$$U_{mf} \quad r_{ft}^2 = \frac{T_{ft}}{T_p} Q_p \quad \text{(A6)}$$

Using the minimum flow expected from the pyrolyzer, the diameter of the reactor should be 6.53 inches. A diameter of 6.5 inches was selected for the actual reactor.

APPENDIX B

FORTRAN PROGRAMS

```
C*************************************************************
C
C   Program to model a fluidized bed reactor
C
C      Declared Variables:
C
C         CB(30,10) = Bubble phase concentration,
C                     moles/cu.cm.
C                     (stage number, component number)
C         CE(30,10) = Emulsion phase concentration,
C                     moles/cu.cm.
C                     (stage number, component number)
C         CC(30,10) = Cloud phase concentration,
C                     moles/cu.cm.
C                     (stage number, component number)
C         D(10)     = Diffusion coefficient for gas
C                     mixture, sq.cm./s
C                     (component number)
C         HT(30)    = Height of a particular stage, cm
C                     (stage number)
C         FCE(10)   = Transfer rate from cloud to
C                     emulsion, 1/s
C                     (component number)
C
C*************************************************************
      REAL CB(30,10),CE(30,10),CC(30,10),D(10),HT(30),
     +     FCE(10)
C*************************************************************
C
C         Common Variables:
C
C             BCOM : Parameters describing the entire bed
C
C             H      = Height of the expanded bed, cm
C             HJ     = Height of the jetting region, cm
C             HC     = Distance from top of jets to start
C                      of bubbling, cm
C             DBO    = Original bubble diameter, cm
C             DBM    = Mean bubble diameter for bed, cm
C
C         SCOM : Paramters describing a particular stage
C
C            E      = Void fraction, unitless
C            VCP    = Volume of cloud phase, cu.cm.
C            VBP    = Volume of bubble phase, cu.cm.
C            VEP    = Volume of emulsion phase, cu.cm.
C            UBS    = Superficial velocity of gas flowing
C                     from the previous stage to current
C                     stage in bubble phase, cm/s
```

```
C            UES    = Superficial velocity of gas flowing
C                     from the previous stage to current
C                     stage in emulsion phase, cm/s
C            UCS    = Superficial velocity of gas flowing
C                     from the previous stage to current
C                     stage in cloud phase, cm/s
C            FBC    = Diffusive transfer from bubble to
C                     cloud phase, 1/s
C            GCE    = Crossflow from cloud to emulsion
C                     phase, cm/s
C            GBC    = Crossflow from bubble to cloud phase,
C                     cm/s
C            UBSN   = Superficial velocity of gas flowing
C                     from the current stage to the next
C                     stage in the bubble phase, cm/s
C            UESN   = Superficial velocity of gas flowing
C                     from the current stage to the next
C                     stage in the emulsion phase, cm/s
C            UCSN   = Superficial velocity of gas flowing
C                     from the current stage to the next
C                     stage in the cloud phase, cm/s
C
C*************************************************************
      COMMON/BCOM/H,HJ,HC,DBC,DBM
      COMMON/SCOM/E,VCP,VBP,VEP,UBS,UES,UCS,FBC,GBC,GCE,
     +            UBSN,UESN,UCSN
C
C     Set stage indicators to the first stage
C
C     HSTAGE = The height of the current stage, cm
C     NSTAGE = The number of the current stage
C
      HSTAGE=0.0
      NSTAGE=1
C
C     Obtain initial data for the current bed.
