

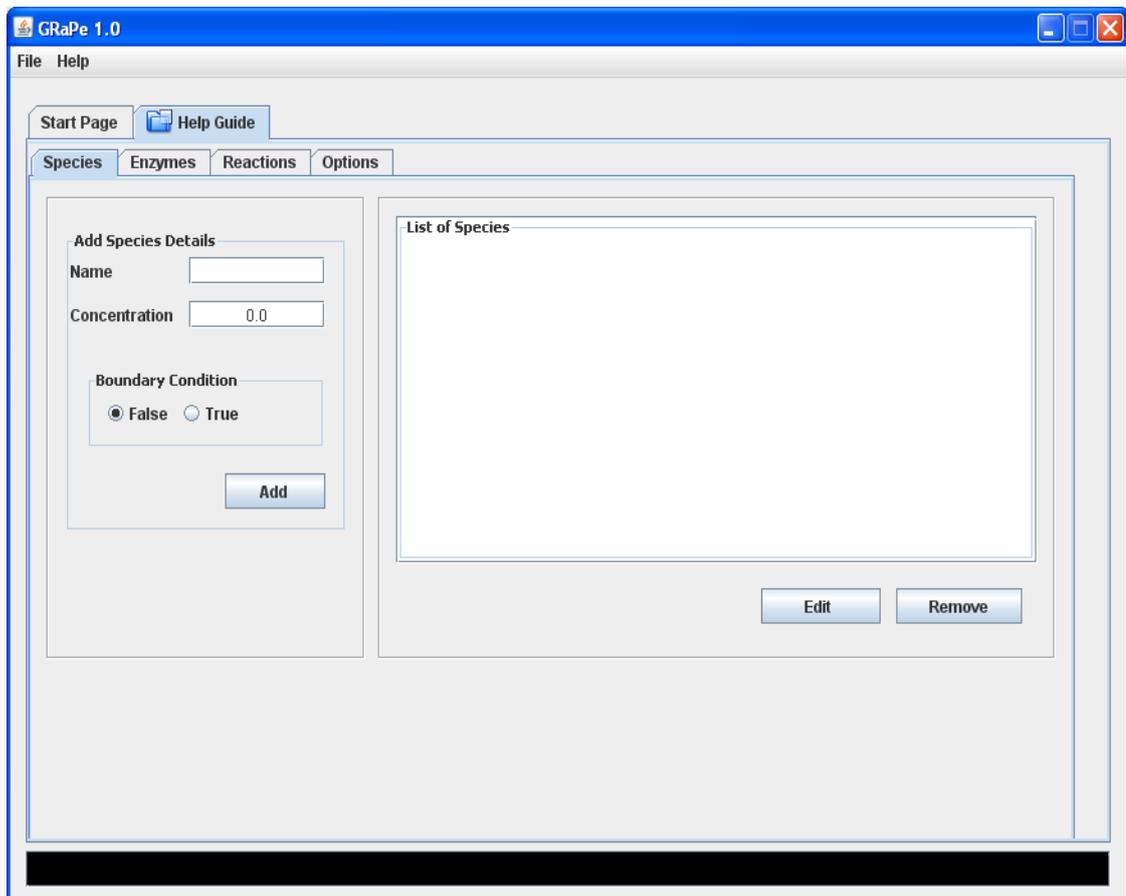
Building A New Model

Models can be constructed using GRaPe in two ways.

