values of K1(1), K1(2), K1(3), K1(4), K1(5), K1(6), K1(7), K1(8), K1(9), K1(10), K1(11) and K1(12) using the IMSL supplied Marquard routine. Go to Line Number 70

540 If required, INK=1, write each of the optimised rate constants and activation energies to File 1

550 If required, INK=1, write overall error to File 1

560 Write Case Number, ICASE, to File 4

```
570 Write number of variables, N, to File 4
580 Write optimised k and E values to File 4
590 Write Marquard convergence criteria achieved to File 4
600 If convergence was not achieved, write Marquard error code to File 4
610 Write total sum of errors squared to File 4
620 End
```

Subroutine INP

```
630 In File 3, read the case number, ICASE
640 In File 2, read the data writing flag, INK
650 In File 2, read the catalyst bed bulk density, RHO
660 In File 2, read the number of components, J1
670 In File 2, read the number of reactions, S
680 In File 2, for each component, I, and each reaction, J, read the stoichiometric coefficient, N1(I,J)
690 In File 2, read the mole mass for each component, I, MOLMAS(I)
700 In File 2, read the number of experiments, M
710 In File 3, read the read the number of variables, N
720 In File 2, read the bed increment height, DZ
730 In File 3, for each reaction read the initial guesses for the rate constants and activation energies, K1(1), K1(2), K1(3), K1(4), K1(5), K1(6), K1(7), K1(8), K1(9), K1(10), K1(11), K1(12)
740 In File 2, for each experiment, M, read the reactor cross sectional area, XSA(M)
750 In File 2, for each experiment, M, read the butene gas flow rate, BUTENE(M)
760 In File 2, for each experiment, M, read the water flow rate, WATER(M)
770 In File 2, for each experiment, M, read the mass of catalyst charged, CAT(M)
780 In File 2, for each experiment, M, and component J, read the feed mole fraction, MOLFR1(J,1,I)
790 In File 2, for each experiment, M, read the total system pressure, P0(M)
800 In File 2, for each experiment, M, read the read the system temperature, T0(M)
810 In File 2, for each experiment, M, read the time on line, TIME(M)
```

820 In File 2, for each experiment, M, and component J read the product mole fraction, DOEL(I,J)

830 For each experiment, M, convert the system temperature from Celsius to Kelvin, T0(M)

840 For each experiment, M, calculate the total inlet concentration, CONCT(M)

850 For each experiment, M, convert the catalyst mass from gram to kilogram, CAT(M)

860 For each experiment, M, calculate the total bed height, ZT(M)

870 For each experiment, M, convert the butene flow rate from $g{\cdot}h^{-1}$ to $g{\cdot}s^{-1}$, BUTENE(M)

880 For each experiment, M, convert the water flow rate from $g{\cdot}h^{-1}$ to $g{\cdot}s^{-1}$, WATER(M)

890 For each experiment, M, calculate the linear velocity, UI(M)

900 Return

A5.2 FORTRAN SOURCE CODE

```
C     KINETICS PROGRAM C:\FORTRAN \ISOMT.FOR
C     MASS ACTION LAW RATE EQUATION
C     MULTI-STEP TYPE RATE EQUATIONS - ONE RATE CONTROLLING STEP
C     MULTI-STEP TYPE RATE EQUATIONS - TWO RATE CONTROLLING STEPS
C      MULTI-STEP TYPE RATE EQUATION - THREE RATE CONTROLLING STEPS
C     POWER LAW - BY-PRODUCT FORMATION
C
      EXTERNAL FUNC
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON MOLMAS(5),MOLFR1(5,1,500),MOLOUT(5,1,500),
     +CIN1(5,1,1),U(500),G,DT,DZ,RHO,ZT(500),FACT(50),ZL,T,
     +SOMC,GX,CNEW(5),UI(500),INK,ICASE,DOEL(500,10),
     +PNC4,PIC4,PPC4,PLTC4,PGTC4,PH2O,CONCT(500),C(500,500,1),
     +K1(50),R1(5),N1(5,5),J1,S,JJ,KK,NZ,NT,CTOT,R1SOM,
     +P0(500),T0(500),MDOEL,II,E,TIME(500),CT
      INTEGER J1,S,JJ,KK,INK,ICASE,II,E,M,N,IXJAC,NSIG,MAXFN,
     +IOPT,I,INFER,IER
```

```
      REAL*8 KA,KR,KD,K1,N1,MOLFR1,MOLOUT,X(150),F(500),PARM(4),
     +XJAC(1500,10),EPS,DELTA,SSQ,XJTJ(1500),WORK(2000),CT
C
      OPEN(2,FILE='ALLT.DAT')
      OPEN(4,FILE='KOUT.DAT')
      OPEN(3,FILE='KIN.DAT')
      CALL INP(M,N)
      IF(INK.EQ.1)OPEN(1,FILE='ISOM.OUT')
      MDOEL=M
      IXJAC=M
      NSIG=10
      EPS=0
      DELTA=0
      MAXFN=1000
      IOPT=1
      DO 1 I=1,N
      X(I)=K1(I)
1     CONTINUE
C
      CALL MARQ(FUNC,M,N,NSIG,EPS,DELTA,MAXFN,IOPT,PARM,
     +X,SSQ,F,XJAC,IXJAC,XJTJ,WORK,INFER,IER)
      WRITE(4,*)ICASE
      WRITE(4,*)N
      DO 7 I=1,N
      WRITE(*,157)I,X(I),FACT(I)
      WRITE(4,*)X(I),FACT(I)
7     CONTINUE
      WRITE(*,*)
      WRITE(*,*)'MARQUARD ERROR CODE INFER (0 IS BAD !) ',INFER
      IF(INFER.EQ.0)WRITE(*,*)'MARQUARD ERROR CODE IER ',IER
      WRITE(*,*)' '
      WRITE(*,*)'SUM OF ERRORS SQUARED =',SSQ
```

```
      WRITE(4,*)' '
      WRITE(4,*)'MARQUARD ERROR CODE INFER (0 IS BAD !) ',INFER
      IF(INFER.EQ.0)WRITE(4,*)'MARQUARD ERROR CODE IER ',IER
      WRITE(4,*)' '
      WRITE(4,*)'SUM OF ERRORS SQUARED =',SSQ
157   FORMAT(5X,'K(',I3,') = ',F10.5,'  *',E10.1)
      END
C
      SUBROUTINE FUNC(X,M,N,F)
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON MOLMAS(5),MOLFR1(5,1,500),MOLOUT(5,1,500),
     +CIN1(5,1,1),U(500),G,DT,DZ,RHO,ZT(500),FACT(50),ZL,T,
     +SOMC,GX,CNEW(5),UI(500),INK,ICASE,DOEL(500,10),
     +PNC4,PIC4,PPC4,PLTC4,PGTC4,PH2O,CONCT(500),C(500,500,1),
     +K1(50),R1(5),N1(5,5),J1,S,JJ,KK,NZ,NT,CTOT,R1SOM,
     +P0(500),T0(500),MDOEL,II,E,TIME(500),CT
C
      INTEGER J1,S,JJ,KK,INK,ICASE,II,E,M,N,IXJAC,NSIG,MAXFN,
     +IOPT,I,INFER,IER
C
      REAL*8 KA,KR,KD,K1,N1,MOLFR1,MOLOUT,X(150),F(500),PARM(4),
     +XJAC(1500,10),EPS,DELTA,SSQ,XJTJ(1500),WORK(2000),CT
C
      DO 10 I=1,N
      IF(X(I).LE.0)X(I)=1E-3
10    CONTINUE
      DO 12 I=1,N
      K1(I)=X(I)
12    CONTINUE
      SOM=0
      SSQQ=0
```

```
      ICOT=ICOT+1
      DO 55 I=1,MDOEL
      U(1)=UI(I)
      CTOT=CONCT(I)
      Z=ZT(I)
      GEMMOL=0
      JJ=0
      DO 5 J=1,J1
      CIN1(J,1,1)=MOLFR1(J,1,I)*CTOT
      GEMMOL=GEMMOL+MOLFR1(J,1,I)*MOLMAS(J)
5     CONTINUE
      G=U(1)*CTOT*GEMMOL/1000
      DO 1 J=1,J1
      C(J,1,1)=CIN1(J,1,1)
1     CONTINUE
1000  JJ=JJ+1
      ZL=DZ*JJ
      DO 13 J=1,J1
      C(J,JJ+1,1)=C(J,JJ,1)
13    CONTINUE
      ITEL=0
1234  ITEL=ITEL+1
      IF(ITEL.GT.500)GO TO 143
      PNC4=C(1,JJ+1,1)/CTOT*P0(I)
      PIC4=C(2,JJ+1,1)/CTOT*P0(I)
      PBP=C(3,JJ+1,1)/CTOT*P0(I)
      PH2O=C(4,JJ+1,1)/CTOT*P0(I)
C
C       KINETIC EQUATIONS
C
      IF(ICASE.EQ.20)GO TO 892
      IF(ICASE.GT.16)GO TO 894
```

```
      IF(ICASE.GE.13)GO TO 893
      IF(ICASE.EQ.1)THEN
      XK1=K1(1)*FACT(1)*EXP(-1*(K1(2)*FACT(2))/(1.987*T0(I)))
      XK2=K1(3)*FACT(3)*EXP(-1*(K1(4)*FACT(4))/(1.987*T0(I)))
      ELSE
      XK1=K1(1)*FACT(1)*EXP(-1*(K1(2)*FACT(2))/(1.987*T0(I)))
      XK2=K1(3)*FACT(3)*EXP(-1*(K1(4)*FACT(4))/(1.987*T0(I)))
      XK3=K1(5)*FACT(5)*EXP(-1*(K1(6)*FACT(6))/(1.987*T0(I)))
      XK4=K1(7)*FACT(7)*EXP(-1*(K1(8)*FACT(8))/(1.987*T0(I)))
      XK5=K1(9)*FACT(9)*EXP(-1*(K1(10)*FACT(10))/(1.987*T0(I)))
      XK6=K1(11)*FACT(11)*EXP(-1*(K1(12)*FACT(12))/(1.987*T0(I)))
      ENDIF
      GO TO 892
893   XK1=K1(1)*FACT(1)*EXP(-1*(K1(2)*FACT(2))/(1.987*T0(I)))
      XK2=K1(3)*FACT(3)*EXP(-1*(K1(4)*FACT(4))/(1.987*T0(I)))
      XK3=K1(5)*FACT(5)*EXP(-1*(K1(6)*FACT(6))/(1.987*T0(I)))
      XK4=K1(7)*FACT(7)*EXP(-1*(K1(8)*FACT(8))/(1.987*T0(I)))
      XK5=K1(9)*FACT(9)*EXP(-1*(K1(10)*FACT(10))/(1.987*T0(I)))
      GO TO 892
891   XK1=K1(1)*FACT(1)*EXP(-1*(K1(2)*FACT(2))/(1.987*T0(I)))
      GO TO 892
 894  XK1=K1(1)*FACT(1)*EXP(-1*(K1(2)*FACT(2))/(1.987*T0(I)))
      XK2=K1(3)*FACT(3)*EXP(-1*(K1(4)*FACT(4))/(1.987*T0(I)))
      XK3=K1(5)*FACT(5)*EXP(-1*(K1(6)*FACT(6))/(1.987*T0(I)))
      XK4=K1(7)*FACT(7)*EXP(-1*(K1(8)*FACT(8))/(1.987*T0(I)))
      XK5=K1(9)*FACT(9)*EXP(-1*(K1(10)*FACT(10))/(1.987*T0(I)))
      XK6=K1(11)*FACT(11)*EXP(-1*(K1(12)*FACT(12))/(1.987*T0(I)))
      XK7=K1(13)*FACT(13)*EXP(-1*(K1(14)*FACT(14))/(1.987*T0(I)))
      XK8=K1(15)*FACT(15)*EXP(-1*(K1(16)*FACT(16))/(1.987*T0(I)))
892   CONTINUE
      CT=1
```

```
C  CASE 1 - POWER LAW
      IF(ICASE.EQ.1)THEN
      XK=XK1/XK2
      RSI=CT*XK1*(PNC4-PIC4/XK)
      ENDIF
C
C CASE 2  - ADSORPTION
      IF(ICASE.EQ.2)THEN
      XK=(XK1*XK2*XK3)/(XK4*XK5*XK6)
      XKA=XK1/XK4
      XKS=XK2/XK5
      XKD=XK3/XK6
      RTL=CT*(PNC4-PIC4/XK)
      RBL1=(1/XK1)
      RBL2=((XKS+1)/(XKS*XK1))*(PIC4/XKD)
      RSI=RTL/(RBL1+RBL2)
      ENDIF
C
C CASE 3 - SURFACE
      IF(ICASE.EQ.3)THEN
      XK=(XK1*XK2*XK3)/(XK4*XK5*XK6)
      XKA=XK1/XK4
      XKS=XK2/XK5
      XKD=XK3/XK6
      RTL=CT*(PNC4-PIC4/XK)
      RBL1=1/(XKA*XK2)
      RBL2=(1/(XKA*XK2))*(XKA*PNC4)
      RBL3=(1/(XKA*XK2))*(PIC4/XKD)
      RSI=RTL/(RBL1+RBL2+RBL3)
      ENDIF
C
C
```

```
C  CASE 4 - DESORPTION
      IF(ICASE.EQ.4)THEN
      XK=(XK1*XK2*XK3)/(XK4*XK5*XK6)
      XKA=XK1/XK4
      XKS=XK2/XK5
      XKD=XK3/XK6
      RTL=CT*(PNC4-PIC4/XK)
      RBL1=1/(XK*XK6)
      RBL2=((1+XKS)/(XK*XK6))*(XKA*PNC4)
      RSI=RTL/(RBL1+RBL2)
      ENDIF
C
C  CASE 5  - SURFACE + DESORPTION
      IF(ICASE.EQ.5)THEN
      XK=(XK1*XK2*XK3)/(XK4*XK5*XK6)
      XKA=XK1/XK4
      XKS=XK2/XK5
      XKD=XK3/XK6
      RTL=(PNC4-PIC4/XK)
      RBL1=(1/XK6)*(1/XK)+(1/XK2)*(1/XKA)
      RBL2=(((1+XKS)/(XK*XK6))+(1/(XK2*XKA)))*XKA*PNC4
      RBL3=(1/(XKA*XK2))*PIC4/XKD
      RSI=RTL/(RBL1+RBL2+RBL3)
      ENDIF
C
C CASE 6  -  ADSORPTION + DESORPTION
C
      IF(ICASE.EQ.6)THEN
      XK=(XK1*XK2*XK3)/(XK4*XK5*XK6)
      XKA=XK1/XK4
      XKS=XK2/XK5
      XKD=XK3/XK6
```

```
      RTL=(PNC4-PIC4/XK)
      RBL1=(1/(XK*XK6))+(1/(XK1))
      RBL2=((1+XKS)/(XK*XK6))*XKA*PNC4
      RBL3=((1+XKS)/(XK1*XKS))*PIC4/XKD
      RSI=RTL/(RBL1+RBL2+RBL3)
      ENDIF
C
C CASE 7  - ADSORPTION + SURFACE
      IF(ICASE.EQ.7)THEN
      XK=(XK1*XK2*XK3)/(XK4*XK5*XK6)
      XKA=XK1/XK4
      XKS=XK2/XK5
      XKD=XK3/XK6
      RTL=(PNC4-PIC4/XK)
      RBL1=(1/(XKA*XK2))+(1/XK1)
      RBL2=((1/(XKA*XK2))+(1+XKS)/(XKS*XK1))*PIC4/XKD
      RBL3=(1/XK2)*PNC4
      RSI=RTL/(RBL1+RBL2+RBL3)
      ENDIF
C
C CASE 8  -  ADSORPTION +SURFACE + DESORPTION
      IF(ICASE.EQ.8)THEN
      XK=(XK1*XK2*XK3)/(XK4*XK5*XK6)
      XKA=XK1/XK4
      XKS=XK2/XK5
      XKD=XK3/XK6
      RTL=CT*(PNC4-PIC4/XK)
      RBL1=(1/XK1)+(1/XK6)*(1/XK)+(1/XK2)*(1/XKA)
      RBL2=(((1+XKS)/(XK*XK6))+(1/(XK2*XKA)))*XKA*PNC4
      RBL3=((1/(XKA*XK2))+((XKS+1)/(XKS*XK1)))*PIC4/XKD
      RSI=RTL/(RBL1+RBL2+RBL3)
      ENDIF
```

```
C BY-PRODUCT FORMATION RATE EQUATION
C
      IF(ICASE.EQ.20)THEN
      XK1=K1(1)*FACT(1)*EXP(-1*(K1(2)*FACT(2))/(1.987*T0(I)))
      XK2=K1(3)*FACT(3)*EXP(-1*(K1(4)*FACT(4))/(1.987*T0(I)))
      XK3=K1(5)*FACT(5)*EXP(-1*(K1(6)*FACT(6))/(1.987*T0(I)))
      XK=XK1/XK2
      RSI=XK1*(PNC4-PIC4/XK)
      RBP=XK3*(PNC4**(K1(7)*FACT(7)))
      ELSE
      XKWGS=(0.07219)*EXP(-(13425)/(T0(I)*1.987))
      RBP=XKWGS*PNC4**(0.778)
      ENDIF
C
C      REACTION RATES
C
      R1(1)=-RSI-RBP
      R1(2)=RSI
      R1(3)=RBP
      R1(4)=0
      R1(5)=0
      R1(6)=0
      R1SOM=0
C
      SOMC=0
      GEMMOL=0
      DO 26 J=1,J1
      CNEW(J)=C(J,JJ,1)+(DZ*RHO*R1(J)/U(1))
      IF(CNEW(J).LT.0)THEN
      CNEW(J)=0.001
      WRITE(*,*)'CNEW LT ZERO'
      ENDIF
```

```
      IF(CNEW(J).GT.CTOT)THEN
      CNEW(J)=CTOT
      WRITE(*,*)'CNEW GT CTOT'
      ENDIF
      SOMC=SOMC+CNEW(J)
      GEMMOL=GEMMOL+MOLMAS(J)*CNEW(J)
26    CONTINUE
      GEMMOL=GEMMOL/SOMC
      DO 27 J=1,J1
      IF(ABS(C(J,JJ+1,1)-CNEW(J)).GT.1E-6)GO TO 28
27    CONTINUE
      GO TO 144
28    DO 29 J=1,J1
      C(J,JJ+1,1)=CNEW(J)
29    CONTINUE
      GO TO 1234
143   WRITE(*,*)'CONVERGENCE WAS NOT ACHIEVED....'
144   DS=ABS(CTOT-SOMC)
      IF(DS.GT.0.01)WRITE(*,*)'CONCENTRATION NOT CONSTANT',CTOT,SOMC
      GX=U(1)*SOMC*GEMMOL/1000
      DX=ABS(G-GX)
      IF(DX.GT.0.01)WRITE(*,*)'MASS FLOW RATE NOT CONSTANT',G,GX
      IF (ZL.LT.Z) GO TO 1000
      DO 1002 J=1,J1
      MOLOUT(J,1,I)=C(J,JJ+1,1)/SOMC
1002  CONTINUE
      DUM1=MOLOUT(1,1,I)*P0(I)
      DUM2=MOLOUT(2,1,I)*P0(I)
      DUM3=MOLOUT(3,1,I)*P0(I)
      DUM4=MOLOUT(4,1,I)*P0(I)
      F1=ABS(DUM1-(DOEL(I,1)*P0(I)))/(DOEL(I,1)*P0(I))
      F2=ABS(DUM2-(DOEL(I,2)*P0(I)))/(DOEL(I,2)*P0(I))
```

```
      IF(ICASE.EQ.20)THEN
      F3=ABS(DUM3-(DOEL(I,3)*P0(I)))/(DOEL(I,3)*P0(I))
      F(I)=F1+F2+F3
      ELSE
      F(I)=F2+F1
      ENDIF
      SOM=SOM+F(I)
      SSQQ=SSQQ+F(I)**2
      WRITE(*,741)I,DOEL(I,1)*P0(I),DUM1,DOEL(I,2)*P0(I),DUM2,
     +DOEL(I,3)*P0(I),DUM3
      IF(INK.EQ.1)THEN
      WRITE(1,741)I,TIME(I),DOEL(I,1)*P0(I),DUM1,DOEL(I,2)*P0(I),
     +DUM2,DOEL(I,3)*P0(I),DUM3,DOEL(I,4)*P0(I),DUM4
      ENDIF
55    CONTINUE
      WRITE(*,748)ICASE,ICOT
      IF(INK.EQ.1)THEN
      DO 71 I=1,N
      WRITE(1,*)I,X(I),FACT(I)
71    CONTINUE
      WRITE(1,*)SSQQ
      ENDIF
      IF(INK.EQ.1)STOP
      RETURN
741   FORMAT(I5,1X,10(F10.5,1X))
748   FORMAT(5X,'FOR CASE ',I5,' COMPLETED LOOP ',I5)
      END
```

```
   SUBROUTINE INP(M,N)
C
    IMPLICIT DOUBLE PRECISION (A-H,O-Z)
    COMMON MOLMAS(5),MOLFR1(5,1,500),MOLOUT(5,1,500),
   +CIN1(5,1,1),U(500),G,DT,DZ,RHO,ZT(500),FACT(50),ZL,T,
   +SOMC,GX,CNEW(5),UI(500),INK,ICASE,DOEL(500,10),
   +PNC4,PIC4,PPC4,PLTC4,PGTC4,PH2O,CONCT(500),C(500,500,1),
   +K1(50),R1(5),N1(5,5),J1,S,JJ,KK,NZ,NT,CTOT,R1SOM,
   +P0(500),T0(500),MDOEL,II,E,TIME(500),CT
C
    INTEGER J1,S,JJ,KK,INK,ICASE,II,E,M,N,IXJAC,NSIG,MAXFN,
   +IOPT,I,INFER,IER
C
    REAL*8 KA,KR,KD,K1,N1,MOLFR1,MOLOUT,X(150),F(500),PARM(4),
   +XJAC(1500,10),EPS,DELTA,SSQ,XJTJ(1500),WORK(2000),CT
C
    READ(3,*)ICASE
    READ(2,*)INK
    READ(2,*)RHO
    READ(2,*)J1
    READ(2,*)S
    DO 100 I=1,J1
    READ(2,*)(N1(I,J),J=1,S)
100 CONTINUE
11  READ(2,*)(MOLMAS(I),I=1,J1)
    READ(2,*)M
    READ(3,*)N
    READ(2,*)DZ
    READ(3,*)(K1(J),FACT(J),J=1,N)
    DO 2 I=1,M
    READ(2,*)XSA,BUTENE,WATER,CAT,(MOLFR1(J,1,I),J=1,J1),
   +P0(I),T0(I),TIME(I),(DOEL(I,J),J=1,J1)
```

```
      T0(I)=T0(I)+273.15
      CONCT(I)=P0(I)/(8.314E-3*T0(I))
      CAT=CAT/1000
      ZT(I)=CAT/(RHO*XSA)
      BUTENE=BUTENE/(3600)
      WATER=WATER/(3600)
      UI(I)=((BUTENE/56)+(WATER/18))*0.008314*T0(I)/(P0(I)*XSA)
2     CONTINUE
      RETURN
      END
C I IS THE EXPERIMENT NUMBER, -
C XSA IS THE REACTOR CROSS SECTIONAL AREA
C BUTENE IS THE N-BUTENE FLOWRATE, G/H
C WATER IS THE WATER FLOW RATE, G/H
C CAT IS THE CATALYST MASS, G
C MOLFR1(1,1,I)=MOLE FRACTION N-C4" IN
C MOLFR1(1,1,I)=MOLE FRACTION I-C4" IN
C MOLFR1(1,1,I)=MOLE FRACTION BP IN
C MOLFR1(1,1,I)=MOLE FRACTION H2O IN
C P0(I) IS THE REACTOR PRESSURE, KPA(A)
C T0(I) IS THE REACTOR TEMPERATURE,°C
C  DOEL(I,1)=MOLE FRACTION N-C4" OUT
C  DOEL(I,2)=MOLE FRACTION I-C4" OUT
C  DOEL(I,3)=MOLE FRACTION BP OUT
C  DOEL(I,4)=MOLE FRACTION H2O OUT
C  DOEL(I,5)=TOTAL CONVERSION
C  DOEL(I,6)=LOSS OF BUTENES
```

