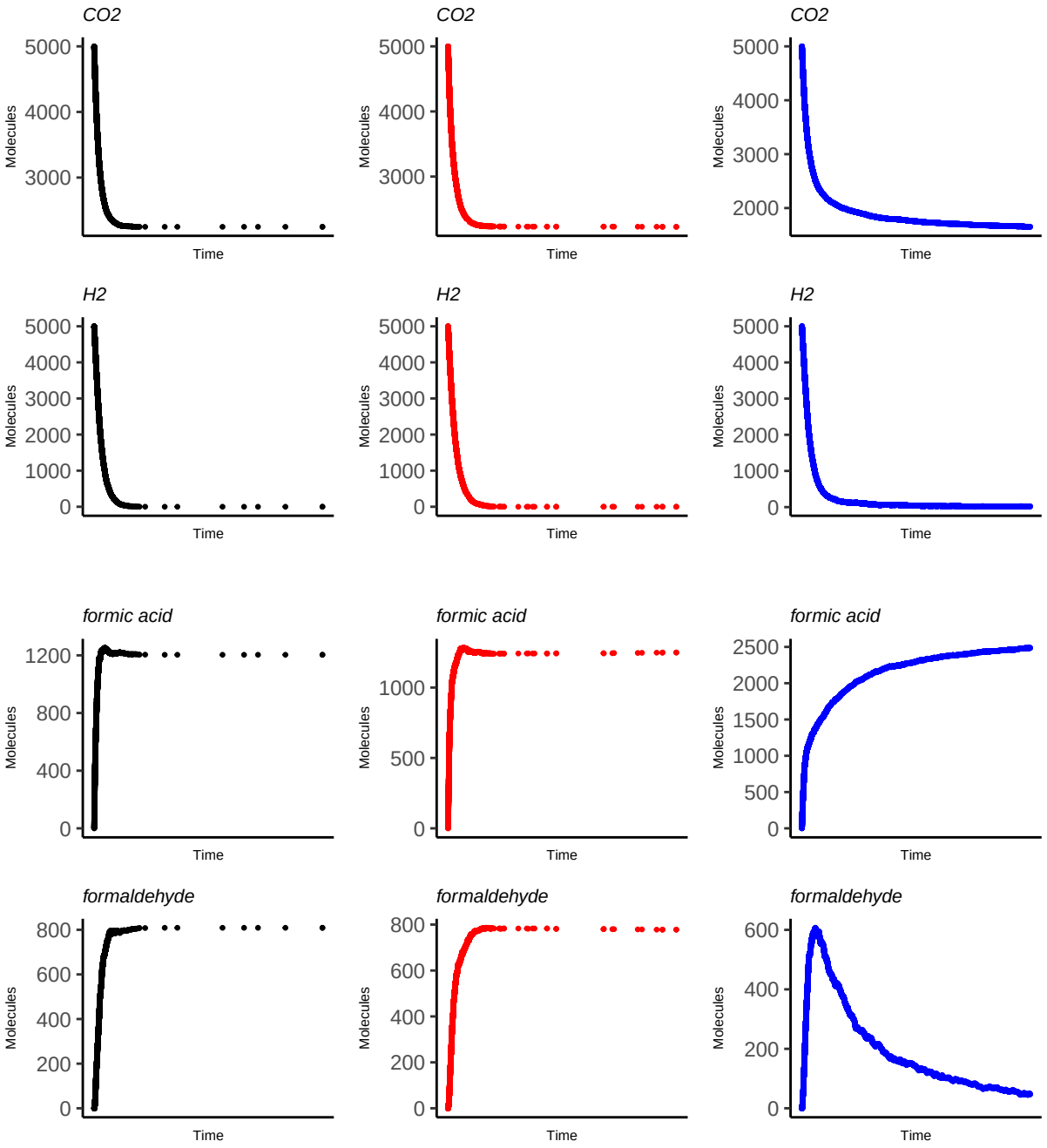
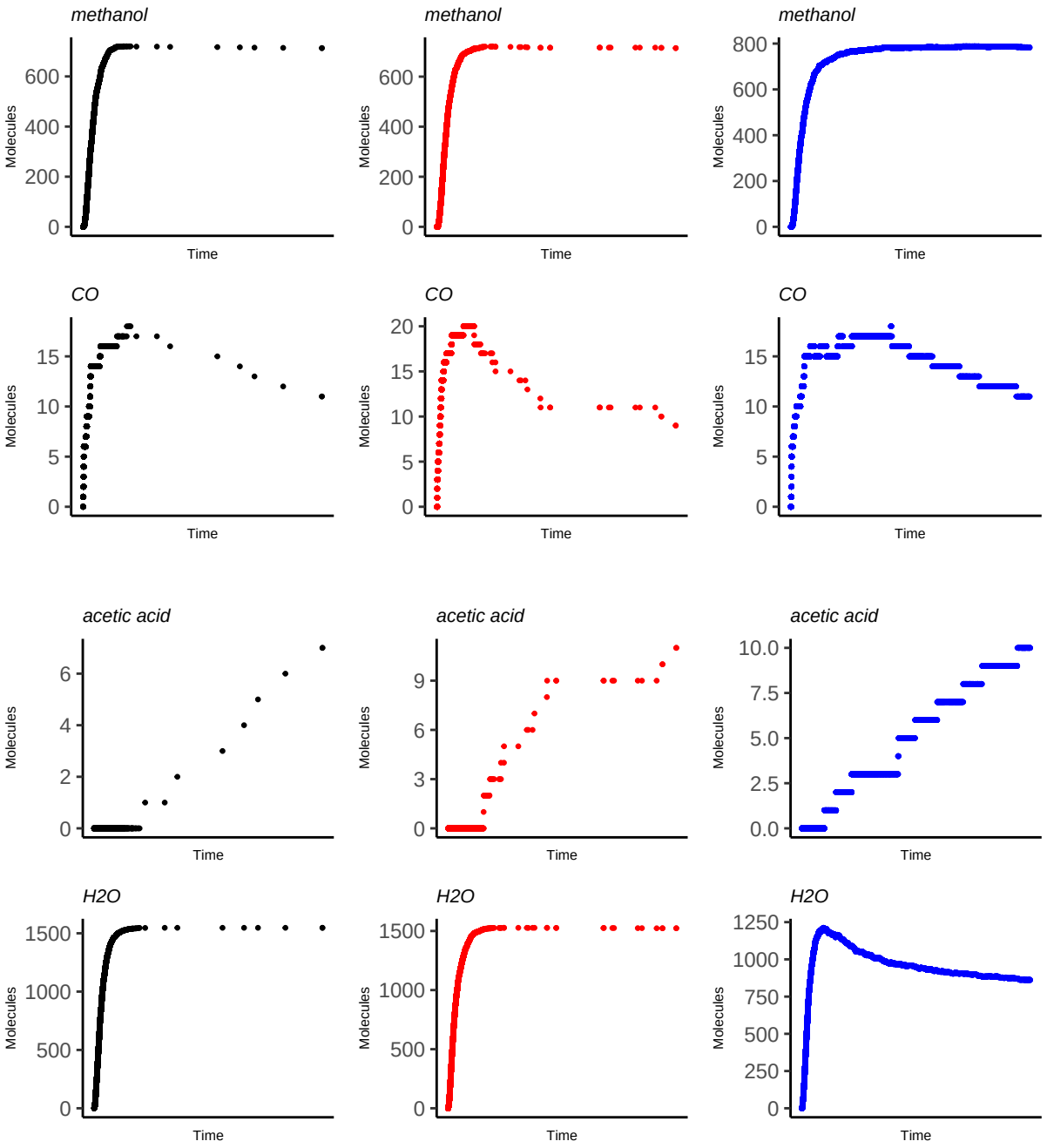
Comparing simulations of irreversible and reversible CO_2 fixation reactions (simplified CO_2 fixation)

