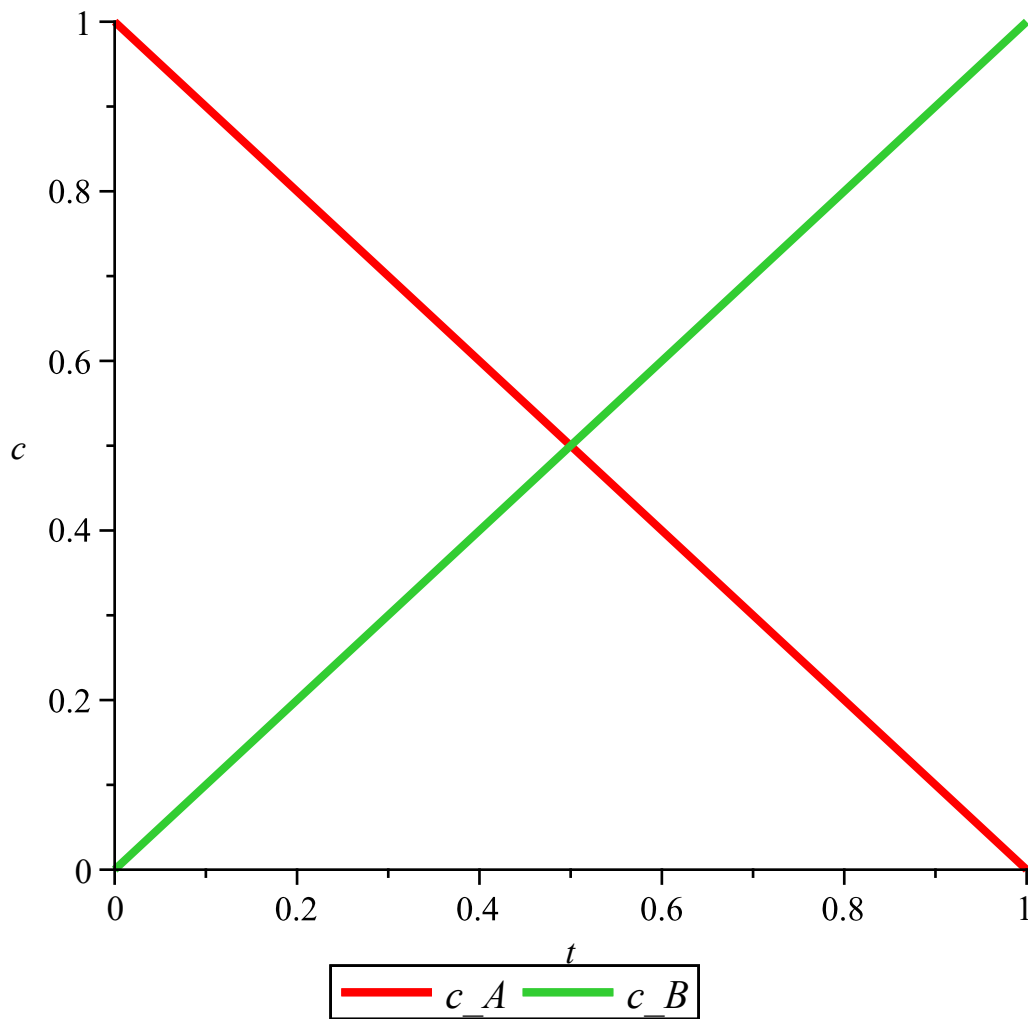


Zero Order

```
> restart;with( DEtools ):with( plots ):with( linalg):
> ode_1:=diff(ca(t),t)=-k_1;ode_2:=diff(cb(t),t)=(k_1);
      ode_1 :=  $\frac{d}{dt} ca(t) = -k_1$ 
      ode_2 :=  $\frac{d}{dt} cb(t) = k_1$ 
(1.1)
> dsolve({ode_1,ca(0)=ca0},ca(t));
      ca(t) = -k_1 t + ca0
> dsolve({ode_2,cb(0)=cb0},cb(t));
      cb(t) = k_1 t + cb0
> sol:= dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0},{ca(t),cb(t)});
      sol := {ca(t) = -k_1 t + ca0, cb(t) = k_1 t + cb0}
> k_1:=1;nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=0}, type=
      numeric, output=listprocedure);#assign(nsol);f:=eval(ca(t),
      sol);f(t=1);
nsol := [t=proc(t) ... end proc, ca(t)=proc(t) ... end proc, cb(t)=proc(t)
      ...
end proc]
> nsol(1);
      [t(1) = 1., ca(t)(1) = 6.93889390390723 10-18, cb(t)(1) = 1.]
(1.2)
> odeplot(nsol, [[t,ca(t)], [t,cb(t)]], 0..1, labels=[t,c], legend=
      [c_A,c_B], thickness=3);
```



>

Prvniho radu A ->B

```
[> restart;with( DEtools ):with( plots ):with( linalg):
```

```
> ode_1:=diff(ca(t),t)=-k_1*ca(t);
```

$$ode_1 := \frac{d}{dt} ca(t) = -k_1 ca(t)$$

```
> ode_2:=diff(cb(t),t)=(k_1)*ca(t);
```

$$ode_2 := \frac{d}{dt} cb(t) = k_1 ca(t)$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = ca0 e^{-k_1 t}$$

```
> dsolve({ode_2,cb(0)=cb0},cb(t));
```

$$cb(t) = \int_0^t k_1 ca(z1) d_z1 + cb0$$

```
> sol := dsolve({ode_1, ca(0)=ca0, ode_2, cb(0)=cb0}, {ca(t), cb(t)});
```

```
sol := {ca(t) = ca0 e-k1t, cb(t) = -ca0 e-k1t + ca0 + cb0}
```

```
> k_1:=1: nsol := dsolve({ode_1, ca(0)=1, ode_2, cb(0)=0}, type=
numeric, output=listprocedure); #assign(nsol); f:=eval(ca(t),
sol); f(t=1);
```

```
nsol := [t=proc(t) ... end proc, ca(t)=proc(t) ... end proc, cb(t)=proc(t)
```

```
...
```

