```
~k
~c

! 1. Rozcvička: reakce 2. řádu (9.26) ===========
T=1163
                                                    1163
c0=101.3/R/T      ! [dm^3 mol^-1]
                                                0.010476
! =================
!      0     tau
! -----------------
! N2O  c0    c0-x  =c
! N2   0     x
! O2   0     x/2
! -----------------
! celk. c0   c0+x/2
! =================
celk=141.3/R/T
                                                0.014613
x=2*(celk-c0)
                                               0.0082732
c=c0-x
                                               0.0022028
k=0.977           ! [dm^3 mol^-1 s^-1]
                                                    0.977
tau=(1/c-1/c0)/k ! [s]
                                                   366.96
!
! 2. Aditivní vlastnost a integrální metoda ===
! == určení řádu reakce=======================
! 1. řád: k=-ln(c1/c2)/(tau1-tau2)
! 2. řád: k=(1/c1-1/c2)/(tau1-tau2)
n_0 =1.3580
                                                     1.358
n_5 =1.3658
                                                    1.3658
n_10=1.3689
                                                    1.3689
n_15=1.3702
                                                    1.3702
n_20=1.3709
                                                    1.3709
nlim=1.3711
                                                    1.3711
! 1. řád: ------------------
ln((n_0-nlim)/(n_5-nlim))/5
                                                   0.18098
ln((n_5-nlim)/(n_10-nlim))/5
                                                   0.17585
ln((n_10-nlim)/(n_15-nlim))/5
                                                   0.17876
ln((n_15-nlim)/(n_20-nlim))/5
                                                   0.30082
! 2. řád: ------------------
k=(1/(n_0-nlim)-1/(n_5-nlim))/5
                                                    22.469
k=(1/(n_5-nlim)-1/(n_10-nlim))/5
                                                    53.173
k=(1/(n_10-nlim)-1/(n_15-nlim))/5
                                                    131.31
k=(1/(n_15-nlim)-1/(n_20-nlim))/5
                                                    777.78
! vyhovuje 1. řád
k=0.18 ! [s^-1]
                                                      0.18
!
! graf a fitovani:
!   sh plot m-7-rad.dat:A:B:-o :"a+b*exp(-c*A)"
!
!
!
! 3. (9.33) Řád reakce metodou poločasů =========
! tau_1/2=[2↑(n-1)-1]/(n-1)*c0↑(1-n)
c01=0.05; tau1=245
                                                     0.05
                                                      245
c02=0.15; tau2=82
                                                     0.15
                                                       82
n=1-ln(tau1/tau2)/ln(c01/c02)
                                                   1.9963
n=2
                                                        2
k=1/c01/tau1 ! [s^-1 dm^3 mol^-1]
                                                 0.081633
k=1/c02/tau2 ! [s^-1 dm^3 mol^-1]
                                                 0.081301
!
!
!
! 4. Následné reakce ============================
k1=ln(2)/14.3     ! [rok^-1]
                                                 0.048472
k2=ln(2)/432      ! [rok^-1]
                                                0.0016045
n=0.1/(241+2*16) ! [mol]
                                                0.0003663
tau=2008-1955     ! [rok]
                                                       53
nA=n*exp(-k1*tau)
                                          2.8063 · 10^-05
nB=n*k1/(k2-k1)*(exp(-k1*tau)-exp(-k2*tau))
                                              0.00031893
nC=n-nA-nB
                                          1.9305 · 10^-05
nC*22.4e3         ! [cm^3]
                                                  0.43243
! b) -------------------------
rok=1955+4/12+ln(k1/k2)/(k1-k2)
                                                   2028.1
!
! graf:
! plot tau=0,100 n*k1/(k2-k1)*(exp(-k1*tau)-exp(-k2
  *tau))
!
!
!
!
!
!
!
!
```

```
! 5. (9.57) Vratné reakce =======================
T=815.6
```
$$815.6$$
```
K=exp(-4.7e3/R/T)
```
$$0.50003$$
```
k2=2.909e-2 ! [min^-1]
```
$$0.02909$$
```
k1=k2*K
```
$$0.014546$$
```
n0=9
```
$$9$$
```
tau=21
```
$$21$$
```
n=n0*(exp(-(k1+k2)*tau)+k2/k1)/(1+k2/k1)
```
$$7.1998$$
```
nS=n0-n
```
$$1.8002$$
```
xS=nS/(n0+3)
```
$$0.15001$$
```
! graf:
! plot tau=0,100 n0*(exp(-(k1+k2)*tau)+k2/k1)/(1+k2
  /k1)
!
!
! 6. (9.53) Bočné reakce + teplotní závislost ===
k1=4.7e-5 ! [s^-1]
```
$$4.7 \cdot 10^{-05}$$
```
k2=2.5e-6 ! [s^-1]
```
$$2.5 \cdot 10^{-06}$$
```
tau=3600  ! [s]
```
$$3600$$
```
n_HCOOH=exp(-(k1+k2)*tau)
```
$$0.83678$$
```
n_H2O=(1-n_HCOOH)*k1/(k1+k2)
```
$$0.15498$$
```
n_CO=n_H2O
```
$$0.15498$$
```
n_H2=(1-n_HCOOH)*k2/(k1+k2)
```
$$0.0082437$$
```
n_CO2=n_H2
```
$$0.0082437$$
```
n=n_HCOOH+n_H2O+n_CO+n_H2+n_CO2
```
$$1.1632$$
```
x_HCOOH=n_HCOOH/n
```
$$0.71936$$
```
x_H2O=n_H2O/n
```
$$0.13323$$
```
! b) ----------------
! rovnice: k1=k2
T0=510
```
$$510$$
```
E1=50.2e3  ! [J mol^-1]
```
$$50200$$
```
E2=102.5e3 ! [J mol^-1]
```
$$1.025 \cdot 10^{+05}$$
```
def k1T=k1*exp(-E1/R/T)/exp(-E1/R/T0)
def k2T=k2*exp(-E2/R/T)/exp(-E2/R/T0)
solve T=500,1000 k1T-k2T
```
$$669.18 \quad f = -1.3 \cdot 10^{-18}$$