A

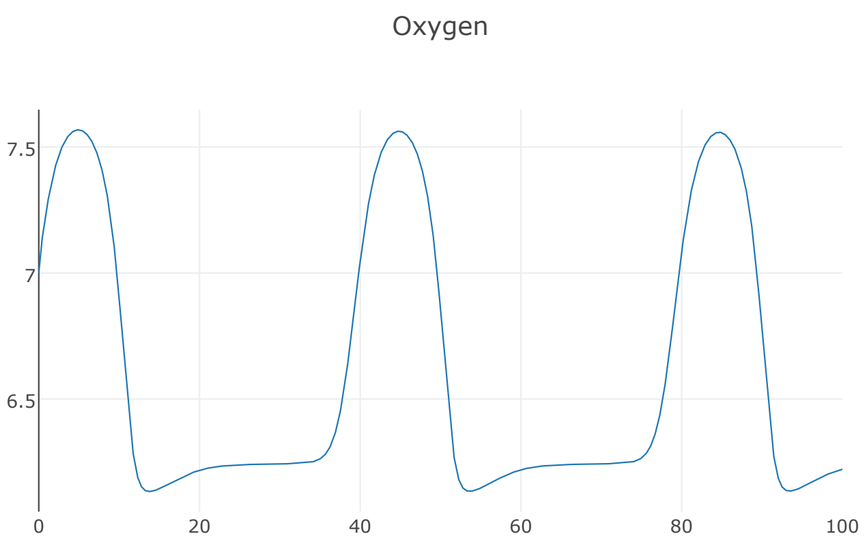
Tellurium notebook with inline OMEX representation of COMBINE archive

```
  ...
  v11a: $C1 + $Hm + N2 => $C2 + $Ho + $N1; \
      c2*k11*N2*oxy/((a*N2 + oxy)*(1 + (hyd/Kh)^m));
  v11a2: $C2 + oxy => $C1 + $H2O; \
      c2*k11*N2*oxy/((a*N2 + oxy)*(1 + (hyd/Kh)^m));
  v16: $A2c + A3m => $A2m + A3c; c2*k16*A3m*A2c;
  v11b: $Ho + $A2m => $Hm + A3m; \
      (c2*3*k11*N2*oxy/((a*N2 + oxy)*(1 + (hyd/Kh)^m)))*A2m/(Ka + A2m);
  ...
// -- End Antimony block

// -- Begin PhraSEDML block converted from main.xml
// Models
wolf2001 = model "wolf2001"

// Simulations / Tasks
sim1 = simulate uniform(0, 100, 1000)
task1  = run sim1 on wolf2001

// Outputs
plot "Oxygen" time vs oxy
```



B

SBML encoding for reaction "v11a2"

```
<reaction id="v11a2" name="vET2" reversible="false" fast="false">
        <listOfReactants>
          <speciesReference species="C2" stoichiometry="1" constant="true"/>
          <speciesReference species="oxy" stoichiometry="1" constant="true"/>
        </listOfReactants>
        <listOfProducts>
          <speciesReference species="C1" stoichiometry="1" constant="true"/>
          <speciesReference species="H2O" stoichiometry="1" constant="true"/>
        </listOfProducts>
        <listOfModifiers>
          <modifierSpeciesReference species="hyd"/>
          <modifierSpeciesReference species="N2"/>
        </listOfModifiers>
        <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
            <apply>
              ...
                  <plus/>
                  <cn type="integer"> 1 </cn>
                  <apply>
                    <power/>
                    <apply>
                      <divide/>
                      <ci> hyd </ci>
                      <ci> Kh </ci>
                    </apply>
                    <ci> m </ci>
                  </apply>
                ...
```

SED-ML encoding of timecourse simulation and plot portion

```
...
<listOfDataGenerators>
  <dataGenerator id="plot_0_0_0" name="time">
    <listOfVariables>
      <variable id="time" symbol="urn:sedml:symbol:time" taskReference="task1"/>
    </listOfVariables>
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <ci> time </ci>
    </math>
  </dataGenerator>
  <dataGenerator id="plot_0_0_1" name="oxy">
    <listOfVariables>
      <variable id="oxy"
        target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='oxy']"
        taskReference="task1" modelReference="wolf2001"/>
    </listOfVariables>
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <ci> oxy </ci>
    </math>
  </dataGenerator>
</listOfDataGenerators>
<listOfOutputs>
  <plot2D id="plot_0" name="Oxygen">
    <listOfCurves>
      <curve id="plot_0__plot_0_0_0__plot_0_0_1" logX="false" logY="false"
        xDataReference="plot_0_0_0" yDataReference="plot_0_0_1"/>
      ...
```

C