

Dynamically Changing Volumes

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Changing Volumes

- ▶ What do we preserve during simulation?
 - ▶ Concentration
 - ▶ Substance
- ▶ What is constant if boundaryCondition = “true”?
 - ▶ Concentration
 - ▶ Substance

Changing Volumes (continued)

► Concentration derivative

$$\begin{aligned}d[A]/dt &= d(A/V)/dt \\ &= 1/V \, dA/dt - A/V^2 \, dV/dt \\ &= 1/V (dA/dt - [A]dV/dt)\end{aligned}$$

Determined by yield,
stoichiometry, and kinetic
laws

Not known for assignments

Different Cases

constant value	boundaryCondition value	can have assignment or rate rule	can be reactant or product	species' quantity can be changed by
true	true	no	yes	(never changes)
false	true	yes	yes	rules and events
true	false	no	no	(never changes)
false	false	yes	yes	reactions <i>or</i> rules (but not both), and events

Determined by:

Constant	Boundary	Rate	Assign	Reaction	none
true	true	NA	NA	NA	???
false	true	flag	flag	NA	???
true	false	NA	NA	NA	???
false	false	flag	flag	substance	???

Some Thoughts

- ▶ We can not use the `hasOnlySubstanceUnits` flag as this would force a complete rewrite of kinetic laws just to keep the substance fix in traditional models.
- ▶ Check whether `initialAmount` or `initialConcentration` is given and keep that value fix.
- ▶ Introduce a new flag.
- ▶ Restrict to substance to avoid changes in the SBML schema.