C (See: Subroutine GETDT)
C
      CALL GETDT(EMF,DR,ND,DP,CB,CE,CC,A,UO,UMF,IC,D,HMF,
     +           RKG,CPS,DENS,CPG,DENG,TR,TAM,VIS,EB,EC)
C
C     Calculate parameters that relate to the current bed
C from the initial data and obtain the height of the first
C stage. (See: Subroutine BED)
C
      CALL BED(EMF,DR,ND,DP,A,UO,UMF,IC,HMF,HSTAGE)
C
C     Save the height of the first stage for latter printing
C
```

```
      HT(1)=HSTAGE
C
C          Calculate the parameters for the first stage.  This
C done so that the cumulative variables will have
C appropriate values when subroutine STAGE is called a
C second time.  Stage 2 is actually the first stage of
C interest
C
      CALL STAGE(NSTAGE,HSTAGE,DR,UO,UMF,A,EMF,D,HMF,EB,
     +           EC,FCE,IC)
C
C     To prepare for calcualtion of values for the next stage:
C          1. Update stage counter
C          2. Set initial concentration profile guess
C
   10 NSTAGE=NSTAGE+1
      DO 20 I=1,IC
            CB(NSTAGE+1,I)= CB(NSTAGE,I)
            CC(NSTAGE+1,I)= CC(NSTAGE,I)
   20    CE(NSTAGE+1,I)= CE(NSTAGE,I)
C
C    Set current UBSN,UCSN,UESN to be the next UBS,UCS,UES
C
      UCS=UCSN
      UBS=UBSN
      UES=UESN
C
C          Calculate values of the parameters for the current
C stage.  (See: Subroutine STAGE)
C
      CALL STAGE(NSTAGE,HSTAGE,DR,UO,UMF,A,EMF,D,HMF,EB,
     +           EC,FCE,IC)
      HT(NSTAGE)=HSTAGE
C
C    This point is jumped to only when calculating the
C compartments concentration and there is backflow.
C
   30 CONTINUE
C
C     Calculate the current concentrations.  Loop ten
C times to insure convergence.
C
      DO 50 J=1,10
          CALL ECON(CB,CE,CC,IC,NSTAGE,A,FCE)
          CALL BCON(CB,CE,CC,IC,NSTAGE,A,FCE)
          CALL CCAN(CB,CE,CC,IC,NSTAGE,A,FCE)
          IF(J.NE.1) GOTO 50
          DO 40 I=1,IC
   40     CE(NSTAGE+1,I)=CE(NSTAGE,I)
```

```
  50      CONTINUE
C
C         Check to see if the total bed has been calculated
C
      IF(HSTAGE.LT.H) GOTO 10
C
C     If the flow in the emulsion was negative, set it to
C the smallest C  value satisfing mass balance constraints
C and recalculate the concentrations in the final stage.
C
      IF(UESN.LT.0.0) THEN
          UESN=0.0
          UESN=GCE
          GOTO 30
      ENDIF
C
C     Print out the concentration profiles
C
      CALL CONPRT(CB,CE,CC,NSTAGE,HSTAGE.IC,HT,UESN,UCSN,
     +            UBSN)
C
C     Calculate heat transfered from the bed to
C surroundings
C
      CALL ENERGY(DP,RKG,CPS,DR,UO,VIS,DENS,CPG,DENG,H,TR,
     +            TAM,HMF,EMF,Q)
C
C    Print out final heat transfered
C
      CALL WRTDT(Q)
      STOP
      END
C*************************************************************
C
C     Subroutine GETDT
C
C          This subroutine obtains data on the properties of
C the bed and the material used to construct it.
C
C*************************************************************
C
C     EMF        = The void fraction of the bed at minimum
C                  fluidization, unitless
C     DR         = The diameter of the reactor, cm
C     ND         = The number of holes in the distributor,
C                  unitless
C     DP         = The diameter of the solid particles, cm
C     CB(30,10) = Bubble phase concentration, moles/cu.cm.
```

```
C                    (stage number, component number)
C     CE(30,10) = Emulsion phase concentration,
C                    moles/cu.cm.
C                        (stage number, component number)
C     CC(30,10) = Cloud phase concentration, moles/cu.cm.
C                    (stage number, component number)
C     A         = Cross-sectional area of the bed, sq.cm.
C     UO        = Initial superficial gas velocity, cm/s
C     UMF       = Superficial gas velocity at minimum
C                    fluidization, sq.cm.
C     IC        = Number of components, unitless
C     D(10)     = Diffusivity of each component, sq.cm./s
C                    (component number)
C     HMF       = Height of the bed at minimum
C                    fluidization gas flow, cm
C     RKG       = Thermal conductivity of the gas, W/m*C
C     CPS       = Heat capacity of solid, kJ/kg*K
C     DENS      = Density of solids, kg/cu.cm.
C     CPG       = Heat capacity of gas, kJ/kg*K
C     DENG      = Density of gas, kg/cu.cm.