1. Building from scratch
2. Importing an SBML document

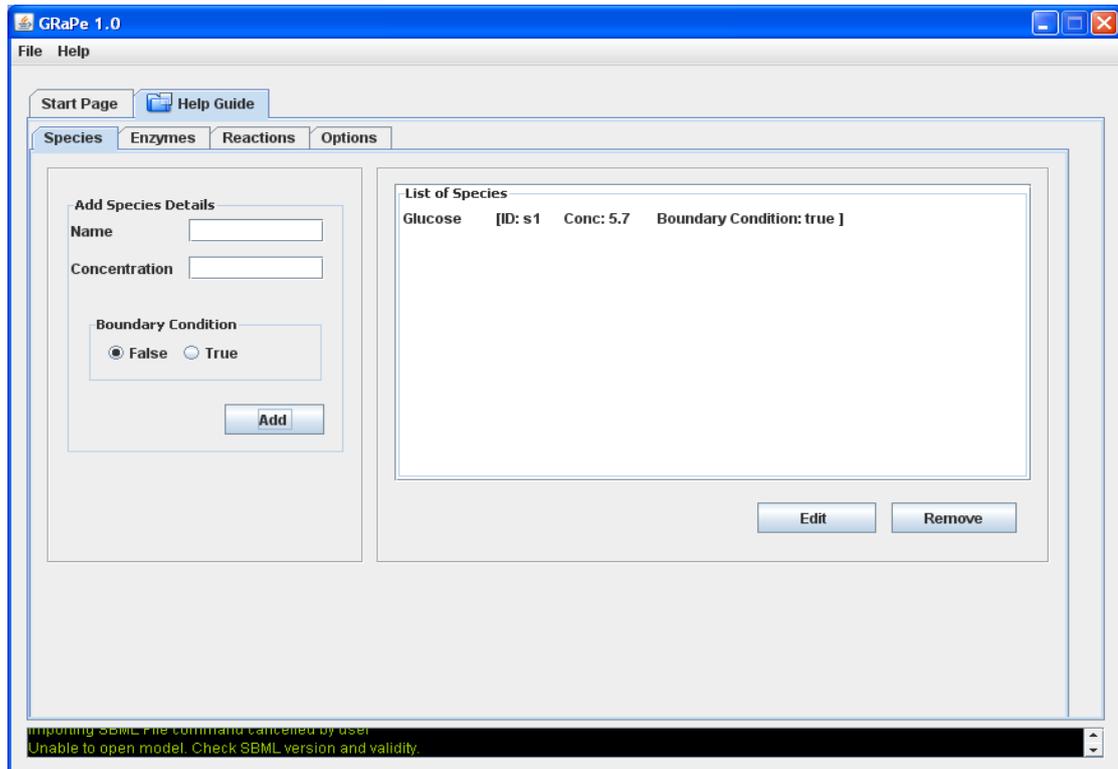
Building from scratch

- Go to “File” -> New
- Type in the name of model then -> “OK”
- A new set of tabs appear (below)
- Use the “Species” tab to add, edit or remove species (metabolites and cofactors in the model)
- Use the “Enzyme” tab to add/edit/remove enzymes (proteins species) in the model
- The “Reaction” tab enables the construction of model reactions
- The “Option” tab provides methods for parameter estimation and also to save the model for simulation.



