

New parameters (N³) and Formelherstellung (8/17/09)

The state equation stays the same:

$$\frac{dC_{iv}^j}{dt} = k_{fi} k_{fadj} [C_{im}^j] S_v - k_{bi} \cdot k_{badj} \cdot C_{iv}^j$$

forward:

Unsaturation forward:

$$un_f = 2^{stdev(un_v)}$$

Charge Forward

$$ch_f = 50^{-|\overline{ch_v} \cdot ch_m|}$$

Curvature Forward

$$cu_f = 10^{stdev(|\log(cu_v)|)}$$

Length Forward

$$l_f = 3^{stdev(l_v)}$$

Complex Formation 1 (CF1; formerly umbrella)

$$CF1_f = 1$$

$$k_{fadj} = un_f \cdot ch_f \cdot cu_f \cdot l_f \cdot CF1_f$$

backward:

unsaturation backward:

$$un_b = 10^{|3.5^{-un_v} - 3.5^{-un_m}|}$$

Charge backward:

$$ch_b = 50^{-|\overline{ch_v} \cdot ch_m|}$$

Curvature backward



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$$cub = 10^{\left| |cu_v-1| - |cu_m-1| \right|}$$

Length backward

$$lb = 3.2^{\left| \bar{l}_v - l_m \right|}$$

Complex Formation 1 (CF1) backward

$$CF1_b = 1.5^{(CF1_v \cdot CF1_m - |CF1_v \cdot CF1_m|)}$$

$$k_{badj} = un_b \cdot ch_b \cdot cub \cdot lb \cdot CF1_b$$

The starting parameters ($k_f = M^{-1}s^{-1}$; $k_b = s^{-1}$)

PC:	$k_f = 3.7 \times 10^6$;	$k_b = 2 \times 10^{-5}$
PE:	$k_f = 2.3 \times 10^6$;	$k_b = 1 \times 10^{-5}$
PS:	$k_f = 3.7 \times 10^6$;	$k_b = 1.25 \times 10^{-5}$
SM:	$k_f = 3.7 \times 10^6$;	$k_b = 3.1 \times 10^{-3} s^{-1}$
CHOL:	$k_f = 5 \times 10^8$;	$k_b = 2.8 \times 10^{-4}$

k_f (PC) taken from Nichols85; **weakness**: NBD-PC; no unlabeled k+ found.

k_f (PE) taken from Abreu04; **NBD-PE**

k_f (PS) and k_f (SM) assumed same as k_f (PC)

k_f (CHOL) is **weak** – basically guessed from k_f (NBD-lysoPE) in Sampaio05 and k_f (PC); try adjustments, probably decrease

k_b (PC) is taken from Wimley90 – radioactive label; LUV, 30° C.

Then, Nichols82 with C6-NBD-PC and other headgroups was used to determine *ratios* of k_b (PC) with other headgroups, and k_b for other headgroups assigned accordingly. k_b (PS) was assumed to be the same as k_b (PG) given by Nichols82 (also ratio from k_b (PC)).

k_b (SM) is taken from k_b (PC) of Wimley90 (radioactive), and then a ratio of k_b (PC)/ k_b (SM) taken from Bai97: = 34/2.2 = 15.45; $2.0 \times 10^{-4} \times 15.45 = 3.1 \times 10^{-3} s^{-1}$.

k_b (CHOL) taken from Jones90 (radioactive; POPC LUV; 37°).

Curvature:

$$PE = 0.8; CHOL = 0.8$$

Charge:

$$PS = -1$$

CF1

SM = 3; PC = 2; CHOL = -1

Initial concentrations:

1×10^{-10} M; gamma distributed with stdev = 10^{-10}