Numerical methods

Amount of the substance

Huge differences between valid concentration values leads to numerical instability of substance accumulation.

$$der(n) = q$$

(1) Accumulated molar flow of the substance with tolerance based on n

The same mathematical expression of the equation (1) can be designed with substitution of "ln = log(n)":

$$der(ln) = \frac{q}{n}$$
$$n = e^{ln}$$

(2) Accumulated molar flow of the substance with tolerance based on ln=log(n)

Expressions (1) and (2) are mathematically the same, but numerically different. Especially, very small concentrations of substances need to have numerical tolerance based on logarithm (2), otherwise ratio between computed value by (1) and correct result can grow up to multiple orders of magnitude. The situations where concentration (mass or amount of substance) fall below typical values of numerical tolerances are in chemistry very common e.g., hormones or equilibria where almost all substrates are converted into products.

Even accumulation in different quantities could lead to the same tolerance. E.g. mass accumulation $der(m) = q_m$, where $m = MM \cdot n$ and MM is molar mass of the substance.

$$der(ln) = \frac{q_m}{m} = \frac{MM \cdot q}{MM \cdot n} = \frac{q}{n}$$
$$m = MM \cdot e^{ln}$$

(3) Accumulated mass flow of the substance with the same tolerance based on ln=log(n)

Chemical inertia of directional flow

As amount of substance also the flows can reach very huge and also very small values.

$$der(q) \cdot L = \Delta r$$

(4) Chemical inertial acceleration with tolerance based on q

The same mathematical expression of the equation (4) can be designed with substitution lq=log(q)

$$der(lq) = \frac{\Delta r}{L \cdot q}$$
$$q = e^{lq}$$

(5) Chemical inertial acceleration with tolerance based on log(q)

However, the flow must be non-zero and positive. So, the user must define these components as directional allowing flow only in forward direction. As initial value we can't set zero, but a number very close to zero. Default initial lq=log(Modelica.Constants.small)/2 caused the flow small enough to be unsignificant for chemical processes and be still representable until value log(Modelica.Constants.small) (e.g. if lq = log(1e-60)/2 = -69 then q = 1e-30 mol/s with representable limits of lq=-138,q=1e-60 mol/s and lq=138,q=1e60 mol/s).

Please note that one mole of substance contains 6.02214076e23 particles (Avogadro's constant). Having positive flow less than 1e-30 mol/s means lower flow than 1 particle per second. And this flow is still representable, significant and inside tolerances of numerical calculation.