A5.3 DATA FILES

The input data required to optimise the values of the various kinetic parameters were read into the program using dedicated data files as shown below. The format of the file used to read in the initial guesses of the various parameters as well as the case number and the number of parameters to be optimised is shown below for Case 8. A complete listing of the optimum values of the parameters considered for each of the eight cases are shown in Table A5.1. (See also Appendix 3 and 4 and Chapter 5 and 6) Text in *italics* did not form part of the original input file but was added, to assist the reader. A key for the various abbreviations is given at the end.

A5.3.1 FILE 3 : KINETIC PARAMETER FILE - CASE 8

8 *Case Number, ICASE*

12 *No of parameters, N*

K1 Values, K1(I)	*Multiplier, FACT(I)*
0.122640795901240	1.00000000000000
0.118504153848820	100000.000000000
0.604317358534415	10.0000000000000
0.522893248211269	10000.0000000000
0.160835053821770	10.0000000000000
0.417533185761222	10000.0000000000
0.443340336917899	1.00000000000000
0.501707405310823	10000.0000000000
0.121204736364146	10.0000000000000
0.505234862192239	10000.0000000000
0.319824775904723	1.00000000000000
0.755424346269017	10000.0000000000

TABLE A5.1 : OPTIMUM VALUES OF K AND E FOR CASE 1 to 8

Case	1	2	3	4	5	6	7	8
k_1	0.0948	0.1195	0.1115	0.0752	0.067	0.118	0.120	0.123
E_1	11785	12015	10975	12396	12034	11921	11962	11850
k_2	0.3613	5.3659	2.6827	3.7872	3.193	5.533	8.153	6.043
E_2	12979	5281	5826	5518	6148	5144	4988	5229
k_3	-	1.0596	1.5293	0.6789	0.926	1.423	1.438	1.608
E_3	-	4569	3533	4980	4416	4172	4703	4175
k_4	-	0.3278	1.4461	0.4561	0.514	0.393	0.401	0.443
E_4	-	5537	3939	5080	4663	5207	5286	5017
k_5	-	1.5046	0.3052	1.8496	0.915	1.471	1.964	1.212
E_5	-	5260	7286	4876	6303	5170	5188	5052
k_6	-	0.2492	0.7313	0.700	0.177	0.262	0.291	0.319
E_6	-	7931	8016	10130	9397	7435	7842	7554

To develop the kinetic equations for the n-butene skeletal isomerisation reaction, all of the data points generated using the bench reactor system were used. The 'best' kinetic rate equation, identified using the procedure discussed above and in Chapter 6, was then used to predict the performance of the pilot plant. The pilot plant data used is also shown below. To develop the formation of by-products, the average result from each of the runs conducted in the bench reactor and the pilot plant were used. A key for the abbreviations used is given at the end in Table A5-2.

A5.3.2 INPUT FILE 2 : BENCH REACTOR DATA

0	*Write results to File 1, 0 = no, 1=yes*
650	*Catalyst density, $kg{\cdot}m^{-3}$*
4	*Number of components*
2	*Number of reactions, -*
-1 -1	*n-Butene Stoichiometric coefficient*
+1 +0	*Isobutene Stoichiometric coefficient*
+0 +1	*By-products Stoichiometric coefficient*
+0 +0	*H_2O Stoichiometric coefficient*
56 56 55 18	*Molar weight of each components, g/mol*
392	*Number of data points, -*
0.0025	*Step size, m*
0.000131	*Reactor cross sectional area, m^2*

Data for Bench Reactor Run M-66

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*$p_T(a)$*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
33.6	20.0	7.35	0.3494	0.0004	0.0006	0.6496	153	523.4	1	0.3049	0.0423	0.0032	0.6496
35.3	20.1	7.35	0.3598	0.0004	0.0006	0.6391	155	524.3	2	0.3190	0.0386	0.0032	0.6391
37.0	19.7	7.35	0.3749	0.0004	0.0007	0.6241	151	524.8	3	0.3319	0.0400	0.0041	0.6241
37.1	19.8	7.35	0.3752	0.0004	0.0007	0.6238	153	525.7	4	0.3299	0.0422	0.0041	0.6238
37.2	19.8	7.35	0.3755	0.0004	0.0007	0.6234	155	524.6	5	0.3330	0.0391	0.0045	0.6234
37.1	19.7	7.35	0.3759	0.0004	0.0007	0.6230	155	524.6	6	0.3318	0.0411	0.0041	0.6230
37.2	19.5	7.35	0.3790	0.0004	0.0007	0.6199	153	524.5	7	0.3346	0.0412	0.0043	0.6199
37.4	19.2	7.35	0.3834	0.0004	0.0007	0.6155	151	526.6	8	0.3342	0.0453	0.0049	0.6155
37.7	19.3	7.35	0.3848	0.0004	0.0007	0.6141	153	524.8	9	0.3339	0.0478	0.0042	0.6141
37.9	18.9	7.35	0.3913	0.0004	0.0007	0.6076	151	525.0	10	0.3405	0.0470	0.0049	0.6076
37.5	18.2	7.35	0.3978	0.0004	0.0007	0.6010	151	525.1	11	0.3457	0.0485	0.0048	0.6010

Data for Bench Reactor Run M-133

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*$p_T(a)$*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
23.3	39.0	13.00	0.1605	0.0002	0.0003	0.8391	150	527.8	1	0.1401	0.0186	0.0022	0.8391
23.2	38.7	13.00	0.1611	0.0002	0.0003	0.8385	150	528.1	2	0.1403	0.0190	0.0022	0.8385
21.3	39.3	13.00	0.1476	0.0001	0.0003	0.8520	150	532.8	3	0.1292	0.0168	0.0021	0.8520
20.8	38.9	13.00	0.1465	0.0001	0.0003	0.8531	152	532.5	4	0.1303	0.0158	0.0009	0.8531
20.8	39.5	13.00	0.1442	0.0001	0.0003	0.8554	153	524.3	5	0.1272	0.0164	0.0009	0.8554
20.6	38.4	13.00	0.1468	0.0001	0.0003	0.8528	152	529.8	6	0.1274	0.0164	0.0034	0.8528
20.4	37.6	13.00	0.1482	0.0001	0.0003	0.8514	153	532.0	7	0.1303	0.0160	0.0023	0.8514
19.7	38.4	13.00	0.1413	0.0001	0.0002	0.8583	153	532.8	8	0.1259	0.0147	0.0011	0.8583

Data for Bench Reactor Run M-76

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*$p_T(a)$*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
21.7	19.0	5.85	0.2679	0.0003	0.0005	0.7313	152	526.4	1	0.2322	0.0327	0.0038	0.7313
23.3	19.0	5.85	0.2812	0.0003	0.0005	0.7180	150	525.7	2	0.2437	0.0352	0.0032	0.7180
22.5	18.6	5.85	0.2783	0.0003	0.0005	0.7209	150	526.0	3	0.2418	0.0331	0.0041	0.7209
21.5	18.5	5.85	0.2710	0.0003	0.0005	0.7283	150	525.4	4	0.2348	0.0339	0.0031	0.7283
20.9	18.5	5.85	0.2656	0.0003	0.0005	0.7336	150	525.3	5	0.2325	0.0311	0.0027	0.7336

Data for Bench Reactor Run M-53

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*$p_T(a)$*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
19.2	13.6	4.35	0.3106	0.0003	0.0006	0.6885	157	522.1	1	0.2716	0.0366	0.0033	0.6885
20.0	13.7	4.35	0.3194	0.0003	0.0006	0.6797	151	523.9	2	0.2788	0.0380	0.0035	0.6797
20.6	13.5	4.35	0.3289	0.0003	0.0006	0.6701	153	524.7	3	0.2834	0.0430	0.0035	0.6701