The output on the next page is generated after manually tweaking Lia's CO2 fixation simulation from the summer. The original simulation is the irreversible CO2 fixation network (output in **black**). In **red**, reversible reactions with negligible backward rates yield simulations which are very similar to the irreversible reaction simulations. In **blue**, the reversible reactions with equal forward and backward reaction rates result in a distinct trajectory.

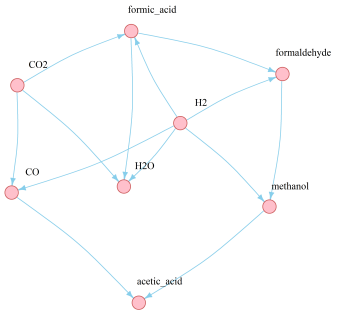
Forward reactants	Forward products	Propensity function	Parameters
$CO_2,\ H_2$	$formic\ acid$	$k_1 * CO_2 * H_2$	$k_1 = 10$
$formic\ acid,\ H_2$	$formaldehyde,\ H2O$	$k_2 * formic\ acid * H_2$	$k_2 = 19.9$
$formaldehyde,\ H_2$	$methanol$	$k_3 * formaldehyde * H_2$	$k_3 = 23.5$
$methanol,\ CO$	$acetic\ acid$	$k_4 * methanol * CO$	$k_4 = 0.869$
$CO_2,\ H_2$	$CO,\ H_2$	$k_5 * CO_2 * H_2$	$k_5 = 0.061$

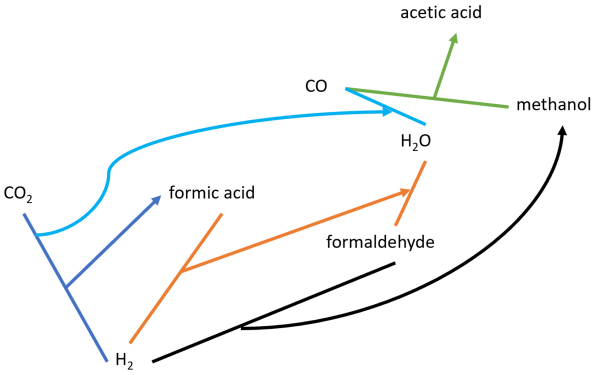

CO2
CO2
CO2
H2
H2
H2
formic acid
formic acid
formic acid
formaldehyde
formaldehyde
formaldehyde
Molecules
Time