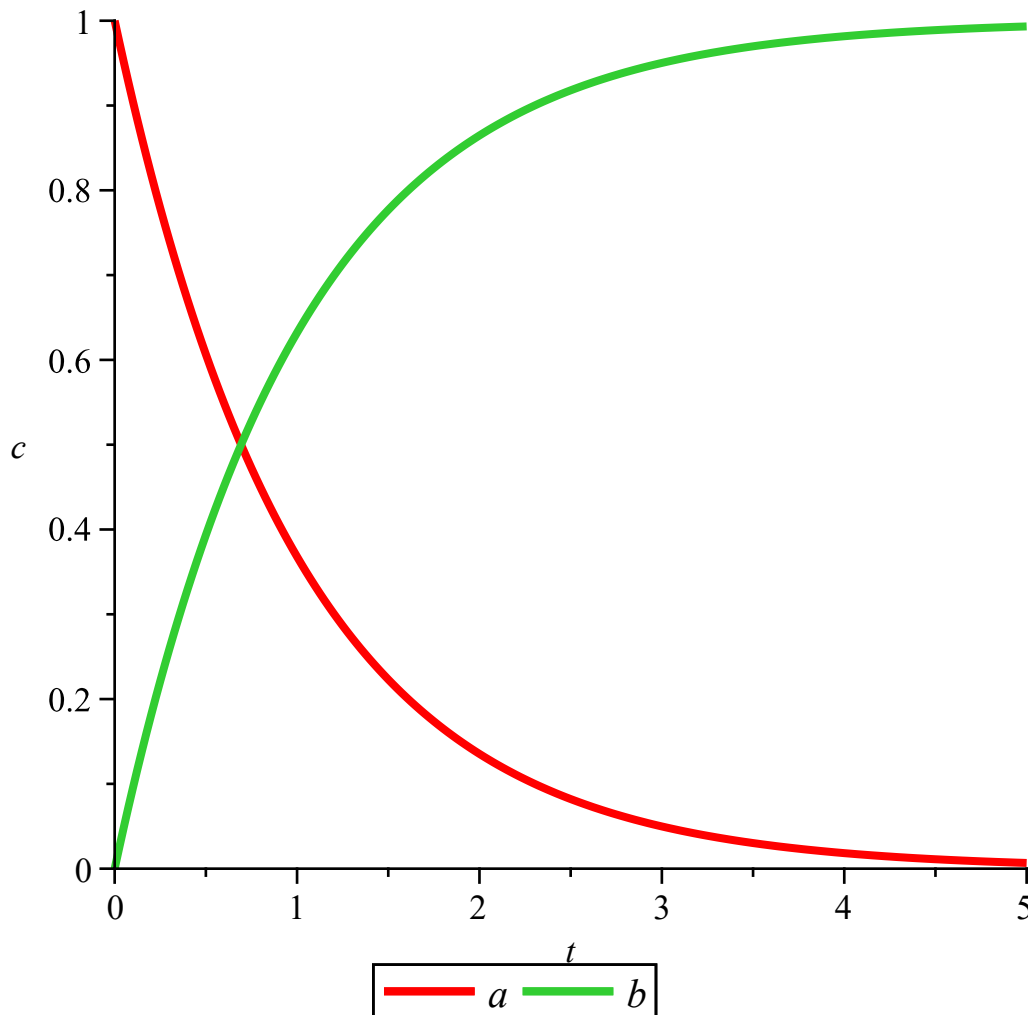
```
end proc]
```

```
> nsol(1);
```

```
[t(1)=1., ca(t)(1)=0.367879361988637, cb(t)(1)=0.632120638011363]
```

(2.1)

```
> odeplot(nsol, [[t, ca(t)], [t, cb(t)]], 0..5, labels=[t, c], legend=
[a, b], thickness=3);
```



Reakce druhého radu 2A→B

```
> restart;with( DEtools ):with( plots ):with( linalg ):
> ode_1:=diff(ca(t),t)=-k_1*(ca(t))^2;

$$\text{ode}_1 := \frac{d}{dt} ca(t) = -k_1 ca(t)^2$$

> ode_2:=diff(cb(t),t)=(k_1)*(ca(t))^2;

$$\text{ode}_2 := \frac{d}{dt} cb(t) = k_1 ca(t)^2$$

> dsolve({ode_1,ca(0)=ca0},ca(t));

$$ca(t) = \frac{ca0}{1 + k_1 t ca0}$$

> dsolve({ode_2,cb(0)=cb0},cb(t));

$$cb(t) = \int_0^t k_1 ca(_z1)^2 d_z1 + cb0$$

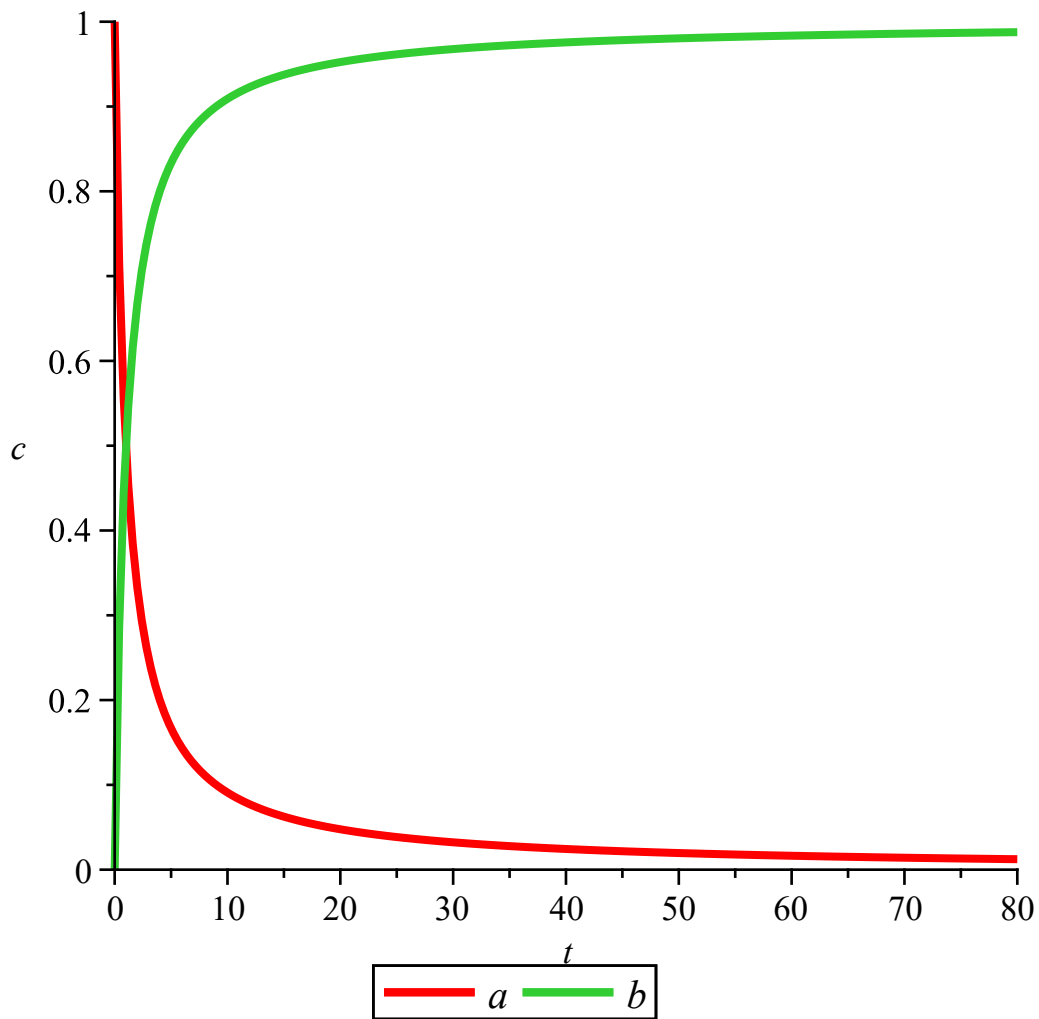
> dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0},{ca(t),cb(t)});

$$\left\{ \begin{array}{l} ca(t) = \frac{1}{k_1 t + \frac{1}{ca0}}, cb(t) = -\frac{1}{k_1 t + \frac{1}{ca0}} + ca0 + cb0 \end{array} \right\}$$

> k_1:=1:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=0}, type=
numeric);

$$nsol := \text{proc}(x\_rkf45) \dots \text{end proc}$$

> odeplot(nsol,[[t,ca(t)],[t,cb(t)]],0..80,labels=[t,c],legend=
[a,b],thickness=3);
```



