

Reversible reaction simulation for simple carbon fixation

My aim was to introduce reversible reactions to the code written by the summer student. Previous attempts to encode reversible reactions seemed to lead to crashes. The results below indicate that the simulation works in principle and that the reversibility of the reactions *per se* does not cause a crash. The simulations of forward reactions (in black) yield plots very similar to simulations of reversible reactions with negligibly small backward reaction rates (in red). The plots below show that when the backward reaction is 10^2 times slower than its forward counterpart, slight differences in the simulation results could be observed, particularly for CO and acetic acid. When the rate of the forward reaction was 10^3 times greater than the backward reaction rate, there was virtually no difference between the unidirectional and reversible simulations. However, when forward and backward reaction rates are equal (in blue), the simulation is truncated early and an error message is displayed, **negative propensity function - coersing to zero**. In other words, we sometimes observe negative values *e.g.* for formaldehyde, methanol, CO , acetate, H_2O . In some simulations, the number of CO_2 and H_2 molecules surpasses the initial input values. This could be caused both by the low numbers of chemical species and by the fact that certain reactants are depleted (and/or replenished) by multiple reactions. Possible solutions would include adjusting the time-step or the relative magnitude of the forward and backward reaction rates to push the system away from chemical equilibrium. *Note that not all features described here might be seen in the plots below, as every simulation yields slightly different results.*

Reactions, Parameters, and Conditions

The reactions and parameters used in the simulations are summarised below:

| Forward reactions | Parameters |
|----------------------------|---------------|
| $k_1 * CO_2 * H_2$ | $k_1 = 10$ |
| $k_2 * formic\ acid * H_2$ | $k_2 = 19.9$ |
| $k_3 * formaldehyde * H_2$ | $k_3 = 23.5$ |
| $k_4 * methanol * CO$ | $k_4 = 0.869$ |
| $k_5 * CO_2 * H_2$ | $k_5 = 0.061$ |
| $20 * formic\ acid$ | |

Conditions kept constant across simulations:

- initial reactants numbers: $CO_2 = H_2 = 500\ mol$
- timestep size: $tf = 0.0005$



