

```
/*
```

This program simultaneously solves the following 5 differential equations:

$$r_A = -k_1c_A - k_2c_A$$

$$r_B = +k_1c_A - k_2c_B - k_4c_B$$

$$r_C = +k_2c_A - k_5c_C$$

$$r_D = +k_3c_B$$

$$r_E = +k_4c_B + k_5c_C$$

where t = time

k_1, k_2, k_3, k_4, k_5 are rate constants

$c_{A0}, c_{B0}, c_{C0}, c_{D0}, c_{E0}$ are initial concentrations of A, B, C, D, E

```
*/
```

```
#include<stdio.h>
#include<math.h>
#include<conio.h>
#include<stdlib.h>
```

```
main()
```

```
{
    FILE *fptr;
    float cAnew, cBnew, cCnew, cDnew, cEnew;
    float cAold, cBold, cCold, cDold, cEold;
    float deltatime, cAend, actualtime;
    float k1, k2, k3, k4, k5;
    int count;
```

```
// Set Constants and Initial Conditions
```

```
cAold = 100.;
cBold = 0.;
cCold = 0.;
cDold = 0.;
cEold = 0.;
```

```
k1 = 0.15;
k2 = 0.14;
k3 = 0.11;
k4 = 0.12;
k5 = 0.08;
```

```
count = 0;
deltatime=0.001;           // value for Delta t - small enough
actualtime=0.;           // (arbitrary) termination point for program
cAend = 0.5;
```

```
// Open File for Output
```

```
fptr = fopen("a:reaction.dat", "w");
```

```
// Central Calculation
```

```
do
```

```
{
    actualtime=actualtime+deltatime;
    cAnew=-(k1+k2)*cAold*deltatime+cAold;
    cBnew=(k1*cAold-(k3+k4)*cBold)*deltatime+cBold;
    cCnew=(k2*cAold-k5*cCold)*deltatime+cCold;
    cDnew=k3*cBold*deltatime+cDold;
    cEnew=(k4*cBold+k5*cCold)*deltatime+cEold;
    cAold=cAnew;
    cBold=cBnew;
    cCold=cCnew;
    cDold=cDnew;
    cEold=cEnew;
    count++;
    if(count==100)
    {
        count=0;
        fprintf(fptr, "%5.2f %5.2f %5.2f %5.2f %5.2f %5.2f\n", actualtime, cAold, cBold, cCold, cDold, cEold);
    }
}
```

```
while(cAnew>=cAend)
```

```
fclose(fptr);
```

```
}
```