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Alternative Forms of Reaction Specification

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1 Introduction

In these meeting minutes we compare some of the solutions developed for specifying reactions using several simple example reactions. These reactions will probably appear as examples in the specification and they have been chosen to demonstrate a wide variety of reaction problems. The solutions developed are discussed in detail in the January 19 meeting minutes.

1.1 XML Formulation One

The **delta_variable** attributes appear on the **<variable_ref>** elements, and there is no **stoichiometry** attributes. All math is defined in a separate **<math>** element.

1.2 XML Formulation Two

Mathematics is moved into each **<variable_ref>** element adjacent to the **<role>** elements. We still have **delta_variable** attributes on **<variable_ref>** elements.

1.3 XML Formulation Three

delta_variable and **stoichiometry** attributes are moved on to the **<role>** elements. No mathematics for calculating the value of the delta variables is needed if both **delta_variable** and **stoichiometry** attributes exist on the same **<role>** element.

2 Simple Reversible Reaction

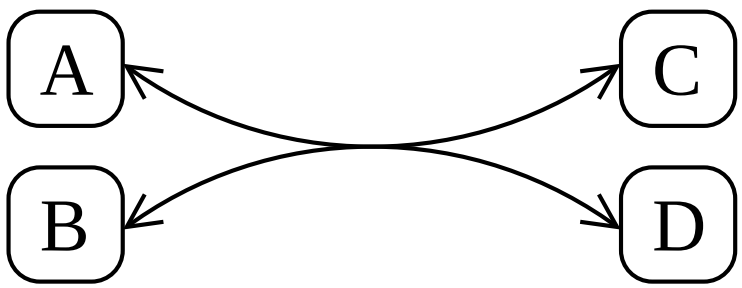
- **Equation**

  `A + B <-> 2C + D`

- **Description**

  A simple reversible reaction.

- **Picture**



- **XML Formulation One**

```
<reaction reversible="yes">

  <variable_ref delta_variable="delta_A" variable="A">
    <role role="reactant" direction="forward" />
  </variable_ref>

  <variable_ref delta_variable="delta_B" variable="B">
    <role role="reactant" direction="forward" />
  </variable_ref>

  <variable_ref delta_variable="delta_C" variable="C">
    <role role="product" direction="forward" />
  </variable_ref>

  <variable_ref delta_variable="delta_D" variable="D">
    <role role="product" direction="forward" />
  </variable_ref>

  <variable_ref variable="r">
    <role role="rate" direction="forward" />
  </variable_ref>

</reaction>
<math xmlns="http://www.w3.org/1998/Math/MathML">
 ...
</math>
```

- **XML Formulation Two**

```
<reaction reversible="yes">

  <variable_ref delta_variable="delta_A" variable="A">
    <role role="reactant" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_A </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> 1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref delta_variable="delta_B" variable="B">
    <role role="reactant" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_B </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> 1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref delta_variable="delta_C" variable="C">
    <role role="product" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_C </ci>
```

```
        <apply><times />
          <cn cellml:units="dimensionless"> -2.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref delta_variable="delta_D" variable="D">
    <role role="product" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_D </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> -1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref variable="r">
    <role role="rate" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      ...
    </math>
  </variable_ref>

</reaction>
```

- **XML Formulation Three**

```
<reaction reversible="yes">

  <variable_ref variable="A">
    <role
        role="reactant"
        direction="forward"
        delta_variable="delta_A"
        stoichiometry="1" />
  </variable_ref>

  <variable_ref variable="B">
    <role
        role="reactant"
        direction="forward"
        delta_variable="delta_B"
        stoichiometry="1" />
  </variable_ref>

  <variable_ref variable="C">
    <role
        role="product"
        direction="forward"
        delta_variable="delta_C"
        stoichiometry="2" />
  </variable_ref>

  <variable_ref variable="D">
    <role
        role="product"
        direction="forward"
        delta_variable="delta_D"
        stoichiometry="1" />
```

```
    </variable_ref>

    <variable_ref variable="r">
      <role role="rate" direction="forward" />
      <math xmlns="http://www.w3.org/1998/Math/MathML">
        ...
      </math>
    </variable_ref>

  </reaction>
```