▼ Reakce druhého radu A+B->C

```
> restart;with( DEtools ):with( plots ):with( linalg ):
```

```
> ode_1:=diff(ca(t),t)=-k_1*(ca(t))*(cb(t));
```

$$ode_1 := \frac{d}{dt} ca(t) = -k_1 ca(t) cb(t)$$

```
> ode_2:=diff(cb(t),t)=-k_1*(ca(t))*(cb(t));
```

$$ode_2 := \frac{d}{dt} cb(t) = -k_1 ca(t) cb(t)$$

```
> ode_3:=diff(cc(t),t)=k_1*(ca(t))*(cb(t));
```

$$ode_3 := \frac{d}{dt} cc(t) = k_1 ca(t) cb(t)$$

(4.1)

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = ca0 e^{\int_0^t (-k_1 cb(z)) dz}$$

```
> dsolve({ode_2,cb(0)=ca0},cb(t));
```

$$cb(t) = ca0 e^{\int_0^t (-k_1 ca(z)) dz}$$

> dsolve({ode_1, ca(0)=ca0, ode_2, cb(0)=cb0, ode_3, cc(0)=cc0}, {ca(t), cb(t), cc(t)});

$$ca(t) = \left((e^{i\pi Z1})^2 e^{t(-cb0k_1 + k_1 ca0)} e^{\frac{\left(\ln\left(\frac{ca0}{cb0k_1}\right) + 2i\pi Z2\right)(-cb0k_1 + k_1 ca0)}{k_1(-cb0 + ca0)}} \right) (-cb0k_1$$

$$+ k_1 ca0) \Bigg) / \left(-1$$

$$+ k_1 ca0) e^{t(-cb0k_1 + k_1 ca0)} e^{\frac{\left(\ln\left(\frac{ca0}{cb0k_1}\right) + 2i\pi Z2\right)(-cb0k_1 + k_1 ca0)}{k_1(-cb0 + ca0)}} \right), cb(t) =$$

$$- \left(\left((e^{i\pi Z1})^2 (-cb0k_1$$

$$+ k_1 ca0) e^{t(-cb0k_1 + k_1 ca0)} e^{\frac{\left(\ln\left(\frac{ca0}{cb0k_1}\right) + 2i\pi Z2\right)(-cb0k_1 + k_1 ca0)}{k_1(-cb0 + ca0)}} \right) / \left(-1$$

$$+ k_{-1} e^{t(-cb_0 k_{-1} + k_{-1} ca_0)} e^{\frac{\left(\ln\left(\frac{ca_0}{cb_0 k_{-1}}\right) + 21\pi_{-Z2}\right) (-cb_0 k_{-1} + k_{-1} ca_0)}{k_{-1} (-cb_0 + ca_0)}}$$

$$a_0) e^{\frac{\left(\ln\left(\frac{ca_0}{cb_0 k_{-1}}\right) + 21\pi_{-Z2}\right) (-cb_0 k_{-1} + k_{-1} ca_0)}{k_{-1} (-cb_0 + ca_0)}} \left(-1 \right)$$

$$+ k_{-1} e^{t(-cb_0 k_{-1} + k_{-1} ca_0)} e^{\frac{\left(\ln\left(\frac{ca_0}{cb_0 k_{-1}}\right) + 21\pi_{-Z2}\right) (-cb_0 k_{-1} + k_{-1} ca_0)}{k_{-1} (-cb_0 + ca_0)}}$$

$$\left(k_{-1} \left(e^{i\pi_{-Z1}} \right)^2 e^{t(-cb_0 k_{-1} + k_{-1} ca_0)} e^{\frac{\left(\ln\left(\frac{ca_0}{cb_0 k_{-1}}\right) + 21\pi_{-Z2}\right) (-cb_0 k_{-1} + k_{-1} ca_0)}{k_{-1} (-cb_0 + ca_0)}} \right) (-cb_0 k_{-1}$$

$$+ k_{-1} ca_0) \Big), cc(t) =$$

$$- \left(\left(e^{i\pi_{-Z1}} \right)^2 e^{t(-cb_0 k_{-1} + k_{-1} ca_0)} e^{\frac{\left(\ln\left(\frac{ca_0}{cb_0 k_{-1}}\right) + 21\pi_{-Z2}\right) (-cb_0 k_{-1} + k_{-1} ca_0)}{k_{-1} (-cb_0 + ca_0)}} \right) (-cb_0 k_{-1}$$

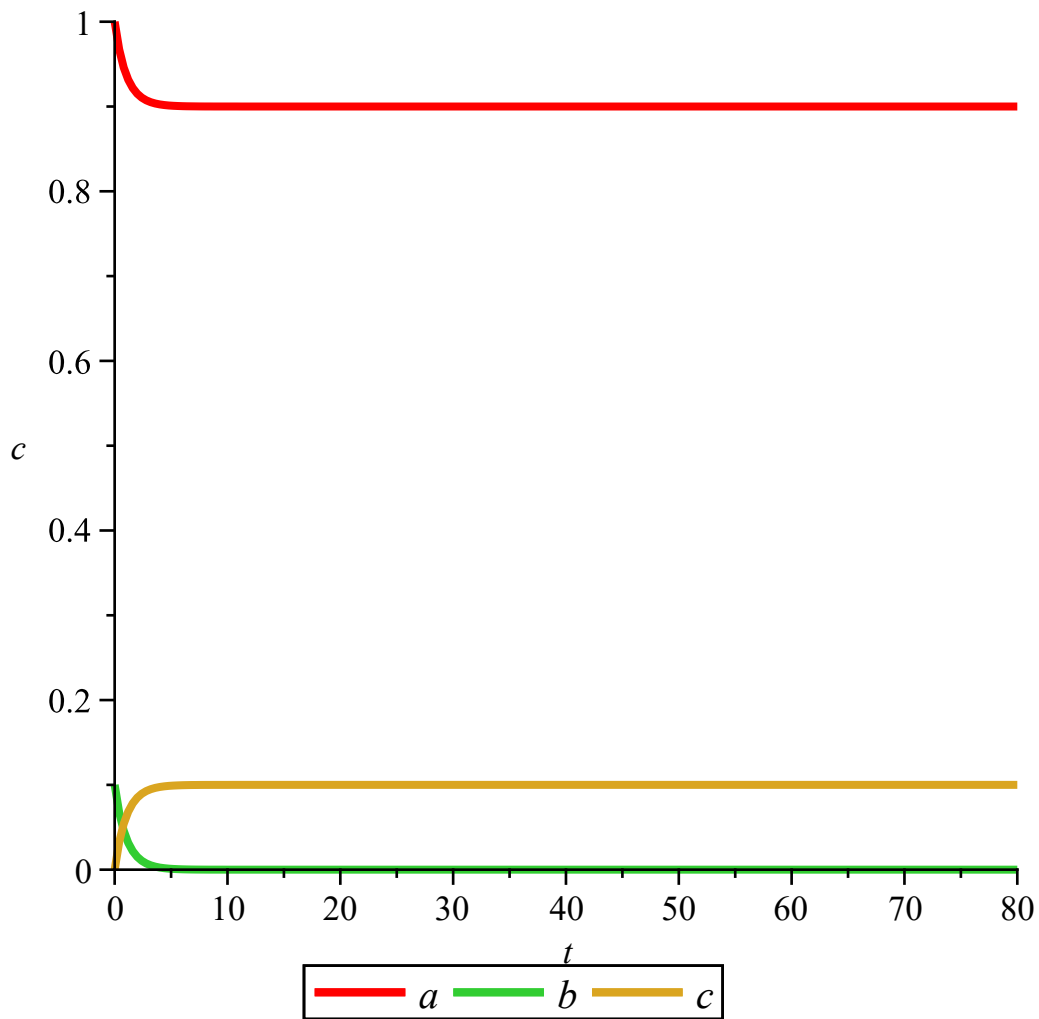
$$+ k_{-1} ca_0) \Big) / \left(-1 \right)$$

