Differential equation has the following physical basis. If x - amount of substance P, formed at time t, then the problem comes from the conditions that this point of time the reaction came substance A and substance B. This in turn means that up to this point and not left reacted substance A and substance B.
According to the law of mass action, for simple chemical reactions, reaction conditions for the first stage, the rate of chemical interaction v is proportional to the concentration of the reactants, ie, either.
For ease up a table matching objectives and conditions designations following entry method Runge-Kutta (tab. 4.2).
Table 4.2. Compliance markings
Terms problem number Runge-Kutta method of discrete analog Analytical Account
1
VI VI + 1 = Δui + y '= f (x, y)
2 x = x (t) VI y = f (x)
3 t xi x
4 x (t0) = x0 yo y (xo) = yo
(t, x)*f*5
To illustrate the calculations by the method of Runge-Kutta for example, when according to the task (all dimensions - conventional): t0 = 0,1; x0 = 0,1; k (t) = 2 · t; ; ; h = 0,01; the observation tmax = 10.
According to Runge-Kutta method for tabular dependence xi perform the following steps.
Initial conditions: i = 0; t0 = 0,1; x0 = 0,1.
· x0) = 2 0,1 (1-1 / 1,5 · 0,1) (0,5-χ / β-β · x0) (χ / α-α (t0, x0) = 2 t0 (*f* 0,5 / 1,5 · 0,1) = 0,0759;
(t0, x0) = 0,01 · 0,0759 = 0,000759;*f*A0 = h ·
· (x0 + A0 / 2)) =χ / β-β · (x0 + A0 / 2)) (χ / αB0 = h · (t0 + h / 2) · (a-
= 0,1 · (0,1 + 0,1 / 2) (1-1 / 1,5 · (0,1 + 0,000759 / 2)) (0,5
-0,5 / 1,5 · (0,1 + 0,000759 / 2)) = 0.0046;
· (x0 + B0 / 2)) =χ / β-β · (x0 + B0 / 2)) (χ / αC0 = h · (t0 + h / 2) · (a-
= 0,1 · (0,1 + 0,1 / 2) (1-1 / 1,5 · (0,1 + 0,0046 / 2)) (0,5-0,5 / 1,5 · (0.1 + 0.0046 / 2)) = 0.0007;
· (x0 + B0)) =χ / β-β · (x0 + B0)) (χ / αD0 = h · (t0 + h / 2) · (a-
= 0,1 · (0,1 + 0,1 / 2) (1-1 / 1,5 · (0,1 + 0,0007)) (0,5-0,5 / 1,5 · (0 , 1 + 0.0007)) = 0.0007;
Δx0 = 1/6 · (A0 + 2V0 + 2S0 + D0) = 1/6 · (0,000759 + 2 · 0,0046 +
+ 2 · 0,0007 + 0,0007) = 0,001214; x1 = x0 + Δx0 = 0,1 + 0,001214 = 0,101214
The next step: i = 1; t1 = t0 + 1 · h = h.
You must complete all the steps again consistently for all nodes i.
Recursive actions require too much computation, so they should perform on a PC in the cyclic calculation algorithms. Calculation program (written in free form location operators) and table IDs (table 4.3.) Provided an example below.
Table 4.3. Table Match identifiers.
For number
In the text

```
Numerical program
Record Type importance
1 t0 T0 0,1 REAL .1
2 h h 0,01 REAL .01
3 k (t) Function Ak (t) calculated REAL -
4
Alpha 1 REAL 1.
5
Beta 0,5 REAL .5
 Chi Calculated REAL -χ6
7 tmax Tmax 10 10 REAL.
8 x0 X0 0,1 REAL .1
Calculated 9 Ai A REAL -
10 Bi B is calculated REAL -
11 Ci C Calculated REAL -
12 Di D calculated REAL -
 (t, x) Function f 13
 (t, x) calculated REAL - f
14 t t calculated REAL -
15 x x Calculated REAL -
16 i i Calculated INTEGER -
17 - Dx calculated REAL -
! The source code program for calculating chemical reaction
Module M1! Expanding the area of variable visibility
Real Alpha /1./, Beta /.5/, Chi
End Module M1
! _____
Function Ak (t)! k (t) - see. task
Ak = 2 * t
End Function Ak
! _____
Function f (t, x)! The right side of the differential equation (see. Diffusion. Model)
USE M1! Access to data module by name
Chi = Alpha + Beta
f = Ak (t) * (Alpha - Alpha / Chi * x) * (Beta - Beta / Chi * x)
End Function f
! _____
Program Chemical! The main program
Data T0 / .1 /, X0 / .1 /, Tmax / 200. /, h / .1 /! Output (see. Task)
Open (1, File = 'Chemi.txt', Status = 'Replase')! File calculation results
Write (1, *) '************ Inputed Data ************'
Write (1, *) 'T0 =', T0
Write (1, *) 'x0 =', X0
Write (1, *) 'Tmax =', Tmax
Write (1, *) 'h =', h
Write (1, *) '************ Solved Resalts ************'
```

```
Write (1, *) 'i t x'! Table caps
i = 0; t = T0; x = X0! The initial conditions
Write (1, *) i, t, x! To file
Do t = T0 + h, Tmax + h, h! Cycle calculation formula Runge-Kutta
i = i + 1
A = h * f (t, x)
B = h * f (t + h / 2, x + A / 2)
C = h * f (t + h / 2, x + B / 2)
D = h * f (t + h / 2, x + C)
Dx = (A + B 2 + 2 * * C + D)
x = x + Dx
Write (1, *) i, t, x! To file
EndDo! End cycle
Write (1, *) '_____'
Stop
End
```

Project MS Dev FPS4 of software code and the calculation results are shown in Figure 4.3.

Fig. 4.3. Project MS Dev FPS4 of software code and the calculation results

Results of calculation of transfer to Excel (Fig. 4.4) for further engineering analysis.

Fig. 4.4. Display Excel chart to change the number of calculations Chemicals reactionin time