APÉNDICE D. DATOS DE ENTRADA AL SIMULADOR DE LOS PROCESOS EVALUADOS

Proceso de Producción de Ciclohexano

```
IN-UNITS ENG

COMPONENTS
   HYDROGEN H2 /
   BENZENE C6H6 /
   CYCLO-01 C6H12-1 /
   NITROGEN N2 /
   METHANE CH4

FLOWSHEET
   BLOCK M-110 IN=FEEDH2 FEEDBZ2 OUT=H2YBZ
   BLOCK P-110 IN=FEEDBZ OUT=FEEDBZ2
   BLOCK M-120 IN=H2YBZ RECICBZ2 SCOMP OUT=EPREHEAT
   BLOCK HE-110 IN=EPREHEAT OUT=EREAC
   BLOCK HE-130 IN=EREAC OUT=SREAC
   BLOCK HE-120 IN=SREAC OUT=EFLASH
   BLOCK CP-110 IN=ECOMP OUT=SCOMP
   BLOCK VV-110 IN=EFLASH OUT=S1FLASH S2FLASH
   BLOCK P-120 IN=RECICBZ1 OUT=RECICBZ2
   BLOCK D-120 IN=S2FLASH OUT=RECICBZ1 ECOLUMNA
   BLOCK D-110 IN=S1FLASH OUT=PURGA ECOMP
   BLOCK TW-110 IN=ECOLUMNA OUT=DEST PRODUCTO

PROPERTIES NRTL

PROP-DATA NRTL-1
   IN-UNITS ENG
   PROP-LIST NRTL
   BPVAL BENZENE CYCLO-01 0.0 328.9580974 .3000000000 0.0 0.0  &
      0.0 171.3200026 177.3500026
   BPVAL CYCLO-01 BENZENE 0.0 -78.01307938 .3000000000 0.0  &
      0.0 0.0 171.3200026 177.3500026

STREAM FEEDBZ
   SUBSTREAM MIXED TEMP=100. PRES=15. MOLE-FLOW=425.
   MOLE-FLOW BENZENE 1.

STREAM FEEDH2
   SUBSTREAM MIXED TEMP=120. PRES=335. MOLE-FLOW=1402.
   MOLE-FLOW HYDROGEN 0.975 / NITROGEN 0.005 / METHANE 0.02

BLOCK M-110 MIXER

BLOCK M-120 MIXER

BLOCK D-110 FSPLIT
   FRAC PURGA 0.08

BLOCK D-120 FSPLIT
   FRAC RECICBZ1 0.3
```

```
BLOCK HE-110 HEATER
   PARAM TEMP=300. PRES=330.

BLOCK HE-120 HEATER
   PARAM TEMP=120. PRES=-5.

BLOCK VV-110 FLASH2
   PARAM TEMP=120. PRES=-5.

BLOCK TW-110 RADFRAC
   PARAM NSTAGE=15 EFF=MURPHREE
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS ECOLUMNA 8
   PRODUCTS DEST 1 V / PRODUCTO 15 L
   P-SPEC 1 200. / 15 250.
   COL-SPECS MOLE-B=420. MOLE-RR=1.2
   STEFF-SEC SECNO=1 2 15 0.5

BLOCK HE-130 RSTOIC
   PARAM TEMP=400. PRES=-15.
   STOIC 1 MIXED BENZENE -1. / HYDROGEN -3. / CYCLO-01 1.
   CONV 1 MIXED BENZENE 0.998

BLOCK P-110 PUMP
   PARAM PRES=315.

BLOCK P-120 PUMP
   PARAM PRES=315.