$$+ k_{-1} e^{t(-cb_0 k_{-1} + k_{-1} ca_0)} e^{\frac{\left(\ln\left(\frac{ca_0}{cb_0 k_{-1}}\right) + 21\pi_{-Z2}\right) (-cb_0 k_{-1} + k_{-1} ca_0)}{k_{-1} (-cb_0 + ca_0)}} \Big) + ca_0 + cc_0 \Big\}$$

```
> k_1:=1:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=.1,ode_3,cc(0)=0}, type=numeric);
```

```
nsol := proc(x_rkf45) ... end proc
```

```
> odeplot(nsol, [[t,ca(t)], [t,cb(t)], [t,cc(t)]], 0..80, labels=[t, c], legend=[a,b,c], thickness=3);
```



Srovnání prvního a druhého ádu

```
> restart;with( DEtools ):with( plots ):with( linalg):
> ode_1:=diff(ca(t),t)=-k_1*ca(t);
```

$$ode_1 := \frac{d}{dt} ca(t) = -k_1 ca(t)$$

```
> ode_2:=diff(cb(t),t)=-k_1*(cb(t))^2;
```

$$ode_2 := \frac{d}{dt} cb(t) = -k_1 cb(t)^2$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = ca0 e^{-k_1 t}$$

```
> dsolve({ode_2,cb(0)=cb0},cb(t));
```

$$cb(t) = \frac{cb0}{1 + k_1 t cb0}$$

```
> sol:= dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0},{ca(t),cb(t)})
;
```


$$sol := \left\{ \begin{array}{l} ca(t) = ca0 e^{-k_1 t}, \\ cb(t) = \frac{1}{k_1 t + \frac{1}{cb0}} \end{array} \right\}$$

```
> k_1:=log(2):nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=1},
type=numeric, output=listprocedure);#assign(nsol);f:=eval(ca
(t), sol);f(t=1);
```

```
nsol := [t=proc(t) ... end proc, ca(t)=proc(t) ... end proc, cb(t)=proc(t)
```

```
...
```

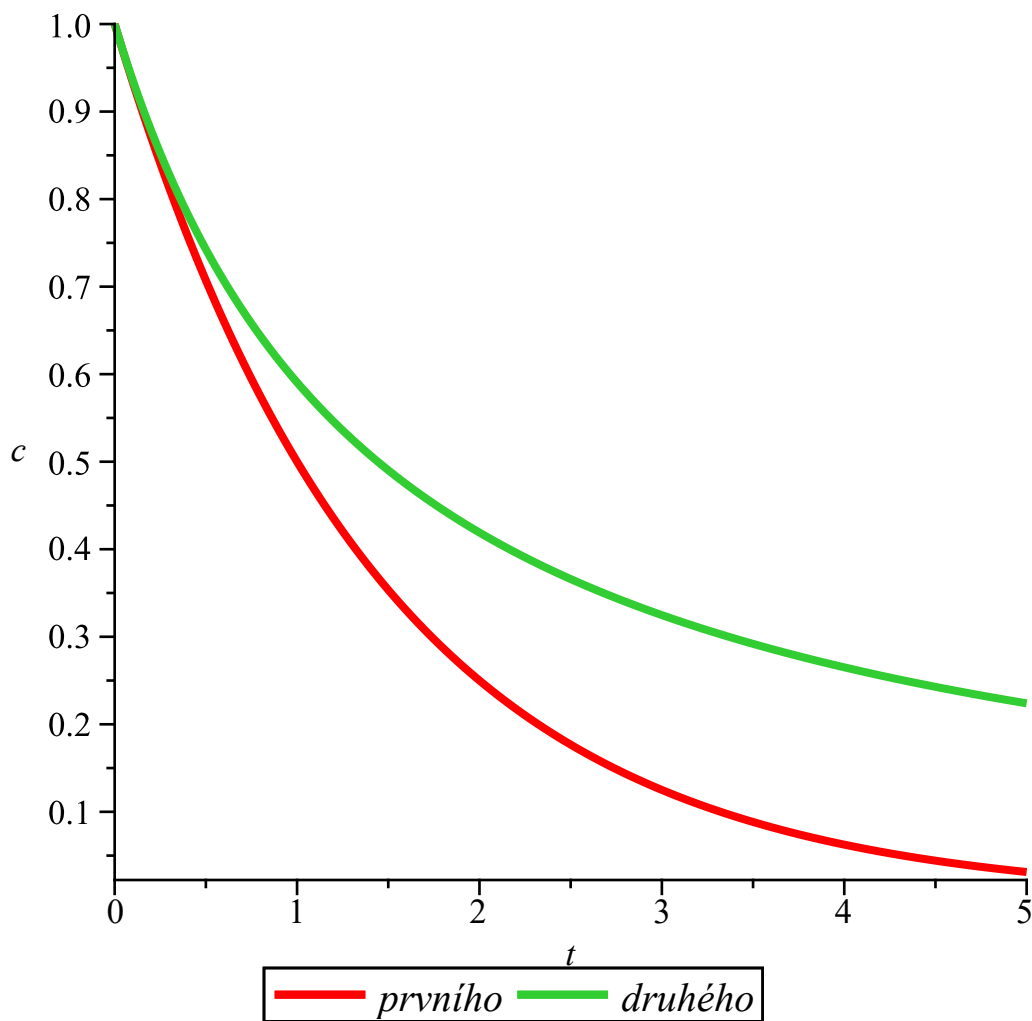
```
end proc]
```

```
> %nsol(1);
```

```
%nsol(1)
```

(5.1)

```
> odeplot(nsol, [[t,ca(t)],[t,cb(t)]],0..5,labels=[t,c],legend=
[prvního,druhého],thickness=3);
```