C     TR        = Temperature of reactor, K
C     TAM       = Ambient temperature, K
C     VIS       = Viscosity of gas, kg/cm*s
C     EB        = Void fraction of in the bubble phase,
C                    unitless
C     EC        = Void fraction in the cloud phase,
C                    unitless
C
C*************************************************************
C
      SUBROUTINE GETDT(EMF,DR,ND,DP,CB,CE,CC,A,UO,UMF,IC,
     +                 D,HMF,RKG,CPS,DENS,CPG,DENG,TR,TAM,
     +                 VIS,EB,EC)
C
C     Declare arrays
C
      REAL CB(30,10),CE(30,10),CC(30,10),D(10)
C
C      Read from input unit, free format, the general
C parameters for the bed
C
      READ(5,*) EMF,DR,DP,HMF,UMF,ND,A,UO
      READ(5,*) IC
C
C      Read initial concentrations
C
      DO 10 I=1,IC
   10 READ(5,*) CB(1,I),CE(1,I),CC(1,I)
C
```

```
C     Initialize all other concentration locations
C
      DO 20 I=3,30
          DO 10 J=1,20
              CE(I,J)=0.0
              CB(I,J)=0.0
 20           CC(I,J)=0.0
C
C         Read in the diffusivities of each component
C
      DO 30 I=1,IC
 30   READ(5,*) D(I)
C
C         Read in thermal characteristics
C
C - of gas
C
      READ(5,*) RKG,CPG,DENG,VIS
C
C     - of solids
C
      READ(5,*) CPS,DENS
C
C         Temperatures
C
      READ(5,*) TR,TAM
C
C         Currently EB and EC are not read in.  EB is 1.0
C because the bubbles are assumed to be free of solids.
C EC is the same as the void fraction in the emulsion.
C
      EB=1.0
      EC=EMF
      RETURN
      END
C*************************************************************
C
C          Subroutine BED
C
C          This subroutine calculates the parameters that are
C constant throughout the bed.
C
C*************************************************************
C
C     EMF     = Void fraction of the bed at minimum
C               fluidization, unitless
C     DR      = Reactor diameter, cm
C     ND      = Number of holes in the distributor,
C               unitless
```

```
C     DP      = Diameter of the particles, cm
C     A       = Cross-sectional area of the bed, sq.cm.
C     UO      = Initial superficial gas velocity, cm/s
C     UMF     = Velocity required for minimum fluidization,
C               cm/s
C     IC      = Number of components
C     HMF     = Height of the bed at minimum fluidizing gas
C               flow, cm
C     HSTAGE  = Height of the current stage, cm
C
C     BCOM common is passed to this subroutine.  See the main
C program for a description of the variables included.
C
C*************************************************************
C
      SUBROUTINE BED(EMF,DR,ND,DP,A,UO,UMF,IC,HMF,IC,HMF,
     +               HSTAGE)
C
      COMMON/BCOM/H,HJ,HC,DBO,DBMAX
C
C     Set constants to be used in subroutine
C
C         G  = Gravitational acceleration, sq.cm./s
C         DBC = Critical bubble diameter, cm
C
      G =980.665
      DBC=0.6
C
C     Use correlation presented in Peters et.al.
C Chem Eng Sci, v.37,no.4, p556, eq 26, to calculate
C expanded bed height
C
C         First calculate the proportionality constant
C             Y=f(Uo,Umf)
C
      Y=0.7585-0.0013*(UO-UMF)+0.0005*(UO-UMF)*(UO-UMF)
C
C         Now calculate average bubble size using the bubble
C size correlation presented in Peters et.al. p555, eq 14.
C To use this correlation the maximum stable bubble size
C and the initial bubble size are both obtained from the
C same source as the average bubble size.
C
C     DBMAX = maximum stable bubble size
C
      DBMAX=0.652*POW(A*(UO-UMF),0.4)
      DBO=0.347*POW(A/ND*(UO-UMF),0.4)
      DBM=DBMAX-(DBMAX-DBO)*EXP(-0.3*(HMF/2)/DR)
C
```

```
C          Now that all preliminary values have been obtained
C it is possible to obtain the expanded bed height
C
      H=HMF/(1-((Y*(UO-UMF)/(UO-UMF+0.71*SQRT(G*DBM))))
C
C          Calculate height of the jetting region.  Use
C correlation presented in Too et.al. , AIChE Winter
C National Meeting, 1984, from Mori and Wen.
