XML format for RBA models

S. Fischer, V. Fromion, A. Goelzer

August 9, 2017

Contents

1 Introduction

In this document we present the XML structures used to define a RBA model. A complete RBA model is composed of the following files:

- metabolism.xml (definition of compartments, metabolic species and metabolic reactions).

- parameters.xml (definition of density constraints and user-defined functions).

- proteins.xml (definition of proteins).

- rnas.xml (definition of RNAs).

- dna.xml (definition of DNA).

- enzymes.xml (definition of enzymatic machineries catalyzing metabolic reactions).

- processes.xml (definition of cell processes necessary to growth and maintenance).

For every file, we present the nodes that composes the XML structure. For every node, we show a class diagram that shows the node's attributes and the children node that it may/must contain. We provide a brief description about the relevance of the node in the RBA model.

2 Conventions

2.1 Naming conventions

2.2 Boolean attributes

3 metabolism.xml

3.1 RBAMetabolism container

The metabolism file is strongly inspired by SBML. More precisely, it is a subpart of an SBML file.

3.1.1 RBAMetabolism

The outermost portion of the metabolism file is an instance of class **RBAMetabolism**, shown in Figure 2.
Currently, **RBAMetabolism** has no simple attributes. It includes exactly one instance of **ListOf** container classes. All **ListOf** classes do not have own attributes, they are merely used to organize a list of instances from another class. This organization was inspired by SBML.
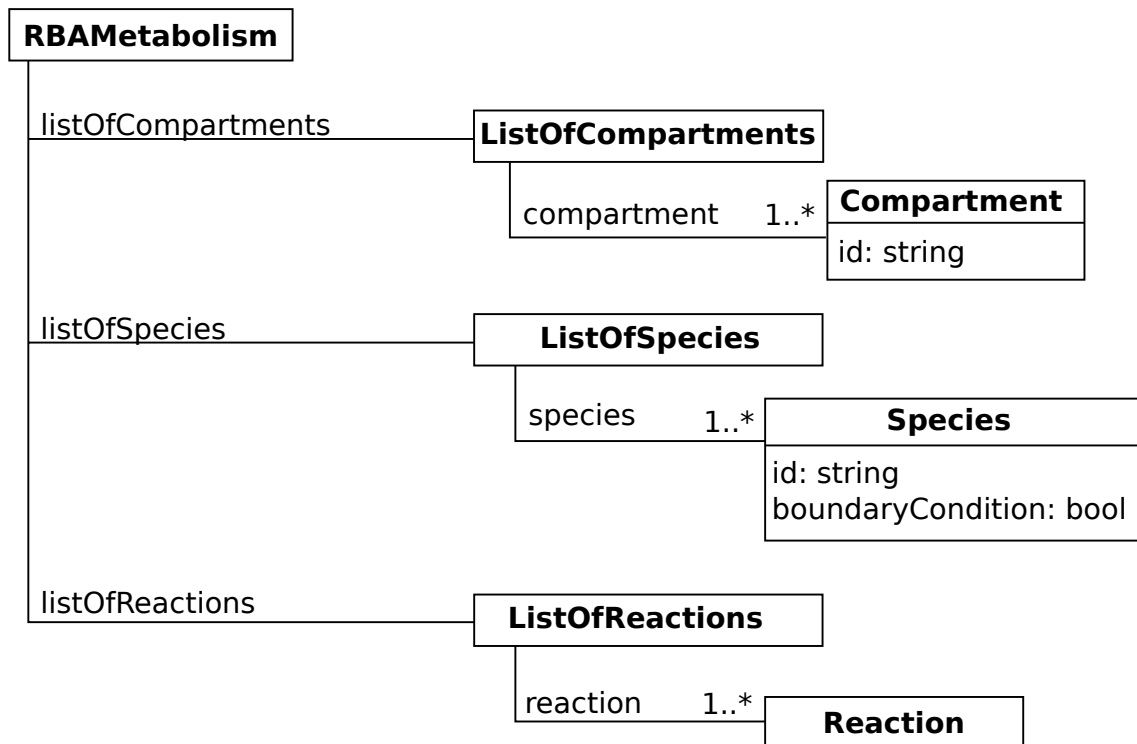
Figure 1: XML structure of metabolism document.

3.1.2 Compartment

The **Compartment** class is used to list existing cell compartments.