▼ Paralelní reakce A→B, A→C

```
> restart;with( DEtools ):with( plots ):with( linalg ):
> ode_1:=diff(ca(t),t)=-(k_1+k_2)*ca(t);
```

$$\text{ode}_1 := \frac{d}{dt} ca(t) = -(k_1 + k_2) ca(t)$$

> **ode_2:=diff(cb(t),t)=(k_1)*ca(t);**

$$\text{ode}_2 := \frac{d}{dt} cb(t) = k_1 ca(t)$$

> **ode_3:=diff(cc(t),t)=(k_2)*ca(t);**

$$\text{ode}_3 := \frac{d}{dt} cc(t) = k_2 ca(t)$$

> **dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0,ode_3,cc(0)=cc0},{ca(t),cb(t),cc(t)});**

$$\left\{ \begin{aligned} ca(t) &= ca0 e^{-(k_1+k_2)t}, cb(t) = -\frac{k_1 ca0 e^{-(k_1+k_2)t}}{k_1+k_2} \\ &+ \frac{k_1 ca0 + cb0 k_1 + cb0 k_2}{k_1+k_2}, cc(t) = -\frac{k_2 ca0 e^{-(k_1+k_2)t}}{k_1+k_2} \\ &+ \frac{k_2 ca0 + cc0 k_1 + cc0 k_2}{k_1+k_2} \end{aligned} \right\}$$

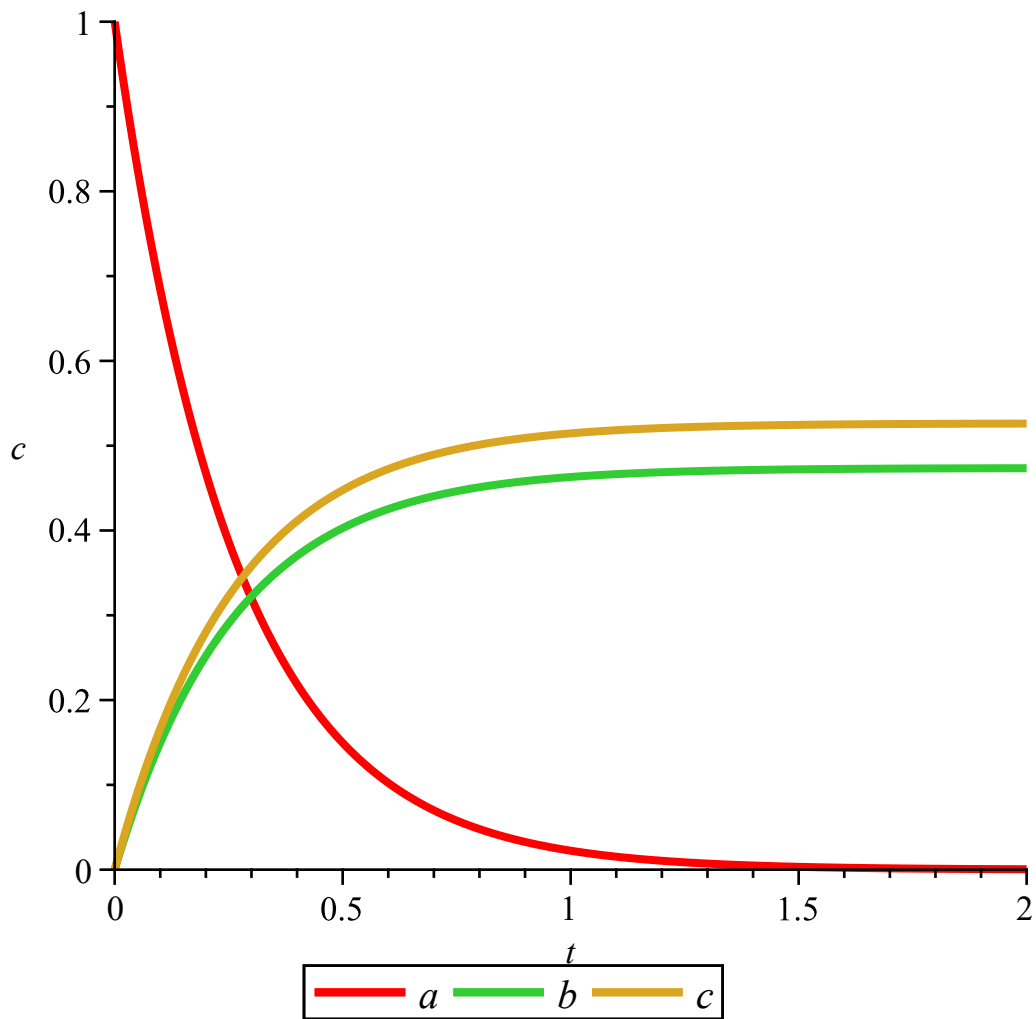
> **dsolve({ode_2,cb(0)=cb0},cb(t));**

$$cb(t) = \int_0^t k_1 ca(z1) dz1 + cb0$$

> **k_1:=1.8:k_2:=2:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=0,ode_3,cc(0)=0}, type=numeric);**

nsol := proc(x_rkf45) ... end proc

> **odeplot(nsol, [[t,ca(t)],[t,cb(t)],[t,cc(t)]],0..2,labels=[t,c],legend=[a,b,c],thickness=3);**



▼ Nasledne reakce

```
> restart;with( DEtools ):with( plots ):with( linalg):
```

```
> ode_1:=diff(ca(t),t)=-k_1*ca(t);
```

$$ode_1 := \frac{d}{dt} ca(t) = -k_1 ca(t)$$

```
> ode_2:=diff(cb(t),t)=k_1*ca(t)-k_2*cb(t);
```

$$ode_2 := \frac{d}{dt} cb(t) = k_1 ca(t) - k_2 cb(t)$$

```
> ode_3:=diff(cc(t),t)=k_2*cb(t);
```

$$ode_3 := \frac{d}{dt} cc(t) = k_2 cb(t)$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = ca0 e^{-k_1 t}$$

```
> dsolve({ode_2,cb(0)=cb0},cb(t));
```

$$cb(t) = \left(\int_0^t k_1 ca(z) e^{k_2 z} dz + cb0 \right) e^{-k_2 t}$$

```
> dsolve({ode_3, cc(0)=cc0}, cc(t));
```