C
      HJ=DP/(0.0007+0.556*DP)*POW(A/ND*(UO-UMF),0.35)
C
C     Calculate the height above the jetting region where
C bubbles begin to form.  This is called the critical
C height and occurs approximately at the location where
C the void fraction in the bed becomes 0.6
C
      HC=DR/0.3*ALOG((DBMAX-DO)/(DBMAX-DBC))

C     Calculate the height of the first stage
C
      IF(HC.LE.0.0) THEN
          HSTAGE=HJ+DBO
      ELSE
          HSTAGE=HJ+HC
      ENDIF
      RETURN
      END
C*************************************************************
C
C Subroutine STAGE
C
C This subroutine calculates the value of parameters that
C change with each stage.
C
C*************************************************************
C
C     NSTAGE  = The number of the current stage
C     HSTAGE  = Height of the current stage, cm
C     DR      = Diameter of the reactor, cm
C     UO      = Initial superficial gas velocity, cm/s
C     UMF     = Superficial gas velocity when bed first
C               becomes fluidized, cm/s
C     A       = Cross-sectional area of the reactor,
C               sq.cm.
C     EMF     = Void fraction of the bed at minimum
C               fluidization
C     D(10)   = Diffusivities of components in the gas
C               phase, sq.cm./s ,(component number)
C     HMF     = Height of the bed when it first begins to
```

```
C                 fluidize, cm
C     EB        =          Void fraction of bubbles
C     EC        = Void fraction of cloud phase
C     FCE(10)   = Diffusive transfer from cloud to emulsion,
C                 1/s (component number)
C     IC        = number of components
C
C*******************************************************
C
      SUBROUTINE STAGE(NSTAGE,HSTAGE,DR,UO,UMF,A,EMF,D,
                       HMF,EB,EC,FCE,IC)
      REAL D(10),FCE(10)
C
C     Both common blocks are passed to this subroutine.
C See the main program for a description of the contents
C of the common blocks.
C
      COMMON/BCOM/H,HJ,HC,DBO,DBMAX
      COMMON/SCOM/E,VCP,VBP,VEP,UBS,UES,UCS,FBC,GBC,GCE,
     +            UBSN,UESN,UCSN
C
C     Set constants
C
C         PI = Pi
C         G  = Gravitational acceleration, cm/sq.s
C
      PI=3.14592
      G=980.665
C
C     Calcualte the size of the current stage.  Use bubble
C diameter from the previous stage in the correlation
C presented by Too et.al..  If this is the first stage set
C DBP to DBO
C
      IF(DBP.LE.0) DBP=DBO
      DH=DBP/(1+0.15*(DBP-DBMAX)/DR)
      HSTAGE=HSTAGE+DH
C
C     Calculate bubble size in current stage.  Correlation
C from Mori and C Wen, AIChE J., v. 21, no 1, p. 109
C (1975)
C
      DBP=DBMAX-(DBMAX-DBO)*EXP(-0.3*(HSTAGE-HJ)/DR)
C
C     Calcualte the distribution of volume in the bed in
C each of the three phases.  First the linear bubble phase
C gas velocity must be calculated from the correlation on
C Too et.al.
C
```

```
      UB=(UO-UMF)+0.71*SQRT(G*DBP)
      IF(HSTAGE.LT.HMF) THEN
          E=1.0-HMF/H*(1.0-EMF)
      ELSE
          E=1.0-(HMF/H)*EXP(-(HSTAGE-HMF)/(H-HMF))
      ENDIF
C
C     Calculate the volume occupied by each phase.  From
C Peters et.al. eq. 22
C
      VBP=DH*(E-EMF)/(1-EMF)
      VCP=VBP*UMF/(EMF*UB-UMF)
      VEP=A*DH-VBP-VCP
C
C     Now calculate the superficial velocity in each phase
C DELB and DELC are the volume fraction in the bubble and
C cloud phase respectively.
C
      DELB=VBP/(A*DH)
      DELC=VCP/(A*DH)
      UBSN=UB*DELB*EB
      UCSN=(DELC*EC)/(DELB*EB)*UBSN
      UESN=UO-UB*(DELB*EB+DELC*EC)
C
C     Calculate the diffusion coefficient for cloud
C emulsion transfer.  Use correlation from Peters et.al.
C eq. 28
C
      DO 10 I=1,IC
   10 FCE(I)=6.78*SQRT(D(I)*EMF*UB/(DBP*DBP*DBP))
C
C     Now calculate the diffusion parameters for bubble to
C cloud transfer, 1/s, from Peters et.al.