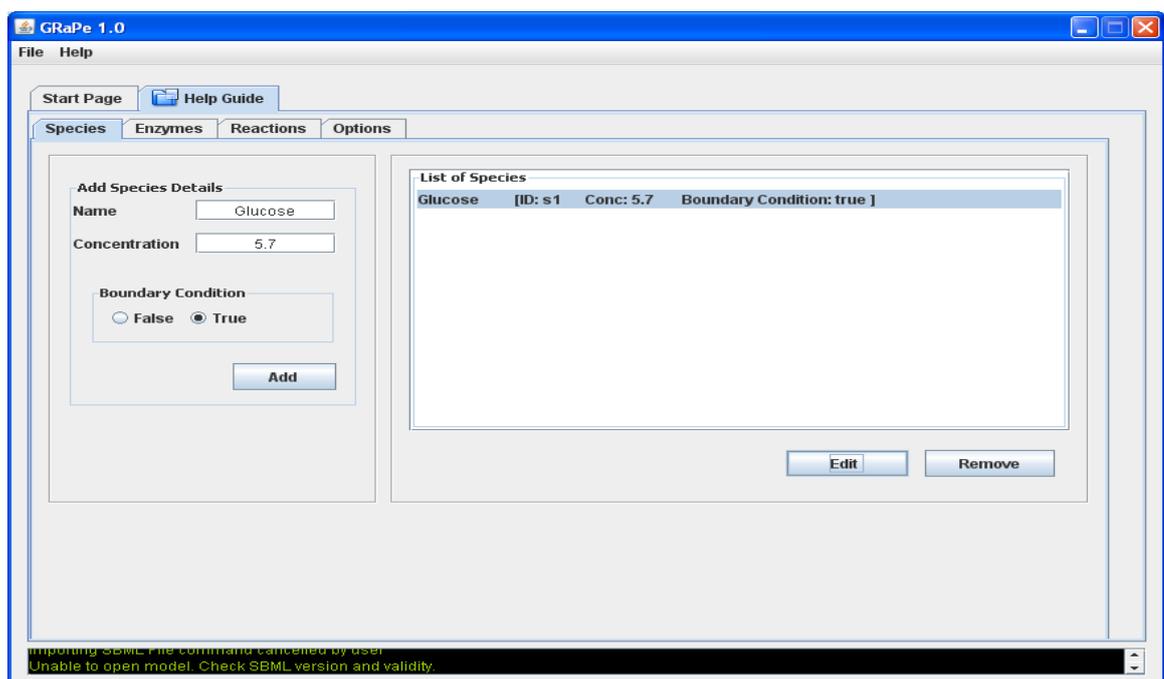
Adding/Editing/Removing Species

- **To Add a species;** from the “Species” tab, enter in the species name, concentration and select its boundary condition then -> “Add”. The boundary condition (BC) is a restriction imposed on a species specifying that its quantity is not determined by the set of reactions but by external constraints. When BC is set to true for a species, its concentration value remains the same as the value specified in the input data.



The newly added species is added to the model and displayed on the “List of Species” canvas

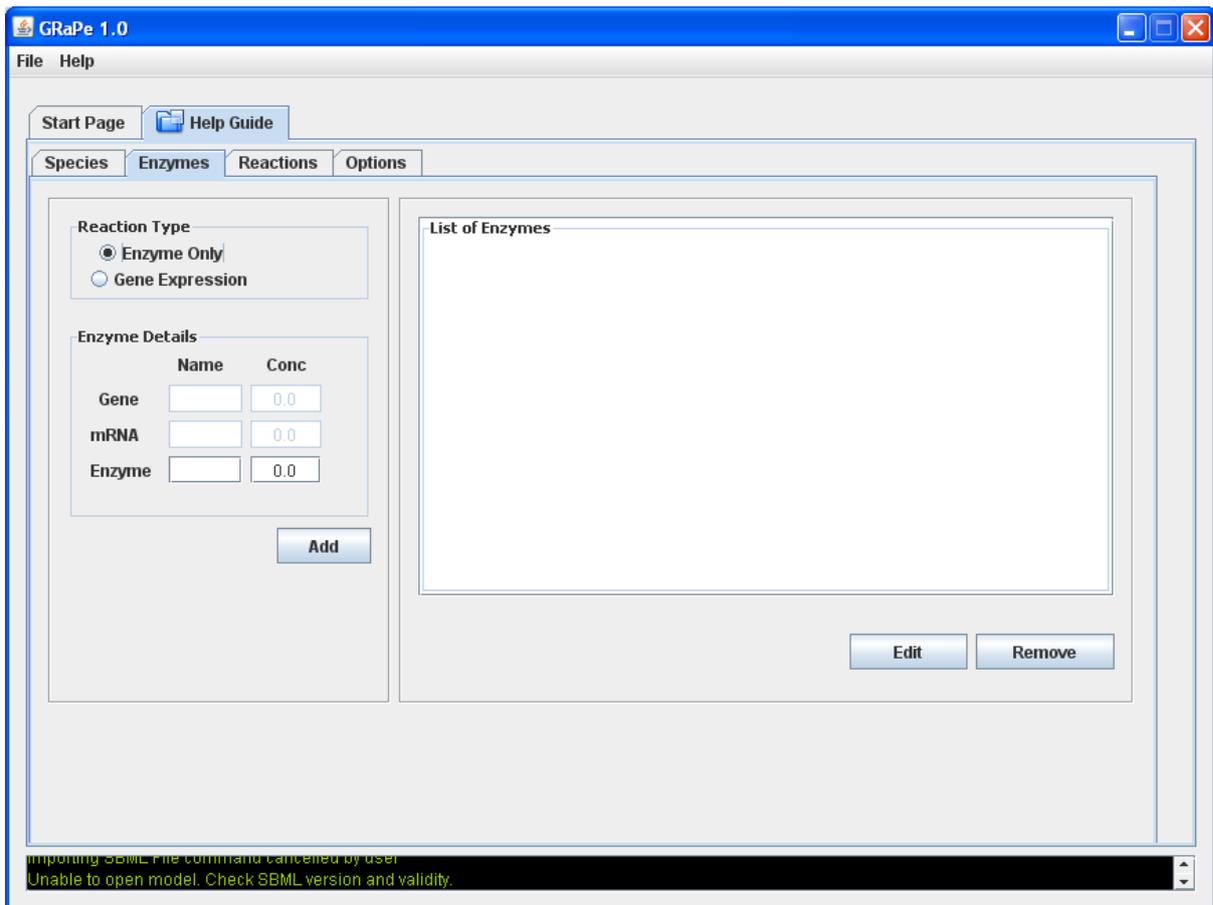
- **To edit** a species, select the species and click -> “Edit”



