1 Solution for the linear system of ODE's presented in Section 2

Although the current application considered a two-dimensional physical model, our proposed framework applies to m-dimensional linear systems of ODE's. Consider the general linear system

$$\frac{d}{dt}\mathbf{c}(t) = \mathbf{W}\mathbf{c}(t) + \mathbf{g}\,, \tag{1}$$

where $\mathbf{c}(t)$ is an $m \times 1$ vector function of t, $\mathbf{W}$ is an $m \times m$ matrix (which may depend upon known and unknown inputs but we suppress them in the notation here) that has m real and distinct eigenvalues and $\mathbf{g}$ is a vector of length m.

When $\mathbf{W}$ has m distinct eigenvalues, we can find a non-singular matrix $\mathbf{P}$ such that $\mathbf{W} = \mathbf{P}\boldsymbol{\Lambda}\mathbf{P}^{-1}$, where the columns of $\mathbf{P}$ are linearly independent eigenvectors. Therefore, $e^{\mathbf{W}} = \mathbf{P}e^{\boldsymbol{\Lambda}}\mathbf{P}^{-1}$, where $\boldsymbol{\Lambda}$ is a diagonal matrix with λ_i as the i-th diagonal element, $i = \{1, 2, \cdots, m\}$. Now, let $\mathbf{G}_i = \mathbf{u}_i\mathbf{v}_i^{\mathrm{T}}$, where $\mathbf{u}_i$ is the i-th column of $\mathbf{P}$ and $\mathbf{v}_i^{\mathrm{T}}$ is the i-th row of $\mathbf{P}^{-1}$. (These are often referred to as the *right* and *left* eigenvectors respectively.) It is straightforward to see that (i) $\mathbf{G}_i^2 = \mathbf{G}_i$, (ii) $\mathbf{G}_i\mathbf{G}_j = 0 \;\; \forall \;\; i \neq j$ and (iii) $\sum_{i=1}^{m} \mathbf{G}_i = \mathbf{I}_m$. Each $\mathbf{G}_i$ is idempotent and is, in fact, the oblique projector onto the null space of $\mathbf{W} - \lambda_i\mathbf{I}_m$ along the column space of $\mathbf{W} - \lambda_i\mathbf{I}_m$. It is also easily verified that $e^{t\mathbf{W}}e^{-t\mathbf{W}} = \mathbf{I}_m$ and $e^{t\mathbf{W}}\mathbf{W}^{-1} = \mathbf{W}^{-1}e^{t\mathbf{W}}$.

From the above properties of the $\mathbf{G}_i$ matrix, it easily follows that $e^{\mathbf{W}} = \sum_{i=1}^{m} e^{\lambda_i}\mathbf{G}_i$. Consequently,

$$\frac{d}{dt}e^{t\mathbf{W}} = \sum_{i=1}^{m} \lambda_i e^{\lambda_i t}\mathbf{G}_i = \sum_{i=1}^{m} \lambda_i e^{\lambda_i t}\mathbf{u}\mathbf{v}_i^{\mathrm{T}} = \mathbf{P}\boldsymbol{\Lambda}e^{t\boldsymbol{\Lambda}}\mathbf{P}^{-1} = \mathbf{P}\boldsymbol{\Lambda}\mathbf{P}^{-1}\mathbf{P}e^{t\boldsymbol{\Lambda}}\mathbf{P}^{-1} = \mathbf{W}e^{t\mathbf{W}}$$

$$\text{and} \quad \int e^{t\mathbf{W}}dt = \sum_{i=1}^{m} \frac{1}{\lambda_i}e^{\lambda_i t}\mathbf{G}_i = \mathbf{P}\boldsymbol{\Lambda}^{-1}e^{t\boldsymbol{\Lambda}}\mathbf{P}^{-1} = \mathbf{P}\boldsymbol{\Lambda}^{-1}\mathbf{P}^{-1}\mathbf{P}e^{t\boldsymbol{\Lambda}}\mathbf{P}^{-1} = \mathbf{W}^{-1}e^{t\mathbf{W}}\,.$$