BLOCK CP-110 COMPR
   PARAM TYPE=ASME-POLYTROP PRES=330. PEFF=0.8

EO-CONV-OPTI

STREAM-REPOR MOLEFLOW
```

Proceso de Producción de Metanol

```
IN-UNITS MET

COMPONENTS
   METHANE CH4 /
   ETHANE C2H6 /
   PROPANE C3H8 /
   CO2 CO2 /
   CO CO /
   H2 H2 /
   OXYGEN O2 /
   WATER H2O /
   METHANOL CH4O /
   ETHANOL C2H6O-2 /
   NITROGEN N2 /
   ARGON AR

PROPERTIES PENG-ROB
   PROPERTIES NRTL

STREAM 1A
   SUBSTREAM MIXED TEMP=35. <C> PRES=27.  &
      MASS-FLOW=65. <tonne/hr>
   MASS-FRAC METHANE 0.88 / ETHANE 0.1 / PROPANE 0.02

STREAM 31
   SUBSTREAM MIXED PRES=40. VFRAC=1. MOLE-FLOW=6000.
   MOLE-FRAC WATER 1.

STREAM 32
   SUBSTREAM MIXED TEMP=25. <C> PRES=1. MASS-FLOW=255000.
   STDVOL-FRAC CO2 0.00036 / OXYGEN 0.1995 / WATER 0.04804 /  &
      NITROGEN 0.7436 / ARGON 0.0085

BLOCK MX-101 MIXER

BLOCK MX-102 MIXER

BLOCK MX-201 MIXER

BLOCK MX-301 MIXER

BLOCK D-101 FSPLIT
   FRAC 3 0.5

BLOCK D-201 FSPLIT
   FRAC 20 0.05 / 21 0.04

BLOCK MM-401 SEP
   FRAC STREAM=37 SUBSTREAM=MIXED COMPS=CO2 WATER FRACS= &
      0.999 0.9999

BLOCK F-101 HEATER
   PARAM TEMP=780. <C> PRES=40.
```

```
BLOCK HE-101 HEATER
   PARAM TEMP=240. <C> PRES=0.

BLOCK HE-201 HEATER
   PARAM TEMP=200. <C> PRES=40.

BLOCK HE-202 HEATER
   PARAM TEMP=20. <C> PRES=60.

BLOCK HE-301 HEATER
   PARAM TEMP=25. <C> PRES=1.
BLOCK HE-401 HEATER
   PARAM TEMP=60. <C> PRES=1.

BLOCK HE-402 HEATER
   PARAM TEMP=15. <C> PRES=6.

BLOCK VV-201 FLASH2
   PARAM PRES=0. DUTY=0.

BLOCK VV-401 FLASH2
   PARAM PRES=0. DUTY=0.

BLOCK HE43 MHEATX
   HOT-SIDE IN=38 OUT=39 TEMP=-67. <C> FREE-WATER=NO
   COLD-SIDE IN=46 OUT=47 FREE-WATER=NO

BLOCK HE44 MHEATX
   HOT-SIDE IN=39 OUT=40 FREE-WATER=NO
   COLD-SIDE IN=42 OUT=43 TEMP=200. <K> FREE-WATER=NO

BLOCK T-301 RADFRAC
   PARAM NSTAGE=7
   COL-CONFIG CONDENSER=NONE
   FEEDS 22 1 ON-STAGE
   PRODUCTS 23 1 V / 24 7 L
   P-SPEC 1 20.
   COL-SPECS MOLE-B=9122.

BLOCK T-302 RADFRAC
   PARAM NSTAGE=69 EFF=MURPHREE
   COL-CONFIG CONDENSER=TOTAL
   FEEDS 24 66
   PRODUCTS 25 1 L / 26 69 L
   P-SPEC 1 1.
   COL-SPECS MOLE-D=2100. MOLE-RR=2.33
   TRAY-SIZE 1 2 68 FLOAT FLOOD-FAC=0.9
   PROPERTIES NRTL
   STEFF-SEC SECNO=1 2 68 0.9

BLOCK T-303 RADFRAC
   PARAM NSTAGE=78 EFF=MURPHREE
   COL-CONFIG CONDENSER=TOTAL
   FEEDS 26 30
   PRODUCTS 28 78 L / 27 1 L
   P-SPEC 1 1.