3 Simple Reversible Reaction with Catalysis

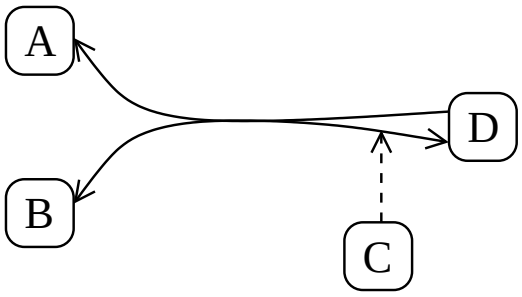
- **Equation**

  `A + B <-> D` (catalyzed in the forward direction by `C`)

- **Description**

  A reversible reaction where `C` acts as a catalyst in the forward direction only.

- **Picture**



- **XML Formulation One**

```
  <reaction reversible="yes">

    <variable_ref delta_variable="delta_A" variable="A">
      <role role="reactant" direction="forward" />
    </variable_ref>

    <variable_ref delta_variable="delta_B" variable="B">
      <role role="reactant" direction="forward" />
    </variable_ref>

    <variable_ref variable="C">
      <role role="catalyst" direction="forward" />
    </variable_ref>

    <variable_ref delta_variable="delta_D" variable="D">
      <role role="product" direction="forward" />
    </variable_ref>

    <variable_ref variable="r">
      <role role="rate" direction="forward" />
    </variable_ref>

  </reaction>
```

```
<math xmlns="http://www.w3.org/1998/Math/MathML">
 ...
</math>
```

- **XML Formulation Two**

```
<reaction reversible="yes">

  <variable_ref delta_variable="delta_A" variable="A">
    <role role="reactant" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_A </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> 1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref delta_variable="delta_B" variable="B">
    <role role="reactant" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_B </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> 1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref variable="C">
    <role role="catalyst" direction="forward" />
  </variable_ref>

  <variable_ref delta_variable="delta_D" variable="D">
    <role role="product" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_D </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> -1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref variable="r">
    <role role="rate" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      ...
    </math>
  </variable_ref>

</reaction>
```

- **XML Formulation Three**

```
<reaction reversible="yes">

  <variable_ref variable="A">
    <role
        role="reactant"
        direction="forward"
        delta_variable="delta_A"
        stoichiometry="1" />
  </variable_ref>

  <variable_ref variable="B">
    <role
        role="reactant"
        direction="forward"
        delta_variable="delta_B"
        stoichiometry="1" />
  </variable_ref>

  <variable_ref variable="C">
    <role role="catalyst" direction="forward" />
  </variable_ref>

  <variable_ref variable="D">
    <role
        role="product"
        direction="forward"
        delta_variable="delta_D"
        stoichiometry="1" />
  </variable_ref>

  <variable_ref variable="r">
    <role role="rate" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      ...
    </math>
  </variable_ref>

</reaction>
```

4 Autophosphorylation

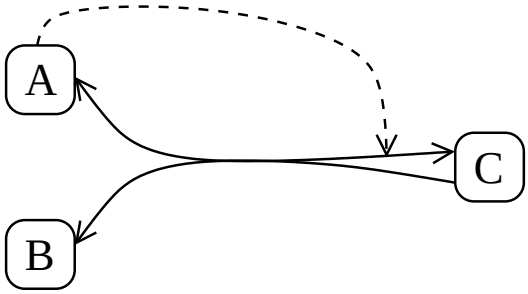
- **Equation**

  A + B <-> C (catalyzed by A in the forward direction)

- **Description**

  A autocatalyzes a reaction (e.g., an autophosphorylation, where B is phosphate).

