

An ODD-Protocol for Agent-Based Model for the Spread of Mpox Through Sexual Contact – The Population Model

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Purpose and Patterns

The purpose of the model is to predict the size of the outbreak (new cases and effective reproductive number denoted by R_e) of an Mpox outbreak in a society in response to variation of multiple parameters: vaccination strategy (the number of people vaccinated, the cohorts vaccinated), the number of superspreader events in a year and the number of imported cases in a year. Some other parameters can also be varied, for example the disease specific parameters: incubation period, infectious period, and the transmission probability. In this model, the society is composed of heterosexual, homosexual and bisexual males and females.

We define the following general patterns as the criteria for its usefulness: The R_e of an outbreak depends on the number of people who are vaccinated, the cohorts who are vaccinated, the number of superspreader events and the number of imported cases in a year.

Entities, State Variables and Scales

The following entities are included in the model: agents representing humans and the global environment representing the society. In total, 10,000 agents are implemented. All state variables of an agent are given in Table 1.

Table 1 State variables of an agent

Agent State Variables	Description
age	Between 16 to 75 years.
Age-days	Between 0 to 365 days.
age-cohort	Each agent has an age-cohort between 0-15. Each cohort is 4 years in size (for example, age-cohort 0 is for agents aged from 16 to 19 years of age).
sex	Biological sex: male or female
sexual-preference	Heterosexual, bisexual or homosexual
new_partners_per_year	An integer that reflects the number of new sexual partners the agent will take on this year
brokenUp?	Set to TRUE if the agent has broken up from a relationship and is currently single, FALSE otherwise.
Vaccinated?	TRUE if the agent is vaccinated, FALSE otherwise

disease-status	Susceptible, Exposed, Infected or Recovered
days_sick	Number of days the agent has been sick. This is set to 0 if the agent is not currently sick (if disease-status is not “Infected”).
days_exposed	An integer that represents the number of days passed since the agent became “Exposed”.
Incubation period	An integer that represents the number of days the agent will stay in the “Exposed” state (when the disease is acquired however no symptoms are yet shown).
sick-period	An integer that represents the number of days the agent will stay in the “infected” state (symptoms showing and/or transmitting disease)
isTravelCase	TRUE if Mpox is acquired through travel (imported case), FALSE otherwise
day_i_got_sick	Records the day on which the agent became “Infected”.
day_infector_got_sick	Records the day on which the infector of the agent became “infected”.
numinfected	Number of other agents who were infected by this agent while it was in the “infected” state.
infected_by	The source of infection. Contains an agent if the infection was spread via community transmission. Contains NULL if the agent acquired infection through travel.

The observer is a single entity that controls the global variables. Observer state variables are global variables that change over time. (Static observer variables—those that do not change over simulated time—are considered parameters. Static observer variables are shown in Table 2.

Table 2 Static Observer Variables (Parameters of the model)

Global Parameters	Description	Value	Source
Society/Sexual-Network Related Global Parameters			
age-mix-agg	Age Mixing matrix. Each cell $C_{r,c}$ represents probability of an agent from age cohort r to form a sexual partnership with an agent from age-cohort c	See Appendix I – (Page Error! Bookmark not defined.)	Calculated using the NATSAL-3 dataset (Mercer, et al., 2013)
lambda-hetero	A 15x2 matrix of Poisson means. Each cell $C_{r,c}$ represents a Poisson mean for an annual number of new opposite-sex sexual partners for heterosexual agents of age cohort r and sex c .	See Appendix I – Parameters (Page 21)	Calculated using the NATSAL-3 dataset

