

Notes on Best Practice for SBML

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Overview

- Aims
- Reactions vs Rules
- Reversible
- Stoichiometry
- Annotations
- Work to be done

Aim

- SBML can encode a given model in a number of ways
- ‘Best Practice’ describes what choices to make to maximize interoperability when encoding a model
- Separate from standard
- Process of defining ‘Best Practice’ may feedback into standard

Reactions versus Rules

- Biochemical networks should be described using reactions and species whenever possible
- **Rules** should be used for
 - _ Describing the behavior of non-biochemical phenomena
 - _ Describing changes in compartment volume
- **Issues**
 - _ Is a rule with no reactant or no product better or worse than a rule controlling species concentration?
 - _ Should the `fast` reaction attribute be used in preference to explicit algebraic constraints?

Reversible reactions

- The use of the `reversible` attribute on reaction should be consistent with the kinetic law (?)

Stoichiometry

- Use the `stoichiometry` attribute on `speciesReference` rather than have more than one `speciesReference` element for the same species in a set of products and reactants

Annotations

- Annotation elements are semantically associated with the element they are enclosed within
- Annotation data should be decomposed and associated with elements at the lowest appropriate level in the element hierarchy
- Annotation schema should avoid duplicating aspects of the SBML schema
- Tools that transform SBML can and should maintain the association between annotations and elements
 - _ delete annotation when deleting element
 - _ move annotation with element

Work to be done

- **Collect documentation on expected forms of SBML**
 - _ ideally developers will document what they expect
 - _ just look at generated SBML (?)
- **Identify common forms**
- **Create document**