$$cc(t) = \int_0^t k_2 cb(z_1) dz_1 + cc0$$

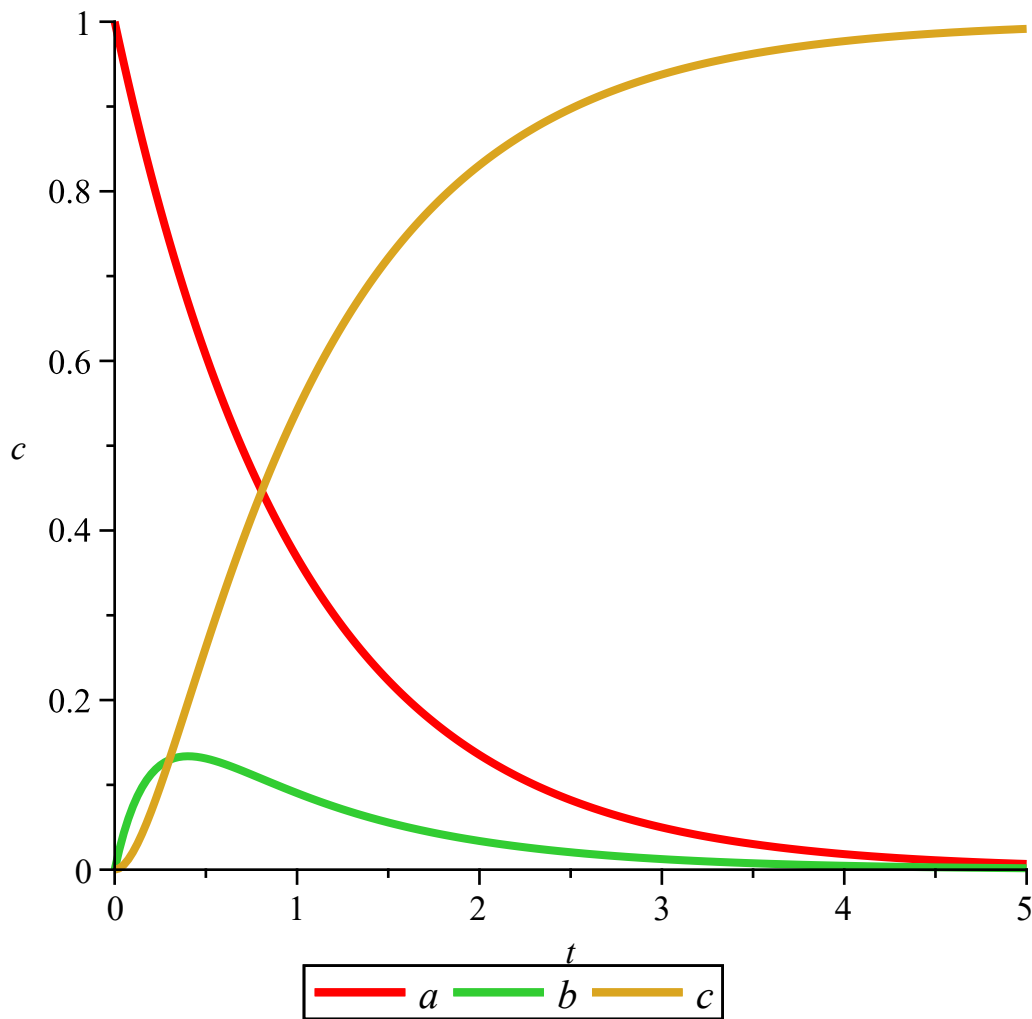
```
> dsolve({ode_1, ca(0)=ca0, ode_2, cb(0)=cb0, ode_3, cc(0)=cc0}, {ca(t), cb(t), cc(t)});
```

$$\left\{ \begin{aligned} ca(t) &= ca0 e^{-k_1 t}, cb(t) = -\frac{1}{k_1 - k_2} \left(\left(-\frac{(-k_2 cb0 + k_1 ca0 + cb0 k_1) k_1}{k_1 - k_2} \right. \right. \\ &+ \left. \left. \frac{(-k_2 cb0 + k_1 ca0 + cb0 k_1) k_2}{k_1 - k_2} \right) e^{-k_2 t} \right) - \frac{k_1 ca0 e^{-k_1 t}}{k_1 - k_2}, cc(t) \\ &= \frac{1}{k_1 - k_2} \left(e^{-k_1 t} ca0 k_2 - \frac{e^{-k_2 t} (-k_2 cb0 + k_1 ca0 + cb0 k_1) k_1}{k_1 - k_2} \right. \\ &+ \left. \frac{e^{-k_2 t} (-k_2 cb0 + k_1 ca0 + cb0 k_1) k_2}{k_1 - k_2} + (cc0 + ca0 + cb0) k_1 - (cc0 + ca0 \right. \\ &\left. + cb0) k_2 \right) \end{aligned} \right\}$$

```
> k_1:=1:k_2:=5:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=0,ode_3,cc(0)=0}, type=numeric);
```

```
nsol := proc(x_rkf45) ... end proc
```

```
> odeplot(nsol, [[t,ca(t)],[t,cb(t)],[t,cc(t)]],0..5,labels=[t,c],legend=[a,b,c],thickness=3);
```



>

Vratná reakce A <--> B

```
> restart;with( DEtools ):with( plots ):with( linalg );
```

```
> ode_1:=diff(ca(t),t)=-k_1*ca(t)+k_2*cb(t);
```

$$ode_1 := \frac{d}{dt} ca(t) = -k_1 ca(t) + k_2 cb(t)$$

```
> ode_2:=diff(cb(t),t)=(k_1)*ca(t)-k_2*cb(t);
```

$$ode_2 := \frac{d}{dt} cb(t) = k_1 ca(t) - k_2 cb(t)$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = \left(\int_0^t k_2 cb(z) e^{k_1 z} dz + ca0 \right) e^{-k_1 t}$$

```
> dsolve({ode_2,cb(0)=cb0},cb(t));
```

$$cb(t) = \left(\int_0^t k_1 ca(z) e^{k_2 z} dz + cb0 \right) e^{-k_2 t}$$

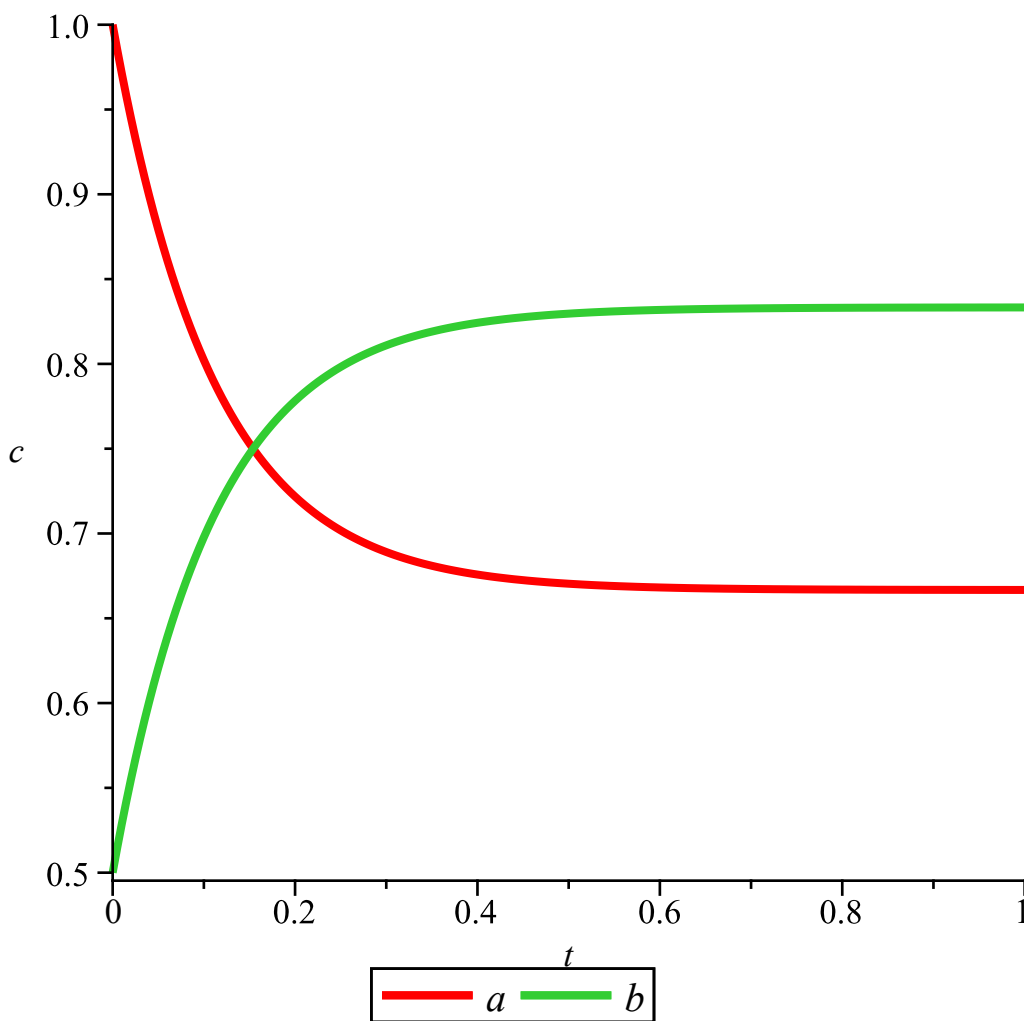
```
> dsolve({ode_1, ca(0)=ca0, ode_2, cb(0)=cb0}, {ca(t), cb(t)});
```