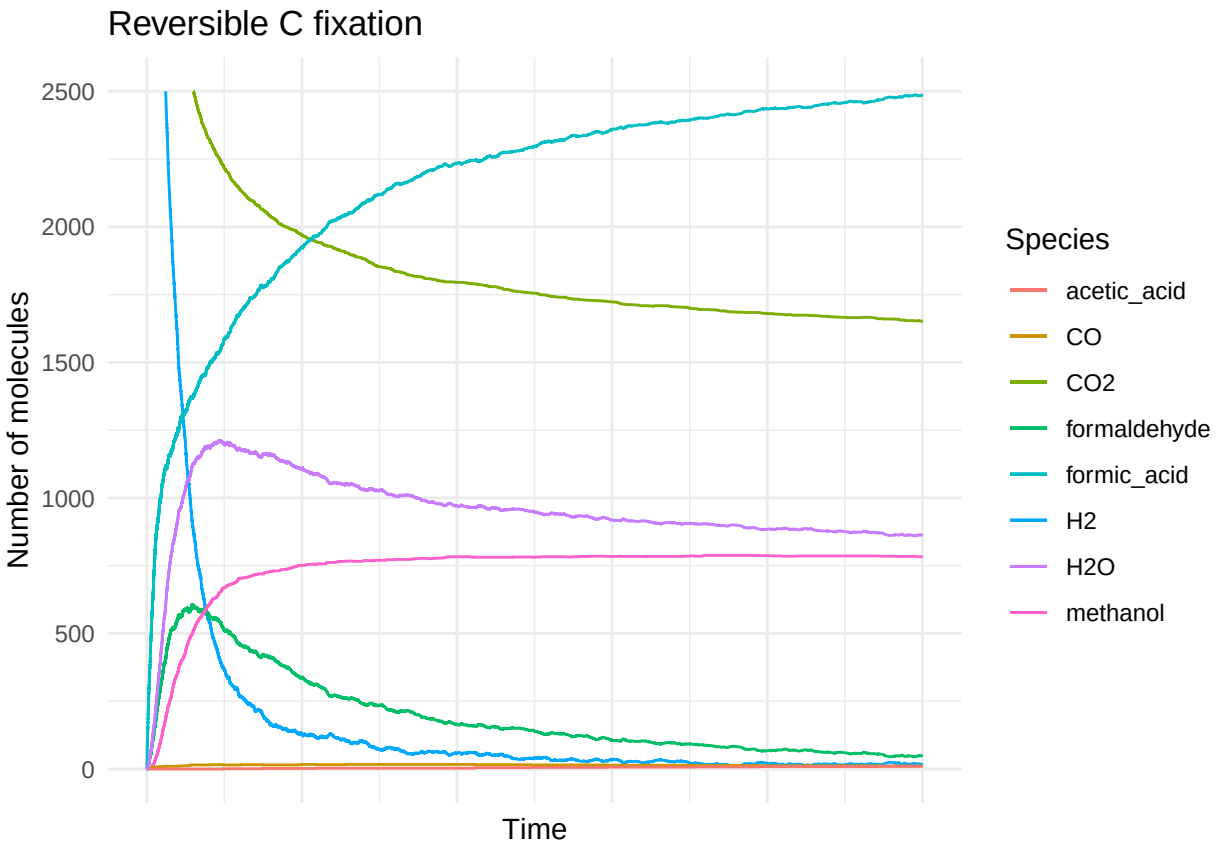

methanol
methanol
methanol
CO
CO
CO
acetic acid
acetic acid
acetic acid
H2O
H2O
H2O
Molecules
Time
0
200
400
600
800
5
10
15
20
2
4
6
9
0.0
2.5
5.0
7.5
10.0
500
1000
1250
750
250