C
      FBC=2.0*UMF/DB
C
C     Finally calculate the crossflows, cm/s
C
      GBC=-(UBS-UBSN)
      GCE=-(UCS-UCSN+GBC)
      RETURN
      END
C*************************************************************
C
C Subroutine ECON
C
C This subroutine calculates the concentration in the
C emulsion phase.
C
```

```
C*************************************************************
C
C     CB(30,10)   = Bubble phase concentration, mole/cu.cm.
C     CE(30,10)   = Emulsion phase concentration,
C                   mole/cu.cm.
C     CC(30,10)   = Cloud phase concentration, mole/cu.cm.
C     IC          = Number of components
C     NSTAGE      = Number of the current stage
C     A           = Cross-sectional area of reactor, sq.cm.
C     FCE(10)     = Cloud to emulsion diffusive transfer
C                   coefficient, 1/s
C
C*************************************************************
C
      SUBROUTINE ECON(CB,CE,CC,IC,NSTAGE,A,FCE)
      REAL CB(30,10),CE(30,10),CC(30,10),FCE(10)
C
C          Common block SCOM is passed to this subroutine.  See
C the main program for a description of the contents of
C the common block.
C
      COMMON/SCOM/E,VCP,VBP,VEP,UBS,UES,UCS,FBC,GBC,GCE,
     +            UBSN,UESN,UCSN
C
C     Check to see if the bulk flow out of this
C compartment is negative.  If it is backflow has occured.
C
      IF(UESN.LT.0.0) THEN
C
C     Check to see if the bulk flow into the compartment
C is negative.  If it is this is not the first backflow
C compartment.
C
          IF(UES.LT.0.0) THEN
C
C     At this point we are dealing with backflow
C compartments that are not not the first such
C compartments.
C
C     Cycle for each component
C
          DO 10 I=1,IC
C
C     Calculate the reaction rate per unit volume
C
              CALL EKINET(CB,CE,CC,I,NSTAGE,RV)
C
C     TOP and BOT are the numerator and denominator in the
C material balance solved for the current concentration
```

```
C
                TOP=ABS(UESN)*A*CE(NSTAGE+1,I)+FCE(I)*
     +              VBP*CC(NSTAGE,I)-VEP*RV
                BOT=ABS(UES)*A+FCE(I)*VBP
C
C     Add on the crossflow depending on the direction it
C is flowing
C
                  IF(GCE.GE.0.0) THEN
                          BOT=BOT+GCE*A
                  ELSE
                          TOP=TOP-GCE*A*CC(NSTAGE,I)
                  ENDIF
C
C     Finally finish the loop by calculating the current
C concentration
C
   10 CE(NSTAGE,I)=TOP/BOT
C
C     This point is reached when we are at the first
C compartment to exhibit back flow
C
      ELSE
C
C     Cycle for each component
C
               DO 20 I=1,IC
C
C     Calculate the reaction rate per unit volume
C
                  CALL EKINET(CB,CE,CC,I,NSTAGE,RV)
C
C     TOP and BOT are the numerator and denominator in the
C material balance solved for the current concentration
C
                  TOP=ABS(UESN)*A*CE(NSTAGE+1,I)+UES*A*
      +               CE(NSTAGE-1,I)+FCE(I)*VBP*CC(NSTAGE,
      +               I)-VEP*RV
                  BOT=ABS(UES)*A
C
C      Add on the crossflow depending on the direction it
C is flowing
C
                  IF(GCE.GE.0.0) THEN
                          BOT=BOT+GCE*A
                  ELSE
                          TOP=TOP-GCE*A*CC(NSTAGE,I)
                  ENDIF
C
```

```
C       Finally finish the loop by calculating the current
C concentration
C
  20  CE(NSTAGE,I)=TOP/BOT
C
C       This point is reached when backflow has not
C occured
C
      ELSE
C
C     Cycle for each component
C
      DO 30 I=1,IC
C
C     Calculate the reaction rate per unit volume
C
          CALL EKINET(CB,CE,CC,I,NSTAGE,RV)
C
C     TOP and BOT are the numerator and denominator in the
C material balance solved for the current concentration
C
              TOP=UESN*A*CE(NSTAGE-1,I)+FCE(I)*VBP*
     +            CC(NSTAGE,I)-VEP*RV
              BOT=UESN*A+FCE(I)*VBP
C
C      Add on the crossflow depending on the direction it
C is flowing
C
                IF(GCE.GE.0.0) THEN
                        BOT=BOT+GCE*A
                ELSE
                        TOP=TOP-GCE*A*CC(NSTAGE,I)
                ENDIF
C
C      Finally finish the loop by calculating the current
C concentration
C
 30         CE(NSTAGE,I)=TOP/BOT
            ENDIF
      RETURN
      END
C*************************************************************
C
C Subroutine EKINET
C
C This subroutine calculates the rate of reaction for the
C emulsion phase
C
C*************************************************************
```

```
C
C     CB(30,10)   = Bubble phase concentration, mole/cu.cm.