   COL-SPECS MOLE-D=1548. MOLE-RR=4.
```

```
   TRAY-SIZE 1 2 77 FLOAT FLOOD-FAC=0.9
   PROPERTIES NRTL
   STEFF-SEC SECNO=1 2 77 0.9

BLOCK T-401 RADFRAC
   PARAM NSTAGE=20 ALGORITHM=STANDARD INIT-OPTION=CRYOGENIC
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 40 13
   PRODUCTS 44 20 L / 41 1 V
   P-SPEC 1 6.
   COL-SPECS MOLE-B=1670. MOLE-RR=2.85

BLOCK T-402 RADFRAC
   PARAM NSTAGE=35 ALGORITHM=STANDARD INIT-OPTION=CRYOGENIC
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 44 26
   PRODUCTS 45 1 V / 46 35 L
   P-SPEC 1 1.
   COL-SPECS MOLE-B=1630. MOLE-RR=60.

BLOCK SM-201 RSTOIC
   PARAM TEMP=250. <C> PRES=70.
   STOIC 1 MIXED H2 -2. / CO -1. / METHANOL 1.
   STOIC 2 MIXED CO2 -1. / H2 -3. / METHANOL 1. / WATER  & 1.
   STOIC 3 MIXED CO2 -2. / H2 -6. / ETHANOL 1. / WATER  & 3.
   CONV 1 MIXED CO 0.55
   CONV 2 MIXED CO2 0.3
   CONV 3 MIXED CO2 0.022

BLOCK SM-202 RSTOIC
   PARAM TEMP=250. <C> PRES=70.
   STOIC 1 MIXED H2 -2. / CO -1. / METHANOL 1.
   STOIC 2 MIXED CO2 -1. / H2 -3. / METHANOL 1. / WATER  & 1.
   STOIC 3 MIXED CO2 -2. / H2 -6. / ETHANOL 1. / WATER  & 3.
   CONV 1 MIXED CO 0.55
   CONV 2 MIXED CO2 0.3
   CONV 3 MIXED CO2 0.022

BLOCK AR-101 RGIBBS
   PARAM TEMP=950. <C> PRES=40.

BLOCK PR-101 RGIBBS
   PARAM TEMP=780. <C> PRES=40.

BLOCK P-301 PUMP
   PARAM PRES=40.

BLOCK P-401 PUMP
   PARAM PRES=40.

BLOCK CP-101 COMPR
   PARAM TYPE=ASME-POLYTROP PRES=40.

BLOCK CP-201 COMPR
   PARAM TYPE=ASME-POLYTROP PRES=70.
```

```
BLOCK CP-202 COMPR
   PARAM TYPE=ASME-POLYTROP PRES=70.

BLOCK TB-401 COMPR
   PARAM TYPE=ISENTROPIC PRES=1. NPHASE=2 MODEL-TYPE=TURBINE
   BLOCK-OPTION FREE-WATER=NO

BLOCK CP-401 MCOMPR
   PARAM NSTAGE=3 TYPE=ASME-POLYTROPIC PRES=6.
   FEEDS 33 1
   PRODUCTS 34 3
   COOLER-SPECS 1 TEMP=100. <C>

BLOCK CP-402 MCOMPR
   PARAM NSTAGE=3 TYPE=ASME-POLYTROPIC PRES=40.
   FEEDS 47 1
   PRODUCTS 48 3
   COOLER-SPECS 3 TEMP=200. <C> / 1 TEMP=200. <C>

BLOCK V-201 VALVE
   PARAM P-OUT=60.

