⇛ **Aim** - Write a program in BASIC to calculate pressure of a gas using
(i) Ideal gas eqⁿ
(ii) Vander waal's eqⁿ
(iii) Dietesici eqⁿ

```
CLS
REM * CALCULATE PRESSURE OF GAS USING DIFFERENT EQUATIONS *
5 INPUT "ENTER 1 FOR IDEAL GAS, 2 FOR VDW GAS AND 3 FOR
        DIETERICI EQUATION" ; M
R = 8.314
INPUT "ENTER AMOUNT OF GAS"; N
INPUT "ENTER TEMPERATURE IN KELVIN"; T
INPUT "ENTER VOLUME OF GAS"; V
REM * FOR IDEAL GOTO 10, FOR VDW GOTO 40, FOR
        DIETERICT GOTO 80 *
ON M GOTO 10, 40, 80
10 P = (N * R * T) / V
20 PRINT "PRESSURE OF AN IDEAL GAS (IN Pa)" ; P
30 GOTO 120.
40 INPUT "ENTER VDW CONSTANTS a,b" ; A, B
50 P = (N*R*T) / (V - N*B) - (A * N^2) / (V^2)
60 PRINT "PRESSURE OF VDW GAS (IN Pa) =" ; P
70 GOTO 120
80 INPUT "ENTER DIETERICI CONSTANT a, b" ; A, B
90 P = (N * R * T) / (V-B) * EXP (A / (R*T*V))
100 PRINT "PRESSURE OF DIETERICI GAS (IN Pa) =" ; P
120 PRINT "DO YOU WANT TO CONTINUE (Y/N)"
```

```
125 INPUT "ENTER Y FOR YES"; Y$
130 IFY$ = "Y" THEN 5
140 END
```

OUTPUT -

```
ENTER 1 FOR IDEAL GAS, 2 FOR VDW GAS AND 3 FOR
  DIETERICI EQUATION? 1
ENTER AMOUNT OF GAS? 1
ENTER TEMPERATURE IN KELVIN? 300
ENTER VOLUME OF GAS? 24
PRESSURE OF AN IDEAL GAS (IN Pa) 103.925
DO YOU WANT TO CONTINUE (Y/N)
ENTER Y FOR YES? Y
ENTER 1 FOR IDEAL GAS, 2 FOR VDW GAS AND 3 FOR
  DIETERICI EQUATION ? 2
ENTER AMOUNT OF GAS ? 1
ENTER TEMPERATURE IN KELVIN ? 300
ENTER VOLUME OF GAS ? 24
ENTER VDW CONSTANT a,b ? 456, 789
PRESSURE OF VDW GAS (IN Pa) = -4.052059
DO YOU WANT TO CONTINUE (Y/N)
  ENTER Y FOR YES ? Y
ENTER 1 FOR IDEAL GAS, 2 FOR VDW GAS AND 3 FOR
  DIETERICI EQUATION ? 3
ENTER AMOUNT OF GAS ? 1
ENTER TEMPERATURE IN KELVIN ? 300
ENTER VOLUME OF GAS ? 24
ENTER DIETERICI CONSTANT a,b ? 987, 654
```

PRESSURE OF DIETERICI GAS (IN Pa) = -4.024867
DO YOU WANT TO CONTINUE (Y/N)
ENTER Y FOR YES ? N

⇒ Aim- Using least square method, write a program to determine slope, intercept, Std. deviation of slope & intercept, corelation coefficient & error parameter.

```
10  CLS
20  REM  * LEAST SQUARE METHOD *
30  INPUT " ENTER NO. OF DATA POINTS " ; N
40  DIM X(50) , Y(50)
50  S=0 : S1 = 0 : S2 = 0 : F=0 : G=0
60  FOR I = 1 TO N
70  READ X(I), Y(I)
80  S = S + X(I) : S1 = S1 + Y(I)
90  S2 = S2 + X(I) * Y(I)
100 F = F + X(I) ^ 2 : G = G + Y(I) ^ 2
110 NEXT I
120 D = N * F - S ^ 2
130 C = (S1 * F - S2 * S) / D
140 M = (N * S2 - S * S1) / D
150 PRINT " INTERCEPT = " ; C
160 PRINT " SLOPE=" ; M
170 VARX = (F - (S^2 / N)) / (N-1)
180 VARY = (G - (S1^2/N)) / (N-1)
190 R = M * SQR( VARX / VARY)
200 E = SQR (( 1 - R^2) / (N-2)) / ABS(R)
```

```
210  SDM = E*M
220  SDC = SDM * SQR(G/N)
230  PRINT "COEFFICIENT OF REGRESSION = "; R
240  PRINT "ERROR PARAMETER = "; E
250  PRINT "SD IN SLOPE = "; SDM
260  PRINT "SD IN INTERCEPT = "; SDC
270  DATA 1, 1.1, 2, 2.2, 3, 3.3, 4, 4.4, 5, 5.5, 6, 6.6,
          7, 7.7, 8, 8.8
280  END
```