Data for Bench Reactor Run M-53 - Continued

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|		
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
21.5	13.5	4.35	0.3369	0.0003	0.0006	0.6621	153	525.1	4	0.2897	0.0446	0.0036	0.6621
22.7	13.3	4.35	0.3530	0.0004	0.0006	0.6460	153	523.7	5	0.3064	0.0445	0.0031	0.6460
23.0	13.5	4.35	0.3524	0.0004	0.0006	0.6466	151	524.0	6	0.3087	0.0421	0.0025	0.6466
22.7	13.6	4.35	0.3473	0.0003	0.0006	0.6518	149	523.2	7	0.3076	0.0380	0.0026	0.6518
22.7	13.4	4.35	0.3506	0.0004	0.0006	0.6484	153	523.3	8	0.3030	0.0439	0.0047	0.6484
23.0	13.5	4.35	0.3527	0.0004	0.0006	0.6463	149	523.8	9	0.3029	0.0465	0.0043	0.6463
23.0	13.5	4.35	0.3518	0.0004	0.0006	0.6472	150	523.0	10	0.3032	0.0446	0.0050	0.6472
23.0	13.2	4.35	0.3570	0.0004	0.0006	0.6420	150	524.6	11	0.3125	0.0410	0.0044	0.6420

Data for Bench Reactor Run M-107

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|		
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
52.6	26.2	8.85	0.3910	0.0004	0.0007	0.6079	150	528.9	1	0.3340	0.0526	0.0055	0.6079
51.7	25.9	8.85	0.3902	0.0004	0.0007	0.6087	153	529.1	2	0.3265	0.0577	0.0071	0.6087
48.0	26.1	8.85	0.3701	0.0004	0.0006	0.6288	150	529.1	3	0.3130	0.0487	0.0095	0.6288
47.6	26.2	8.85	0.3680	0.0004	0.0006	0.6310	150	529.1	4	0.3134	0.0480	0.0076	0.6310
47.2	25.5	8.85	0.3717	0.0004	0.0006	0.6272	150	528.1	5	0.3179	0.0478	0.0070	0.6272
46.6	25.9	8.85	0.3659	0.0004	0.0006	0.6330	150	528.3	6	0.3138	0.0468	0.0064	0.6330
45.9	26.7	8.85	0.3550	0.0004	0.0006	0.6440	151	528.3	7	0.3052	0.0451	0.0057	0.6440
45.8	26.1	8.85	0.3591	0.0004	0.0006	0.6399	151	525.9	8	0.3138	0.0416	0.0047	0.6399
46.1	25.9	8.85	0.3627	0.0004	0.0006	0.6363	150	526.2	9	0.3194	0.0395	0.0049	0.6363
47.8	27.3	8.85	0.3595	0.0004	0.0006	0.6395	150	526.3	10	0.3158	0.0384	0.0063	0.6395
48.7	26.3	8.85	0.3725	0.0004	0.0006	0.6265	150	525.6	11	0.3262	0.0430	0.0043	0.6265

Data for Bench Reactor Run M-132

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|		
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
24.4	17.2	13.00	0.3128	0.0003	0.0006	0.6863	150	503.6	1	0.2472	0.0428	0.0237	0.6863
24.4	17.1	13.00	0.3134	0.0003	0.0005	0.6858	150	503.6	2	0.2674	0.0431	0.0037	0.6858
23.8	17.2	13.00	0.3070	0.0003	0.0005	0.6921	150	501.3	3	0.2605	0.0420	0.0054	0.6921
22.5	17.4	13.00	0.2923	0.0003	0.0005	0.7068	150	500.7	4	0.2477	0.0387	0.0067	0.7068
22.4	17.5	13.00	0.2909	0.0003	0.0005	0.7083	150	499.9	5	0.2493	0.0401	0.0024	0.7083
23.3	17.7	13.00	0.2964	0.0003	0.0005	0.7028	150	500.5	6	0.2524	0.0414	0.0034	0.7028
23.5	17.5	13.00	0.3012	0.0003	0.0005	0.6980	150	502.2	7	0.2574	0.0400	0.0046	0.6980
23.9	16.6	13.00	0.3150	0.0003	0.0005	0.6841	150	500.9	8	0.2679	0.0424	0.0056	0.6841

Data for Bench Reactor Run M-125

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|		
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
16.7	21.3	13.00	0.2009	0.0002	0.0004	0.7985	182	524.2	1	0.1576	0.0416	0.0023	0.7985
26.4	20.6	13.00	0.2915	0.0003	0.0005	0.7077	183	513.7	2	0.2453	0.0439	0.0031	0.7077
27.3	22.2	13.00	0.2825	0.0003	0.0005	0.7167	182	520.3	3	0.2341	0.0449	0.0043	0.7167
25.1	22.2	13.00	0.2664	0.0003	0.0005	0.7329	183	524.5	4	0.2309	0.0334	0.0029	0.7329
26.5	20.1	13.00	0.2969	0.0003	0.0005	0.7023	182	527.4	5	0.2540	0.0398	0.0039	0.7023
29.4	21.3	13.00	0.3070	0.0003	0.0005	0.6922	183	524.5	6	0.2594	0.0438	0.0047	0.6922
29.2	23.3	13.00	0.2864	0.0003	0.0005	0.7128	183	520.1	7	0.2513	0.0359	0.0010	0.7128
29.6	23.4	13.00	0.2884	0.0003	0.0005	0.7108	182	521.5	8	0.2526	0.0351	0.0014	0.7108

Data for Bench Reactor Run M-129

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|		
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
20.0	19.9	13.00	0.2427	0.0002	0.0004	0.7566	182	516.2	1	0.2106	0.0294	0.0034	0.7566
20.7	19.4	13.00	0.2549	0.0003	0.0004	0.7443	183	517.0	2	0.2026	0.0458	0.0073	0.7443
23.0	19.2	13.00	0.2774	0.0003	0.0005	0.7218	182	513.1	3	0.2349	0.0384	0.0049	0.7218
21.8	19.1	13.00	0.2669	0.0003	0.0005	0.7323	182	515.2	4	0.2192	0.0430	0.0055	0.7323

Data for Bench Reactor Run M-129 - Continued

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*p_T(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
23.9	20.3	13.00	0.2736	0.0003	0.0005	0.7256	183	519.5	6	0.2283	0.0374	0.0087	0.7256
23.4	20.1	13.00	0.2721	0.0003	0.0005	0.7272	183	518.6	7	0.2285	0.0391	0.0053	0.7272
23.8	20.7	13.00	0.2685	0.0003	0.0005	0.7307	183	519.1	8	0.2218	0.0355	0.0119	0.7307

Data for Bench Reactor Run M-135

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*p_T(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
19.7	16.9	13.00	0.2721	0.0003	0.0005	0.7271	85	533.5	1	0.2214	0.0485	0.0030	0.7271
19.5	16.4	13.00	0.2757	0.0003	0.0005	0.7235	85	532.5	2	0.2270	0.0466	0.0029	0.7235
19.5	17.1	13.00	0.2681	0.0003	0.0005	0.7312	85	533.2	3	0.2217	0.0442	0.0029	0.7312
20.8	17.9	13.00	0.2713	0.0003	0.0005	0.7279	85	532.8	4	0.2255	0.0436	0.0030	0.7279
20.6	17.6	13.00	0.2720	0.0003	0.0005	0.7272	85	532.8	5	0.2262	0.0438	0.0029	0.7272
19.6	16.9	13.00	0.2716	0.0003	0.0005	0.7276	85	536.3	6	0.2240	0.0453	0.0031	0.7276
19.7	16.6	13.00	0.2752	0.0003	0.0005	0.7240	85	535.8	7	0.2225	0.0499	0.0036	0.7240
19.8	16.9	13.00	0.2732	0.0003	0.0005	0.7260	85	534.3	8	0.2231	0.0475	0.0034	0.7260

Data for Bench Reactor Run M-124

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*p_T(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
23.8	10.3	13.00	0.4243	0.0004	0.0008	0.5745	117	520.8	1	0.3538	0.0682	0.0036	0.5745
23.6	11.3	13.00	0.3998	0.0004	0.0007	0.5991	119	519.0	2	0.3410	0.0571	0.0027	0.5991
23.3	13.9	13.00	0.3487	0.0003	0.0006	0.6503	117	525.6	3	0.2882	0.0596	0.0019	0.6503
23.0	13.8	13.00	0.3479	0.0003	0.0006	0.6511	117	525.7	4	0.2901	0.0560	0.0028	0.6511
22.9	11.6	13.00	0.3866	0.0004	0.0007	0.6124	117	521.5	5	0.2938	0.0847	0.0090	0.6124
22.8	8.6	13.00	0.4574	0.0005	0.0008	0.5414	117	521.5	6	0.3531	0.0982	0.0074	0.5414
23.2	11.2	13.00	0.3986	0.0004	0.0007	0.6003	117	520.3	7	0.3074	0.0859	0.0064	0.6003
23.0	11.2	13.00	0.3965	0.0004	0.0007	0.6024	117	521.1	8	0.3066	0.0863	0.0048	0.6024

Data for Bench Reactor Run M-64

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*p_T(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
8.9	6.5	5.85	0.3052	0.0003	0.0006	0.6939	153	522.9	1	0.2217	0.0649	0.0195	0.6939
8.7	6.4	5.85	0.3050	0.0003	0.0005	0.6941	153	523.4	2	0.2227	0.0643	0.0189	0.6941
10.6	6.8	5.85	0.3328	0.0003	0.0006	0.6663	153	523.2	3	0.2442	0.0695	0.0200	0.6663
12.7	7.0	5.85	0.3679	0.0004	0.0006	0.6311	153	523.4	4	0.2733	0.0748	0.0209	0.6311
13.0	6.7	5.85	0.3820	0.0004	0.0007	0.6170	151	525.9	5	0.2872	0.0755	0.0204	0.6170
11.8	6.9	5.85	0.3532	0.0004	0.0006	0.6458	151	524.4	6	0.2623	0.0718	0.0201	0.6458
10.5	6.9	5.85	0.3257	0.0003	0.0006	0.6733	85	525.7	8	0.2486	0.0631	0.0149	0.6733
10.9	6.9	5.85	0.3342	0.0003	0.0006	0.6648	85	525.7	9	0.2650	0.0597	0.0105	0.6648
10.9	7.0	5.85	0.3310	0.0003	0.0006	0.6680	85	525.1	10	0.2620	0.0601	0.0099	0.6680
10.6	7.2	5.85	0.3204	0.0003	0.0006	0.6787	85	524.6	11	0.2531	0.0592	0.0090	0.6787

Data for Bench Reactor Run M-137

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*p_T(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
27.2	15.6	13.00	0.3583	0.0004	0.0006	0.6407	213	529.8	1	0.2739	0.0761	0.0093	0.6407
27.7	17.0	13.00	0.3432	0.0003	0.0006	0.6559	215	528.6	2	0.2636	0.0693	0.0112	0.6559
27.8	16.4	13.00	0.3525	0.0004	0.0006	0.6465	215	530.3	3	0.2721	0.0675	0.0138	0.6465
24.9	15.4	13.00	0.3417	0.0003	0.0006	0.6574	215	531.6	4	0.2609	0.0662	0.0156	0.6574
25.6	15.3	13.00	0.3494	0.0004	0.0006	0.6497	215	532.3	5	0.2545	0.0764	0.0195	0.6497
28.9	16.2	13.00	0.3635	0.0004	0.0006	0.6354	215	531.2	6	0.2840	0.0690	0.0115	0.6354
29.0	16.4	13.00	0.3617	0.0004	0.0006	0.6373	215	499.8	7	0.2803	0.0719	0.0105	0.6373
29.7	16.5	13.00	0.3653	0.0004	0.0006	0.6337	215	531.2	8	0.2712	0.0682	0.0269	0.6337

Data for Bench Reactor Run M-138

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
30.0	14.4	13.00	0.4000	0.0004	0.0007	0.5989	149	527.3	1	0.2841	0.0951	0.0219	0.5989
30.0	16.3	13.00	0.3708	0.0004	0.0006	0.6281	150	530.4	2	0.2994	0.0626	0.0098	0.6281
29.8	18.8	13.00	0.3362	0.0003	0.0006	0.6628	150	531.4	3	0.2640	0.0672	0.0059	0.6628
27.2	17.1	13.00	0.3371	0.0003	0.0006	0.6619	150	530.0	4	0.2763	0.0554	0.0064	0.6619
27.4	15.3	13.00	0.3642	0.0004	0.0006	0.6348	150	532.6	5	0.2763	0.0789	0.0100	0.6348
30.1	17.0	13.00	0.3613	0.0004	0.0006	0.6377	149	531.4	6	0.2717	0.0817	0.0089	0.6377
30.4	18.4	13.00	0.3458	0.0003	0.0006	0.6533	149	532.5	7	0.2803	0.0614	0.0051	0.6533
30.8	18.1	13.00	0.3533	0.0004	0.0006	0.6457	150	533.2	8	0.2502	0.0931	0.0110	0.6457

Data for Bench Reactor Run M-109

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
21.9	14.5	14.25	0.3264	0.0003	0.0006	0.6727	153	527.1	1	0.2315	0.0718	0.0239	0.6727
22.3	14.1	14.25	0.3361	0.0003	0.0006	0.6629	152	528.2	2	0.2411	0.0771	0.0189	0.6629
22.9	14.2	14.25	0.3396	0.0003	0.0006	0.6595	150	529.7	3	0.2482	0.0772	0.0151	0.6595
22.9	14.3	14.25	0.3388	0.0003	0.0006	0.6602	150	530.3	4	0.2533	0.0757	0.0108	0.6602
23.1	14.2	14.25	0.3426	0.0003	0.0006	0.6564	150	529.5	5	0.2544	0.0776	0.0116	0.6564
23.3	14.0	14.25	0.3473	0.0003	0.0006	0.6518	150	527.4	6	0.2616	0.0760	0.0107	0.6518
23.1	14.0	14.25	0.3453	0.0003	0.0006	0.6537	150	528.1	7	0.2581	0.0751	0.0131	0.6537
23.1	14.2	14.25	0.3415	0.0003	0.0006	0.6575	150	528.3	8	0.2566	0.0751	0.0108	0.6575
23.2	14.5	14.25	0.3387	0.0003	0.0006	0.6604	150	528.3	9	0.2549	0.0743	0.0104	0.6604
22.9	14.5	14.25	0.3365	0.0003	0.0006	0.6626	150	528.3	10	0.2548	0.0726	0.0100	0.6626
22.4	14.5	14.25	0.3309	0.0003	0.0006	0.6682	150	528.3	11	0.2500	0.0711	0.0107	0.6682

Data for Bench Reactor Run M-81

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
10.0	7.7	7.35	0.2935	0.0003	0.0005	0.7057	150	547.6	1	0.2221	0.0631	0.0091	0.7057
9.9	7.8	7.35	0.2897	0.0003	0.0005	0.7095	150	544.2	2	0.2164	0.0650	0.0091	0.7095
9.3	8.0	7.35	0.2713	0.0003	0.0005	0.7279	149	544.9	3	0.2053	0.0583	0.0084	0.7279
10.1	7.9	7.35	0.2904	0.0003	0.0005	0.7088	149	544.9	4	0.2195	0.0631	0.0086	0.7088
10.8	7.7	7.35	0.3086	0.0003	0.0005	0.6905	151	544.9	5	0.2324	0.0677	0.0094	0.6905
10.5	7.9	7.35	0.2993	0.0003	0.0005	0.6999	151	545.3	6	0.2222	0.0690	0.0089	0.6999
11.5	8.0	7.35	0.3152	0.0003	0.0005	0.6839	151	543.9	7	0.2335	0.0724	0.0102	0.6839
11.5	7.9	7.35	0.3183	0.0003	0.0006	0.6808	151	545.4	8	0.2353	0.0728	0.0111	0.6808

Data for Bench Reactor Run M-111

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
18.5	11.4	20.00	0.3413	0.0003	0.0006	0.6577	150	406.7	1	0.2709	0.0655	0.0059	0.6577
18.1	11.6	20.00	0.3327	0.0003	0.0006	0.6664	150	427.9	2	0.2610	0.0528	0.0199	0.6664
17.6	10.8	20.00	0.3428	0.0003	0.0006	0.6562	153	474.7	3	0.2506	0.0731	0.0201	0.6562
17.7	10.3	20.00	0.3543	0.0004	0.0006	0.6447	152	479.6	4	0.2401	0.0948	0.0204	0.6447
18.7	11.2	20.00	0.3476	0.0003	0.0006	0.6514	151	479.5	5	0.2377	0.0878	0.0231	0.6514
18.9	11.2	20.00	0.3508	0.0004	0.0006	0.6482	151	476.1	6	0.2452	0.0897	0.0169	0.6482
19.0	11.2	20.00	0.3520	0.0004	0.0006	0.6470	150	479.4	7	0.2419	0.0919	0.0192	0.6470
18.8	11.4	20.00	0.3453	0.0003	0.0006	0.6537	150	480.9	8	0.2376	0.0875	0.0212	0.6537
18.8	11.4	20.00	0.3447	0.0003	0.0006	0.6543	150	479.4	9	0.2345	0.0884	0.0228	0.6543
18.9	11.3	20.00	0.3480	0.0003	0.0006	0.6511	150	480.1	10	0.2340	0.0901	0.0249	0.6511