EO-CONV-OPTI

CONV-OPTIONS
   WEGSTEIN MAXIT=80

STREAM-REPOR MOLEFLOW MOLEFRAC
```

Proceso de Producción de Dimetil-Éter

```
IN-UNITS MET

COMPONENTS
   METANOL CH4O /
   AGUA H2O /
   DMT C2H6O-1

FLOWSHEET
   BLOCK V-200 IN=8 OUT=9
   BLOCK E-202 IN=6 4 OUT=7 5
   BLOCK V-201 IN=15 OUT=16
   BLOCK E-208 IN=14 OUT=15
   BLOCK E-203 IN=7 OUT=8
   BLOCK R-201 IN=5 OUT=6
   BLOCK E-201 IN=3 OUT=4
   BLOCK P-201 IN=1 OUT=2
   BLOCK P-202 IN=13 OUT=13-A
   BLOCK M-201 IN=2 13-A OUT=3
   BLOCK T-201 IN=9 OUT=10 11
   BLOCK T-202 IN=11 OUT=13 14

PROPERTIES UNIQUAC

ESTIMATE ALL
   IN-UNITS ENG
   UNIQ ALL ALL UNIFAC

PROP-DATA UNIQ-1
   IN-UNITS ENG
   PROP-LIST UNIQ
   BPVAL METANOL AGUA -1.066200000 779.1812938 0.0 0.0  &
      76.98200338 212.0000023 0.0
   BPVAL AGUA METANOL .6437000000 -579.8361554 0.0 0.0  &
      76.98200338 212.0000023 0.0
   BPVAL METANOL DMT 0.0 -627.8180350 0.0 0.0 32.00000374  &
      32.00000374 0.0
   BPVAL DMT METANOL 0.0 -45.17999964 0.0 0.0 32.00000374  &
      32.00000374 0.0
   BPVAL AGUA DMT 0.0 -689.4514079 0.0 0.0 77.00000338  &
      77.00000338 *
   BPVAL DMT AGUA 0.0 275.6147252 0.0 0.0 77.00000338  &
      77.00000338 *

PROP-SET IPE-1
   IN-UNITS ENG
   PROPNAME-LIS MASSVFRA MASSSFRA MASSFLMX VOLFLMX TEMP PRES  &
      MWMX MASSFLOW SUBSTREAM=ALL

PROP-SET IPE-2
   IN-UNITS ENG
   PROPNAME-LIS VOLFLMX MASSFLMX KMX SIGMAMX MUMX CPMX MWMX  &
      UNITS='kJ/kg-K' SUBSTREAM=MIXED PHASE=L
```

```
PROP-SET IPE-3
   IN-UNITS ENG
   PROPNAME-LIS VOLFLMX MASSFLMX KMX MUMX CPMX MWMX UNITS= &
      'kJ/kg-K' SUBSTREAM=MIXED PHASE=V

STREAM 1
   IN-UNITS ENG
   SUBSTREAM MIXED TEMP=25. <C> PRES=1. <bar>  &
      MOLE-FLOW=246.919968 <kmol/hr>
   MOLE-FRAC METANOL 1.

BLOCK M-201 MIXER
   IN-UNITS ENG
   PARAM PRES=-0.3 <bar>

BLOCK E-201 HEATER
   IN-UNITS ENG
   PARAM TEMP=154. <C> PRES=15.1 <bar>

BLOCK E-203 HEATER
   IN-UNITS ENG
   PARAM TEMP=100. <C> PRES=13.4 <bar>

BLOCK E-208 HEATER
   IN-UNITS ENG
   PARAM TEMP=50. <C> PRES=-0.5 <bar>

BLOCK E-202 HEATX
   IN-UNITS ENG
   PARAM T-COLD=250. <C> PRES-COLD=14.7 <bar> U-OPTION=PHASE  &
      F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
   FEEDS HOT=6 COLD=4
   PRODUCTS HOT=7 COLD=5
   HOT-SIDE DP-OPTION=CONSTANT
   COLD-SIDE DP-OPTION=CONSTANT

BLOCK T-201 RADFRAC
   IN-UNITS SI MASS-FLOW='tonne/year' MOLE-FLOW='kmol/hr'  &
      PRESSURE=bar TEMPERATURE=C DELTA-T=C PDROP=bar
   PARAM NSTAGE=22
   COL-CONFIG CONDENSER=TOTAL
   FEEDS 9 16
   PRODUCTS 11 22 L / 10 1 L
   P-SPEC 1 10.3
   COL-SPECS D:F=0.3974927 DP-COL=0.2 MOLE-RR=0.41701745
   SPEC 1 MOLE-FRAC 0.9991 COMPS=DMT STREAMS=10
   VARY 1 MOLE-RR 0.3 5.