	<p>The agent state variable <code>new_partners_per_year</code> for each heterosexual agent of age-cohort r and sex c is calculated by drawing a random number from Poisson distribution with mean equal to $C_{r,c}$.</p>		
lambda-homo	<p>A 15x2 matrix of Poisson means. Each cell $C_{r,c}$ represents a Poisson mean for an annual number of new same-sex sexual partners for homosexual agents of age cohort r and sex c.</p> <p>The agent state variable <code>new_partners_per_year</code> for each homosexual agent of age-cohort r and sex c is calculated by drawing a random number from Poisson distribution with mean equal to $C_{r,c}$.</p>	See Appendix I – Parameters (Page 21)	Calculated using the NATSAL-3 dataset
lambda-bi-same-sex	<p>A 15x2 matrix of Poisson means. Each cell $C_{r,c}$ represents a Poisson mean for an annual number of new same-sex sexual partners for bi-sexual agents of age cohort r and sex c.</p> <p>The agent state variable <code>new_partners_per_year</code> for each bi-sexual agent of age-cohort r and sex c is calculated by drawing a random number from Poisson distribution with mean equal to $C_{r,c}$.</p>	See Appendix I – Parameters (Page 21)	Calculated using the NATSAL-3 dataset
lambda-bi-opp-sex	<p>A 15x2 matrix of Poisson means. Each cell $C_{r,c}$ represents a Poisson mean for an annual number of new opposite-sex sexual partners for bi-sexual agents of age cohort r and sex c.</p>	See Appendix I – Parameters (Page 22)	Calculated using the NATSAL-3 dataset

	The agent state variable $\text{new_partners_per_year}$ for each bi-sexual agent of age-cohort r and sex c is calculated by drawing a random number from Poisson distribution with mean equal to $C_{r,c}$.		
bi_prob_same_sex	A 15x2 matrix. Each cell $C_{r,c}$ represents probability of an agent of age-cohort r and sex c selecting a same sex partner. The probability of the agent selecting an opposite sex partner is $1 - C_{r,c}$. During calculation from the NATSAL-3 data, some values were missing. There were changed to 0.5.	See Appendix I – Parameters (Page 22)	Calculated using the NATSAL-3 dataset
total_population	Represents the total number of agents in the model.	10,000	Assumed
min-age	Represents the minimum age for the agents.	16	Calculated using the NATSAL-3 dataset
max-age	Represents the maximum age for the agents.	74	Calculated using the NATSAL-3 dataset
%homosexual_males	Percentage of homosexual males among all males	1.144%	Calculated using the NATSAL-3 dataset
%bi_males	Percentage of bi-sexual males among all males	3.924%	Calculated using the NATSAL-3 dataset
%homosexual_females	Percentage of homosexual females among all females	0.304%	Calculated using the NATSAL-3 dataset
%bi_females	Percentage of bisexual females among all females	6.043%	Calculated using the NATSAL-3 dataset
weekly_contact	Number of weekly sexual encounters between each long-term sexual partnership.	3/7	Assumed
Initially_infected_MSM	Represents the number of MSM who are infected at the start of the simulation (Seed cases)	5	Assumed

Initially_infected_others	Represents the number of non-MSM who are infected at the start of the simulation (Seed cases)	0	Assumed
People_vaccinated	Number of people vaccinated	0 or 200	Assumed
Vaccination_Programme	If set to "None", it means that no agents are vaccinated. If set to "RandomAll", it means that random agents from the entire population are vaccinated. If set to "RandomMSM", it means that random MSM agents are vaccinated.	None, RandomAll, RandomMSM	Assumed
SuperSpreaderEventsPerYear	Represents the number of superspreader events in the year.	0 or 30	Assumed
ImportedCasesPerYear	Represents the number of imported cases in a year	0 or 30	Assumed
Mpox Related Global Parameters			
Vaccine_efficacy	Vaccine efficacy refers to the percentage reduction in disease incidence among vaccinated individuals compared to those who are unvaccinated, indicating how well the vaccine prevents illness. Vaccine_efficacy of 1 means all vaccinated individuals are protected, while 0 means none of the vaccinated individuals are protected against the disease.	85%	(Rimoin, et al., 2010; Grant, Nguyen, & Breban, 2020)
mean_infectious_period	Represents the mean of the infectious period for Mpox. For each agent who is infected, an individualised "sick-period" is calculated by drawing a random number from a normal distribution with this mean and a standard deviation (sd) of 3 days.	2-4 weeks We assume a normal distribution with mean = 21 days and sd = 3 days.	(CDC, 2023)
Transmission_probability	Probability of acquiring infection after sexual	1/8	Assumed