Data for Bench Reactor Run M-71

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
13.9	6.8	8.85	0.3948	0.0004	0.0007	0.6041	151	521.6	1	0.2969	0.0883	0.0107	0.6041
13.5	6.9	8.85	0.3838	0.0004	0.0007	0.6151	151	526.6	2	0.2854	0.0879	0.0116	0.6151

Data for Bench Reactor Run M-71 - Continued

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
13.3	7.0	8.85	0.3757	0.0004	0.0007	0.6232	153	526.4	3	0.2762	0.0880	0.0126	0.6232
13.0	7.1	8.85	0.3680	0.0004	0.0006	0.6309	151	525.5	4	0.2642	0.0887	0.0162	0.6309
12.7	7.2	8.85	0.3598	0.0004	0.0006	0.6392	150	525.6	5	0.2577	0.0871	0.0160	0.6392
13.1	6.9	8.85	0.3773	0.0004	0.0007	0.6216	153	526.3	6	0.2698	0.0918	0.0168	0.6216
12.5	6.6	8.85	0.3766	0.0004	0.0007	0.6223	153	529.0	7	0.2790	0.0851	0.0136	0.6223
12.1	6.8	8.85	0.3604	0.0004	0.0006	0.6386	153	530.6	8	0.2644	0.0821	0.0149	0.6386
11.9	7.2	8.85	0.3455	0.0003	0.0006	0.6535	153	531.9	9	0.2510	0.0794	0.0160	0.6535
12.1	7.1	8.85	0.3535	0.0004	0.0006	0.6455	151	523.0	10	0.2646	0.0772	0.0127	0.6455
13.1	7.1	8.85	0.3708	0.0004	0.0006	0.6282	153	527.6	11	0.2797	0.0800	0.0121	0.6282

Data for Bench Reactor Run M-136

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
22.3	12.3	13.00	0.3670	0.0004	0.0007	0.6319	150	533.2	1	0.2541	0.0975	0.0165	0.6319
22.8	14.0	13.00	0.3422	0.0003	0.0006	0.6569	150	534.5	2	0.2467	0.0832	0.0133	0.6569
22.8	14.0	13.00	0.3428	0.0003	0.0006	0.6562	150	532.9	3	0.2578	0.0732	0.0128	0.6562
22.4	16.5	13.00	0.3030	0.0003	0.0005	0.6962	150	531.2	4	0.2332	0.0617	0.0089	0.6962
21.9	16.9	13.00	0.2938	0.0003	0.0005	0.7054	149	526.4	5	0.2163	0.0630	0.0154	0.7054
22.6	14.1	13.00	0.3380	0.0003	0.0006	0.6611	150	532.2	6	0.2510	0.0745	0.0134	0.6611
22.7	14.5	13.00	0.3333	0.0003	0.0006	0.6658	150	533.1	7	0.2497	0.0755	0.0091	0.6658
22.6	15.0	13.00	0.3259	0.0003	0.0006	0.6732	150	532.3	8	0.2431	0.0728	0.0109	0.6732

Data for Bench Reactor Run M-134

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
18.6	11.4	13.00	0.3418	0.0003	0.0006	0.6573	147	496.2	1	0.2528	0.0761	0.0138	0.6573
18.9	11.3	13.00	0.3492	0.0004	0.0006	0.6498	150	530.0	2	0.2591	0.0767	0.0143	0.6498
19.4	11.8	13.00	0.3451	0.0003	0.0006	0.6539	150	529.5	3	0.2558	0.0774	0.0129	0.6539
19.2	11.7	13.00	0.3446	0.0003	0.0006	0.6544	150	529.1	4	0.2537	0.0763	0.0156	0.6544
18.4	11.3	13.00	0.3429	0.0003	0.0006	0.6561	150	529.9	5	0.2507	0.0750	0.0182	0.6561
17.7	11.7	13.00	0.3270	0.0003	0.0006	0.6721	150	529.4	6	0.2284	0.0793	0.0201	0.6721
17.2	11.8	13.00	0.3185	0.0003	0.0006	0.6806	150	529.2	7	0.2161	0.0795	0.0238	0.6806
18.5	11.6	13.00	0.3385	0.0003	0.0006	0.6606	150	524.7	8	0.2450	0.0773	0.0171	0.6606

Data for Bench Reactor Run M-69

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
15.1	10.2	8.85	0.3202	0.0003	0.0006	0.6789	151	527.0	1	0.2277	0.0813	0.0121	0.6789
15.4	10.2	8.85	0.3245	0.0003	0.0006	0.6746	151	524.7	2	0.2313	0.0825	0.0116	0.6746
17.0	10.3	8.85	0.3461	0.0003	0.0006	0.6529	150	523.2	3	0.2513	0.0850	0.0108	0.6529
17.8	10.3	8.85	0.3549	0.0004	0.0006	0.6441	153	522.4	4	0.2592	0.0851	0.0116	0.6441
17.6	10.3	8.85	0.3540	0.0004	0.0006	0.6450	151	525.5	5	0.2603	0.0845	0.0101	0.6450
17.7	10.4	8.85	0.3530	0.0004	0.0006	0.6460	149	526.3	6	0.2594	0.0836	0.0109	0.6460
18.3	10.3	8.85	0.3618	0.0004	0.0006	0.6372	153	524.8	7	0.2556	0.0867	0.0205	0.6372
18.0	9.8	8.85	0.3705	0.0004	0.0006	0.6285	149	525.5	8	0.2775	0.0814	0.0126	0.6285
16.8	9.8	8.85	0.3549	0.0004	0.0006	0.6441	149	528.7	9	0.2592	0.0820	0.0147	0.6441
17.1	10.1	8.85	0.3513	0.0004	0.0006	0.6477	150	526.6	10	0.2599	0.0796	0.0129	0.6477
16.8	10.3	8.85	0.3438	0.0003	0.0006	0.6552	150	526.2	11	0.2575	0.0763	0.0109	0.6552

Data for Bench Reactor Run M-112

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
6.9	6.9	13.00	0.2442	0.0002	0.0004	0.7551	150	525.0	1	0.1724	0.0608	0.0118	0.7551
27.3	17.2	13.00	0.3367	0.0003	0.0006	0.6623	150	526.2	2	0.2449	0.0812	0.0117	0.6623
27.0	17.2	13.00	0.3336	0.0003	0.0006	0.6655	150	528.0	3	0.2430	0.0794	0.0122	0.6655

Data for Bench Reactor Run M-112 - Continued

Feed flow		*Mass*	*Feed Gas Composition*				*Parameters*		*Run*	*Product Gas Composition*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
27.0	17.1	13.00	0.3355	0.0003	0.0006	0.6635	153	527.0	5	0.2367	0.0812	0.0185	0.6635
27.5	17.0	13.00	0.3417	0.0003	0.0006	0.6574	150	525.7	6	0.2463	0.0837	0.0126	0.6574
27.7	17.4	13.00	0.3383	0.0003	0.0006	0.6608	146	526.7	7	0.2497	0.0772	0.0123	0.6608
27.6	17.9	13.00	0.3307	0.0003	0.0006	0.6683	148	526.9	8	0.2391	0.0771	0.0154	0.6683

Data for Bench Reactor Run M-73

Feed flow		*Mass*	*Feed Gas Composition*				*Parameters*		*Run*	*Product Gas Composition*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
13.9	8.7	8.85	0.3366	0.0003	0.0006	0.6625	151	524.1	1	0.2378	0.0854	0.0143	0.6625
13.3	8.8	8.85	0.3247	0.0003	0.0006	0.6744	151	523.7	2	0.2296	0.0805	0.0155	0.6744
13.3	8.8	8.85	0.3267	0.0003	0.0006	0.6724	150	524.0	3	0.2365	0.0778	0.0133	0.6724
13.1	8.7	8.85	0.3247	0.0003	0.0006	0.6744	150	526.0	4	0.2296	0.0805	0.0155	0.6744
13.4	8.9	8.85	0.3254	0.0003	0.0006	0.6737	152	526.2	5	0.2338	0.0783	0.0142	0.6737
13.8	8.9	8.85	0.3317	0.0003	0.0006	0.6674	151	522.9	6	0.2397	0.0789	0.0140	0.6674
13.9	8.6	8.85	0.3403	0.0003	0.0006	0.6588	150	523.3	7	0.2470	0.0799	0.0143	0.6588
13.9	8.8	8.85	0.3362	0.0003	0.0006	0.6628	150	522.7	8	0.2432	0.0797	0.0143	0.6628
13.8	9.1	8.85	0.3264	0.0003	0.0006	0.6727	150	523.1	9	0.2385	0.0752	0.0135	0.6727
14.2	9.3	8.85	0.3277	0.0003	0.0006	0.6714	150	524.0	10	0.2376	0.0763	0.0147	0.6714

Data for Bench Reactor Run M-65

Feed flow		*Mass*	*Feed Gas Composition*				*Parameters*		*Run*	*Product Gas Composition*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
12.6	8.3	7.35	0.3254	0.0003	0.0006	0.6737	151	524.6	1	0.2365	0.0797	0.0102	0.6737
12.6	8.6	7.35	0.3188	0.0003	0.0006	0.6803	151	524.3	2	0.2368	0.0740	0.0089	0.6803
12.6	8.5	7.35	0.3200	0.0003	0.0006	0.6791	150	524.8	3	0.2355	0.0774	0.0080	0.6791
12.5	8.6	7.35	0.3170	0.0003	0.0006	0.6821	150	524.8	4	0.2311	0.0787	0.0081	0.6821
12.5	8.1	7.35	0.3296	0.0003	0.0006	0.6694	150	524.6	5	0.2380	0.0839	0.0086	0.6694
12.2	8.1	7.35	0.3248	0.0003	0.0006	0.6743	150	524.8	6	0.2367	0.0797	0.0093	0.6743
11.9	8.5	7.35	0.3093	0.0003	0.0005	0.6899	150	525.4	7	0.2212	0.0799	0.0091	0.6899
11.9	8.5	7.35	0.3103	0.0003	0.0005	0.6889	151	525.6	8	0.2264	0.0760	0.0087	0.6889
12.1	8.5	7.35	0.3130	0.0003	0.0005	0.6862	151	525.3	9	0.2318	0.0731	0.0089	0.6862
12.2	8.6	7.35	0.3120	0.0003	0.0005	0.6872	152	526.3	10	0.2269	0.0761	0.0099	0.6872
12.2	8.6	7.35	0.3110	0.0003	0.0005	0.6881	151	527.1	11	0.2244	0.0772	0.0102	0.6881

Data for Bench Reactor Run M-116

Feed flow		*Mass*	*Feed Gas Composition*				*Parameters*		*Run*	*Product Gas Composition*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
27.8	14.8	13.00	0.3750	0.0004	0.0007	0.6239	150	534.0	2	0.2783	0.0823	0.0155	0.6239
29.3	14.0	13.00	0.4017	0.0004	0.0007	0.5972	150	533.2	3	0.2951	0.0933	0.0144	0.5972
32.3	14.4	13.00	0.4175	0.0004	0.0007	0.5813	150	533.1	4	0.3079	0.0956	0.0152	0.5813
33.8	14.9	13.00	0.4203	0.0004	0.0007	0.5785	153	533.2	5	0.3133	0.0944	0.0138	0.5785
33.8	14.4	13.00	0.4286	0.0004	0.0007	0.5702	153	533.6	6	0.3154	0.0991	0.0153	0.5702
33.5	14.4	13.00	0.4265	0.0004	0.0007	0.5723	150	534.1	7	0.3163	0.0973	0.0142	0.5723
31.5	14.6	13.00	0.4089	0.0004	0.0007	0.5900	150	534.8	8	0.3045	0.0915	0.0140	0.5900

Data for Bench Reactor Run M-128

Feed flow		*Mass*	*Feed Gas Composition*				*Parameters*		*Run*	*Product Gas Composition*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
19.4	10.5	13.00	0.3710	0.0004	0.0007	0.6279	118	532.7	1	0.2616	0.0990	0.0115	0.6279
19.3	10.0	13.00	0.3820	0.0004	0.0007	0.6169	118	529.9	2	0.2691	0.1014	0.0126	0.6169
19.4	9.7	13.00	0.3901	0.0004	0.0007	0.6088	119	530.9	3	0.2724	0.1039	0.0149	0.6088
20.0	9.5	13.00	0.4014	0.0004	0.0007	0.5975	119	531.8	4	0.2804	0.1076	0.0146	0.5975
20.1	9.4	13.00	0.4079	0.0004	0.0007	0.5910	117	532.9	5	0.2850	0.1100	0.0140	0.5910
19.6	9.6	13.00	0.3946	0.0004	0.0007	0.6043	119	523.4	6	0.2873	0.0968	0.0116	0.6043
19.8	10.1	13.00	0.3856	0.0004	0.0007	0.6133	118	531.2	7	0.2915	0.0846	0.0106	0.6133

Data for Bench Reactor Run M-80

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
11.0	7.4	7.35	0.3204	0.0003	0.0006	0.6787	157	526.6	1	0.2283	0.0794	0.0136	0.6787
11.2	7.4	7.35	0.3247	0.0003	0.0006	0.6744	153	525.3	2	0.2292	0.0814	0.0150	0.6744
11.1	7.4	7.35	0.3231	0.0003	0.0006	0.6760	153	525.0	3	0.2298	0.0781	0.0161	0.6760
12.6	7.6	7.35	0.3472	0.0003	0.0006	0.6518	150	525.0	4	0.2451	0.0870	0.0161	0.6518
13.5	7.5	7.35	0.3668	0.0004	0.0006	0.6321	143	526.4	5	0.2591	0.0886	0.0202	0.6321
12.9	7.4	7.35	0.3576	0.0004	0.0006	0.6414	149	525.5	6	0.2424	0.0916	0.0246	0.6414
13.0	7.3	7.35	0.3620	0.0004	0.0006	0.6370	151	524.3	7	0.2460	0.0901	0.0269	0.6370
12.8	7.2	7.35	0.3604	0.0004	0.0006	0.6386	149	525.4	8	0.2432	0.0909	0.0272	0.6386

Data for Bench Reactor Run M-121

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
19.6	16.8	13.00	0.2727	0.0003	0.0005	0.7265	185	544.3	1	0.2060	0.0591	0.0083	0.7265
19.7	15.5	13.00	0.2889	0.0003	0.0005	0.7103	185	545.2	2	0.2096	0.0686	0.0115	0.7103
19.8	14.3	13.00	0.3077	0.0003	0.0005	0.6914	185	544.9	3	0.2173	0.0778	0.0135	0.6914
19.8	13.5	13.00	0.3198	0.0003	0.0006	0.6793	185	549.8	4	0.2164	0.0871	0.0172	0.6793
19.8	13.9	13.00	0.3141	0.0003	0.0005	0.6850	185	545.1	5	0.2176	0.0843	0.0131	0.6850
20.0	15.1	13.00	0.2977	0.0003	0.0005	0.7014	185	548.2	6	0.2126	0.0732	0.0128	0.7014
19.6	15.3	13.00	0.2918	0.0003	0.0005	0.7074	185	545.4	7	0.2124	0.0688	0.0114	0.7074
19.7	14.5	13.00	0.3024	0.0003	0.0005	0.6967	185	546.5	8	0.2093	0.0791	0.0149	0.6967

Data for Bench Reactor Run M-120

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
19.6	16.8	13.00	0.2727	0.0003	0.0005	0.7265	185	544.3	1	0.2060	0.0591	0.0083	0.7265
19.7	15.5	13.00	0.2889	0.0003	0.0005	0.7103	185	545.2	2	0.2096	0.0686	0.0115	0.7103
19.8	14.3	13.00	0.3077	0.0003	0.0005	0.6914	185	544.9	3	0.2173	0.0778	0.0135	0.6914
19.8	13.5	13.00	0.3198	0.0003	0.0006	0.6793	185	549.8	4	0.2164	0.0871	0.0172	0.6793
19.8	13.9	13.00	0.3141	0.0003	0.0005	0.6850	185	545.1	5	0.2176	0.0843	0.0131	0.6850
20.0	15.1	13.00	0.2977	0.0003	0.0005	0.7014	185	548.2	6	0.2126	0.0732	0.0128	0.7014
19.6	15.3	13.00	0.2918	0.0003	0.0005	0.7074	185	545.4	7	0.2124	0.0688	0.0114	0.7074
19.7	14.5	13.00	0.3024	0.0003	0.0005	0.6967	185	546.5	8	0.2093	0.0791	0.0149	0.6967

