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Appendix

Listing of the Virtual Basic program

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'****TOTAL DEUTERATION AND SPECIES CONCENTRATION IN AN EXCHANGE REACTION****

DECLARE SUB DispBarGraph (SPECIES() AS INTEGER, M AS INTEGER, Index!)
DECLARE FUNCTION DeutPercent (Sample() AS ANY, M AS INTEGER, S AS INTEGER) AS SINGLE

CONST Deut = 1 '***A deuterium atom is modeled as a one ***
CONST Prot = 0 '***A proton is modeled as a zero ***
CONST Tolerance = .1 '***Used to test for convergence ***
CONST MaxIterations = 500 '***Max # of iterations in event of no convergence ***
CONST Enough = 3 '***Number of Consecutive Convergences needed to end***
CONST MaxMolecules = 4000
CONST MaxSites = 8

DIM Molecule(1 TO MaxMolecules, 1 TO MaxSites) AS INTEGER
DIM Coverage(0 TO MaxSites) AS INTEGER

'***Note: The Molecule() array is limited to 32,767 array elements;***
'***consequently, MaxMolecules * MaxSites may not exceed this value***

SCREEN 0
Start:
 CLS
 INPUT "What is the desired total % deuteration "; a!
 DeutEnd = a!
 ProtEnd = 100 - DeutEnd
 DO
 PRINT
 INPUT "How many molecules in the modeled system (#<=4000) "; b%
 NumMolec% = b%

 INPUT "How many deuteration sites @ molecule (#<=8)"; c%
 NumOfSites% = c%
 LOOP UNTIL (NumMolec% <= 4000 AND NumOfSites% <= 8)
 CLS

FillArray: '***Fills the Molecule() array with Protons***
 FOR i = 1 TO NumMolec%
 FOR j = 1 TO NumOfSites%
 Molecule(i, j) = Prot
 NEXT j
 NEXT i

