

$X_i = X_{i-1} + k_d \, C_{A_0} \left((1 - X_{i-1})^2 - X_{i-1}^2 / k_e ight) \Delta t$

$$-r_A = k_d \left(C_{A0}^{\alpha+\beta} (1-X)^{\alpha} (\theta_B - X)^{\beta} - \frac{C_{A0}^2 X^2}{K_e} \right)$$

 $rac{\mathrm{d}X}{\mathrm{d}V} = rac{-r_A}{F_{A\,0}}$