Data for Bench Reactor Run M-127

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
22.0	11.4	13.00	0.3819	0.0004	0.0007	0.6171	150	544.3	1	0.2707	0.1006	0.0116	0.6171
22.2	11.3	13.00	0.3866	0.0004	0.0007	0.6123	150	542.8	2	0.2782	0.0919	0.0176	0.6123
22.0	11.8	13.00	0.3749	0.0004	0.0007	0.6240	150	540.7	3	0.2699	0.0910	0.0151	0.6240
21.6	12.2	13.00	0.3620	0.0004	0.0006	0.6370	150	542.2	4	0.2607	0.0896	0.0127	0.6370
22.1	11.9	13.00	0.3726	0.0004	0.0006	0.6263	151	542.9	5	0.2659	0.0949	0.0129	0.6263
23.1	12.0	13.00	0.3810	0.0004	0.0007	0.6180	150	540.6	6	0.2693	0.0997	0.0130	0.6180
23.4	11.9	13.00	0.3868	0.0004	0.0007	0.6121	150	542.3	7	0.2763	0.0984	0.0132	0.6121
23.3	11.4	13.00	0.3964	0.0004	0.0007	0.6025	150	542.0	8	0.2731	0.1014	0.0231	0.6025

Data for Bench Reactor Run M-79

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
13.1	7.3	7.35	0.3668	0.0004	0.0007	0.6322	149	525.2	1	0.2577	0.0992	0.0110	0.6322
13.0	7.3	7.35	0.3646	0.0004	0.0006	0.6344	149	526.6	2	0.2567	0.0973	0.0116	0.6344
12.0	7.0	7.35	0.3551	0.0004	0.0006	0.6439	151	525.8	3	0.2460	0.0978	0.0122	0.6439
11.5	6.9	7.35	0.3468	0.0003	0.0006	0.6523	153	519.9	4	0.2442	0.0926	0.0110	0.6523
12.7	7.3	7.35	0.3564	0.0004	0.0006	0.6426	153	527.4	5	0.2483	0.0966	0.0125	0.6426
13.3	7.4	7.35	0.3663	0.0004	0.0006	0.6327	150	526.7	6	0.2567	0.0996	0.0110	0.6327
13.0	7.2	7.35	0.3646	0.0004	0.0006	0.6344	150	525.0	7	0.2576	0.0957	0.0123	0.6344

Data for Bench Reactor Run M-139

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
18.3	13.4	13.00	0.3051	0.0003	0.0006	0.6940	149	569.6	1	0.1977	0.0907	0.0177	0.6940
22.7	12.9	13.00	0.3607	0.0004	0.0006	0.6383	151	567.7	2	0.2401	0.0967	0.0249	0.6383
22.6	13.1	13.00	0.3556	0.0004	0.0006	0.6434	150	564.3	3	0.2300	0.0971	0.0295	0.6434
21.7	13.7	13.00	0.3369	0.0003	0.0006	0.6621	150	567.1	4	0.2249	0.0903	0.0227	0.6621
23.1	13.9	13.00	0.3484	0.0003	0.0006	0.6506	150	564.2	5	0.2414	0.0878	0.0202	0.6506
23.9	13.9	13.00	0.3561	0.0004	0.0006	0.6429	150	562.9	6	0.2365	0.0879	0.0327	0.6429
23.5	13.6	13.00	0.3564	0.0004	0.0006	0.6426	150	562.2	7	0.2463	0.0898	0.0214	0.6426
24.0	13.5	13.00	0.3638	0.0004	0.0006	0.6352	150	561.5	8	0.2442	0.0948	0.0258	0.6352

Data for Bench Reactor Run M-46

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
11.7	4.5	2.85	0.4536	0.0005	0.0008	0.5452	150	528.1	1	0.3933	0.0561	0.0054	0.5452
11.2	4.5	2.85	0.4435	0.0004	0.0008	0.5552	150	521.1	2	0.3901	0.0502	0.0044	0.5552
12.6	3.8	2.85	0.5142	0.0005	0.0009	0.4844	150	521.5	3	0.4547	0.0554	0.0055	0.4844
12.4	3.9	2.85	0.5064	0.0005	0.0009	0.4922	150	522.1	4	0.4465	0.0558	0.0055	0.4922
12.0	4.4	2.85	0.4677	0.0005	0.0008	0.5310	153	522.6	5	0.4118	0.0521	0.0051	0.5310
12.3	4.2	2.85	0.4862	0.0005	0.0008	0.5124	153	523.2	6	0.4249	0.0577	0.0050	0.5124
12.4	4.2	2.85	0.4889	0.0005	0.0009	0.5097	153	523.8	7	0.4249	0.0603	0.0051	0.5097
12.2	4.4	2.85	0.4737	0.0005	0.0008	0.5250	151	523.8	8	0.4111	0.0588	0.0051	0.5250
12.4	4.4	2.85	0.4766	0.0005	0.0008	0.5220	150	524.1	9	0.4130	0.0596	0.0054	0.5220
12.7	4.4	2.85	0.4823	0.0005	0.0008	0.5164	151	524.0	10	0.4231	0.0553	0.0052	0.5164

Data for Bench Reactor Run M-51

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
7.0	5.2	4.35	0.3035	0.0003	0.0005	0.6956	150	524.9	1	0.2180	0.0765	0.0099	0.6956
7.2	5.1	4.35	0.3129	0.0003	0.0005	0.6862	151	522.9	2	0.2203	0.0830	0.0105	0.6862
7.3	5.1	4.35	0.3165	0.0003	0.0006	0.6827	151	524.1	3	0.2262	0.0808	0.0103	0.6827
6.7	5.1	4.35	0.2974	0.0003	0.0005	0.7018	149	524.0	4	0.2158	0.0730	0.0095	0.7018
6.2	5.0	4.35	0.2856	0.0003	0.0005	0.7136	149	523.8	5	0.2083	0.0690	0.0091	0.7136
6.2	5.1	4.35	0.2827	0.0003	0.0005	0.7165	149	523.9	6	0.2072	0.0672	0.0091	0.7165
6.7	5.1	4.35	0.2981	0.0003	0.0005	0.7011	149	523.8	7	0.2197	0.0697	0.0096	0.7011
7.5	5.1	4.35	0.3177	0.0003	0.0006	0.6814	150	523.9	8	0.2353	0.0730	0.0103	0.6814
7.7	5.1	4.35	0.3242	0.0003	0.0006	0.6749	151	523.9	9	0.2382	0.0760	0.0109	0.6749
7.5	5.2	4.35	0.3167	0.0003	0.0006	0.6825	153	523.9	10	0.2309	0.0757	0.0109	0.6825
7.4	5.2	4.35	0.3122	0.0003	0.0005	0.6869	153	523.9	11	0.2293	0.0733	0.0105	0.6869

Data for Bench Reactor Run M-52

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
8.0	5.0	4.35	0.3402	0.0003	0.0006	0.6588	150	525.3	1	0.2467	0.0835	0.0110	0.6588
8.0	4.9	4.35	0.3424	0.0003	0.0006	0.6566	151	525.7	2	0.2504	0.0825	0.0106	0.6566
8.2	5.0	4.35	0.3439	0.0003	0.0006	0.6552	150	524.9	3	0.2494	0.0844	0.0111	0.6552
8.3	5.1	4.35	0.3400	0.0003	0.0006	0.6590	151	524.5	4	0.2446	0.0849	0.0114	0.6590
8.3	5.0	4.35	0.3478	0.0003	0.0006	0.6513	150	524.0	5	0.2532	0.0838	0.0117	0.6513
8.4	5.0	4.35	0.3501	0.0004	0.0006	0.6489	153	524.6	6	0.2581	0.0812	0.0118	0.6489
8.3	5.1	4.35	0.3439	0.0003	0.0006	0.6551	152	524.8	7	0.2534	0.0805	0.0110	0.6551
8.3	4.9	4.35	0.3510	0.0004	0.0006	0.6480	152	524.7	8	0.2585	0.0829	0.0106	0.6480
8.1	5.1	4.35	0.3375	0.0003	0.0006	0.6616	153	524.6	9	0.2487	0.0795	0.0103	0.6616
7.7	5.2	4.35	0.3230	0.0003	0.0006	0.6761	153	524.5	10	0.2382	0.0758	0.0099	0.6761
7.8	5.1	4.35	0.3282	0.0003	0.0006	0.6709	153	524.5	11	0.2400	0.0788	0.0102	0.6709

Data for Bench Reactor Run M-54

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
6.6	4.8	4.35	0.3060	0.0003	0.0006	0.6932	152	524.6	1	0.2220	0.0743	0.0105	0.6932
7.0	4.9	4.35	0.3149	0.0003	0.0005	0.6842	152	525.1	2	0.2305	0.0747	0.0107	0.6842
7.2	4.7	4.35	0.3281	0.0003	0.0006	0.6710	153	525.4	3	0.2350	0.0815	0.0126	0.6710
6.9	4.6	4.35	0.3237	0.0003	0.0006	0.6754	150	525.3	4	0.2331	0.0785	0.0129	0.6754
7.1	4.6	4.35	0.3299	0.0003	0.0006	0.6692	150	524.4	5	0.2403	0.0787	0.0118	0.6692
7.5	4.6	4.35	0.3457	0.0003	0.0006	0.6534	150	526.1	6	0.2500	0.0820	0.0147	0.6534
7.5	4.6	4.35	0.3438	0.0003	0.0006	0.6553	149	525.9	7	0.2468	0.0810	0.0169	0.6553
7.2	4.4	4.35	0.3411	0.0003	0.0006	0.6580	150	525.9	8	0.2470	0.0821	0.0129	0.6580
7.0	4.6	4.35	0.3286	0.0003	0.0006	0.6705	150	526.1	9	0.2375	0.0797	0.0123	0.6705
7.0	4.8	4.35	0.3170	0.0003	0.0006	0.6821	150	526.7	10	0.2294	0.0759	0.0125	0.6821
7.0	4.6	4.35	0.3244	0.0003	0.0006	0.6747	150	525.8	11	0.2351	0.0767	0.0135	0.6747

Data for Bench Reactor Run M-62

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
9.4	5.8	5.85	0.3412	0.0003	0.0006	0.6579	153	525.2	1	0.2493	0.0718	0.0211	0.6579
9.5	5.7	5.85	0.3497	0.0004	0.0006	0.6493	149	525.0	2	0.2550	0.0732	0.0225	0.6493
9.0	5.6	5.85	0.3385	0.0003	0.0006	0.6606	149	524.2	3	0.2464	0.0704	0.0226	0.6606
8.5	5.5	5.85	0.3339	0.0003	0.0006	0.6651	149	524.7	4	0.2424	0.0702	0.0223	0.6651
8.6	5.6	5.85	0.3314	0.0003	0.0006	0.6676	150	524.9	5	0.2399	0.0704	0.0221	0.6676
8.5	5.7	5.85	0.3245	0.0003	0.0006	0.6746	153	525.6	6	0.2338	0.0705	0.0211	0.6746
8.2	5.4	5.85	0.3271	0.0003	0.0006	0.6720	153	524.7	7	0.2347	0.0726	0.0207	0.6720
8.5	5.7	5.85	0.3228	0.0003	0.0006	0.6763	150	524.5	8	0.2304	0.0712	0.0222	0.6763
8.8	5.8	5.85	0.3289	0.0003	0.0006	0.6702	150	525.6	9	0.2335	0.0720	0.0243	0.6702
8.8	5.6	5.85	0.3362	0.0003	0.0006	0.6629	153	525.2	10	0.2403	0.0727	0.0242	0.6629
8.8	5.6	5.85	0.3353	0.0003	0.0006	0.6638	150	525.9	11	0.2413	0.0715	0.0234	0.6638

Data for Bench Reactor Run M-67

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
10.4	7.2	7.35	0.3168	0.0003	0.0006	0.6823	153	523.9	1	0.2234	0.0811	0.0133	0.6823
10.5	6.9	7.35	0.3278	0.0003	0.0006	0.6712	151	524.1	2	0.2316	0.0827	0.0145	0.6712
10.4	7.0	7.35	0.3227	0.0003	0.0006	0.6764	150	524.2	3	0.2301	0.0809	0.0127	0.6764
10.2	7.0	7.35	0.3181	0.0003	0.0006	0.6810	150	524.2	4	0.2290	0.0791	0.0109	0.6810
10.2	7.1	7.35	0.3170	0.0003	0.0006	0.6821	150	524.1	5	0.2278	0.0787	0.0114	0.6821
10.5	7.1	7.35	0.3220	0.0003	0.0006	0.6771	150	523.9	6	0.2310	0.0798	0.0122	0.6771
10.4	7.1	7.35	0.3202	0.0003	0.0006	0.6789	149	523.7	7	0.2293	0.0792	0.0126	0.6789

Data for Bench Reactor Run M-55

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
4.3	2.6	4.35	0.3464	0.0003	0.0006	0.6526	149	523.7	1	0.2245	0.1028	0.0201	0.6526
4.2	2.7	4.35	0.3383	0.0003	0.0006	0.6608	150	523.3	2	0.2249	0.0948	0.0195	0.6608
4.3	2.8	4.35	0.3311	0.0003	0.0006	0.6680	151	523.2	3	0.2256	0.0873	0.0191	0.6680
4.9	2.7	4.35	0.3667	0.0004	0.0006	0.6323	150	524.1	4	0.2499	0.0983	0.0196	0.6323
5.3	2.7	4.35	0.3898	0.0004	0.0007	0.6091	151	524.4	5	0.2574	0.1083	0.0253	0.6091
5.0	2.7	4.35	0.3770	0.0004	0.0007	0.6220	150	524.2	6	0.2461	0.1067	0.0253	0.6220
4.9	2.6	4.35	0.3743	0.0004	0.0007	0.6247	151	524.5	7	0.2416	0.1078	0.0259	0.6247
4.7	2.6	4.35	0.3726	0.0004	0.0006	0.6263	150	524.1	8	0.2408	0.1069	0.0259	0.6263
4.9	2.6	4.35	0.3820	0.0004	0.0007	0.6169	149	524.9	9	0.2476	0.1081	0.0274	0.6169
5.2	2.6	4.35	0.3931	0.0004	0.0007	0.6058	150	524.0	10	0.2681	0.1025	0.0236	0.6058
5.2	2.6	4.35	0.3938	0.0004	0.0007	0.6051	150	523.6	11	0.2716	0.1016	0.0217	0.6051

Data for Bench Reactor Run M-72

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
7.0	5.6	8.85	0.2879	0.0003	0.0005	0.7113	150	524.7	1	0.1857	0.0871	0.0158	0.7113
6.6	5.6	8.85	0.2731	0.0003	0.0005	0.7261	151	525.1	2	0.1763	0.0827	0.0149	0.7261
6.8	5.6	8.85	0.2775	0.0003	0.0005	0.7218	151	524.6	3	0.1785	0.0858	0.0139	0.7218
6.9	5.6	8.85	0.2814	0.0003	0.0005	0.7178	150	525.3	4	0.1816	0.0852	0.0154	0.7178
7.0	5.7	8.85	0.2833	0.0003	0.0005	0.7159	152	524.9	5	0.1834	0.0845	0.0161	0.7159
6.9	5.7	8.85	0.2780	0.0003	0.0005	0.7212	150	525.2	6	0.1784	0.0840	0.0164	0.7212
7.0	5.6	8.85	0.2856	0.0003	0.0005	0.7136	150	525.5	7	0.1856	0.0853	0.0155	0.7136
7.6	5.7	8.85	0.3005	0.0003	0.0005	0.6986	150	526.7	8	0.1953	0.0901	0.0160	0.6986
8.0	5.8	8.85	0.3047	0.0003	0.0005	0.6944	150	527.1	9	0.1976	0.0903	0.0177	0.6944
7.9	5.8	8.85	0.3027	0.0003	0.0005	0.6965	153	525.1	10	0.1973	0.0889	0.0173	0.6965
7.8	5.8	8.85	0.3026	0.0003	0.0005	0.6965	153	525.5	11	0.1963	0.0899	0.0173	0.6965