C     CE(30,10)   = Emulsion phase concentration,
C                   mole/cu.cm.
C     CC(30,10)   = Cloud phase concentration, mole/cu.cm.
C     I           = Number of component
C     NSTAGE      = Number of the current stage
C     RV          = Reaction rate, mole/s*cu.cm
C
C*************************************************************
C
      SUBROUTINE EKINET(CB,CE,CC,I,NSTAGE,RV)
C
      REAL K(10),CB(30,10),CE(30,10),CC(30,10)
      INTEGER N(10)
C
C     K = rate constants and N = reaction order for each
C component.  The values are given in the data statements.
C
      DATA K/94.56,94.56,-94.11,-94.11,0,0,0,0,0,0/
      DATA N/10*1/
C
C Only the first four components are considered reactive.
C
      IF(I.GT.4) GOTO 10
      RV=K(1)*CE(NSTAGE,1)*CE(NSTAGE,2)+K(3)*CE(NSTAGE,3)*
     +   CE(NSTAGE,4)
C
C Change the sign of the rate if we are dealing with the
C products
C
      IF(I.GT.2) RV=-RV
      RETURN
   10 RV=0.0
      RETURN
      END
C*************************************************************
C
C Subroutine CCON
C
C This subroutine calculates the concentrations in the
C cloud phase
C
C*************************************************************
C
C     CB(30,10)   = Concentration in the bubble phase,
C                   mole/cu.cm.
C     CE(30,10)   = Concentration in the emulsion phase,
C                   mole/cu.cm.
C     CC(30,10)   = Concentration in the cloud phase,
```

```
C                     mole/cu.cm
C     IC            = Number of components
C     NSTAGE        = Number of the current stage
C     A             = Cross-sectional area of reactor,sq.cm
C     FCE(10)       = Diffusion coefficient for cloud to
C                     emulsion transfer 1/s
C
C*************************************************************
C
      SUBROUTINE CCON(CCB,CE,CC,IC,NSTAGE,A,FCE)
      REAL CB(30,10),CE(30,10),CC(30,10)FCE(10)
C
C     Common block SCOM is passed to the subroutine.  See
C the main program for a description of the contents of
C the common.
C
      COMMON/SCOM/E,VCP,VBP,VEP,UBS,UES,UCS,FBC,GBC,GCE,
     +            UBSN,UESN,UCSN
C
C     Loop for each component
C
      DO 10 I=1,IC
C
C     Calcualte the reaction rate per unit volume
C
      CALL CKINET(CB,CE,CC,I,NSTAGE,RV)
C
C     Calculate the material balance terms
C
      TOP=UCS*A*CC(NSTAGE-1,I)+FCE(I)*VBP*CE(NSTAGE,I)+FBC
     +    *VBP*CB(NSTAGE,I)-VCP*RV
      BOT=UCSN*A+FCE(I)*VBP+FBC*VBP
C
C     Account for the cross flow terms
C
      IF(GBC.GE.0) THEN
          BOT=BOT+GBC*A
      ELSE
          TOP=TOP-GBC*A*CB(NSTAGE,I)
      ENDIF
      IF(GCE.GE.0) THEN
          TOP=TOP+GCE*A*CE(NSTAGE,I)
      ELSE
          BOT=BOT-GCE*A
      ENDIF
C
C         Calculate final concentration
C
   10 CC(NSTAGE,I)=TOP/BOT
```

```
      RETURN
      END
C*************************************************************
C
C Subroutine CKINET
C
C      This subroutine calculates the reation rate in the
C cloud phase.
C
C*************************************************************
C
C     CB(30,10)   = Bubble phase concentration, mole/cu.cm.