	contact with an infected agent		
TP_multiplier_for_msm	This parameter is used to increase the transmission probability in an MSM contact. If set to 1, transmission probability in an MSM sexual contact is same as the transmission probability in a non-MSM sexual contact.	1	Assumed

Scales. Geographical aspect is not considered for this model. Therefore, the location of the agents on a grid does not mean anything and hence, holds no significance.

In our model, the temporal scale is set as days. One tick is equal to 1 day. Any event, for example, sexual contact, breaking up of a current relationship, new partnership formation, attending an event, acquiring disease through travel, disease-transmission, etc. is modelled to occur at maximum once a day. The current setting for simulation time is 180 days, however this can be changed as per the need.

Process Overview and Scheduling

Processes: The model is developed to cover the transmission of Mpox in a society for 180 days after the introduction of seed cases. It is structured into the following different processes:

At each timestep, the processes are executed in the exact same order:

- 1) Ageing
On each tick, all agents grow old by one-day. If an agent reaches the maximum age, it exits the model and to replace it, another agent of minimum age is added to the model.
- 2) Dissolution of (some of) the current long-term sexual partnerships
Each agent in a long-term relationship has a probability of breaking up the current relationship at each time-step. If the agent is to break up with its current long-term sexual partner, link between the agent and its partner is removed.
- 3) Formation of new long-term sexual partnerships
If the agent is seeking new long-term sexual partnership, a suitable partner is selected for it. A new link is formed between the agent and the new partner.
- 4) Formation of short-term sexual contacts through superspreader events
If there is a superspreader event on the day (tick), some agents from a specific cohort travel to attend that event. On the day of the event, each agent attending the event forms a short-term link with every other agent who attended the event.
- 5) Mpox case importation through travel
If theres an imported case on the day (tick), one of the susceptible agents from a specific cohort enter the “Exposed” state.
- 6) SEIR model for Mpox transmission

These processes are explained in detail in Section Sub-models.

Schedule: The simulation starts at day 0. The processes related to the sexual network are scheduled first because the subsequent process of disease transmission depend on the sexual network.

Design Concepts

Basic Principles

We use computer software Netlogo to implement our agent-based model of MonkeyPox spread in a closed population. This model takes an agent-based perspective of the SEIR model for Mpox transmission. An agent-based model for the spread of an infection has typically 4 main components: disease, society, transportation, and environment. To simplify, we are modelling the spread of Mpox through sexual contact only.

The disease component is modelled like an SEIR model. Agents can be in one of the following states: susceptible, exposed, infected, and recovered. The society component is structured to simulate a population using the NATSAL-3 survey data (Mercer, et al., 2013). Each agent is randomly assigned an age from a uniform distribution between 16 and 74 years. Agents are also assigned an age cohort. There are 15 age-cohorts, each with a size of 4 years. These upper and lower limits correspond to the minimum and the maximum ages of the respondents of the NATSAL-3 dataset.