BLOCK T-202 RADFRAC
   IN-UNITS SI MASS-FLOW='tonne/year' MOLE-FLOW='kmol/hr'  &
      PRESSURE=bar TEMPERATURE=C DELTA-T=C PDROP=bar
   PARAM NSTAGE=26
   COL-CONFIG CONDENSER=TOTAL
   FEEDS 11 19
   PRODUCTS 14 26 L / 13 1 L
   P-SPEC 1 7.3
   COL-SPECS D:F=0.3402385 DP-COL=0.3 MOLE-RR=2.44502269
```

```
BLOCK R-201 RPLUG
   IN-UNITS ENG
   PARAM TYPE=ADIABATIC LENGTH=13. <meter> DIAM=0.7 <meter>  &
      PDROP=0.8 <bar> CAT-PRESENT=NO
   REACTIONS RXN-IDS=R-1

BLOCK P-201 PUMP
   IN-UNITS ENG
   PARAM PRES=15.5 <bar>

BLOCK P-202 PUMP
   IN-UNITS ENG
   PARAM PRES=15.5 <bar>

BLOCK V-200 VALVE
   IN-UNITS ENG
   PARAM P-OUT=10.4 <bar>

BLOCK V-201 VALVE
   IN-UNITS ENG
   PARAM P-OUT=1.2 <bar>

EO-CONV-OPTI

CONV-OPTIONS
   PARAM SPEC-METHOD=BROYDEN
   WEGSTEIN MAXIT=100
   BROYDEN MAXIT=100

STREAM-REPOR PROPERTIES=IPE-1 IPE-2 IPE-3

REACTIONS R-1 POWERLAW
   IN-UNITS ENG
   REAC-DATA 1 PHASE=V
   RATE-CON 1 PRE-EXP=0.336 ACT-ENERGY=80480. <kJ/kmol>  &
      T-REF=25. <C>
   STOIC 1 MIXED METANOL -2. / AGUA 1. / DMT 1.
   POWLAW-EXP 1 MIXED METANOL 8.4
```

Proceso de Producción de Dimetiletanolamina

```
IN-UNITS MET

COMPONENTS
   ETHYL-01 C2H4O-2 /
   DIMET-01 C2H7N-2 /
   DIMET-02 C4H11NO

FLOWSHEET
   BLOCK REACTOR IN=ALIM-R OUT=SAL-R
   BLOCK MEZCLADO IN=DMA OET DMA-R TORRE-R OUT=MEZCLA
   BLOCK ENFRIADO IN=MEZCLA OUT=ALIM-R
   BLOCK EVAP IN=SAL-R OUT=ALIM-T
   BLOCK TANQUE IN=ALIM-T OUT=DMA-R LIQ-T
   BLOCK TORRE IN=LIQ-T OUT=TORRE-R PRODUCTO

PROPERTIES NRTL
   PROPERTIES AMINES

PROP-SET IPE-1
   IN-UNITS ENG
   PROPNAME-LIS MASSVFRA MASSSFRA MASSFLMX VOLFLMX TEMP PRES  &
      MWMX MASSFLOW SUBSTREAM=ALL

PROP-SET IPE-2
   IN-UNITS ENG
   PROPNAME-LIS VOLFLMX MASSFLMX KMX SIGMAMX MUMX CPMX MWMX  &
      UNITS='kJ/kg-K' SUBSTREAM=MIXED PHASE=L

PROP-SET IPE-3
   IN-UNITS ENG
   PROPNAME-LIS VOLFLMX MASSFLMX KMX MUMX CPMX MWMX UNITS= &
      'kJ/kg-K' SUBSTREAM=MIXED PHASE=V

STREAM DMA
   IN-UNITS MET
   SUBSTREAM MIXED TEMP=25. <C> PRES=1. MOLE-FLOW=118.98
   MOLE-FRAC ETHYL-01 0. / DIMET-01 1. / DIMET-02 0.