$$\left\{ \begin{aligned} ca(t) &= \frac{k_2 (cb0 + ca0)}{k_1 + k_2} + \frac{(k_1 ca0 - k_2 cb0) e^{-(k_1 + k_2)t}}{k_1 + k_2}, \\ cb(t) &= -\frac{(k_1 ca0 - k_2 cb0) e^{-(k_1 + k_2)t}}{k_1 + k_2} + \frac{k_1 (cb0 + ca0)}{k_1 + k_2} \end{aligned} \right\}$$

```
> k_1:=5:k_2:=4:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=.5},
type=numeric);
```

```
nsol := proc(x_rkf45) ... end proc
```

```
> odeplot(nsol, [[t,ca(t)],[t,cb(t)]],0..1,labels=[t,c],legend=
[a,b],thickness=3);
```



```
>
```

▼ řešení využívající piblížení

▼ Reakce druhého řádu $A+B \rightarrow C$, pevedená na pseudoprvní řád

```
> restart;with( DEtools ):with( plots ):with( linalg ):
```

```
> ode_1:=diff(ca(t),t)=-k_1*(ca(t))*(cb(t));
```

$$ode_1 := \frac{d}{dt} ca(t) = -k_1 ca(t) cb(t)$$

```
> ode_2:=diff(cb(t),t)=-k_1*(ca(t))*(cb(t));
```

$$ode_2 := \frac{d}{dt} cb(t) = -k_1 ca(t) cb(t)$$

```
> ode_3:=diff(cc(t),t)=k_1*(ca(t))*(cb(t));
```

$$ode_3 := \frac{d}{dt} cc(t) = k_1 ca(t) cb(t)$$

(9.1.1)

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = ca0 e^{\int_0^t (-k_1 cb(z1)) dz1}$$

```
> dsolve({ode_2,cb(0)=cb0},cb(t));
```

$$cb(t) = cb0 e^{\int_0^t (-k_1 ca(z1)) dz1}$$

```
> dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0,ode_3,cc(0)=cc0},
{ca(t),cb(t),cc(t)});
```

$$ca(t) = \left(e^{i\pi Z1} \right)^2 e^{t(-cb0k_1 + k_1 ca0)} e^{\frac{\left(\ln\left(\frac{ca0}{cb0k_1} \right) + 2i\pi Z2 \right) (-cb0k_1 + k_1 ca0)}{k_1 (-cb0 + ca0)}} \quad ($$

$$-cb0k_1 + k_1 ca0) \Big/ \left(-1 \right)$$

$$+ k_1 e^{t(-cb0k_1 + k_1 ca0)} e^{\frac{\left(\ln\left(\frac{ca0}{cb0k_1} \right) + 2i\pi Z2 \right) (-cb0k_1 + k_1 ca0)}{k_1 (-cb0 + ca0)}} \Big), cb(t) =$$

$$- \left[\left(e^{1\pi_{Z1\sim}} \right)^2 (-cb_0 k_{-1} + k_{-1} ca_0)^2 e^{t(-cb_0 k_{-1} + k_{-1} ca_0)} e^{\frac{\left(\ln\left(\frac{ca_0}{cb_0 k_{-1}}\right) + 21\pi_{Z2\sim} \right) (-cb_0 k_{-1} + k_{-1} ca_0)}{k_{-1} (-cb_0 + ca_0)}} \right) / \left(-1 \right.$$

$$\left. + k_{-1} e^{t(-cb_0 k_{-1} + k_{-1} ca_0)} e^{\frac{\left(\ln\left(\frac{ca_0}{cb_0 k_{-1}}\right) + 21\pi_{Z2\sim} \right) (-cb_0 k_{-1} + k_{-1} ca_0)}{k_{-1} (-cb_0 + ca_0)}} \right)$$

$$e^{\frac{\left(\ln\left(\frac{ca_0}{cb_0 k_{-1}}\right) + 21\pi_{Z2\sim} \right) (-cb_0 k_{-1} + k_{-1} ca_0)}{k_{-1} (-cb_0 + ca_0)}} \right)^2 \left(-1 \right.$$

$$\left. + k_{-1} e^{t(-cb_0 k_{-1} + k_{-1} ca_0)} e^{\frac{\left(\ln\left(\frac{ca_0}{cb_0 k_{-1}}\right) + 21\pi_{Z2\sim} \right) (-cb_0 k_{-1} + k_{-1} ca_0)}{k_{-1} (-cb_0 + ca_0)}} \right) /$$

$$\left(k_{-1} \left(e^{1\pi_{Z1\sim}} \right)^2 e^{t(-cb_0 k_{-1} + k_{-1} ca_0)} e^{\frac{\left(\ln\left(\frac{ca_0}{cb_0 k_{-1}}\right) + 21\pi_{Z2\sim} \right) (-cb_0 k_{-1} + k_{-1} ca_0)}{k_{-1} (-cb_0 + ca_0)}} \right) ($$