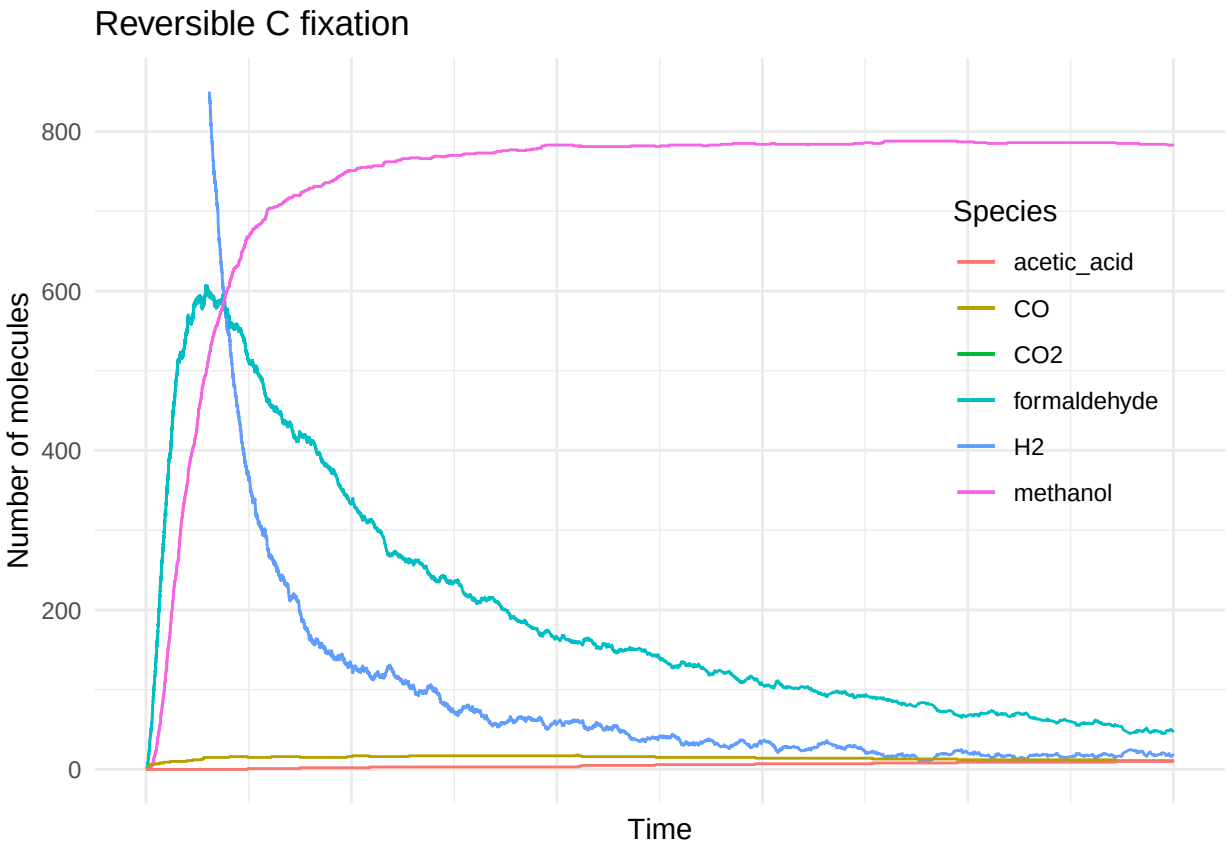
Inspecting the reversible network

The network diagram below shows the relationship between the differrent reactants and products.