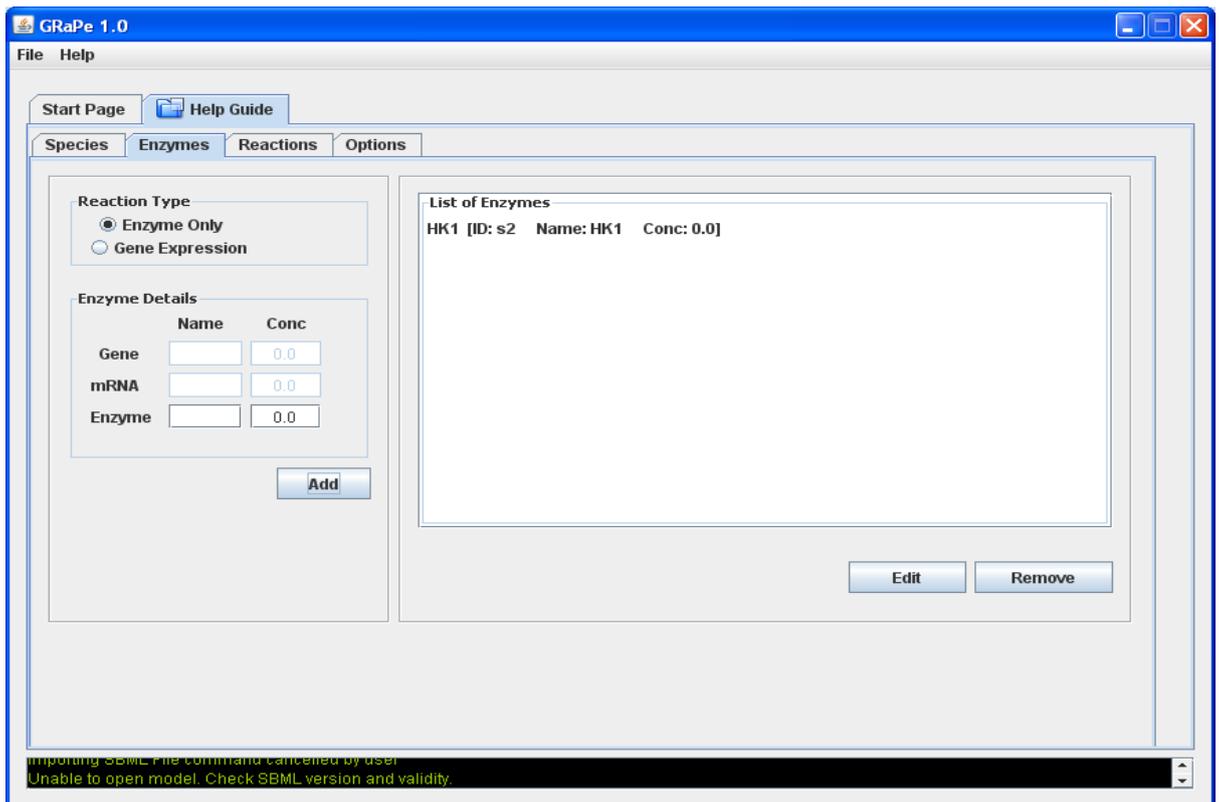
- After editing, click -> “Add” to add the species back to the list. NOTE: The species ID does not change after editing.
- **To remove a species;** select the species and click -> “Remove”. The species is removed from the model and on-screen list.