All agents are given a biological sex: male and female. The sex is also assigned randomly, with a 50% probability of being a male. Each agent is also assigned a sexual-preference. There are three types of sexual preferences modelled: heterosexual, homosexual or bi-sexual. The percentages of males and females in these categories of sexual preferences are derived from the NATSAL-3 dataset and are mentioned in Table 1. These percentages are calculated in the following way: the percentage of heterosexual men in the model is equal to the percentage of men in NATSAL-3 survey who reported sexual contact only with the opposite sex in their lifetime, percentage of homosexual men is equal to the percentage of men in NATSAL-3 survey who reported having only same-sex sexual contact in their lifetime and percentage of bi-sexual men is equal to the percentage of men who reported having sexual contact with both sexes in their lifetime. The same method is applied to calculate percentage of heterosexual, homosexual and bi-sexual women. All the parameters that define the structure of the society are shown in **Error! Reference source not found.**

The Netlogo world is a two-dimensional grid where the squares that make up the grid are referred to as patches. None of our agents physically move within the Netlogo world. Changes in sexual partners is represented by the links between the agents. Who an agent selects as a sexual partner is dependent on the age-cohort and sex of the agent and the potential partners. The probabilities of an agents having a sexual contact with another agent is based on parameters learned from the NATSAL-3 survey data (Table 2). The age mixing matrices for each cohort is calculated from the NATSAL-3 survey data. An age-mixing matrix represents the probability of a person from an age-cohort having a sexual partnership with another person in the same or another age-cohort.

The infection spread part of the model is based on an SEIR (susceptible-exposed-infected-recovered) model. This model is widely used within infectious disease modelling. The idea behind an SEIR model is that when a susceptible agent comes in contact with an infected agent, there is a certain probability that the agent will be exposed to the disease. This probability is the transmission probability and assumed to be $1/8$ in our model. The weekly sexual contact rate is set to 3 times a

week, this means that agents in long-term partnerships have on average 3 sexual encounters in a week.

Agents forms sexual partnership with other agents based on age-mixing matrix, which is calculated from the NATSAL dataset. Two factors decide if agents have a sexual contact with other agents. Each agent has a "number of new partners each year" parameter (denoted by k in this paper), which is based on its age, sex and sexual preference. This parameter is equal to a random Poisson number which is generated using the means calculated from NATSAL-3 data for each sex, sexual preference and age-cohort. A discrete random variable is said to have a Poisson distribution, with parameter $\lambda_{s,a,p} > 0$ if it has a probability mass function given by:

$$f(k; \lambda_{s,a,p}) = Pr(X = k) = \frac{\lambda_{s,a,p}^k \times e^{-\lambda_{s,a,p}}}{k!}$$

where k is the number of annual new partners ($k \geq 0$), e is the Euler's constant ($e = 2.718..$) and $\lambda_{s,a,p}$ is the average number of new partners of sex $s = [\text{male, female}]$, age-cohort $a = [0, 1, \dots, 15]$ and sexual preference $p = [\text{homosexual, bi-sexual, heterosexual}]$ as calculated from the NATSAL-3 survey data. In our model, there are 90 such means (15 age cohorts, 2 sexes and 3 sexual preferences).

For agents who are bi-sexual, the probability of finding a same-sex partner, denoted by $P(\text{SameSexPartner}, a, s)$ is based on the relative frequency of same-sex partners out of all the partners in the previous year for each cohort (age, sex) within the bi-sexual group calculated from the NATSAL-3 dataset. For example, the probability of finding a same-sex and opposite sex partner for a bi-sexual agent $p = \text{bi-sexual}$ of age cohort $a : a \in [0, 1, \dots, 15]$ and sex $s : s \in \text{male, female}$ is given by:

$$P(\text{SameSexPartner}, a, s) = \sum_{i \in C_{\text{bisexual}, a, s}} \frac{N_{\text{SameSexPartners}}}{N_{\text{AllPartners}}}$$

$$P(\text{OppositeSexPartner}, a, s) = 1 - P(\text{SameSexPartner}, a, s).$$

Here, $N_{\text{SameSexPartners}}$ represents the number of same-sex partners and $N_{\text{AllPartners}}$ represents the total number of partners in last 12 months of each agent in the cohort $C_{\text{bisexual}, a, s}$.