Data for Bench Reactor Run M-68

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
5.7	4.4	7.35	0.2947	0.0003	0.0005	0.7045	150	523.8	2	0.1871	0.0922	0.0162	0.7045
5.9	4.5	7.35	0.2957	0.0003	0.0005	0.7035	152	523.9	3	0.1919	0.0902	0.0145	0.7035
6.7	4.4	7.35	0.3270	0.0003	0.0006	0.6721	153	523.7	4	0.2113	0.0994	0.0172	0.6721
6.7	4.4	7.35	0.3271	0.0003	0.0006	0.6720	153	523.7	5	0.2129	0.0982	0.0169	0.6720
7.3	4.4	7.35	0.3473	0.0003	0.0006	0.6517	150	523.9	6	0.2278	0.1028	0.0177	0.6517
7.5	4.4	7.35	0.3526	0.0004	0.0006	0.6464	153	526.6	7	0.2309	0.1028	0.0199	0.6464
6.9	4.4	7.35	0.3329	0.0003	0.0006	0.6661	149	530.5	8	0.2104	0.0999	0.0235	0.6661
6.5	4.4	7.35	0.3227	0.0003	0.0006	0.6764	149	527.3	9	0.2081	0.0964	0.0191	0.6764
6.5	4.3	7.35	0.3250	0.0003	0.0006	0.6741	149	523.2	10	0.2111	0.0979	0.0169	0.6741
6.5	4.3	7.35	0.3289	0.0003	0.0006	0.6702	149	524.6	11	0.2139	0.0970	0.0189	0.6702

Data for Bench Reactor Run M-82

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
6.9	6.9	5.85	0.2442	0.0002	0.0004	0.7551	150	525.0	1	0.1724	0.0608	0.0118	0.7551
8.6	6.7	5.85	0.2918	0.0003	0.0005	0.7074	147	525.4	2	0.2081	0.0728	0.0117	0.7074
10.3	6.6	5.85	0.3321	0.0003	0.0006	0.6670	150	525.1	3	0.2344	0.0826	0.0160	0.6670
10.3	6.8	5.85	0.3258	0.0003	0.0006	0.6733	151	525.8	4	0.2324	0.0813	0.0131	0.6733
10.9	6.8	5.85	0.3392	0.0003	0.0006	0.6598	149	525.9	5	0.2388	0.0860	0.0153	0.6598
9.4	6.7	5.85	0.3082	0.0003	0.0005	0.6910	149	525.5	6	0.2183	0.0770	0.0137	0.6910
9.9	6.7	5.85	0.3199	0.0003	0.0006	0.6792	149	525.5	7	0.2268	0.0801	0.0139	0.6792
10.1	6.7	5.85	0.3252	0.0003	0.0006	0.6739	150	525.6	8	0.2303	0.0814	0.0144	0.6739

Data for Bench Reactor Run M-115

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
21.0	12.7	13.00	0.3464	0.0003	0.0006	0.6527	215	501.5	2	0.2635	0.0706	0.0133	0.6527
20.1	12.4	13.00	0.3411	0.0003	0.0006	0.6579	215	497.9	3	0.2571	0.0678	0.0173	0.6579
19.1	12.3	13.00	0.3309	0.0003	0.0006	0.6682	215	500.0	4	0.2488	0.0655	0.0175	0.6682
18.7	12.5	13.00	0.3244	0.0003	0.0006	0.6746	215	500.1	5	0.2436	0.0680	0.0138	0.6746
19.1	12.5	13.00	0.3280	0.0003	0.0006	0.6711	215	499.1	6	0.2484	0.0662	0.0143	0.6711
20.3	11.9	13.00	0.3526	0.0004	0.0006	0.6464	215	498.3	7	0.2693	0.0685	0.0158	0.6464
20.2	11.8	13.00	0.3546	0.0004	0.0006	0.6444	215	500.4	8	0.2628	0.0723	0.0206	0.6444

Data for Bench Reactor Run M-119

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	p_T*(a)*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
25.6	10.9	13.00	0.4288	0.0004	0.0008	0.5700	185	540.9	1	0.2901	0.1208	0.0191	0.5700
29.8	10.4	13.00	0.4775	0.0005	0.0008	0.5212	182	541.3	2	0.3189	0.1357	0.0243	0.5212
29.1	10.3	13.00	0.4747	0.0005	0.0008	0.5240	183	539.4	3	0.3218	0.1291	0.0251	0.5240

Data for Bench Reactor Run M-119 - Continued

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*$p_T(a)$*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
29.6	10.1	13.00	0.4828	0.0005	0.0008	0.5158	183	538.8	4	0.3199	0.1317	0.0326	0.5158
30.9	10.2	13.00	0.4920	0.0005	0.0009	0.5066	183	538.4	5	0.3367	0.1313	0.0254	0.5066
31.2	10.2	13.00	0.4944	0.0005	0.0009	0.5042	183	540.1	6	0.3398	0.1294	0.0266	0.5042
30.0	10.2	13.00	0.4851	0.0005	0.0008	0.5136	183	539.6	7	0.3280	0.1297	0.0288	0.5136

Data for Bench Reactor Run M-130

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*$p_T(a)$*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
32.5	28.2	13.00	0.2700	0.0003	0.0005	0.7293	119	550.3	1	0.2276	0.0366	0.0065	0.7293
32.1	28.7	13.00	0.2637	0.0003	0.0005	0.7356	118	547.0	2	0.2199	0.0410	0.0035	0.7356
32.2	27.2	13.00	0.2745	0.0003	0.0005	0.7247	116	547.9	3	0.2289	0.0419	0.0044	0.7247
27.1	25.1	13.00	0.2567	0.0003	0.0004	0.7426	117	544.7	4	0.2140	0.0385	0.0049	0.7426
25.0	25.3	13.00	0.2403	0.0002	0.0004	0.7590	123	545.7	5	0.2004	0.0360	0.0046	0.7590
30.9	24.7	13.00	0.2862	0.0003	0.0005	0.7130	125	549.0	6	0.2358	0.0453	0.0060	0.7130

A5.3.3 INPUT FILE 2 : PILOT REACTOR DATA

0	*Write results to File 1, 0 = no, 1=yes*
650	*Catalyst density, kg·m^{-3}*
4	*Number of components*
2	*Number of reactions, -*
-1 -1	*n-Butene Stoichiometric coefficient*
+1 +0	*Isobutene Stoichiometric coefficient*
+0 +1	*By-products Stoichiometric coefficient*
+0 +0	*H_2O Stoichiometric coefficient*
56 56 55 18	*Molar weight of each components, g/mol*
270	*Number of data points, -*
0.0025	*Step size, m*
0.000475	*Reactor cross sectional area, m^2*

Data for Pilot Plant Run Isom-221

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*$p_T(a)$*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
93.1	55.2	50	0.2747	0.0303	0.0460	0.6489	151.5	519.8	2	0.2110	0.0761	0.0648	0.6481
93.1	55.2	50	0.2747	0.0303	0.0460	0.6489	151.5	519.8	4	0.2111	0.0757	0.0654	0.6478
93.1	55.2	50	0.2747	0.0303	0.0460	0.6489	151.5	519.8	6	0.2179	0.0719	0.0623	0.6480
93.1	55.2	50	0.2747	0.0303	0.0460	0.6489	151.5	519.8	8	0.2214	0.0691	0.0611	0.6483
93.1	55.2	50	0.2747	0.0303	0.0460	0.6489	151.5	519.8	10	0.2201	0.0692	0.0627	0.6481
93.1	55.2	50	0.2747	0.0303	0.0460	0.6489	151.5	519.8	12	0.2183	0.0691	0.0658	0.6467
93.1	55.2	50	0.2747	0.0303	0.0460	0.6489	151.5	519.8	16	0.2293	0.0607	0.0616	0.6484
93.1	55.2	50	0.2747	0.0303	0.0460	0.6489	151.5	519.8	20	0.2326	0.0586	0.0604	0.6484
93.1	55.2	50	0.2747	0.0303	0.0460	0.6489	151.5	519.8	24	0.2359	0.0566	0.0591	0.6484
93.1	55.2	50	0.2747	0.0303	0.0460	0.6489	151.5	519.8	28	0.2310	0.0580	0.0627	0.6483
93.1	55.2	50	0.2747	0.0303	0.0460	0.6489	151.5	519.8	32	0.2329	0.0551	0.0637	0.6483

Data for Pilot Plant Run Isom-222

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	*$p_T(a)$*	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
94.8	59.1	50	0.2654	0.0288	0.0452	0.6606	149.9	523.7	2	0.2056	0.0760	0.0582	0.6601
94.8	59.1	50	0.2654	0.0288	0.0452	0.6606	149.9	523.7	4	0.2071	0.0757	0.0573	0.6599
94.8	59.1	50	0.2654	0.0288	0.0452	0.6606	149.9	523.7	6	0.2098	0.0740	0.0563	0.6599
94.8	59.1	50	0.2654	0.0288	0.0452	0.6606	149.9	523.7	8	0.1961	0.0821	0.0628	0.6590
94.8	59.1	50	0.2654	0.0288	0.0452	0.6606	149.9	523.7	10	0.2052	0.0764	0.0590	0.6593
94.8	59.1	50	0.2654	0.0288	0.0452	0.6606	149.9	523.7	12	0.2052	0.0756	0.0613	0.6580

Data for Pilot Plant Run Isom-222 - Continued

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
94.8	59.1	50	0.2654	0.0288	0.0452	0.6606	149.9	523.7	16	0.2059	0.0750	0.0598	0.6593
94.8	59.1	50	0.2654	0.0288	0.0452	0.6606	149.9	523.7	20	0.2148	0.0690	0.0564	0.6598
94.8	59.1	50	0.2654	0.0288	0.0452	0.6606	149.9	523.7	24	0.2224	0.0621	0.0557	0.6598
94.8	59.1	50	0.2654	0.0288	0.0452	0.6606	149.9	523.7	28	0.2198	0.0628	0.0577	0.6598
94.8	59.1	50	0.2654	0.0288	0.0452	0.6606	149.9	523.7	32	0.2252	0.0587	0.0562	0.6599

Data for Pilot Plant Run Isom-226

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
92.0	97.8	50	0.1817	0.0199	0.0303	0.7681	147.5	521.2	2	0.1454	0.0510	0.0359	0.7677
92.0	97.8	50	0.1817	0.0199	0.0303	0.7681	147.5	521.2	4	0.1453	0.0515	0.0355	0.7678
92.0	97.8	50	0.1817	0.0199	0.0303	0.7681	147.5	521.2	6	0.1459	0.0500	0.0364	0.7677
92.0	97.8	50	0.1817	0.0199	0.0303	0.7681	147.5	521.2	8	0.1465	0.0486	0.0373	0.7676
92.0	97.8	50	0.1817	0.0199	0.0303	0.7681	147.5	521.2	10	0.1472	0.0471	0.0382	0.7675
92.0	97.8	50	0.1817	0.0199	0.0303	0.7681	147.5	521.2	12	0.1476	0.0456	0.0404	0.7664
92.0	97.8	50	0.1817	0.0199	0.0303	0.7681	147.5	521.2	16	0.1505	0.0432	0.0387	0.7676
92.0	97.8	50	0.1817	0.0199	0.0303	0.7681	147.5	521.2	20	0.1531	0.0408	0.0383	0.7678
92.0	97.8	50	0.1817	0.0199	0.0303	0.7681	147.5	521.2	24	0.1533	0.0408	0.0382	0.7678
92.0	97.8	50	0.1817	0.0199	0.0303	0.7681	147.5	521.2	28	0.1534	0.0408	0.0380	0.7678

Data for Pilot Plant Run Isom-229

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
139.7	60.7	50	0.3277	0.0401	0.0583	0.5739	119.2	494.3	2	0.2778	0.0728	0.0781	0.5713
139.7	60.7	50	0.3277	0.0401	0.0583	0.5739	119.2	494.3	4	0.2783	0.0731	0.0772	0.5714
139.7	60.7	50	0.3277	0.0401	0.0583	0.5739	119.2	494.3	6	0.2796	0.0714	0.0777	0.5714
139.7	60.7	50	0.3277	0.0401	0.0583	0.5739	119.2	494.3	8	0.2802	0.0721	0.0763	0.5714
139.7	60.7	50	0.3277	0.0401	0.0583	0.5739	119.2	494.3	10	0.2793	0.0717	0.0778	0.5712
139.7	60.7	50	0.3277	0.0401	0.0583	0.5739	119.2	494.3	12	0.2785	0.0720	0.0794	0.5701
139.7	60.7	50	0.3277	0.0401	0.0583	0.5739	119.2	494.3	16	0.2778	0.0730	0.0780	0.5711
139.7	60.7	50	0.3277	0.0401	0.0583	0.5739	119.2	494.3	20	0.2774	0.0727	0.0789	0.5709
139.7	60.7	50	0.3277	0.0401	0.0583	0.5739	119.2	494.3	24	0.2769	0.0724	0.0799	0.5708
139.7	60.7	50	0.3277	0.0401	0.0583	0.5739	119.2	494.3	28	0.2784	0.0722	0.0784	0.5710
139.7	60.7	50	0.3277	0.0401	0.0583	0.5739	119.2	494.3	32	0.2803	0.0722	0.0761	0.5714

Data for Pilot Plant Run Isom-241

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
89.0	58.4	50	0.2285	0.0262	0.0803	0.6651	149.2	522.8	1	0.1753	0.0729	0.0853	0.6665
89.0	58.4	50	0.2285	0.0262	0.0803	0.6651	149.2	522.8	3	0.1805	0.0656	0.0884	0.6656
89.0	58.4	50	0.2285	0.0262	0.0803	0.6651	149.2	522.8	5	0.1891	0.0613	0.0836	0.6661
89.0	58.4	50	0.2285	0.0262	0.0803	0.6651	149.2	522.8	7	0.1901	0.0603	0.0838	0.6658
89.0	58.4	50	0.2285	0.0262	0.0803	0.6651	149.2	522.8	9	0.1916	0.0599	0.0823	0.6662
89.0	58.4	50	0.2285	0.0262	0.0803	0.6651	149.2	522.8	11	0.1911	0.0589	0.0841	0.6659
89.0	58.4	50	0.2285	0.0262	0.0803	0.6651	149.2	522.8	13	0.1882	0.0598	0.0885	0.6635
89.0	58.4	50	0.2285	0.0262	0.0803	0.6651	149.2	522.8	17	0.1895	0.0566	0.0904	0.6634
89.0	58.4	50	0.2285	0.0262	0.0803	0.6651	149.2	522.8	21	0.1965	0.0531	0.0862	0.6641
89.0	58.4	50	0.2285	0.0262	0.0803	0.6651	149.2	522.8	25	0.1988	0.0507	0.0870	0.6635
89.0	58.4	50	0.2285	0.0262	0.0803	0.6651	149.2	522.8	29	0.1988	0.0507	0.0870	0.6635
89.0	58.4	50	0.2285	0.0262	0.0803	0.6651	149.2	522.8	33	0.1988	0.0507	0.0870	0.6635

Data for Pilot Plant Run Isom-245

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
94.4	58.8	50	0.2364	0.0271	0.0831	0.6534	85.0	521.7	1	0.1939	0.0678	0.0835	0.6548

Data for Pilot Plant Run Isom-245 - Continued

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
94.4	58.8	50	0.2364	0.0271	0.0831	0.6534	85.0	521.7	3	0.1939	0.0678	0.0835	0.6548
94.4	58.8	50	0.2364	0.0271	0.0831	0.6534	85.0	521.7	5	0.1955	0.0670	0.0826	0.6549
94.4	58.8	50	0.2364	0.0271	0.0831	0.6534	85.0	521.7	7	0.1969	0.0669	0.0812	0.6549
94.4	58.8	50	0.2364	0.0271	0.0831	0.6534	85.0	521.7	9	0.1969	0.0656	0.0826	0.6549
94.4	58.8	50	0.2364	0.0271	0.0831	0.6534	85.0	521.7	11	0.1975	0.0652	0.0824	0.6549
94.4	58.8	50	0.2364	0.0271	0.0831	0.6534	85.0	521.7	13	0.1970	0.0647	0.0857	0.6527
94.4	58.8	50	0.2364	0.0271	0.0831	0.6534	85.0	521.7	17	0.1964	0.0640	0.0872	0.6524
94.4	58.8	50	0.2364	0.0271	0.0831	0.6534	85.0	521.7	21	0.2000	0.0614	0.0860	0.6526
94.4	58.8	50	0.2364	0.0271	0.0831	0.6534	85.0	521.7	25	0.1996	0.0614	0.0854	0.6535
94.4	58.8	50	0.2364	0.0271	0.0831	0.6534	85.0	521.7	29	0.1993	0.0615	0.0848	0.6544
94.4	58.8	50	0.2364	0.0271	0.0831	0.6534	85.0	521.7	33	0.1973	0.0610	0.0868	0.6549