Adding/Editing/Removing Enzymes

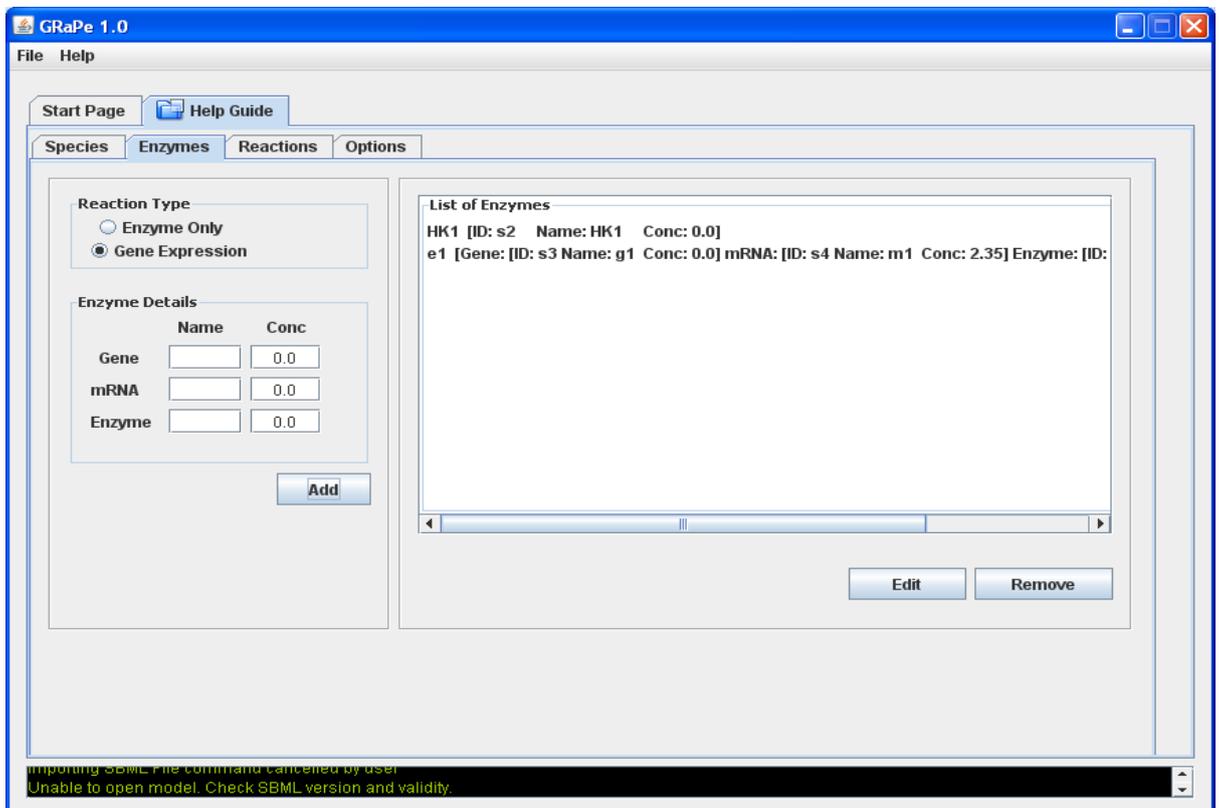
- From the “Enzymes” tab, choose whether to add the gene expression for the reaction or just the enzyme species (when the gene expression process is unknown).



- **If only the enzyme** is to be added. Simply select “Enzyme Only”
- Enter the enzyme’s name and concentration and click -> “Add”