Initialization:
 percent = DeutPercent(Molecule(), NumMolec%, NumOfSites%) '***Initial % Deuteration***
 OldDeutPercent = percent
 NumConvs = 0 '***Set # of convergences to 0***
 k = 0 '***Set iteration counter k = 0***
 MaxStop = MaxIterations
```

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```
LOCATE 1, 1
PRINT "Iter#: "; FORMAT$(k, "0000"); " %Deut: "; FORMAT$(percent, "00.00"); " Old %Deut: ";
FORMAT$(OldDeutPercent, "00.00"); " Diff: "; FORMAT$(Diff, "0.000"); " Desired Deut "; FORMAT$(DeutEnd,
"000"); "% "
GOSUB Display

Iteration:
 '***Iteration is the subroutine in which one pass of each molecule is***
 '***conducted. One site is randomly selected for each molecule. ***
 '***The atom in the site is then replaced by a proton (0) or a ***
 '***deuterium (1) determined by probability. ***

 k = k + 1 '***Increment iteration counter by one***
 RANDOMIZE TIMER '***Reset Random # generator***

 FOR i = 1 TO NumMolec%
 SiteNum = INT(RND * NumOfSites%) + 1 '***Pick a site***
 RandNum = INT(RND * 100) '***# for Prot/Deut Decision***
 IF RandNum < DeutEnd THEN AtomChoice = Deut ELSE AtomChoice = Prot
 Molecule(i, SiteNum) = AtomChoice '***Replace SiteNum on ith molecule with AtomChoice***
 NEXT i

 percent = DeutPercent(Molecule(), NumMolec%, NumOfSites%) '***Determine Deut %***
 Diff = ABS(percent - OldDeutPercent)

 LOCATE 1, 1
 PRINT "Iter#: "; FORMAT$(k, "0000"); " %Deut: "; FORMAT$(percent, "00.00"); " Old %Deut: ";
FORMAT$(OldDeutPercent, "00.00");
 PRINT " Diff: "; FORMAT$(Diff, "0.000"); " Desired Deut "; FORMAT$(DeutEnd, "000"); "% "
 GOSUB Display '***Display Bar Graph and Sample Molecules***

 IF Diff < Tolerance THEN NumConvs = NumConvs + 1 ELSE NumConvs = 0 '***Test for Convergence***
 IF NumConvs = Enough THEN '***If system has converged within Tolerance for Enough iterations...***
 PRINT "Convergence within "; FORMAT$(Tolerance, "0.000"); "% Tolerance"
 PRINT "With a final % deuteration of "; FORMAT$(percent, "##0.0"); "%."
 PRINT "Press a Key to Resume..."
 DO
 LOOP UNTIL INKEY$ <> ""
 GOTO Start
 END IF

 IF k = MaxStop THEN
 PRINT "No convergence in "; MaxStop; " iterations! Continue? (y/n)"
 DO
 a$ = INKEY$
 LOOP UNTIL a$ <> ""
 IF UCASE$(a$) = "Y" THEN MaxStop = MaxStop + MaxIterations ELSE GOTO Start
 END IF
 OldDeutPercent = percent
 GOTO Iteration '***Perform another iteration***

Display: '***Display a Bar Graph and a symbolic representation of molecules***
 LOCATE 2, 76
 PRINT " "
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```
 LOCATE 1 + NumOfSites%, 76
 PRINT " "
 FOR i = 0 TO NumOfSites%
 Coverage(i) = 0
 NEXT i

 FOR i = 1 TO NumMolec%
 SiteTotal = 0
 FOR j = 1 TO NumOfSites%
 SiteTotal = SiteTotal + Molecule(i, j)
 NEXT j
 Coverage(SiteTotal) = Coverage(SiteTotal) + 1
 NEXT i
 FOR i! = 0 TO NumOfSites%
 CALL DispBarGraph(Coverage(), NumMolec%, i!)
 NEXT i!

 RoomOnScreen = 20 - (4 + NumOfSites%) '***How many rows of symbolic molecules will be displayed***
 LOCATE (4 + NumOfSites%), 24
 PRINT "Sample Molecules"
 FOR i = 1 TO RoomOnScreen '***Display Column One of Molecules***
 Site$ = ""
 LOCATE (4 + NumOfSites% + i), 5
 FOR j = 1 TO NumOfSites%
 IF Molecule(i, j) = Prot THEN Site$ = Site$ + "P" ELSE Site$ = Site$ + "D"
 NEXT j
 PRINT Site$
 NEXT i
 FOR i = 1 TO RoomOnScreen '***Display Column Two of Molecules***
 Site$ = ""
 LOCATE 4 + NumOfSites% + i, 30
 FOR j = 1 TO NumOfSites%
 IF Molecule(i + RoomOnScreen, j) = Prot THEN Site$ = Site$ + "P" ELSE Site$ = Site$ + "D"
 NEXT j
 PRINT Site$
 NEXT i
 FOR i = 1 TO RoomOnScreen '***Display Column Three of Molecules***
 Site$ = ""
 LOCATE 4 + NumOfSites% + i, 55
 FOR j = 1 TO NumOfSites%
 IF Molecule(i + 2 * RoomOnScreen, j) = Prot THEN Site$ = Site$ + "P" ELSE Site$ = Site$ + "D"
 NEXT j
 PRINT Site$
 NEXT i
RETURN
END

FUNCTION DeutPercent (Sample() AS INTEGER, M AS INTEGER, S AS INTEGER) AS SINGLE

 '*****************************************************
 '*** The total % deuteration = DeutPercent is given ***
 '*** by Total/(M*S) where M = # of molecules, ***
 '*** S = # of sites on each molecule, and Total = ***
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```
 '*** a sum of all deuterium atoms on all sites. ***
 '*****************************************************


 TOTAL = 0
 FOR Counter1 = 1 TO M
 FOR Counter2 = 1 TO S
 TOTAL = TOTAL + Sample(Counter1, Counter2)
 NEXT Counter2
 NEXT Counter1
 DeutPercent = TOTAL / (S * M) * 100
END FUNCTION

SUB DispBarGraph (SPECIES() AS INTEGER, M AS INTEGER, Index!)
 PercentVal = (SPECIES(Index!) / M * 100)
 LOCATE Index! + 2, 11
 PRINT STRING$(58, " ")
 LOCATE Index! + 2, 1
 PRINT FORMAT$(Index!, "00"); " Deuts: "; STRING$(VAL(FORMAT$((PercentVal * .58), "##")), "X")
 LOCATE Index! + 2, 70
 PRINT FORMAT$(PercentVal, "00.00"); "%"
END SUB
```