OUTPUT-

```
ENTER NO. OF DATA POINTS ? 8
INTERCEPT = -2.724784E-07
SLOPE = 1.1
COEFFICIENT OF REGRESSION = .9999999
ERROR PARAMETER = 1.9934E-04
SD IN SLOPE = 2.19274E-04
SD IN INTERCEPT = 1.218007E-03
```

⇒ AIM - Write a program to solve numerically vander waal's equation of state using iterative method

$$\left(P + \frac{an^2}{V^2}\right)(V - nb) = nRT$$

In cubic form : $V = nRT / \left(P + \frac{an^2}{V^2}\right) + nb$

```
10 CLS
20 REM "ITERATIVE METHOD"
30 INPUT "PRESSURE IN ATM" ; P
40 INPUT "TEMPERATURE IN KELVIN" ; T
50 INPUT "NO. OF MOLES" ; N
60 INPUT "NO. OF ITERATIONS" ; M
70 A = 1.5 : B = .02 : R = .082
80 V = N * R * T / P
90 PRINT "INITIAL VALUE OF V =" ; V
100 FOR I = 1 TO M
110 V1 = N * R * T / (P + (A * N^2) / (V^2)) + N * B
120 IF ABS ((V1 - V) / V) < .0001 THEN 170
130 V = V1
140 NEXT I
150 PRINT "THE VALUES HAVE NOT CONVERGED"
160 GOTO 180
170 PRINT "THE VOLUME OF GAS IS=" ; V1
180 END
```

OUTPUT -

```
PRESSURE IN ATM ? 1
TEMPERATURE IN KELVIN ? 300
NO. OF MOLES ? 1
NO. OF ITERATIONS ? 50
  INITIAL VALUE OF V = 24.6
THE VOLUME OF GAS IS = 24.55897
```

03/04/2023

⇒ AIM- Write a program to solve eq^n $x^5 + 2x^4 + 4x = 5$ using binary bisection method for the root that lies b/w 0 and 1.

```
10  CLS
20  REM  * BINARY BISECTION METHOD *
30  INPUT " LOWER LIMIT " ; X1
40  INPUT " UPPER LIMIT " ; XMAX
50  INPUT "STEP" ; S
60  DEF FNA (X) = X^5 + 2 * X^4 + 4 * X - 5
70   X2 = X1 + S
80  IF X2 > XMAX THEN PRINT "NO ROOTS IN THE RANGE": END
90   Y1 = FNA ( X1) : Y2 = FNA (X2)
100 IF Y1 = 0 THEN PRINT " ROOT = " ; X1 : END
110 IF X2 = 0 THEN PRINT " ROOT= " ; X2 : END
120 IF SGN (Y1) = SGN (Y2) THEN 130 ELSE 150
130  X1 = X2
140 GOTO 70
150  X3 = (X1 + X2) / 2
160  Y3 = FNA ( X3)
170 IF Y3 = 0 THEN 220
180 IF ABS ((X2-X1)/X3) < = .00001 THEN 220
190 IF SGN ( Y3) = SGN (Y1) THEN 220 ELSE 210
200 X1 = X3 : Y1 = Y3 : GOTO 130
210 X2 = X3 : Y2 = Y3 : GOTO 150
220 PRINT " ROOT = " ; X3
230 END
```