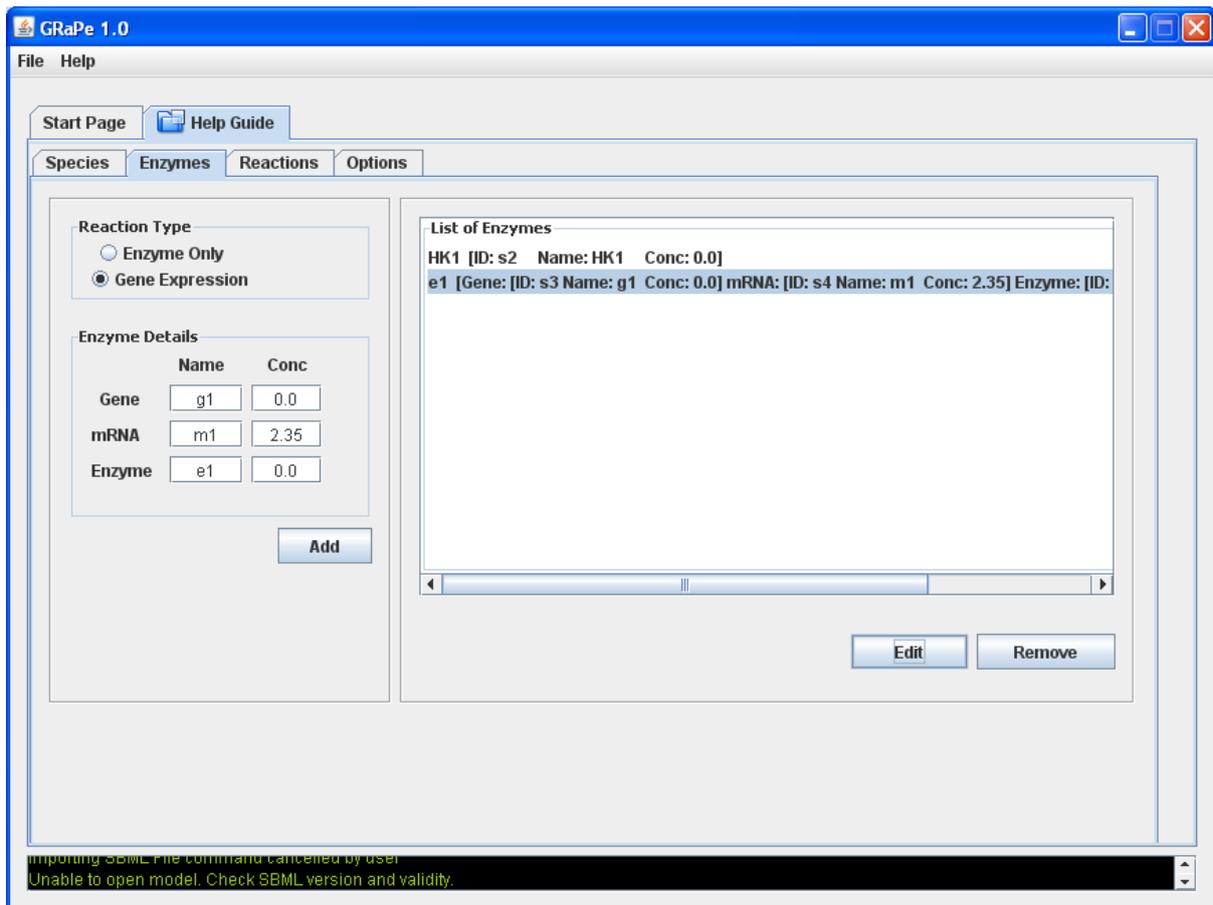


- **To enter the gene expression** for a reaction
- Select “Gene Expression”, enter the names and concentration amounts of the gene(s), mRNA and enzyme species then click-> “Add”
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- **To edit the enzyme or gene expression species**, simply select the enzyme/gene expression species and click -> “Edit”.
- Once editing is complete, click “Add” to add the enzyme/gene expression back.

- **To remove an enzyme or gene expression species**, select the enzyme/gene expression species and click ->”Remove”.

