2. Reverse Catalytic Model

$$S \underset{\sigma}{\overset{\lambda(t)}{\rightleftharpoons}} P$$

$S + P = 1$

$S = 1 - P$

Part 1 – $\lambda(t)$ is some function of 't' – no assumptions made.

$$\frac{dP}{dt} = \lambda(t) S - \sigma P$$

$$= \lambda(t)(1-P) - \sigma P$$

$$= \lambda(t) - \lambda(t)P - \sigma P$$

$$= \lambda(t) - P(\lambda(t) - \sigma)$$

$$\frac{dP}{dt} + (\lambda(t) - \sigma)P = \lambda(t)$$

integrating factor $\mu(t) = e^{\int (\lambda(t) - \sigma)\,dt}$

or $= e^{\int_0^t \lambda(t)\,dt - \sigma t}$

Multiply both sides by integrating factor.

$$\frac{dP}{dt} e^{\int_0^t \lambda(t) - \sigma \, dt} + (\lambda(t) - \sigma) P e^{\int_0^t \lambda(t) - \sigma \, dt} = \lambda(t) e^{\int_0^t \lambda(t) - \sigma \, dt}$$

Simplify LHS. using product rule trick.

$$\frac{d}{dt}\left(P e^{\int_0^t \lambda(t) - \sigma \, dt}\right) = \lambda(t) e^{\int_0^t \lambda(t) - \sigma \, dt}$$

Integrate both sides wrt 't'

$$P e^{\int_0^t \lambda(t) - \sigma \, dt} = \int \lambda(t) e^{\int_0^t \lambda(t) - \sigma \, dt} \, dt$$

$$\boxed{P(t) = \frac{\int \left(\lambda(t) e^{\int_0^t \lambda(t) - \sigma \, dt} \right) dt}{e^{\int_0^t \lambda(t) - \sigma \, dt}}} \quad 1$$

Part 2 – $\lambda(t) = \lambda$ – is a constant.

* we will now simplify 1 under the assumption of constant λ.

$$P(t) = \frac{\int \lambda e^{\int \lambda - \sigma \, dt} \, dt}{e^{\int (\lambda - \sigma) dt}}$$

$$= \frac{\int \lambda e^{(\lambda - \sigma)t} \, dt}{e^{(\lambda - \sigma)t}}$$

$$= \frac{\frac{\lambda}{\lambda - \sigma} e^{(\lambda - \sigma)t} + C_1}{e^{(\lambda - \sigma)t}}$$

we finally integrated, so we get a constant. Generally speaking, you ignore the integration constant from the integrating factor, since in can be absorbed into this constant

$P(0) = 0$, solve for C_1 using initial condition

$$0 = \frac{\frac{\lambda}{\lambda - \sigma} \cancel{e^{0}}^{\,1} + C_1}{\cancel{e^{0}}^{\,1}}$$

$$C_1 = -\frac{\lambda}{\lambda - \sigma}$$

$$P(t) = \frac{\frac{\lambda}{\lambda-\sigma} e^{(\lambda-\sigma)t} - \frac{\lambda}{\lambda-\sigma}}{e^{(\lambda-\sigma)t}}$$

$$= \frac{\lambda}{\lambda-\sigma}\left[1 - \frac{1}{e^{(\lambda-\sigma)t}}\right]$$

$$\boxed{P(t) = \frac{\lambda}{\lambda-\sigma}\left(1 - e^{-(\lambda-\sigma)t}\right)} \quad (2)$$

solution in commings I think

Two things to note

(1) Getting (2) would be faster if we never derived (1) first, and assumed $\lambda(t)=\lambda$ from the beginning. Just an FYI.

(2) Is (2) salvagable given λ changes with 't'. I think maybe there is an argument that λ changes with 'a' age or 't' time only, and we can say we are integrating w.r.t. the other constant, <u>or</u> we just assume its constant.

③ Two-Stage Catalytic Model.

← there are some differences between the Muench model and Ferguson/Cummings, Munch wants P_1 and P_2 while F/C wants P_2

$$S \xrightarrow{\lambda_1(t)} P_1 \xrightarrow{\lambda_2(t)} P_2$$

Goal - solve for P_2., solving P_1+P_2 would take a different approach

Part 1 - λ's are functions of 't', no assumptions made.

$$\frac{dS}{dt} = -\lambda(t)\,S \qquad\qquad S+P_1+P_2 = 1$$

separation of variables & integrate.

$$\frac{1}{S}\,dS = -\lambda(t)\,dt$$

$$\ln(S) + C_1 = -\int \lambda(t)\,dt$$

note, usually we ignore this integration constant and absorbe it by the constant on the right-hand-side (RHS). But since we are not integrating the RHS, we will include the constant on the left-hand-side (LHS)

$$\ln(S) = -\int \lambda(t)\,dt - C_1$$

$$S = e^{-\int \lambda(t)\,dt - C_1}$$

$$= \cancel{e}^{\cancel{C_1}\,C_1}\, e^{-\int \lambda(t)\,dt}$$

$$S = C_2\, e^{-\int \lambda(t)\,dt}$$

I think this is legit. instead of $\int_0^t$ we sub in $t=0$, and $\int_0^0 = 0$

$S(0) = 1$, solve for constant

$$S(0) = 1 = C_2\, \cancel{e^{\int_0^0 \lambda(t)\,dt}}^{=1}$$

$$C_2 = 1$$

$$\boxed{S(t) = e^{-\int \lambda(t)\,dt}} \quad ③$$

Note, if $\lambda(t)=\lambda$, is a constant, then $\boxed{S(t) = e^{-\lambda t}}$ 3.5