$$-cb_0 k_{-1} + k_{-1} ca_0) \Big), cc(t) =$$

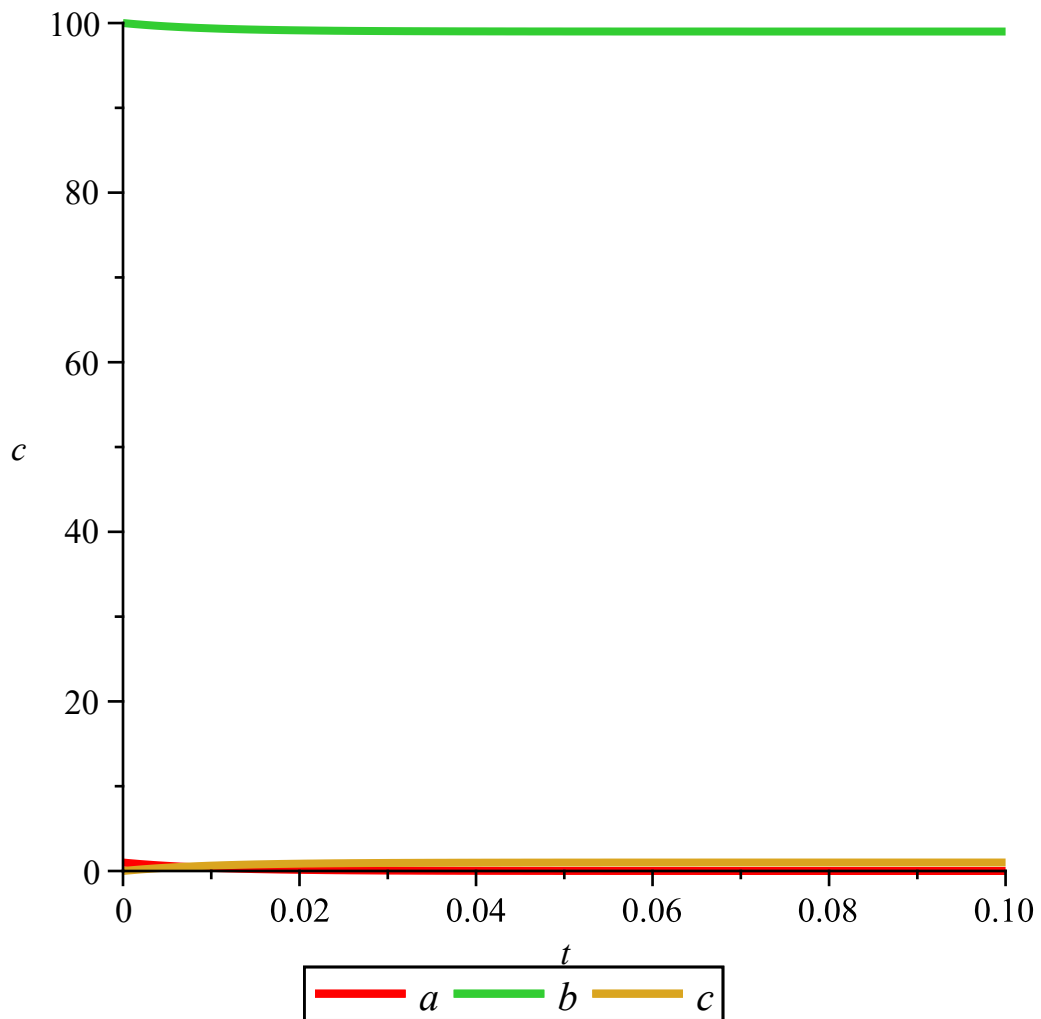
$$- \left(\left(e^{1\pi_{Z1\sim}} \right)^2 e^{t(-cb_0 k_{-1} + k_{-1} ca_0)} e^{\frac{\left(\ln\left(\frac{ca_0}{cb_0 k_{-1}}\right) + 21\pi_{Z2\sim} \right) (-cb_0 k_{-1} + k_{-1} ca_0)}{k_{-1} (-cb_0 + ca_0)}} \right) (-cb_0 k_{-1}$$

$$\left. \begin{aligned} &+ k_{-1} ca0) \Big/ \left(-1 \right. \\ &\left. + k_{-1} e^{t(-cb0k_{-1} + k_{-1}ca0)} e^{\frac{\left(\ln\left(\frac{ca0}{cb0k_{-1}} \right) + 21\pi_{Z2\sim} \right) (-cb0k_{-1} + k_{-1}ca0)}{k_{-1}(-cb0 + ca0)}} \right) + ca0 + cc0 \Big\} \end{aligned} \right\}$$

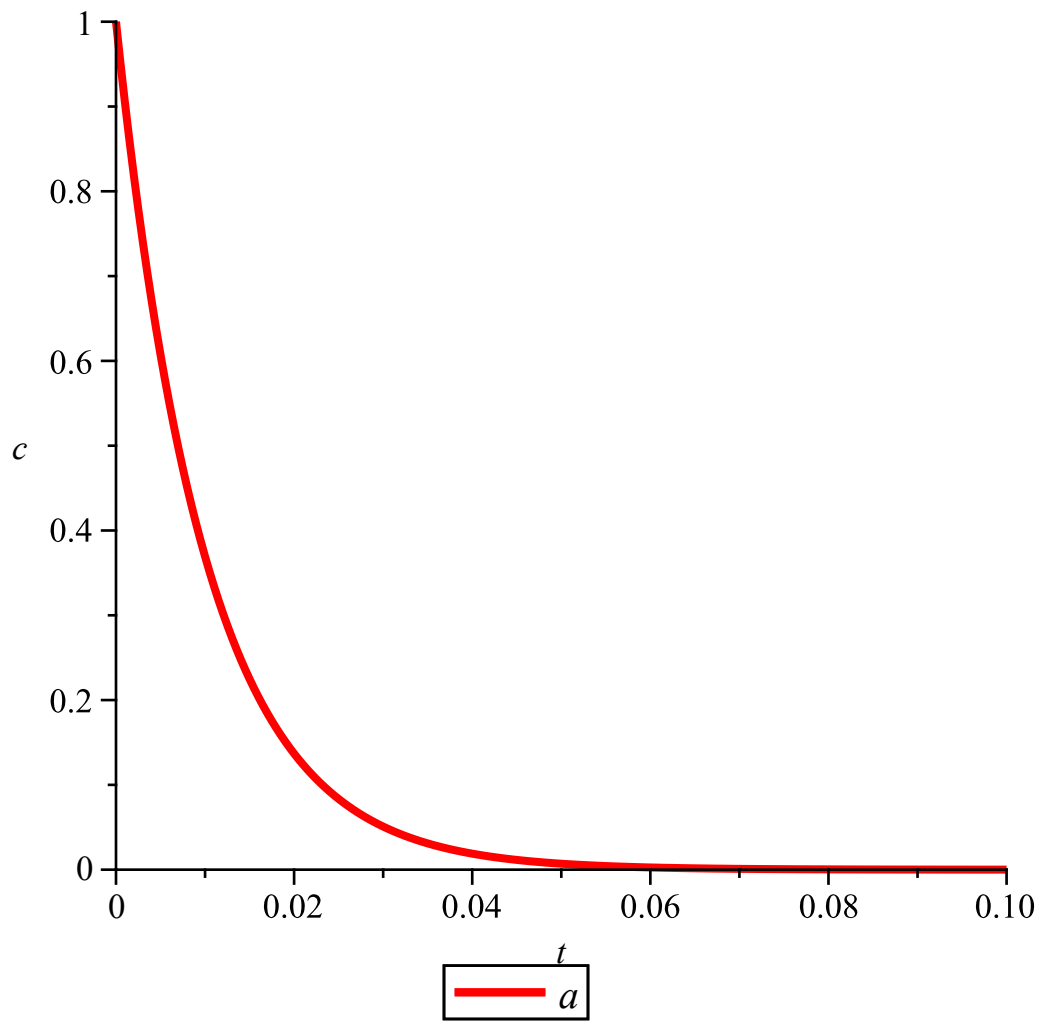
```
> k_1:=1:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=100,ode_3,
cc(0)=0}, type=numeric);
```

```
nsol := proc(x_rkf45) ... end proc
```

```
> odeplot(nsol, [[t,ca(t)],[t,cb(t)],[t,cc(t)]],0..0.1,labels=
[t,c],legend=[a,b,c],thickness=3);
```



```
> odeplot(nsol, [[t,ca(t)]],0..0.1,labels=[t,c],legend=[a],
thickness=3);
```



```
> odeplot(nsol, [[t, cb(t)], 0..0.1, labels=[t, c], legend=[b],  
thickness=3, color=[green]);
```