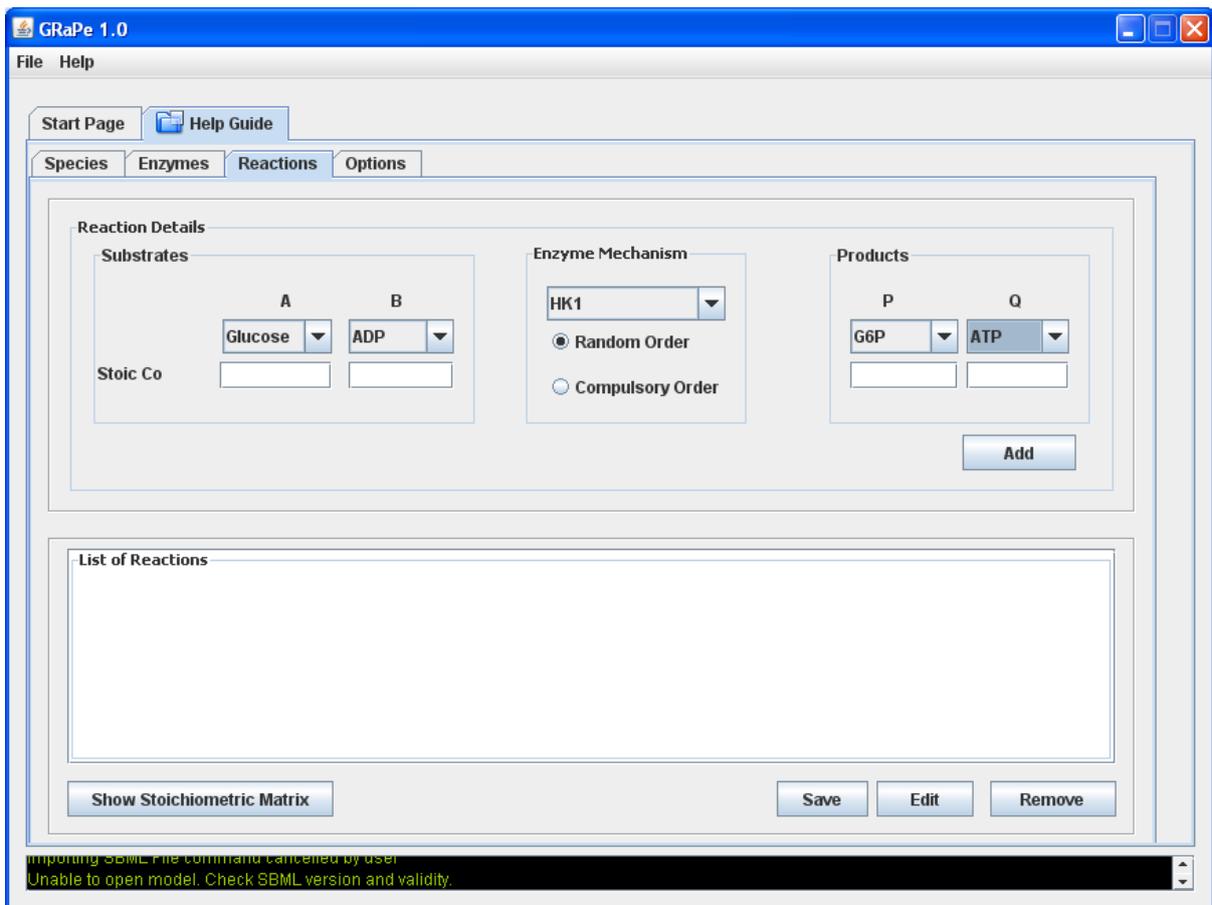


Construction a reaction

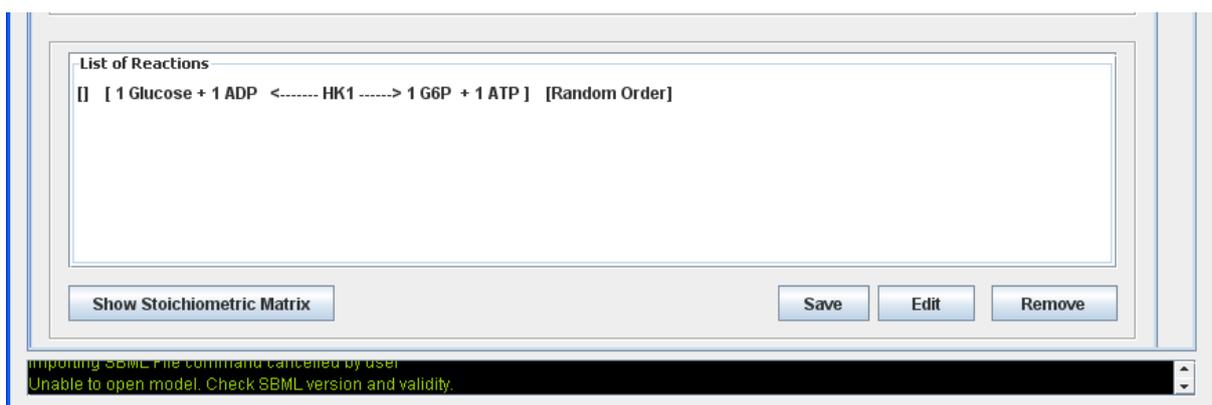
- From the “Reaction” tab, there are five (5) combo boxes. The first 2 allows for the addition of substrates and the last 2 enables the addition of products to a reaction. The middle one allows the user to select the enzyme/gene expression species for the reaction.