Sexual partnerships are formed probabilistically using the $\lambda_{s,a,p}$ parameter derived from the NATSAL-3 dataset. Each agent has a parameter that defines the number of new partners that agent will take in a year. To get a new long term partner, the agent has to break-up with the existing partner first. The probability that an agent will breakup on a particular day is drawn from the following exponential distribution function (scaled to a day from a year):

$$P(\text{BreakupToday}) = 1 - e^{(-1 \times \frac{(\text{NewPartnersPerYear} + 0.1)}{365})}$$

Here, a small number ($0.1/365$) is added as a large number of agents will end up with zero probability of finding a new partner otherwise. For each agent, at each timestep/day, a random uniform number is drawn between 0 and 1. If the drawn random number is less than $P(\text{BreakupToday})$, the link between the agent's current long term partner, if any, is removed, and a new partner is sought for this agent.

The other component of the model is the contact matrix. This matrix gives the probability that an agent in an age-cohort will form a sexual partnership with another agent in the same or a different age cohort. The age of the partner is recorded within the NATSAL-3. Therefore, an age-mixing matrix is calculated from the NATSAL-3 dataset, using the method presented by Datta et al. (2018) (these methods are explained in detailed in our paper). The following equation is used to calculate the age-mixing matrix. C_{ij} represents probability that an agent in cohort C_i will have sexual partnership with an agent in cohort C_j . The probability that an agent in cohort C_i will seek a sexual partnership with an agent in cohort C_j , $P(P_{C_i C_j})$ is based on the relative frequency counts obtained from the NATSAL-3 dataset, described by the following equation:

$$P(P_{C_i C_j}) = \frac{\sum \theta_{i,j}}{\sum \theta_i},$$

where $\theta_{i,j}$ is the sum of weights of all respondents in NATSAL-3 survey in cohort i who had a past or a current partnership with a person in age cohort j . Similarly, θ_i is the sum of weights of all respondents in age-cohort i reporting any sexual relationship with people of any age cohort. The entire matrix of probabilities is represented by:

$$AgeMix = \begin{bmatrix} P_{C1,C1} & \cdots & P_{C1,C15} \\ \vdots & \ddots & \vdots \\ P_{C15,C1} & \cdots & P_{C15,C15} \end{bmatrix}$$

Here, N is the total number of age cohorts.

Emergence

The emerging result from the model is the course that the infection takes. Based on the type of agent that is initially infectious, the other agents come into contact with the infectious agent, the length of the contact, patterns can emerge how an outbreak can spread. For example, if an agent from a specific cohort is infected, and the probability of that agent having a sexual contact with other agent(s) from the same cohort is high, then that cohort will see a higher outbreak compared to others. The outcome (daily new infections) emerges from the number of vaccinated individuals, the type of vaccination programme, the number of superspreader events and the number of imported cases and multiple other factors.

At the end of the simulation, an effective reproduction number, R_e , is calculated. A time-varying reproduction number, R_t is also calculated retrospectively. R_e represents average number of secondary infections caused by a single infected individual in a population where not everyone is susceptible to the disease (R_e is different from the basic reproductive number, R_0 , which represents the average number of new infections caused by a single infected individual in a completely susceptible population). R_t refers to the average number of secondary infections caused by a single infected individual at a specific time during an outbreak or epidemic. In other words, it is an estimation of R_e at a single specific point in time during the outbreak.

Adaptation, Objectives, Learning, Prediction

Adaptive behaviours are not yet modelled. The agents do not change their behaviour after infection or exposure. There is consequently no inherent pursuit of specific objectives, learning (how agents change their decision-making methods), implicit or explicit prediction and sensing.

Interaction

Two types of sexual contacts are possible in this model: long-term and short-term. Long-term sexual contact that is continued towards the end of a relationship. It is represented by a breed of links named “lt-links”. The short-term contact is a once-only contact modelled to mimic the transmission through super spreader events or travel. It is represented by a breed of links called the “st-links”. The model assumes direct interaction between agents. If two agents are connected to each other through links, it means there is a sexual relationship between them. An interaction may lead to the infection of an agent if one is susceptible, and one is infected.

