
Title: README file for supplemental data files to define model detailed in “Distinguishing multiple roles of T cell and macrophage involvement in determining lymph node fates during *Mycobacterium tuberculosis* infection”

Author: Kathryn C. Krupinsky

Date: 02/07/25

The ODE component of the model is given in **LN_Blood_coupled_ODEs_SBML.xml**. By itself, this model description assumes that all lung APCs are zero; addition of Mtb and APCs must be pulsed given the user’s ODE solver framework. This model has ODEs for all five LNs plus the Blood as a single, coupled ODE representation. Parameters that are the same mechanism split between different LNs have unique parameter names, like “k3” becomes “LN1_k3”, “LN2_k3”, etc. The parameter names in this SBML file correspond to the parameters in the parameter range and matrix CSVs. This SBML file was generated in part using the MOCCASIN software developed by Michael Hucka (<https://doi.org/10.22002/D1.965>).

We have included a MATLAB file, **CaliPro.m**, which can be adapted to the user’s solver framework. CaliPro is a published procedure to calibrate parameter ranges to various user-specified constraints—in this case, to keep model outcomes near experimental datasets. Although this MATLAB class is incomplete by itself, it can be easily treated as pseudocode or adapted for implementation in other object-oriented languages. Details for usage are in the header comments of this file.

For each of the following csv files, each row represents an individual host after performing a LHS. Each column represents a model state aside from the first column (hostNum) that contains the host number.

1. **icMatrix_involved_active.csv** contains the initial conditions of all model states for the involved case of hosts for actively infected pulmonary hosts.
2. **icMatrix_involved_latent.csv** contains the initial conditions of all model states for the involved case of hosts for LTBI hosts.
3. **icMatrix_uninfected_active.csv** contains the initial conditions of all model states for the uninfected case of hosts for actively infected pulmonary hosts.
4. **icMatrix_uninfected_latent.csv** contains the initial conditions of all model states for the uninfected case of hosts for LTBI hosts.
5. **icMatrix_uninvolved_active.csv** contains the initial conditions of all model states for the uninvolved case of hosts for actively infected pulmonary hosts.
6. **icMatrix_uninvolved_latent.csv** contains the initial conditions of all model states for the uninvolved case of hosts for LTBI hosts.

For each of the following csv files, each row represents an individual host after performing a LHS. Each column represents a model parameter aside from the first column (hostNum) that contains the host number.

7. **paramMatrix_involved_active.csv** contains all parameter values for the involved case of hosts for actively infected pulmonary hosts.
8. **paramMatrix_involved_latent.csv** contains all parameter values for the involved case of hosts for LTBI hosts.

9. **paramMatrix_uninfected_active.csv** contains all parameter values for the uninfected case of hosts for actively infected pulmonary hosts.
10. **paramMatrix_uninfected_latent.csv** contains all parameter values for the uninfected case of hosts for LTBI hosts.
11. **paramMatrix_uninvolved_active.csv** contains all parameter values for the uninvolved case of hosts for actively infected pulmonary hosts.
12. **paramMatrix_uninvolved_latent.csv** contains all parameter values for the uninvolved case of hosts for LTBI hosts.

Lastly, this file contains a machine readable format of **S1 Appendix**. Each row represents a unique parameter or initial condition for cell populations levels in the blood used within the model and each column represents the parameter/initial condition name, distribution used during LHS, and minimum/maximum values of parameter/initial condition sampling range.

13. **paramRanges.csv** contains all parameter/initial condition ranges used in LHS sampling for model runs.

We have additionally included all necessary raw data files to produce all figures:

Figure 1 –image

Figure 2 – image

Figure 3

1. **activeApcVector.csv**
2. **latentApcVector.csv**

Figure 4

1. **uninvolved-latent-result.rds**
2. **involved-latent-result.rds**

Figure 5

1. **involved-latent-result-uninvolved-ln-prcc.rds**
2. **involved-latent-result-involved-ln-prcc.rds**

Figure 6

1. **involved-latent-result-prcc-sterilization.rds**

Figure 7

1. **involved-latent-results.rds**
2. **involved-latent-result-geo.rds**

Figure 8

1. **involved-latent-result-fdg.rds**
2. **involved-latent-result-involved-ln-prcc.rds**
3. **involved-latent-result-uninvolved-ln-prcc.rds**

4. **involved-active-result-involved-ln-prcc.rds**
5. **involved-active-result-uninvolved-ln-prcc.rds**

Figure 9

1. **involved-latent-result-fdg.rds**
2. **involved-latent-result-involved-ln-prcc.rds**
3. **involved-latent-result-uninvolved-ln-prcc.rds**

Figure 10

1. **involved-latent-result-involved-ln-prcc.rds**
2. **involved-latent-result-uninvolved-ln-prcc.rds**
3. **involved-active-result-involved-ln-prcc.rds**
4. **involved-active-result-uninvolved-ln-prcc.rds**

Figure S1

1. **activeHostGrans.csv**

Figure S2

1. **uninfected-latent-result.rds**
2. **uninvolved-latent-result.rds**
3. **involved-latent-result.rds**
4. **uninfected-active-result.rds**
5. **uninvolved-active-result.rds**
6. **involved-active-result.rds**

Figure S3

1. **uninfected-latent-result.rds**
2. **uninfected-active-result.rds**

Figure S4

1. **uninvolved-active-result.rds**
2. **involved-active-result.rds**

Figure S5

3. **involved-active-result-uninvolved-ln-prcc.rds**
4. **involved-active-result-involved-ln-prcc.rds**

Figure A

1. **involved-active-result-prcc-sterilization.rds**

Figure B

1. **involved-active-result-fdg.rds**

Figure C

1. **involved-active-result-fdg.rds**
2. **involved-active-result-involved-ln-prcc.rds**
3. **involved-active-result-uninvolved-ln-prcc.rds**

For additional questions, please contact Denise Kirschner at kirschne@umich.edu