CoRC Worksheet

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This document shows some of the functionality of CoRC, the Copasi R Connector. CoRC can be downloaded from jpahle.github.io/CoRC. There, you will also find the documentation, further examples, complete function reference and more.

Load the CoRC library and, possibly, other utility libraries, such as the ones contained in tidyverse:

```
library(CoRC)
library(tidyverse) # autoplot()
```

Model creation / editing

Create an empty model:

```
newModel()
```

```
## # A COPASI model reference:
## Model name: "New Model"
## Number of compartments: 0
## Number of species: 0
## Number of reactions: 0
```

Change model name (and, possibly, other model properties):

```
setModelName("Michaelis-Menten scheme")
getCurrentModel()
```

```
## # A COPASI model reference:
## Model name: "Michaelis-Menten scheme"
## Number of compartments: 0
## Number of species: 0
## Number of reactions: 0
```

Create a reversible reaction (note: "=" for reversible, and "->" for irreversible reactions):

```
newReaction("S + E = C", name = "Complex formation")
```

```
## [1] "(Complex formation)"
```

Show all compartments (note: COPASI created one default compartment simply called "compartment"):

```
getCompartments()
```

```
## # A tibble: 1 x 10
##   key                  name  type  dimensionality unit  initial_size  size  rate
##   <chr>                <chr> <chr>          <int> <chr>        <dbl> <dbl> <dbl>
## 1 Compartments[compar~ comp~ fixed              3 l                1   NaN     0
## # i 2 more variables: initial_expression <chr>, expression <chr>
```

Show all species (note: COPASI auto-created all species implicitly defined in a reaction):

```
getSpecies()
```

```
## # A tibble: 3 x 13
##   key         name  compartment type  unit  initial_concentration initial_number
##   <chr>       <chr> <chr>       <chr> <chr>                 <dbl>          <dbl>
## 1 C{compartm~ C     compartment reac~ mol/l                     1        6.02e23
## 2 E{compartm~ E     compartment reac~ mol/l                     1        6.02e23
## 3 S{compartm~ S     compartment reac~ mol/l                     1        6.02e23
## # i 6 more variables: concentration <dbl>, number <dbl>, rate <dbl>,
## #   number_rate <dbl>, initial_expression <chr>, expression <chr>
```

Show all reactions:

```
getReactions()
```

```
## # A tibble: 1 x 6
##   key                 name              reaction  rate_law      flux number_flux
##   <chr>               <chr>             <chr>     <chr>        <dbl>       <dbl>
## 1 (Complex formation) Complex formation S + E = C FunctionDB.~     0           0
```

Create a reaction for product formation:

```
newReaction("C -> E + P", name = "Product formation")
```

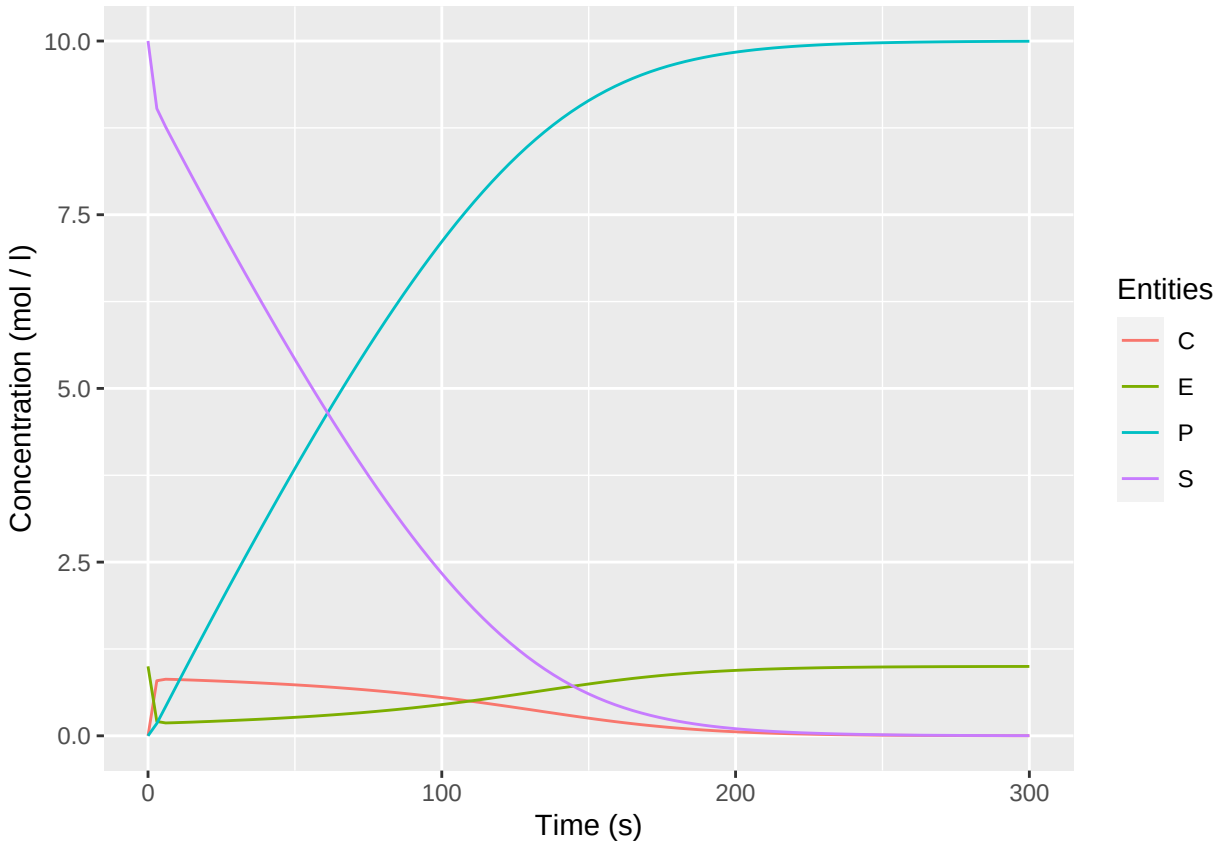
```
## [1] "(Product formation)"
```

Set initial concentrations for all species

```
setSpecies("S", initial_concentration = 10)
setSpecies("C", initial_concentration = 0)
setSpecies("P", initial_concentration = 0)
```

Simulate: calculate a timecourse for the first 300 seconds, and plot:

```
timecourse <- runTimeCourse(300)
autoplot.copasi_ts(timecourse)
```



If you have COPASI installed, you can quickly open the GUI to manually inspect and work with your model:

```
openCopasi()
```

If you want to free memory space, you can unload the model (CoRC allows you to have an arbitrary number of models opened at the same time):

```
unloadModel()
```