OUTPUT -

```
LOWER LIMIT ? 0
UPPER LIMIT ? 1
STEP ? .01
ROOT =  .8549995
```

⇒ AIM - Write a program in BASIC to solve numerically the exact expression for acid dissociation to calculate the pH of a weak acid, using Newton-Raphson method

$$pH = -\log 10[H^+]$$

$$Ka = \frac{[H^+]\left\{[H^+] - \frac{Kw}{[H^+]}\right\}}{Ca - [H^+] + \frac{Kw}{[H^+]}}$$

$$\Rightarrow [H^+]^3 + Ka[H^+]^2 - (Kw + KaCa)[H^+] - KaKw = 0$$

```
10 CLS
20 REM " PH OF WEAK ACID "
30 KW = 1E-14
40 INPUT " DISSOCIATION CONSTANT OF ACID " ; KA
50 INPUT " INITIAL CONCENTRATION OF ACID " ; CA
60 DEF FNA(H) = H^3 + KA * H^2 - (KW + KA * CA) * H
                - KA * KW
70 DEF FND(H) = 3 * H^2 + 2 * KA * H - (KW + KA * CA)
80 H = SQR(KA * CA)
```

```
90  FOR T = 1 TO 100
100 HO = H
110 Y = FNA(HO) : D = FND(HO)
120 H = HO - Y/D
130 IF ABS((H-HO)/HO) < .0001 THEN 150
140 NEXT T
150 PRINT "CONC. OF H+ IS "; H
160 PH = -LOG(H) / LOG(10)
170 PRINT "PH OF ACID IS "; PH
180 END
```

OUTPUT -

```
DISSOCIATION CONSTANT OF ACID ? 1.80E-3
INITIAL CONCENTRATION OF ACID ? .01
CONCENTRATION OF H+ IS 3.43705E-03
PH OF ACID IS 2.463814
```

03/04/2023

⇒ AIM- Write a program in BASIC to evaluate using trapezoidal method the following integral:

$$I = \int_0^1 x \ln(1+x)\, dx$$

```
10  CLS
20  REM "TREPEZOIDAL METHOD"
30  INPUT "LOWER LIMIT "; A
40  INPUT "UPPER LIMIT "; B
50  DEF FNA(X) = X * LOG(1 + X)
60  H = (B-A) / 2 : N=2
70  S = 0
80  FOR J = 1 TO N-1
90  S = S + FNA( A + J * H)
100   NEXT J
110 I = (H /2) * ( FNA(A) + FNA(B)) + H * S
120 IF ABS ((I - I1) / I )  <= .00001 THEN 160
130 I1 = I
140 H = H/2 : N = N*2
150 GOTO 70
160 PRINT " INTEGRAL=" ; I
170 END
```

OUTPUT -

```
LOWER LIMIT ? 0
UPPER LIMIT ? 1
 INTEGRAL =  .2500004
```

⇒ **AIM** - Write a program in BASIC to evaluate the following integral using Simpson's rule and compare the result with the exact value, $\frac{\sqrt{\pi}}{2}$

$$I = \int_0^{\infty} e^{-x^2} dx$$

```
10  CLS
20  REM "SIMPSON'S RULE"
30  INPUT "LOWER LIMIT" ; A
40  B=0 : I1=0 : I2 = 0
50  DEF FNA(X) = EXP(-X^2)
60  B = B + .1
70  H = (B-A)/2 : N=2
80  S=0 : S1 = 0
90  FOR J = 1 TO N-1
100 IF INT(J/2) = J/2 THEN 110 ELSE 120
110 S = S + FNA(A + J*H) : GOTO 130
120 S1 = S1 + FNA(A + J*H)
130 NEXT J
140 I = (H/3) * (FNA(A) + 2*S + 4*S1 + FNA(B))
150 IF ABS( (I-I1)/I) <= .00001 THEN 190.
160 I1 = I
170 H = H/2 : N = N*2
180 GOTO 80
190 IF ABS (( I-I2)/I) <= .00001 THEN 210
200 I2 = I : GOTO 60
210 PRINT "INTEGRAL=" ; I
220 E = SQR (3.14159) / 2
```

```
230 PRINT " EXACT VALUE = " ; E
240 END
```