Now can we skip right to P_2.

$$\frac{dP_2}{dt} = \lambda_2(t) P_1 \longleftarrow$$

But $S + P_1 + P_2 = 1$

$P_1 = 1 - S - P_2$

$$\frac{dP_2}{dt} = \lambda_2(t)\left(1 - S - P_2\right)$$

$\longleftarrow$ and we knew that

$$S = e^{-\int \lambda_1(t)\,dt} \quad (3)$$

$$\frac{dP_2}{dt} = \lambda_2(t)\left(1 - e^{-\int \lambda_1(t)\,dt} - P_2\right)$$

only two variables now P_2 and t.

$$\frac{dP_2}{dt} = \lambda_2(t) - \lambda_2(t) e^{-\int \lambda_1(t)\,dt} - P_2 \lambda_2(t)$$

Get this in the "integrating factor" form.

$$\frac{dP_2}{dt} + P_2 \lambda_2(t) = \lambda_2(t)\left(1 - e^{-\int \lambda_1(t)\,dt}\right)$$

Multiply everything by $\mu(t)$ and simplify

integrating factor is

$$\mu(t) = e^{\int \lambda_2\,dt}$$

$$\frac{d}{dt}\left(P_2\, e^{\int \lambda_2 dt}\right) = \lambda_2(t)\left(1 - e^{-\int \lambda_1(t)\,dt}\right) e^{\int \lambda_2\,dt}$$

integrate both sides wrt t....

$$P_2 e^{\int \lambda_2(t)dt} = \int \lambda_2(t) e^{\int \lambda_2(t)dt}\left(1 - e^{-\int \lambda_1(t)dt}\right)dt$$

$$④ \quad \boxed{P_2(t) = e^{-\int \lambda_2(t)\,dt}\left[\int \lambda_2(t) e^{\int \lambda_2(t)dt}\left(1 - e^{-\int \lambda_1(t)\,dt}\right)dt\right]}$$

notice I have not integrated anything, so no integration constant.

Part 2. $\rightarrow$ $\lambda_1(t) = \lambda_1$, $\lambda_2(t) = \lambda_2$ $\rightarrow$ they are both constants over whatever range we are integrating.

simplifying 4 ...

$$P_2(t) = e^{-\lambda_2 t}\left[\int \lambda_2 e^{\lambda_2 t}\left(1 - e^{-\lambda_1 t}\right)dt\right]$$

$$= e^{-\lambda_2 t}\left[\lambda_2 \int e^{\lambda_2 t} - e^{(\lambda_2 - \lambda_1)t}\, dt\right]$$

$$= e^{-\lambda_2 t}\left[\lambda_2\left(\frac{e^{\lambda_2 t}}{\lambda_2} - \frac{e^{(\lambda_2 - \lambda_1)t}}{\lambda_2 - \lambda_1} + c_1\right)\right]$$

$P_2(0) = 0$

$$0 = \cancel{e^0}^{\,1}\left(\lambda_2\left(\frac{\cancel{e^0}^{\,1}}{\lambda_2} - \frac{\cancel{e^0}^{\,1}}{\lambda_2 - \lambda_1} + c_1\right)\right)$$

$$0 = 1 - \frac{\lambda_2}{2_2 - \lambda_1} + C \quad \rightarrow \quad C = \frac{\lambda_2}{\lambda_2 - \lambda_1} - 1$$

$$= \frac{\cancel{\lambda_2} - \cancel{\lambda_2} + \lambda_1}{\lambda_2 - \lambda_1}$$

$$= \frac{\lambda_1}{\lambda_2 - \lambda_1}$$

$$P_2(t) = e^{-\lambda_2 t}\left[\lambda_2\left(\frac{e^{\lambda_2 t}}{\lambda_2} - \frac{e^{(\lambda_2-\lambda_1)t}}{\lambda_2 - \lambda_1} + \frac{\lambda_1}{\lambda_2 - \lambda_1}\right)\right.$$

$$= \frac{\cancel{\lambda_2} \cancel{e^{\lambda_2 t}}\, \cancel{e^{-\lambda_2 t}}}{\cancel{\lambda_2}} - \frac{e^{(\lambda_2-\lambda_1)t}\, e^{-\lambda_2 t}}{\lambda_2 - \lambda_1} + \frac{\lambda_1}{\lambda_2 - \lambda_1} e^{-\lambda_2 t}$$

Did you forget to multiply lambda_2 by the second 2 terms in this expression?

$$= 1 - \frac{e^{\cancel{\lambda_2 t} - \lambda_1 t - \cancel{\lambda_2 t}}}{\lambda_2 - \lambda_1} + \frac{\lambda_1}{\lambda_2 - \lambda_1} e^{-\lambda_2 t}$$

$$\boxed{P_2(t) = 1 - \left(\frac{1}{\lambda_2 - \lambda_1}\right) e^{-\lambda_1 t} + \frac{\lambda_1}{\lambda_2 - \lambda_1} e^{-\lambda_2 t}}$$

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What happens if we make the assumption that lambda_2 = lambda_1 (or at least that we cannot distinguish them)? This is what F/C do when writing as lambda_i.