Data for Pilot Plant Run Isom-192

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
61.4	33.2	50	0.2876	0.0294	0.0576	0.6254	121.2	494.7	1	0.2451	0.0661	0.0635	0.6253
61.4	33.2	50	0.2876	0.0294	0.0576	0.6254	121.2	494.7	3	0.2432	0.0683	0.0631	0.6253
61.4	33.2	50	0.2876	0.0294	0.0576	0.6254	121.2	494.7	5	0.2421	0.0692	0.0634	0.6253
61.4	33.2	50	0.2876	0.0294	0.0576	0.6254	121.2	494.7	7	0.2399	0.0706	0.0643	0.6252
61.4	33.2	50	0.2876	0.0294	0.0576	0.6254	121.2	494.7	9	0.2388	0.0705	0.0657	0.6250
61.4	33.2	50	0.2876	0.0294	0.0576	0.6254	121.2	494.7	11	0.2382	0.0718	0.0648	0.6252
61.4	33.2	50	0.2876	0.0294	0.0576	0.6254	121.2	494.7	13	0.2366	0.0718	0.0683	0.6233
61.4	33.2	50	0.2876	0.0294	0.0576	0.6254	121.2	494.7	17	0.2365	0.0723	0.0659	0.6253
61.4	33.2	50	0.2876	0.0294	0.0576	0.6254	121.2	494.7	21	0.2371	0.0716	0.0660	0.6252
61.4	33.2	50	0.2876	0.0294	0.0576	0.6254	121.2	494.7	25	0.2377	0.0710	0.0662	0.6251
61.4	33.2	50	0.2876	0.0294	0.0576	0.6254	121.2	494.7	29	0.2386	0.0704	0.0657	0.6253
61.4	33.2	50	0.2876	0.0294	0.0576	0.6254	121.2	494.7	33	0.2386	0.0702	0.0660	0.6252

Data for Pilot Plant Run Isom-198

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
90.4	60.9	50	0.2602	0.0281	0.0349	0.6768	150.2	471.0	1	0.2389	0.0448	0.0401	0.6762
90.4	60.9	50	0.2602	0.0281	0.0349	0.6768	150.2	471.0	3	0.2400	0.0445	0.0393	0.6762
90.4	60.9	50	0.2602	0.0281	0.0349	0.6768	150.2	471.0	5	0.2403	0.0444	0.0391	0.6762
90.4	60.9	50	0.2602	0.0281	0.0349	0.6768	150.2	471.0	7	0.2392	0.0452	0.0393	0.6762
90.4	60.9	50	0.2602	0.0281	0.0349	0.6768	150.2	471.0	9	0.2405	0.0444	0.0389	0.6763
90.4	60.9	50	0.2602	0.0281	0.0349	0.6768	150.2	471.0	11	0.2402	0.0446	0.0390	0.6762
90.4	60.9	50	0.2602	0.0281	0.0349	0.6768	150.2	471.0	13	0.2414	0.0436	0.0392	0.6758
90.4	60.9	50	0.2602	0.0281	0.0349	0.6768	150.2	471.0	17	0.2410	0.0438	0.0390	0.6762
90.4	60.9	50	0.2602	0.0281	0.0349	0.6768	150.2	471.0	21	0.2394	0.0449	0.0395	0.6762
90.4	60.9	50	0.2602	0.0281	0.0349	0.6768	150.2	471.0	25	0.2395	0.0449	0.0393	0.6762
90.4	60.9	50	0.2602	0.0281	0.0349	0.6768	150.2	471.0	29	0.2392	0.0450	0.0397	0.6761
90.4	60.9	50	0.2602	0.0281	0.0349	0.6768	150.2	471.0	33	0.2394	0.0448	0.0397	0.6762

Data for Pilot Plant Run Isom-201

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p* H_2O
32.3	20.9	50	0.2671	0.0289	0.0359	0.6682	150.0	521.0	1	0.1849	0.0912	0.0571	0.6669
32.3	20.9	50	0.2671	0.0289	0.0359	0.6682	150.0	521.0	3	0.1819	0.0922	0.0590	0.6668
32.3	20.9	50	0.2671	0.0289	0.0359	0.6682	150.0	521.0	5	0.1780	0.0940	0.0615	0.6665
32.3	20.9	50	0.2671	0.0289	0.0359	0.6682	150.0	521.0	7	0.1754	0.0945	0.0638	0.6663
32.3	20.9	50	0.2671	0.0289	0.0359	0.6682	150.0	521.0	9	0.1738	0.0936	0.0661	0.6665
32.3	20.9	50	0.2671	0.0289	0.0359	0.6682	150.0	521.0	11	0.1802	0.0917	0.0614	0.6666
32.3	20.9	50	0.2671	0.0289	0.0359	0.6682	150.0	521.0	13	0.1803	0.0888	0.0699	0.6611
32.3	20.9	50	0.2671	0.0289	0.0359	0.6682	150.0	521.0	17	0.1799	0.0902	0.0634	0.6664

Data for Pilot Plant Run Isom-201 - Continued

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
32.3	20.9	50	0.2671	0.0289	0.0359	0.6682	150.0	521.0	21	0.1774	0.0901	0.0661	0.6664
32.3	20.9	50	0.2671	0.0289	0.0359	0.6682	150.0	521.0	25	0.1805	0.0873	0.0650	0.6672
32.3	20.9	50	0.2671	0.0289	0.0359	0.6682	150.0	521.0	29	0.1738	0.0895	0.0717	0.6650
32.3	20.9	50	0.2671	0.0289	0.0359	0.6682	150.0	521.0	33	0.1738	0.0895	0.0717	0.6650

Data for Pilot Plant Run Isom-204

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
84.4	59.1	50	0.2503	0.0282	0.0372	0.6843	85.0	522.2	1	0.2170	0.0586	0.0401	0.6843
84.4	59.1	50	0.2503	0.0282	0.0372	0.6843	85.0	522.2	3	0.2176	0.0583	0.0397	0.6844
84.4	59.1	50	0.2503	0.0282	0.0372	0.6843	85.0	522.2	5	0.2203	0.0555	0.0398	0.6844
84.4	59.1	50	0.2503	0.0282	0.0372	0.6843	85.0	522.2	7	0.2206	0.0552	0.0398	0.6844
84.4	59.1	50	0.2503	0.0282	0.0372	0.6843	85.0	522.2	9	0.2209	0.0550	0.0397	0.6844
84.4	59.1	50	0.2503	0.0282	0.0372	0.6843	85.0	522.2	11	0.2209	0.0548	0.0400	0.6843
84.4	59.1	50	0.2503	0.0282	0.0372	0.6843	85.0	522.2	13	0.2205	0.0547	0.0411	0.6836
84.4	59.1	50	0.2503	0.0282	0.0372	0.6843	85.0	522.2	17	0.2206	0.0547	0.0404	0.6843
84.4	59.1	50	0.2503	0.0282	0.0372	0.6843	85.0	522.2	21	0.2212	0.0546	0.0398	0.6844
84.4	59.1	50	0.2503	0.0282	0.0372	0.6843	85.0	522.2	25	0.2199	0.0557	0.0400	0.6844
84.4	59.1	50	0.2503	0.0282	0.0372	0.6843	85.0	522.2	29	0.2229	0.0529	0.0398	0.6844
84.4	59.1	50	0.2503	0.0282	0.0372	0.6843	85.0	522.2	33	0.2228	0.0530	0.0398	0.6844

Data for Pilot Plant Run Isom-205

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
87.8	60.5	50	0.2542	0.0285	0.0364	0.6810	149.4	529.6	1	0.2030	0.0696	0.0469	0.6805
87.8	60.5	50	0.2542	0.0285	0.0364	0.6810	149.4	529.6	3	0.2046	0.0688	0.0462	0.6805
87.8	60.5	50	0.2542	0.0285	0.0364	0.6810	149.4	529.6	5	0.2036	0.0673	0.0483	0.6807
87.8	60.5	50	0.2542	0.0285	0.0364	0.6810	149.4	529.6	7	0.2058	0.0672	0.0467	0.6803
87.8	60.5	50	0.2542	0.0285	0.0364	0.6810	149.4	529.6	9	0.2112	0.0631	0.0451	0.6806
87.8	60.5	50	0.2542	0.0285	0.0364	0.6810	149.4	529.6	11	0.2103	0.0635	0.0456	0.6805
87.8	60.5	50	0.2542	0.0285	0.0364	0.6810	149.4	529.6	13	0.2087	0.0638	0.0492	0.6783
87.8	60.5	50	0.2542	0.0285	0.0364	0.6810	149.4	529.6	17	0.2077	0.0652	0.0468	0.6804
87.8	60.5	50	0.2542	0.0285	0.0364	0.6810	149.4	529.6	21	0.2028	0.0666	0.0506	0.6800
87.8	60.5	50	0.2542	0.0285	0.0364	0.6810	149.4	529.6	25	0.2084	0.0634	0.0478	0.6804
87.8	60.5	50	0.2542	0.0285	0.0364	0.6810	149.4	529.6	29	0.2097	0.0617	0.0483	0.6804
87.8	60.5	50	0.2542	0.0285	0.0364	0.6810	149.4	529.6	33	0.2097	0.0617	0.0483	0.6804

Data for Pilot Plant Run Isom-214

-Feed flow-		Mass	---- Feed Gas Composition ----				Parameters		Run	--- Product Gas Composition ---			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
93.4	50.7	50	0.2856	0.0330	0.0538	0.6276	150.8	506.3	1	0.2107	0.0928	0.0706	0.6260
93.4	50.7	50	0.2856	0.0330	0.0538	0.6276	150.8	506.3	3	0.2109	0.0922	0.0707	0.6261
93.4	50.7	50	0.2856	0.0330	0.0538	0.6276	150.8	506.3	5	0.2112	0.0917	0.0709	0.6262
93.4	50.7	50	0.2856	0.0330	0.0538	0.6276	150.8	506.3	7	0.2064	0.0920	0.0759	0.6258
93.4	50.7	50	0.2856	0.0330	0.0538	0.6276	150.8	506.3	9	0.2098	0.0911	0.0728	0.6263
93.4	50.7	50	0.2856	0.0330	0.0538	0.6276	150.8	506.3	11	0.2133	0.0903	0.0696	0.6268
93.4	50.7	50	0.2856	0.0330	0.0538	0.6276	150.8	506.3	13	0.2102	0.0889	0.0796	0.6213
93.4	50.7	50	0.2856	0.0330	0.0538	0.6276	150.8	506.3	17	0.2154	0.0876	0.0701	0.6268
93.4	50.7	50	0.2856	0.0330	0.0538	0.6276	150.8	506.3	21	0.2209	0.0862	0.0651	0.6278
93.4	50.7	50	0.2856	0.0330	0.0538	0.6276	150.8	506.3	25	0.2134	0.0866	0.0727	0.6274
93.4	50.7	50	0.2856	0.0330	0.0538	0.6276	150.8	506.3	29	0.2138	0.0855	0.0731	0.6276
93.4	50.7	50	0.2856	0.0330	0.0538	0.6276	150.8	506.3	33	0.2087	0.0856	0.0783	0.6274

Data for Pilot Plant Run Isom-216

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
85.5	59.3	50	0.2430	0.0281	0.0458	0.6832	151.6	522.2	2	0.1903	0.0710	0.0567	0.6820
85.5	59.3	50	0.2430	0.0281	0.0458	0.6832	151.6	522.2	4	0.1870	0.0731	0.0579	0.6821
85.5	59.3	50	0.2430	0.0281	0.0458	0.6832	151.6	522.2	6	0.1837	0.0751	0.0591	0.6821
85.5	59.3	50	0.2430	0.0281	0.0458	0.6832	151.6	522.2	8	0.1881	0.0722	0.0574	0.6823
85.5	59.3	50	0.2430	0.0281	0.0458	0.6832	151.6	522.2	10	0.1894	0.0717	0.0565	0.6823
85.5	59.3	50	0.2430	0.0281	0.0458	0.6832	151.6	522.2	12	0.1883	0.0710	0.0616	0.6791
85.5	59.3	50	0.2430	0.0281	0.0458	0.6832	151.6	522.2	16	0.1888	0.0709	0.0582	0.6821
85.5	59.3	50	0.2430	0.0281	0.0458	0.6832	151.6	522.2	20	0.1879	0.0677	0.0616	0.6829
85.5	59.3	50	0.2430	0.0281	0.0458	0.6832	151.6	522.2	24	0.1931	0.0674	0.0572	0.6823
85.5	59.3	50	0.2430	0.0281	0.0458	0.6832	151.6	522.2	28	0.1922	0.0680	0.0575	0.6823
85.5	59.3	50	0.2430	0.0281	0.0458	0.6832	151.6	522.2	32	0.1936	0.0670	0.0569	0.6825

Data for Pilot Plant Run Isom-217

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
85.2	60.1	50	0.2403	0.0278	0.0452	0.6867	151.3	521.4	2	0.1882	0.0730	0.0527	0.6861
85.2	60.1	50	0.2403	0.0278	0.0452	0.6867	151.3	521.4	4	0.1877	0.0723	0.0541	0.6859
85.2	60.1	50	0.2403	0.0278	0.0452	0.6867	151.3	521.4	6	0.1871	0.0716	0.0554	0.6858
85.2	60.1	50	0.2403	0.0278	0.0452	0.6867	151.3	521.4	8	0.1994	0.0594	0.0554	0.6859
85.2	60.1	50	0.2403	0.0278	0.0452	0.6867	151.3	521.4	10	0.1948	0.0625	0.0571	0.6856
85.2	60.1	50	0.2403	0.0278	0.0452	0.6867	151.3	521.4	12	0.1895	0.0655	0.0618	0.6832
85.2	60.1	50	0.2403	0.0278	0.0452	0.6867	151.3	521.4	16	0.1983	0.0610	0.0544	0.6862
85.2	60.1	50	0.2403	0.0278	0.0452	0.6867	151.3	521.4	20	0.1987	0.0595	0.0558	0.6860
85.2	60.1	50	0.2403	0.0278	0.0452	0.6867	151.3	521.4	24	0.2012	0.0575	0.0553	0.6861
85.2	60.1	50	0.2403	0.0278	0.0452	0.6867	151.3	521.4	28	0.2000	0.0577	0.0563	0.6860
85.2	60.1	50	0.2403	0.0278	0.0452	0.6867	151.3	521.4	32	0.1998	0.0569	0.0573	0.6860

Data for Pilot Plant Run Isom-163

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
90.8	56.9	50	0.3319	0.0063	0.0006	0.6612	154.9	522.3	1	0.2453	0.0789	0.0152	0.6607
90.8	56.9	50	0.3319	0.0063	0.0006	0.6612	154.9	522.3	3	0.2460	0.0787	0.0147	0.6606
90.8	56.9	50	0.3319	0.0063	0.0006	0.6612	154.9	522.3	5	0.2484	0.0767	0.0144	0.6604
90.8	56.9	50	0.3319	0.0063	0.0006	0.6612	154.9	522.3	7	0.2482	0.0761	0.0153	0.6604
90.8	56.9	50	0.3319	0.0063	0.0006	0.6612	154.9	522.3	9	0.2497	0.0742	0.0155	0.6606
90.8	56.9	50	0.3319	0.0063	0.0006	0.6612	154.9	522.3	11	0.2509	0.0728	0.0157	0.6606
90.8	56.9	50	0.3319	0.0063	0.0006	0.6612	154.9	522.3	13	0.2489	0.0745	0.0162	0.6604
90.8	56.9	50	0.3319	0.0063	0.0006	0.6612	154.9	522.3	17	0.2491	0.0732	0.0173	0.6604
90.8	56.9	50	0.3319	0.0063	0.0006	0.6612	154.9	522.3	21	0.2517	0.0702	0.0177	0.6605
90.8	56.9	50	0.3319	0.0063	0.0006	0.6612	154.9	522.3	25	0.2569	0.0659	0.0166	0.6606
90.8	56.9	50	0.3319	0.0063	0.0006	0.6612	154.9	522.3	29	0.2582	0.0645	0.0168	0.6604
90.8	56.9	50	0.3319	0.0063	0.0006	0.6612	154.9	522.3	33	0.2650	0.0604	0.0138	0.6607