STREAM OET
   IN-UNITS MET
   SUBSTREAM MIXED TEMP=25. <C> PRES=1. MOLE-FLOW=39.66
   MOLE-FRAC ETHYL-01 1. / DIMET-01 0. / DIMET-02 0.

BLOCK MEZCLADO MIXER
   IN-UNITS MET

BLOCK ENFRIADO HEATER
   IN-UNITS MET
   PARAM PRES=0. VFRAC=0.

BLOCK EVAP HEATER
   IN-UNITS MET
   PARAM PRES=0. VFRAC=0.65
```

```
BLOCK TANQUE FLASH2
   IN-UNITS MET
   PARAM PRES=0. DUTY=0.

BLOCK TORRE RADFRAC
   IN-UNITS MET
   PARAM NSTAGE=5
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS LIQ-T 2
   PRODUCTS TORRE-R 1 V / PRODUCTO 5 L
   P-SPEC 1 1.
   COL-SPECS D:F=0.12 MOLE-RR=1.

BLOCK REACTOR RCSTR
   IN-UNITS ENG
   PARAM VOL=200. <l> TEMP=40. <C> PRES=1. <atm> NPHASE=1  &
      PHASE=L CAT-PRESENT=NO
   BLOCK-OPTION FREE-WATER=NO
   REACTIONS RXN-IDS=R-1

DESIGN-SPEC DS-1
   IN-UNITS MET
   DEFINE FDMA MOLE-FLOW STREAM=ALIM-R SUBSTREAM=MIXED  &
      COMPONENT=DIMET-01
   DEFINE FOXET MOLE-FLOW STREAM=ALIM-R SUBSTREAM=MIXED  &
      COMPONENT=ETHYL-01
   SPEC "FDMA/FOXET" TO "3"
   TOL-SPEC ".05"
   VARY STREAM-VAR STREAM=DMA SUBSTREAM=MIXED  &
      VARIABLE=MOLE-FLOW
   LIMITS "30" "120"

EO-CONV-OPTI

SENSITIVITY S-1
   IN-UNITS MET
   DEFINE FDMEA MOLE-FLOW STREAM=ALIM-T SUBSTREAM=MIXED  &
      COMPONENT=DIMET-02
   DEFINE LDMEA MOLE-FLOW STREAM=LIQ-T SUBSTREAM=MIXED  &
      COMPONENT=DIMET-02
   DEFINE XDMEA MOLE-FRAC STREAM=LIQ-T SUBSTREAM=MIXED  &
      COMPONENT=DIMET-02
   TABULATE 1 "FDMEA"
   TABULATE 2 "LDMEA"
   TABULATE 4 "XDMEA"
   TABULATE 3 "LDMEA/FDMEA"
   VARY BLOCK-VAR BLOCK=EVAP VARIABLE=VFRAC SENTENCE=PARAM
   RANGE LOWER="0" UPPER="1" INCR=".05"

STREAM-REPOR MOLEFLOW MOLEFRAC PROPERTIES=IPE-1 IPE-2 IPE-3

REACTIONS R-1 GENERAL
   IN-UNITS ENG
   REAC-DATA 1 NAME=RX1 REAC-CLASS=EQUILIBRIUM DELT=25. <C>
   STOIC 1 MIXED ETHYL-01 -1. / DIMET-01 -1. / DIMET-02 1.
```