The *id* attribute   The **id** attribute is a string defining the identifier of a compartment.

3.1.3 Species

The **Species** class is used to list *metabolic* species.

The *id* attribute   The **id** attribute is a string defining the identifier of a metabolite.

The *boundaryCondition* attribute   The **boundaryCondition** attribute is a boolean. If the attribute is set to true, the metabolite is considered to be at a constant concentration. In other words, it is not affected by reactions. This is typical for metabolites in the external medium.
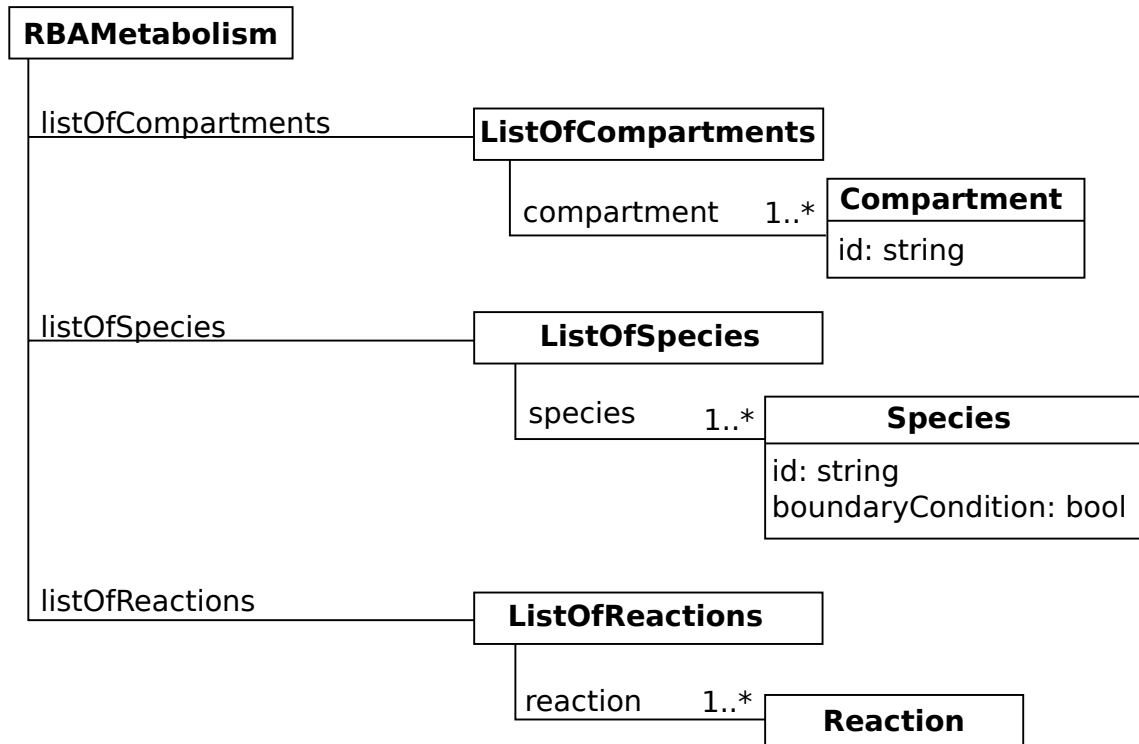
Figure 2: XML structure of metabolism document.

4 parameters.xml

4.1 RBAMetabolism container

The metabolism file is strongly inspired by SBML. More precisely, it is a subpart of an SBML file.

4.1.1 RBAMetabolism

The outermost portion of the metabolism file is an instance of class **RBAMetabolism**, shown in Figure 2.

Currently, **RBAMetabolism** has no simple attributes. It includes exactly one instance of **ListOf** container classes. All **ListOf** classes do not have own attributes, they are merely used to organize a list of instances from another class. This organization was inspired by SBML.

4.1.2 Compartment

The **Compartment** class is used to list existing cell compartments.

The *id* attribute   The **id** attribute is a string defining the identifier of a compartment.

5

4.1.3 Species

The **Species** class is used to list *metabolic* species.

The *id* attribute　　The **id** attribute is a string defining the identifier of a metabolite.

The *boundaryCondition* attribute　　The **boundaryCondition** attribute is a boolean. If the attribute is set to true, the metabolite is considered to be at a constant concentration. In other words, it is not affected by reactions. This is typical for metabolites in the external medium.