Data for Pilot Plant Run Isom-165

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	*p H_2O*
93.2	57.5	50	0.3158	0.0268	0.0002	0.6572	152.4	523.5	1	0.2395	0.0894	0.0147	0.6564
93.2	57.5	50	0.3158	0.0268	0.0002	0.6572	152.4	523.5	3	0.2397	0.0889	0.0151	0.6564
93.2	57.5	50	0.3158	0.0268	0.0002	0.6572	152.4	523.5	5	0.2443	0.0853	0.0140	0.6564
93.2	57.5	50	0.3158	0.0268	0.0002	0.6572	152.4	523.5	7	0.2445	0.0843	0.0146	0.6567
93.2	57.5	50	0.3158	0.0268	0.0002	0.6572	152.4	523.5	9	0.2444	0.0840	0.0150	0.6566
93.2	57.5	50	0.3158	0.0268	0.0002	0.6572	152.4	523.5	11	0.2467	0.0820	0.0146	0.6567
93.2	57.5	50	0.3158	0.0268	0.0002	0.6572	152.4	523.5	13	0.2390	0.0898	0.0152	0.6559
93.2	57.5	50	0.3158	0.0268	0.0002	0.6572	152.4	523.5	16	0.2464	0.0809	0.0162	0.6565
93.2	57.5	50	0.3158	0.0268	0.0002	0.6572	152.4	523.5	20	0.2470	0.0799	0.0166	0.6565

Data for Pilot Plant Run Isom-165 - Continued

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
93.2	57.5	50	0.3158	0.0268	0.0002	0.6572	152.4	523.5	24	0.2471	0.0793	0.0172	0.6564
93.2	57.5	50	0.3158	0.0268	0.0002	0.6572	152.4	523.5	27	0.2474	0.0783	0.0180	0.6563
93.2	57.5	50	0.3158	0.0268	0.0002	0.6572	152.4	523.5	31	0.2499	0.0777	0.0161	0.6563

Data for Pilot Plant Run Isom-168

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
91.9	52.6	50	0.2227	0.0025	0.1315	0.6433	152.0	517.3	1	0.1670	0.0491	0.1413	0.6426
91.9	52.6	50	0.2227	0.0025	0.1315	0.6433	152.0	517.3	3	0.1667	0.0501	0.1407	0.6425
91.9	52.6	50	0.2227	0.0025	0.1315	0.6433	152.0	517.3	5	0.1675	0.0492	0.1407	0.6426
91.9	52.6	50	0.2227	0.0025	0.1315	0.6433	152.0	517.3	7	0.1656	0.0505	0.1415	0.6424
91.9	52.6	50	0.2227	0.0025	0.1315	0.6433	152.0	517.3	9	0.1681	0.0473	0.1422	0.6424
91.9	52.6	50	0.2227	0.0025	0.1315	0.6433	152.0	517.3	11	0.1699	0.0470	0.1406	0.6425
91.9	52.6	50	0.2227	0.0025	0.1315	0.6433	152.0	517.3	13	0.1693	0.0470	0.1413	0.6425
91.9	52.6	50	0.2227	0.0025	0.1315	0.6433	152.0	517.3	19	0.1717	0.0443	0.1414	0.6426
91.9	52.6	50	0.2227	0.0025	0.1315	0.6433	152.0	517.3	23	0.1695	0.0457	0.1424	0.6424
91.9	52.6	50	0.2227	0.0025	0.1315	0.6433	152.0	517.3	27	0.1754	0.0426	0.1394	0.6426
91.9	52.6	50	0.2227	0.0025	0.1315	0.6433	152.0	517.3	30	0.1724	0.0443	0.1408	0.6425
91.9	52.6	50	0.2227	0.0025	0.1315	0.6433	152.0	517.3	34	0.1959	0.0226	0.1383	0.6432

Data for Pilot Plant Run Isom-178

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
89.9	57.1	50	0.2568	0.0271	0.0528	0.6633	151.3	520.6	1	0.2054	0.0699	0.0628	0.6619
89.9	57.1	50	0.2568	0.0271	0.0528	0.6633	151.3	520.6	3	0.2030	0.0720	0.0628	0.6622
89.9	57.1	50	0.2568	0.0271	0.0528	0.6633	151.3	520.6	5	0.2011	0.0726	0.0643	0.6621
89.9	57.1	50	0.2568	0.0271	0.0528	0.6633	151.3	520.6	7	0.2031	0.0716	0.0633	0.6620
89.9	57.1	50	0.2568	0.0271	0.0528	0.6633	151.3	520.6	9	0.2019	0.0716	0.0646	0.6619
89.9	57.1	50	0.2568	0.0271	0.0528	0.6633	151.3	520.6	11	0.2034	0.0704	0.0640	0.6622
89.9	57.1	50	0.2568	0.0271	0.0528	0.6633	151.3	520.6	15	0.2034	0.0697	0.0647	0.6622
89.9	57.1	50	0.2568	0.0271	0.0528	0.6633	151.3	520.6	19	0.2090	0.0657	0.0631	0.6622
89.9	57.1	50	0.2568	0.0271	0.0528	0.6633	151.3	520.6	23	0.2169	0.0609	0.0598	0.6623
89.9	57.1	50	0.2568	0.0271	0.0528	0.6633	151.3	520.6	27	0.2078	0.0664	0.0637	0.6622
89.9	57.1	50	0.2568	0.0271	0.0528	0.6633	151.3	520.6	31	0.2095	0.0645	0.0638	0.6622
89.9	57.1	50	0.2568	0.0271	0.0528	0.6633	151.3	520.6	35	0.2093	0.0638	0.0647	0.6622

Data for Pilot Plant Run Isom-183

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	p_T(a)	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
123.8	61.8	50	0.3015	0.0317	0.0597	0.6071	185.0	544.9	1	0.2234	0.0900	0.0806	0.6061
123.8	61.8	50	0.3015	0.0317	0.0597	0.6071	185.0	544.9	3	0.2260	0.0874	0.0807	0.6058
123.8	61.8	50	0.3015	0.0317	0.0597	0.6071	185.0	544.9	5	0.2269	0.0860	0.0811	0.6059
123.8	61.8	50	0.3015	0.0317	0.0597	0.6071	185.0	544.9	7	0.2248	0.0860	0.0835	0.6058
123.8	61.8	50	0.3015	0.0317	0.0597	0.6071	185.0	544.9	9	0.2353	0.0736	0.0856	0.6056
123.8	61.8	50	0.3015	0.0317	0.0597	0.6071	185.0	544.9	11	0.2458	0.0612	0.0876	0.6054
123.8	61.8	50	0.3015	0.0317	0.0597	0.6071	185.0	544.9	13	0.2560	0.0550	0.0831	0.6059
123.8	61.8	50	0.3015	0.0317	0.0597	0.6071	185.0	544.9	17	0.2629	0.0480	0.0832	0.6059
123.8	61.8	50	0.3015	0.0317	0.0597	0.6071	185.0	544.9	21	0.2732	0.0413	0.0792	0.6063
123.8	61.8	50	0.3015	0.0317	0.0597	0.6071	185.0	544.9	25	0.2797	0.0369	0.0769	0.6066
123.8	61.8	50	0.3015	0.0317	0.0597	0.6071	185.0	544.9	29	0.2838	0.0340	0.0756	0.6066
123.8	61.8	50	0.3015	0.0317	0.0597	0.6071	185.0	544.9	33	0.2847	0.0331	0.0757	0.6066

Data for Pilot Plant Run Isom-190

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	$p_T(a)$	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
124.2	60.2	50	0.3071	0.0314	0.0615	0.6000	118.5	496.5	1	0.2845	0.0499	0.0657	0.5999
124.2	60.2	50	0.3071	0.0314	0.0615	0.6000	118.5	496.5	3	0.2750	0.0575	0.0678	0.5997
124.2	60.2	50	0.3071	0.0314	0.0615	0.6000	118.5	496.5	5	0.2728	0.0602	0.0672	0.5997
124.2	60.2	50	0.3071	0.0314	0.0615	0.6000	118.5	496.5	7	0.2747	0.0591	0.0664	0.5998
124.2	60.2	50	0.3071	0.0314	0.0615	0.6000	118.5	496.5	9	0.2737	0.0587	0.0678	0.5999
124.2	60.2	50	0.3071	0.0314	0.0615	0.6000	118.5	496.5	11	0.2755	0.0585	0.0663	0.5997
124.2	60.2	50	0.3071	0.0314	0.0615	0.6000	118.5	496.5	13	0.2725	0.0600	0.0687	0.5987
124.2	60.2	50	0.3071	0.0314	0.0615	0.6000	118.5	496.5	17	0.2778	0.0569	0.0655	0.5998
124.2	60.2	50	0.3071	0.0314	0.0615	0.6000	118.5	496.5	21	0.2778	0.0569	0.0655	0.5998
124.2	60.2	50	0.3071	0.0314	0.0615	0.6000	118.5	496.5	25	0.2756	0.0570	0.0679	0.5995
124.2	60.2	50	0.3071	0.0314	0.0615	0.6000	118.5	496.5	29	0.2785	0.0553	0.0666	0.5996
124.2	60.2	50	0.3071	0.0314	0.0615	0.6000	118.5	496.5	33	0.2791	0.0556	0.0656	0.5998

Data for Pilot Plant Run Isom-144

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	$p_T(a)$	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
129.9	61.5	50	0.2961	0.0348	0.0720	0.5971	205.7	518.3	1	0.2225	0.0934	0.0880	0.5960
129.9	61.5	50	0.2961	0.0348	0.0720	0.5971	205.7	518.3	3	0.2230	0.0933	0.0876	0.5960
129.9	61.5	50	0.2961	0.0348	0.0720	0.5971	205.7	518.3	5	0.2223	0.0930	0.0886	0.5961
129.9	61.5	50	0.2961	0.0348	0.0720	0.5971	205.7	518.3	7	0.2232	0.0924	0.0883	0.5961
129.9	61.5	50	0.2961	0.0348	0.0720	0.5971	205.7	518.3	9	0.2235	0.0922	0.0884	0.5959
129.9	61.5	50	0.2961	0.0348	0.0720	0.5971	205.7	518.3	11	0.2250	0.0909	0.0879	0.5961
129.9	61.5	50	0.2961	0.0348	0.0720	0.5971	205.7	518.3	13	0.2262	0.0898	0.0879	0.5962
129.9	61.5	50	0.2961	0.0348	0.0720	0.5971	205.7	518.3	17	0.2254	0.0912	0.0874	0.5959
129.9	61.5	50	0.2961	0.0348	0.0720	0.5971	205.7	518.3	21	0.2165	0.0941	0.0941	0.5954
129.9	61.5	50	0.2961	0.0348	0.0720	0.5971	205.7	518.3	25	0.2168	0.0944	0.0933	0.5955
129.9	61.5	50	0.2961	0.0348	0.0720	0.5971	205.7	518.3	29	0.2196	0.0928	0.0923	0.5953
129.9	61.5	50	0.2961	0.0348	0.0720	0.5971	205.7	518.3	33	0.2209	0.0901	0.0936	0.5953

Data for Pilot Plant Run Isom-151

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	$p_T(a)$	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	1	0.1762	0.0796	0.0651	0.6791
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	3	0.1765	0.0795	0.0650	0.6790
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	5	0.1766	0.0792	0.0652	0.6790
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	7	0.1766	0.0790	0.0654	0.6790
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	9	0.1752	0.0795	0.0662	0.6790
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	11	0.1733	0.0805	0.0675	0.6787
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	13	0.1753	0.0787	0.0669	0.6790
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	17	0.1735	0.0786	0.0691	0.6788
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	21	0.1757	0.0773	0.0684	0.6787
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	25	0.1778	0.0749	0.0683	0.6791
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	29	0.1794	0.0736	0.0680	0.6790
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	33	0.1787	0.0737	0.0687	0.6789
59.4	40.5	50	0.2424	0.0268	0.0511	0.6797	174.9	520.7	37	0.1747	0.0752	0.0714	0.6787

Data for Pilot Plant Run Isom-157

|-Feed flow-|		Mass	|---- Feed Gas Composition ----|				|Parameters|		Run	|--- Product Gas Composition ---|			
n-C4	H2O	Cat.	p n-C4	p i-C4	p bp	p H_2O	$p_T(a)$	Temp.	time	p n-C4	p i-C4	p bp	p H_2O
75.6	53.2	50	0.2324	0.0250	0.0535	0.6890	154.4	521.9	1	0.1734	0.0733	0.0647	0.6885
75.6	53.2	50	0.2324	0.0250	0.0535	0.6890	154.4	521.9	3	0.1734	0.0732	0.0648	0.6886
75.6	53.2	50	0.2324	0.0250	0.0535	0.6890	154.4	521.9	5	0.1694	0.0766	0.0659	0.6881
75.6	53.2	50	0.2324	0.0250	0.0535	0.6890	154.4	521.9	7	0.1689	0.0762	0.0667	0.6882
75.6	53.2	50	0.2324	0.0250	0.0535	0.6890	154.4	521.9	9	0.1685	0.0758	0.0674	0.6883
75.6	53.2	50	0.2324	0.0250	0.0535	0.6890	154.4	521.9	11	0.1692	0.0759	0.0669	0.6880

Data for Pilot Plant Run Isom-157 - Continued

|-Feed flow-|		*Mass*	*|---- Feed Gas Composition ----|*				*|Parameters|*		*Run*	*|--- Product Gas Composition ---|*			
n-C4	*H2O*	*Cat.*	*p n-C4*	*p i-C4*	*p bp*	$p\ H_2O$	$p_T(a)$	*Temp.*	*time*	*p n-C4*	*p i-C4*	*p bp*	$p\ H_2O$
75.6	53.2	50	0.2324	0.0250	0.0535	0.6890	154.4	521.9	13	0.1689	0.0760	0.0671	0.6879
75.6	53.2	50	0.2324	0.0250	0.0535	0.6890	154.4	521.9	17	0.1703	0.0751	0.0668	0.6878
75.6	53.2	50	0.2324	0.0250	0.0535	0.6890	154.4	521.9	21	0.1734	0.0732	0.0657	0.6876
75.6	53.2	50	0.2324	0.0250	0.0535	0.6890	154.4	521.9	25	0.1765	0.0714	0.0646	0.6875
75.6	53.2	50	0.2324	0.0250	0.0535	0.6890	154.4	521.9	29	0.1768	0.0709	0.0646	0.6877

TABLE A5.2 : INPUT FILE KEY

Feed flow : n-C4	Hydrocarbon Feed Rate, g/h
Feed flow : H2O	Water Flow Rate, g/h
Mass : Cat.	Catalyst Mass, g
Feed Gas Composition : p n-C4	n-Butene Mole Fraction in the Combined Feed
Feed Gas Composition : p i-C4	Isobutene Mole Fraction in the Combined Feed
Feed Gas Composition : p bp	Mole Fraction of Light (<C4), Heavy (>C4), Paraffinic (n-Butane and Isobutane) and 1,3-Butadiene in the Combined Feed
Feed Gas Composition : $p\ H_2O$	Mole Fraction of Water in the Combined Feed
Parameters : $p_T(a)$	Absolute Total System Pressure, kPa(a)
Parameters : Temp.	System Temperature, °C
Run : Time	Time On Line, h
Product Gas Composition : p n-C4	Mole Fraction of n-Butene in the Combined Product Gas
Product Gas Composition : p i-C4	Mole Fraction of Isobutene in the Combined Product Gas
Product Gas Composition : p bp	Mole Fraction of Light (<C4), Heavy (>C4), Paraffinic (n-Butane and Isobutane) and 1,3-Butadiene in the Combined Product Gas
Product Gas Composition : $p\ H_2O$	Mole Fraction of Water in the Combined Product Gas