OUTPUT -

```
LOWER LIMIT ? 0
INTEGRAL =  .8862216
EXACT VALUE =  .8862266
```

⇒ AIM - The maxwell- boltzman distribution function for the speed (v) of molecule is :

$$f(v)\,dv = \frac{4}{\sqrt{\pi}}\, e^{-w^2}\, w^2\, dw$$

$$w = \frac{v}{\sqrt{2RT/M}}$$

T = Temp. of Gas
M = Molar Mass
R = 8.314 $JK^{-1}\,mol^{-1}$

Write a program in BASIC to evaluate the fraction of oxygen molecules with speed b/w 200 & 400 $m\,s^{-1}$ at 1000 K.

```
10 CLS
20 INPUT "MINIMUM SPEED "; V1
30 INPUT "MAXIMUM SPEED " ; V2
40 INPUT " TEMPERATURE " ; T
50 R = 8.314 : M = 0.032
```

```
60  DEF FNA(W) = 4/SQR(3.14) * EXP(-W^2) * W^2
70  W1 = V1 / SQR((2*R*T)/M) : W2=V2/SQR((2*R*T)/M)
80  N = 2
90  H = (W2- W1)/2
100 S = FNA(W1) + FNA(W2)
110 REM "LOWER LIMIT OF INTEGRAL IS W1, UPPER LIMIT IS W2"
120 FOR J = 1 TO N-1
130 IF INT (J/2) = J/2 THEN 140 ELSE 150
140 S = S+2 * FNA (W1 +J*H) : GOTO 160
150 S = S+4 * FNA(W1 + J*H)
160 NEXT J
170 I = (H/3) * S
180 IF ABS((I-I1)/I) <= .00001 THEN 220
190  I1 = I
200  H = H/2 : N= N * 2
210  GOTO 100
220 PRINT "FRACTION OF MOLECULE=" ; I
230 END
```

OUTPUT -

```
MINIMUM SPEED ? 200
MAXIMUM SPEED ? 400
 TEMPERATURE ? 1000
FRACTION OF MOLECULE =  9.187955E-02
```

⇒ **AIM**- Write a program in BASIC to calculate the change in entropy 'S' of a substance over a given temp. range by the method of integration using the trapezoidal approximation.
It is expressed in terms of the heat capacity at constant pressure as:

$$\int_{S1}^{S2} dS = \int_{T1}^{T2} \frac{C_p}{T} dT$$

→ The heat capacity values at various temp for CO are as follows:

T (°C)	0	10	20	30	40	50	60	70
C_p (J/deg mol)	28.912	28.902	29.118	29.151	29.184	29.299	29.361	29.392

```
10  CLS
20  REM "TRAPEZOIDAL APPROXIMATION"
30  INPUT "NO. OF DATA POINTS "; N
40  DIM T(N), CP(N)
50  FOR T = 1 TO N
60  READ T, CP(I)
70  T(I) = T + 273.15
80  NEXT I
90  DATA 0, 28.912, 10, 28.902, 20, 29.118, 30, 29.151, 40, 29.184,
        50, 29.299, 60, 29.361, 70, 29-392
100 S = CP(1) / T(1) + CP(N) / T(N)
110 FOR T = 2 TO N-1
```

```
120 S = S + 2 * (P(T) / T(I)
130 NEXT T
140 DS = (10/2) * S
150 PRINT " ENTROPY CHANGE = " ; DS
160 END
```

OUTPUT -

```
NO. OF DATA POINTS ? 8
ENTROPY CHANGE = 6.653048
```

⇒ Aim- Write a program in BASIC to plot exponential curve

$$Y = \exp(-a^2 / bx)$$

```
10 CLS
20 REM * EXPONENTIAL CURVE *
30 INPUT A, B, N
40 SCREEN 2
50 VIEW (60,60) - (400,170)
60 WINDOW (0,0) - (N,1)
70 LINE (0,0) - (N,0) : LINE (0,0) - (0,1)
80 LOCATE 15,10 : PRINT "Y- AXIS"
90 LOCATE 23,24 : PRINT "X- AXIS"
100 LOCATE 2,20 : PRINT "PLOT OF EXPONENTIAL CURVE"
110 FOR X = .1 TO N STEP .1
120 Y = EXP ( (-A^2)/ (B * X))
130 PSET (X, Y)
140 NEXT X
150 END
```

OUTPUT -

? 2,4,6

⇒ AIM - Write a program in BASIC to plot cosine curve.

```
10  CLS
20  REM * PLOTTING COSINE CURVE  Y=COSX *
30  YMAX = 1.1 : YMIN = -1.1
40  SCREEN 2
50  VIEW (60,60) - (500, 170)
60  WINDOW (0, YMIN) - (360, YMAX)
70  LINE (0,0) - (360,0) : LINE (0, YMIN) - (0, YMAX)
80  LOCATE 23,30 : PRINT "ANGLE IN DEGREE"
90  LOCATE 12,1 : PRINT " COS X "
100 LOCATE 2,22 : PRINT " PLOT OF COSINE CURVE "
110 FOR X = 0 TO 360
120 Y = COS ( 3.14 * X / 180 )
130 PSET (X, Y)
140 NEXT X
150 END
```