Multiplying both sides of (1) by $e^{-t\mathbf{W}}$ from the left yields:

$$e^{-t\mathbf{W}}\left[\frac{d}{dt}\mathbf{c}(t) - \mathbf{W}\mathbf{c}(t)\right] = e^{-t\mathbf{W}}\mathbf{g} \Longrightarrow \frac{d}{dt}\left[e^{-t\mathbf{W}}\mathbf{c}(t)\right] = e^{-t\mathbf{W}}\mathbf{g}\,. \tag{2}$$

Integrating out both sides of (2), we obtain $e^{-t\mathbf{W}}\mathbf{c}(t) = -\mathbf{W}^{-1}e^{-t\mathbf{W}}\mathbf{g} + \mathbf{k}$, where $\mathbf{k}$ is a constant vector. The initial condition at $t = 0$ yields $\mathbf{c}(0) = -\mathbf{W}^{-1}\mathbf{g}+\mathbf{k}$, so $\mathbf{k} = \mathbf{c}(0)+\mathbf{W}^{-1}\mathbf{g}$. Consequently, $\mathbf{c}(t) = e^{t\mathbf{W}}\mathbf{c}(0) + \mathbf{W}^{-1}\left[e^{t\mathbf{W}} - \mathbf{I}_m\right]\mathbf{g}$ is the solution to (1).

The two-zone model (Section 2) fits into the above framework with $m = 2$. Therefore, to use the result just derived, we have to guarantee that $\mathbf{W}$ has 2 distinct eigenvalues. The eigenvalues of $\mathbf{W}$ determine the numerical stability and the physical interpretability of the two-zone model. The two eigenvalues of $\mathbf{W}$ are the roots of the characteristic polynomial $\lambda^2 + \left(\frac{\beta}{V_N} + \frac{\beta+Q}{V_F}\right)\lambda + \frac{\beta Q}{V_N V_F} = 0$. Note that $\det(\mathbf{W}) = \dfrac{\beta Q}{V_N V_F}$, which means that $\mathbf{W}$ is nonsingular as long as β and Q are not zero. The eigenvalues are available in closed form as

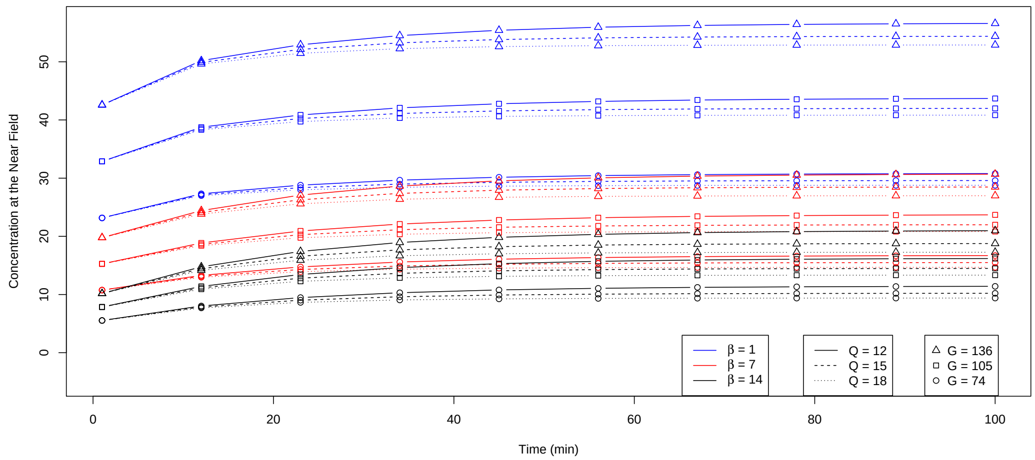
$$\begin{aligned}
\lambda_1 &= \tfrac{1}{2}\left[-\left(\tfrac{\beta V_F+(\beta+Q)V_N}{V_N V_F}\right) + \sqrt{\left(\tfrac{\beta V_F+(\beta+Q)V_N}{V_N V_F}\right)^2 - 4\left(\tfrac{\beta Q}{V_N V_F}\right)}\right], \\
\lambda_2 &= \tfrac{1}{2}\left[-\left(\tfrac{\beta V_F+(\beta+Q)V_N}{V_N V_F}\right) - \sqrt{\left(\tfrac{\beta V_F+(\beta+Q)V_N}{V_N V_F}\right)^2 - 4\left(\tfrac{\beta Q}{V_N V_F}\right)}\right].
\end{aligned} \tag{3}$$