- **Picture**



- **XML Formulation One**

```
<reaction reversible="yes">

  <variable_ref delta_variable="delta_A" variable="A">
    <role role="reactant" direction="forward" />
  </variable_ref>

  <variable_ref delta_variable="delta_B" variable="B">
    <role role="reactant" direction="forward" />
  </variable_ref>

  <variable_ref variable="C">
    <role role="catalyst" direction="forward" />
  </variable_ref>

  <variable_ref delta_variable="delta_D" variable="D">
    <role role="product" direction="forward" />
  </variable_ref>

  <variable_ref variable="r">
    <role role="rate" direction="forward" />
  </variable_ref>

</reaction>
<math xmlns="http://www.w3.org/1998/Math/MathML">
 ...
</math>
```

- **XML Formulation Two**

```
<reaction reversible="yes">

  <variable_ref delta_variable="delta_A" variable="A">
    <role role="reactant" direction="forward" />
    <role role="catalyst" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_A </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> 1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref delta_variable="delta_B" variable="B">
```

```
    <role role="reactant" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_B </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> 1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref delta_variable="delta_C" variable="C">
    <role role="product" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_C </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> -1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref variable="r">
    <role role="rate" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      ...
    </math>
  </variable_ref>

</reaction>
```

- **XML Formulation Three**

```
<reaction reversible="yes">

  <variable_ref variable="A">
    <role
        role="reactant"
        direction="forward"
        delta_variable="delta_A"
        stoichiometry="1" />
    <role role="catalyst" direction="forward" />
  </variable_ref>

  <variable_ref variable="B">
    <role
        role="reactant"
        direction="forward"
        delta_variable="delta_B"
        stoichiometry="1" />
  </variable_ref>

  <variable_ref variable="C">
    <role
        role="product"
```

```
        direction="forward"
        delta_variable="delta_C"
        stoichiometry="1" />
    </variable_ref>

    <variable_ref variable="r">
      <role role="rate" direction="forward" />
    </variable_ref>

  </reaction>
```

5 Simple Reaction with Catalysis and Substrate Inhibition

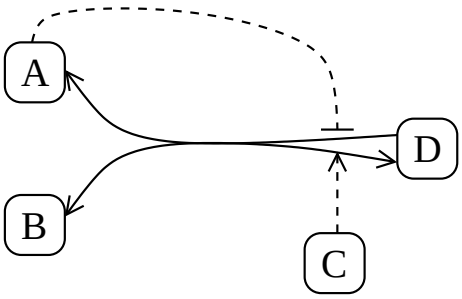
- **Equation**

  A + B <-> D (catalyzed by C, inhibited by A)

- **Description**

  A reversible reaction in which the reverse reaction is inhibited by one of the substrates.

- **Picture**



- **XML Formulation One**

```
<reaction reversible="yes">

  <variable_ref delta_variable="delta_A" variable="A">
    <role role="reactant" direction="forward" />
    <role role="inhibitor" direction="reverse" />
  </variable_ref>

  <variable_ref delta_variable="delta_B" variable="B">
    <role role="reactant" direction="forward" />
  </variable_ref>

  <variable_ref variable="C">
    <role role="catalyst" direction="forward" />
  </variable_ref>

  <variable_ref variable="D">
    <role role="product" direction="forward" />
  </variable_ref>

  <variable_ref variable="r">
    <role role="rate" direction="forward" />
  </variable_ref>
```

```
</reaction>
<math xmlns="http://www.w3.org/1998/Math/MathML">
 ...
</math>
```

- **XML Formulation Two**

```
<reaction reversible="yes">
  <variable_ref delta_variable="delta_A" variable="A">
    <role role="reactant" direction="forward" />
    <role role="inhibitor" direction="reverse" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_A </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> 1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref delta_variable="delta_B" variable="B">
    <role role="reactant" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_B </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> 1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref variable="C">
    <role role="catalyst" direction="forward" />
  </variable_ref>

   <variable_ref delta_variable="delta_D" variable="D">
    <role role="product" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_D </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> -1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref variable="r">
    <role role="rate" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      ...
    </math>
  </variable_ref>
```

```
</reaction>
```