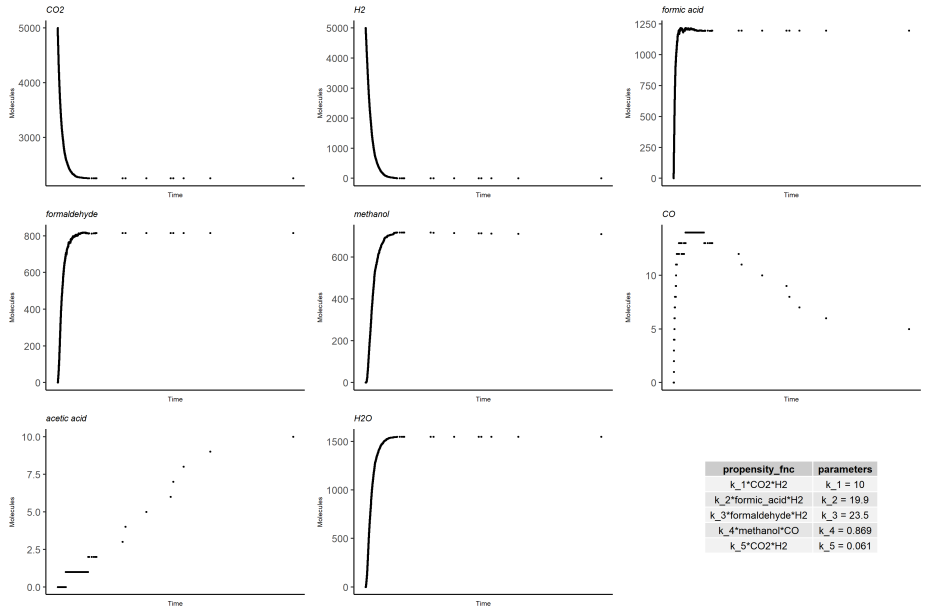




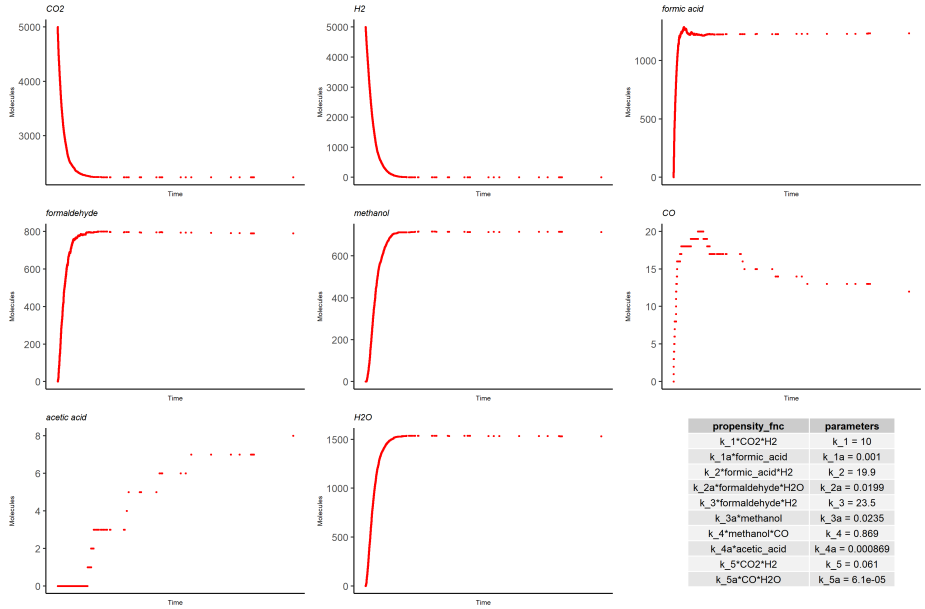



Reversible C fixation
Number of molecules
800
600
400
200
0
Time
Species
acetic_acid
CO
CO2
formaldehyde
H2
methanol

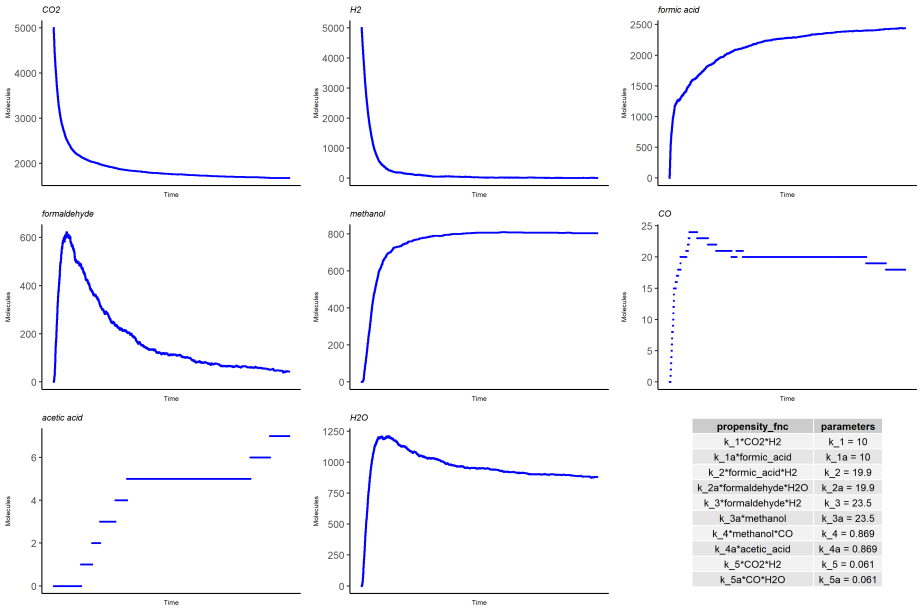
Compare to Lia's simulations



propensity_fnc	parameters
k_1*CO2*H2	k_1 = 10
k_2*formic_acid*H2	k_2 = 19.9
k_3*formaldehyde*H2	k_3 = 23.5
k_4*methanol*CO	k_4 = 0.869
k_5*CO2*H2	k_5 = 0.061



propensity_fnc	parameters
k_1*CO2*H2	k_1 = 10
k_1a*formic_acid	k_1a = 0.001
k_2*formic_acid*H2	k_2 = 19.9
k_2a*formaldehyde*H2O	k_2a = 0.0199
k_3*formaldehyde*H2	k_3 = 23.5
k_3a*methanol	k_3a = 0.0235
k_4*methanol*CO	k_4 = 0.869
k_4a*acetic_acid	k_4a = 0.000869
k_5*CO2*H2	k_5 = 0.061
k_5a*CO*H2O	k_5a = 6.1e-05



propensity_fnc	parameters
k_1*CO2*H2	k_1 = 10
k_1a*formic_acid	k_1a = 10
k_2*formic_acid*H2	k_2 = 19.9
k_2a*formaldehyde*H2O	k_2a = 19.9
k_3*formaldehyde*H2	k_3 = 23.5
k_3a*methanol	k_3a = 23.5
k_4*methanol*CO	k_4 = 0.869
k_4a*acetic_acid	k_4a = 0.869
k_5*CO2*H2	k_5 = 0.061
k_5a*CO*H2O	k_5a = 0.061