# Creating an PBK model in SBML

## A guide to implement models in Antimony and convert them to SBML

### Introduction

‘Since the advent of SBML (the Systems Biology Markup Language) computer models of biological systems have been able to be transferred easily between different labs and different computer programs without loss of specificity. But SBML was not designed to be readable or writable by humans, only by computer programs, so other programs have sprung up to allow users to more easily create the models they need.’[[1]](https://tellurium.readthedocs.io/en/latest/antimony.html)

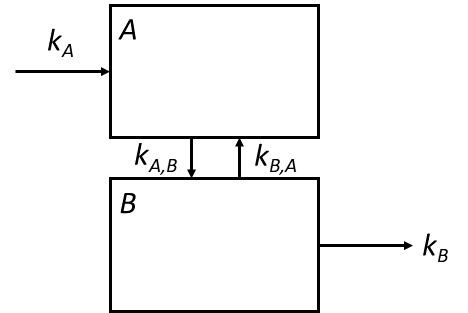
[Antimony](https://tellurium.readthedocs.io/en/latest/antimony.html) is such a program. ‘Antimony is designed to interconvert between the SBML format and a shorthand form that allows editing without the structure and overhead of working with SBML directly. In Antimony, users can easily define substance species, reactions, compartments, events, and other elements of a biological model.’ [[1]](https://tellurium.readthedocs.io/en/latest/antimony.html) Essentially, Antimony is a relatively easy way of defining models that can be subsequently converted into SBML files using [Tellurium](http://tellurium.analogmachine.org/). Thus, Antimony provides a way of harmonizing the way in which PBK models are defined within the PARC project.

In this guidance document, we will describe how to use antimony, provide basic coding examples and discuss more complex elements that may be present in your PBK models. The goal of this guidance is not to provide a detailed overview of all functionalities of Antimony, as that can already be found [here](https://tellurium.readthedocs.io/en/latest/antimony.html). Instead, this guidance focus on distilling the aspects of Antimony that may be relevant when building your own PBK models within PARC.

### Basics of antimony

* Reactions

Antimony uses reactions to define the transfer of a substance to one compartment to the other. Hence, instead of using differential equations to describe the rate of change within a given compartment, modelers should specify the rate with which compounds migrate from one compartment to the other. Consider this two compartment model below (Fig. ):



Example of a two-compartment model

In terms of differential equations, this model would be defined as:

In contrast, in antimony this model is described with the following reactions:

-> A; D(t)   
A -> B; k\_{A,B} \* A(t)   
B -> A; k\_{B,A} \* B(t)   
B -> ; Eliminated

Basically, instead of specifying the rate at which the amount in a compartment changes, modelers should define the ‘arrows’ representing the transfer of a compound.

* Compartments In order to define the transfer of a compound to and from a compartment, compartments need to be defined in Antimony. This can be done by using the compartment keyword
* Species

### Advanced antimony

* Assignment rules
  + Piecewise assignment
  + Time-dependent parameters
* Probabilistic modelling and random sampling from distribution
* Custom functions
* Events

### Conversion to SBML using Tellurium

* Basic syntax
* Changing parameter values

### Exporting SMBL to other software packages

* R (mrgsolve package)
* R (deSolve): Not possible yet
* MCsim: not possible yet?

### Tips and tricks

* Common errors

### References

[1] <https://tellurium.readthedocs.io/en/latest/antimony.html>