- **XML Formulation Three**

```
<reaction reversible="yes">

  <variable_ref variable="A">
    <role
        role="reactant"
        direction="forward"
        delta_variable="delta_A"
        stoichiometry="1" />
    <role
        role="inhibitor"
        direction="reverse"
        delta_variable="delta_A"
        stoichiometry="1" />
  </variable_ref>

  <variable_ref variable="B">
    <role
        role="reactant"
        direction="forward"
        delta_variable="delta_B"
        stoichiometry="1" />
  </variable_ref>

  <variable_ref variable="C">
    <role role="catalyst" direction="forward" />
  </variable_ref>

  <variable_ref variable="D">
    <role
        role="product"
        direction="forward"
        delta_variable="delta_D"
        stoichiometry="1" />
  </variable_ref>

  <variable_ref variable="r">
    <role role="rate" direction="forward" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      ...
    </math>
  </variable_ref>

</reaction>
```

6 Simple Reaction with Catalysis and Product Inhibition

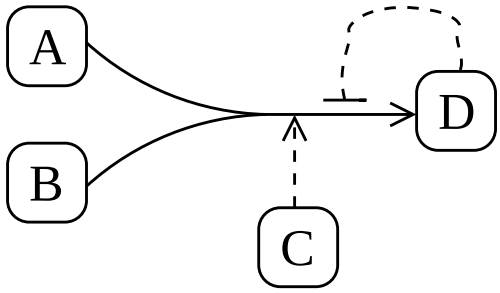
- **Equation**

  `A + B -> D` (catalyzed by `C`, inhibited by `D`)

- **Description**

  An irreversible, catalyzed reaction that exhibits product-inhibition.

- **Picture**



- **XML Formulation One**

```
<reaction reversible="no">
  <variable_ref delta_variable="delta_A" variable="A">
    <role role="reactant" />
  </variable_ref>
  <variable_ref delta_variable="delta_B" variable="B">
    <role role="reactant" />
  </variable_ref>
  <variable_ref variable="C">
    <role role="catalyst" />
  </variable_ref>
  <variable_ref delta_variable="delta_D" variable="D">
    <role role="product" />
    <role role="inhibitor" />
  </variable_ref>
  <variable_ref variable="r">
    <role role="rate" />
  </variable_ref>
</reaction>
<math xmlns="http://www.w3.org/1998/Math/MathML">
 ...
</math>
```

- **XML Formulation Two**

```
<reaction reversible="no">

  <variable_ref delta_variable="delta_A" variable="A">
    <role role="reactant" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_A </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> 1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref delta_variable="delta_B" variable="B">
    <role role="reactant" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
```

```
        <ci> delta_B </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> 1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref variable="C">
    <role role="catalyst" direction="forward" />
  </variable_ref>

  <variable_ref delta_variable="delta_D" variable="D">
    <role role="product" />
    <role role="inhibitor" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply><eq />
        <ci> delta_D </ci>
        <apply><times />
          <cn cellml:units="dimensionless"> -1.0 </cn>
          <ci> r </ci>
        </apply>
      </apply>
    </math>
  </variable_ref>

  <variable_ref variable="r">
    <role role="rate" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      ...
    </math>
  </variable_ref>

</reaction>
```

- **XML Formulation Three**

```
<reaction reversible="no">

  <variable_ref variable="A">
    <role role="reactant" delta_variable="delta_A" stoichiometry="1" />
  </variable_ref>

  <variable_ref variable="B">
    <role role="reactant" delta_variable="delta_B" stoichiometry="1" />
  </variable_ref>

  <variable_ref variable="C">
    <role role="catalyst" />
  </variable_ref>

  <variable_ref variable="D">
    <role role="product" delta_variable="delta_D" stoichiometry="1" />
    <role role="inhibitor" stoichiometry="1" />
  </variable_ref>

  <variable_ref variable="r">
```

```
    <role role="rate" />
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      ...
    </math>
  </variable_ref>

</reaction>
```
