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

The state equation stays the same:

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

forward:

Unsaturation forward:

$$un_f = 2^{[1+stdev(un_v)]}$$

Charge Forward

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

Curvature Forward

$$cu_f = 3^{stdev(\left|cu_v - 1\right|)}$$

Length Forward

$$l_f = 3^{[1+stdev(l_v)]}$$

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:

$$un_b = 10^{\left|3.5^{-\overline{un_v}} - 3.5^{-un_m}\right|}$$

Charge backward:

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

Curvature backward

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

Length backward

$$l_b = 3.2^{|\bar{l}_v - l_m|}$$

Complex Formation 1 (CF1) backward

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

$$k_{badj} = un_b \cdot ch_b \cdot cu_b \cdot l_b \cdot CF1_b$$

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; 2.0×10^{-4} x 15.45 = 3.1×10^{-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 x 10^{-10} M; gamma distributed with stdev = 10^{-10}