NOTE: A reaction MUST have an enzyme species/gene expression.

- The user must also specify the type of enzyme mechanism for the reaction. The default selection is “Random order” mechanism. (example below)

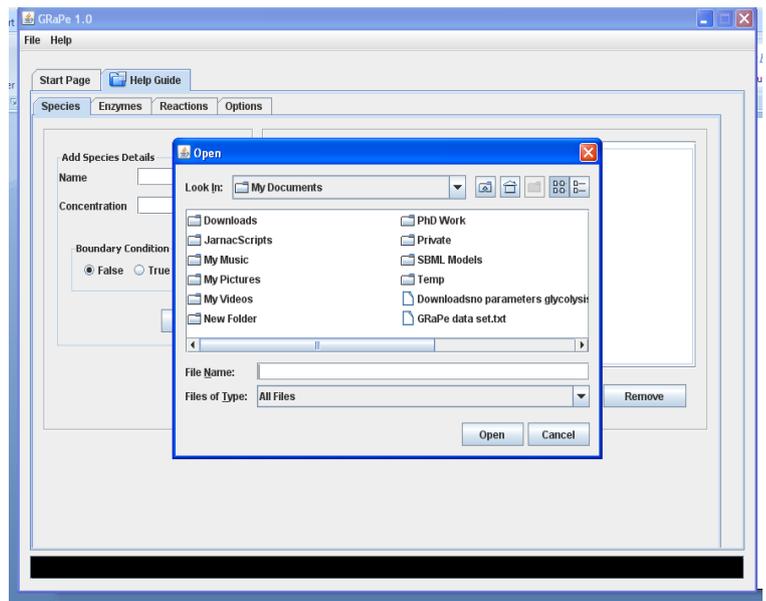


- Once the substrates, products and enzymes have been selected using the combo boxes simply click -> “Add” to add the reaction to the model. (below)

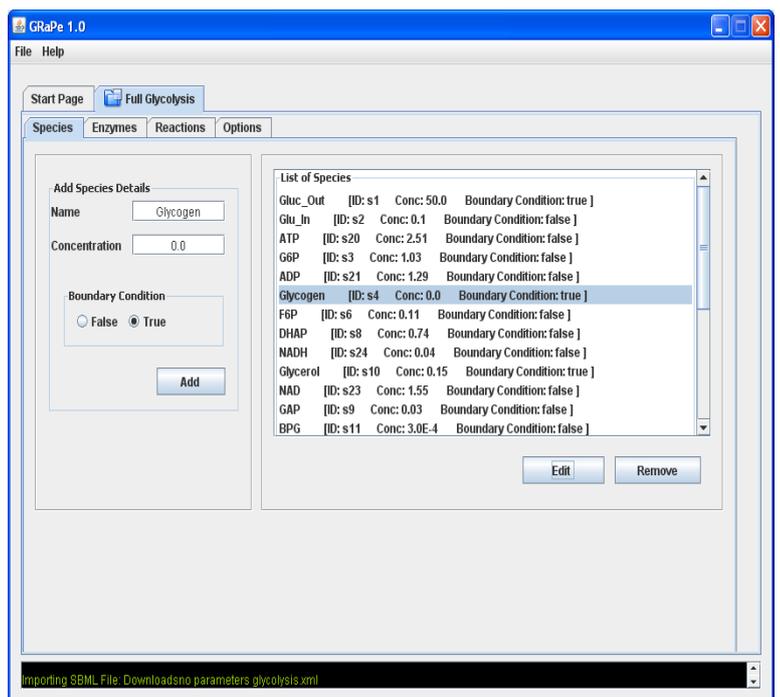


Importing an SBML document

- Go to “File” -> “Open File”
- Select the file (in SBML) and click -> “Open”



- Again, the model appears as a list of tabs and provides functionalities for editing the model.
- The “Species” tab list all species in the model
- The “Enzyme” tab lists all enzymes (proteins species in the model)
- The “Reaction” tab contains a list of all reactions
- The “Options” tab provides methods for parameter estimation



- **To edit a species/enzyme/reaction**, simply select the entity and click -> “Edit”.
- After editing, click on -> “Add” to add them back
- **To remove a species/enzyme/reaction**, simply select the appropriate entity and click -> “Remove”. GPaPe allows for multiple deletion of species (metabolites), enzymes and reactions