Furthermore, since β, Q, V_F and V_N are all strictly positive, we find

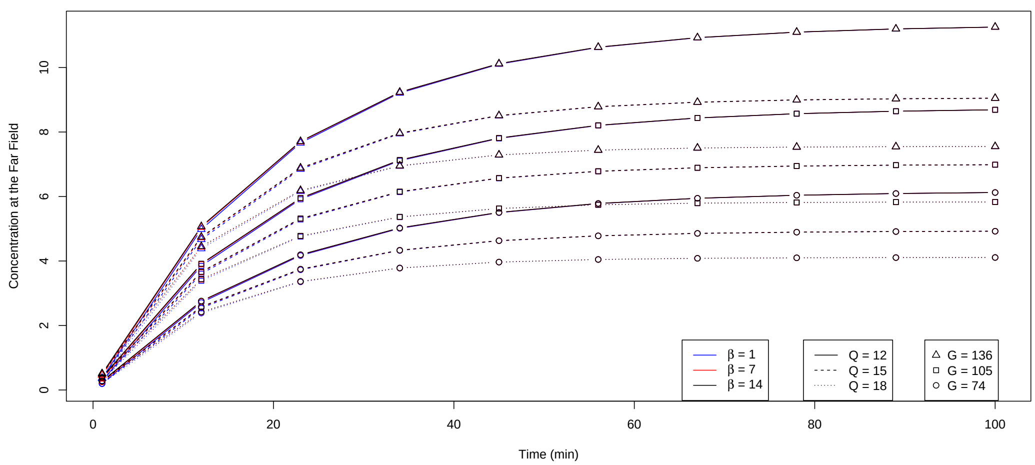
$$\begin{aligned}
\left(\frac{\beta V_F + (\beta+Q)V_N}{V_N V_F}\right)^2 - 4\left(\frac{\beta Q}{V_N V_F}\right) &= \frac{\beta^2 V_F^2 + 2\beta V_F(\beta+Q)V_N + (\beta+Q)^2 V_N^2}{(V_N V_F)^2} - 4\frac{\beta Q}{V_N V_F} \\
&= \frac{(\beta V_F - Q V_N)^2 + 2\beta^2 V_F V_N + (\beta^2 + 2\beta Q)V_N^2}{(V_N V_F)^2} > 0\,.
\end{aligned}$$

This implies that the eigenvalues in (3) are real and distinct. The latter two quantities are volumes of a chamber and clearly positive. Physical considerations ensure that the same is true for β and Q. Assigning priors with positive support is all that is needed to ensure a stable system with real solutions.

We conclude this section with two figures that may offer further insight into the behavior of the two-zone model for varying values of the parameters. Figures 1(a) and 1(b) depict the trajectories of the exposures contrations over time in the near and far fields respectively. We consider three possible values for each parameter: $(a)\beta = \{3, 7, 14\}$, (b) $Q = \{12, 15, 18\}$ and (c) $G = \{74, 105, 136\}$. We then plot the trajectories of the exposure concentrations over time at the near and far fields obtained for each combination of the parameters β, Q and G. This results in 27 trajectories. Here, the volumes at the near and far fields are respectively 1.1m^3 and 240m^3.



(a) Near Field



(b) Far Field

Figure 1: Trajectories of the exposures concentrations at the near and far fields for different two-zone model parameters.