⇒ AIM - Write a program in BASIC to plot the graph of particle in a 1-D box of length 'a'.

$$\Psi = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

```
10  CLS
20  REM * PARTICLE IN A 1-D BOX *
30  INPUT " VALUE OF A ": A
40  INPUT " ENERGY LEVEL N ": N
50  YM = SQR(2/A)
60  YMAX = YM + .1*YM : YMIN = -YM - .1*YM
70  CLS : SCREEN 2
80  VIEW (50,50) - (380,150)
90  WINDOW (0,YMIN) - (A,YMAX)
100 LINE (0,YMAX) - (0,YMIN)
110 LINE (0,0) - (A,0)
120 LOCATE 5,10
130 PRINT " PLOT OF PARTICLE IN A 1-D BOX AT ENERGY LEVEL=";N
140 FOR X = 0 TO A STEP .001
150 Y = YM * SIN(N * 3.14 * X / A)
160 PSET (X,Y)
170 NEXT X
180 END
```

⇒ AIM - Write a program in BASIC to plot the graph of Maxwell Boltzmann distribution curve for a gas at two temp.

$$\frac{1}{N}\frac{dN}{du} = 4\pi\left(\frac{M}{2MRT}\right)^{3/2} \exp(-Mu^2/2RT)\,u^2$$

```
10  CLS
20  INPUT G$
30  INPUT "MOLAR MASS IN KG "; M
40  INPUT "TWO TEMPERATURES "; T1,T2
50  R = 8.314 : PI = 3.14
60  M1 = M / (2*R)
70  IF T1 > T2 THEN T=T2 ELSE T=T1
80  UM = SQR(T/M1)
90  DEF FNA(U) = 4 * PI * (M1/(PI * T1)^3/2) * EXP(-
                (M1 * U^2) / T) * (U^2)
100 YMAX = FNA(UM) + .1 * FNA(UM)
110 SCREEN 2 : CLS
120 VIEW (60, 50) - (500, 170)
130 WINDOW (0,0) - (1500, YMAX)
140 LINE (0,0) - (1500,0)
150 LINE (0,0) - (0, YMAX)
160 LOCATE 23, 30 : PRINT " VELOCITY IN M/S "
170 LOCATE 12, 2 : PRINT " 1/dN "
180 LOCATE 2, 10 : PRINT "PLOT OF MAXWELL BOLTZMANN
                DISTRIBUTION CURVE FOR "; G$ ; " AT
                TEMPERATURE "; T1 ; "AND" ; T2
190 T = T1
200 FOR U = 1 TO 1500
```

```
210   Y = FNA(U)
220   PSET (U,Y)
230   NEXT U
240   IF T=T2 THEN 260 ELSE 250
250   T=T2 : GOTO 200
260   END
```

⇒ AIM- Write a program in BASIC to find the root of the given polynomial in the range [1,2] using Regula Falsi method

$f(x) = x^3 + 3x - 5$

Take the degree of accuracy as 0.001.

```
10  CLS
20  REM  * REGULA FALSI METHOD *
30  INPUT "LOWER VALUE OF THE RANGE"; A
40  INPUT "UPPER VALUE OF THE RANGE"; B
50  DEF FNA(X) = X^3 + 3 * X - 5
60  FA = FNA(A) : FB = FNA(B)
70  IF FA = 0 THEN PRINT "ROOT = "; A
80  IF FB = 0 THEN PRINT "ROOT = "; B
90  IF FA * FB > 0 THEN 100 ELSE 130
100 PRINT " NO ROOTS IN THE RANGE"
110 PRINT " CHOOSE DIFFERENT RANGE"
120 GOTO 30
130 X1 = A - (B-A) * FA / (FB-FA)
140  Y1 = FNA(X1)
150 IF Y1 = 0 THEN 170
160 IF ABS(Y1) <= .001 THEN 170 ELSE 180
170  PRINT "ROOT = "; X1 = END
180  IF Y1 * FA > 0 THEN 190 ELSE 210
190  A = X1 : FA = Y1
200  GOTO 130
210  B = X1 : FB = Y1
220  GOTO 130
```

```
230 PRINT "ROOT = "; X3
240 END
```