C     CE(30,10)   = Emulsion phase concentration,
C                   mole/cu.cm.
C     CC(30,10)   = Cloud phase concentration, mole/cu.cm.
C     I           = Number of component
C     NSTAGE      = Number of the current stage
C     RV          = Reaction rate, mole/s*cu.cm
C
C*************************************************************
C
      SUBROUTINE CKINET(CB,CE,CC,I,NSTAGE,RV)
C
      REAL K(10),CB(30,10),CE(30,10),CC(30,10)
      INTEGER N(10)
C
C     K = rate constants and N = reaction order for each
C component.  The values are given in the data statements.
C
      DATA K/94.56,94.56,-94.11,-94.11,0,0,0,0,0,0/
      DATA N/10*1/
C
C Only the first component are considered reactive.
C
      IF(I.GT.4) GOTO 10
      RV=K(1)*CE(NSTAGE,1)*CE(NSTAGE,2)+K(3)*CE(NSTAGE,3)*
     +   CE(NSTAGE,4)
C
C     Change the sign of the rate if we are dealing with
C the products
C
      IF(I.GT.2) RV=-RV
      RETURN
   10 RV=0.0
      RETURN
      END
C*************************************************************
C
C Subroutine BCON
```

```
C
C This subroutine calculates the concentrations in the
C bubble phase
C
C*************************************************************
C
C     CB(30,10)   = Concentration in the bubble phase,
C                   mole/cu.cm.
C     CE(30,10)   = Concentration in the emulsion phase,
C                   mole/cu.cm.
C     CC(30,10)   = Concentration in the cloud phase,
C                   mole/cu.cm
C     IC          = Number of components
C     NSTAGE      = Number of the current stage
C     A           = Cross-sectional area of reactor,sq.cm
C     FCE(10)     = Diffusion coefficient for cloud to
C                   emulsion transfer  1/s
C
C*************************************************************
C
      SUBROUTINE BCON(CCB,CE,CC,IC,NSTAGE,A,FCE)
      REAL CB(30,10),CE(30,10),CC(30,10)FCE(10)
C
C     Common block SCOM is passed to the subroutine.  See
C the main program for a description of the contents of
C the common.
C
      COMMON/SCOM/E,VCP,VBP,VEP,UBS,UES,UCS,FBC,GBC,GCE,
     +           UBSN,UESN,UCSN
C
C     Loop for each component
C
      DO 10 I=1,IC
C
C     Calcualte the reaction rate per unit volume
C
      CALL BKINET(CB,CE,CC,I,NSTAGE,RV)
C
C     Calculate the material balance terms
C
      TOP=UBS*A*CB(NSTAGE-1,I)+FBC(I)*VBP*CC(NSTAGE,I)-VBP
     +    *RV
      BOT=UBSN*A+FBC*VBP
C
C     Account for the cross flow terms
C
      IF(GBC.GE.0) THEN
          TOP=TOP+GBC*A*CC(NSTAGE,I)
      ELSE
```

```
          BOT=BOT-GSC*A
        ENDIF
C
C           Calculate final concentration
C
  10  CB(NSTAGE,I)=TOP/BOT
      RETURN
      END
C*************************************************************
C
C Subroutine BKINET
C
C     This subroutine calculates the reation rate in the
C bubble phase.
C
C*************************************************************
C
C     CB(30,10)   = Bubble phase concentration, mole/cu.cm.
C     CE(30,10)   = Emulsion phase concentration,
C                   mole/cu.cm.
C     CC(30,10)   = Cloud phase concentration, mole/cu.cm.
C     I           = Number of component
C     NSTAGE      = Number of the current stage
C     RV          = Reaction rate, mole/s*cu.cm
C
C*************************************************************
C
      SUBROUTINE BKINET(CB,CE,CC,I,NSTAGE,RV)
C
      REAL K(10),CB(30,10),CE(30,10),CC(30,10)
      INTEGER N(10)
C
C     K = rate constants and N = reaction order for each
C component.  The values are given in the data statements.
C
      DATA K/10*0/
      DATA N/10*1/
C
C     There is no reation occuring in the bubbles
C
      RV=K(I)*CB(NSTAGE,1)**N(I)
      RETURN
      END
C*************************************************************
C
C Subroutine CONPRT
C
C      This subroutine prints the concentration profiles
C
```