Stochasticity

Agent relationships, breakup and new partner selections are random based on predefined distributions. Whether a agent will break up today and find a new sexual partner is based on a probability that is calculated through predefined distributions. From which age-cohort an agent will find a new partner from also depends on a pre-defined probability distribution based on age mixing matrix. When an infectious agent comes in contact with a susceptible agent, there is a certain probability that determines if the susceptible agent will become exposed. Once exposed, the length of time an agent will stay in ‘exposed’ state before it becomes infectious is also determined by a probability distribution: incubation period is drawn from a Weibull distribution with scale parameter $\eta = 8.4$ and the shape parameter $\beta = 1.5$ (Ward, Christie, Paton, Cumming, & Overton, 2022). Once in an infectious state, the length of time this agent will stay infectious before its recovered is also determined by a probability distribution: normal distribution with mean = 21 and sd = 3 days.

Observation

Every run of the model, data is collected on the number of agents who are infected that day (this can be update later). We also collect data of number of agents from each age-cohort who are infected at that day.

Collectives

Collectives are not explicitly modelled. However, the agents state-variables define who they are: age-cohort, sex and sexual preference.

Observation

Graphical output of the model shoes the daily number of new infections. Other summary statistics can be gathered via the output files. These include number of new infections in each age-cohort, sex and sexual preference groups. The Re and Rt are also written in separate output files.

Initialisation

To initialise, we create a population of agents, global parameters and initial setting conditions. By default, the population is set to 10000, this however can be changed for any run. Minimum age of an agent in the population is 16 and maximum is 74. Each agent is randomly assigned an age sampled from a uniform distribution between 16 to 74 years of age. Sex (male/female) is also assigned to agents randomly from a uniform distribution. Sexual preference of each agent is based on the user inputs. The user of the model can select number of homosexuals, bi-sexual males and females in the population. We have calculated them from the NATSAL-3 dataset as mentioned in Table 2.

The number of new sexual partner an agent takes each year is based on a probability distribution calculated from the NATSAL-3 survey data, explained already in the design concepts section. This probability distribution is based on the age, sex and sexual preference of the agent.

Setting Global Parameters

The values for the global parameters are shown in Table 1 and Table 2.

Setting Initial Conditions

The initial conditions of the model are set to make the start of the simulation. These are given following categories:

Disease Conditions:

We assume that there are no exposed or recovered agents at the start of the simulation. Only 5 agents who are MSM (sex = male and sexual-preference = homosexual or bi-sexual) are set to be in infected state.

Vaccination Parameters:

The user can select a Vaccination_programme and Vaccinated_people. The former describes the type of vaccination strategy to be implemented. The latter represents the number of agents who will be vaccinated. If the vaccination_programme is set to “none”, no agents are vaccinated. If it is set to “RandomAll”, random “Vaccinated_people” agents are vaccinated. If the vaccination_programme is set to “RandomMSM”, random “Vaccinated_people” MSM agents are vaccinated.

The vaccination is set to be 85% effective. This means if 100 people are vaccinated, only 85 of them will have complete protection against the disease.

Sexual Network Parameters

At the start of the simulation, there is 0.5 probability that each single agent will be in a relationship. This leads to a different number of turtles in long-term partnerships for each simulation (roughly around 75% each time).

All other global parameters are set to values shown in Table 2. Each agent is initialised based on these global parameters, for example, an agent’s sex, sexual preference and ages are drawn from distribution described in Table 2.

Input data

No data is fed into the model as such, several global variables that are shown in Table 2 are calculated from the NATSAL-3 dataset and hardcoded into the model. These variables are also printed in Appendix I – Parameters.

Sub-models

Sub-models for initialisation

1. Setup

This is the main sub-model for initialisation of the model. The following sub-sub-models are called in it.

a. set-global-vars

Sets the values of all the global variables except the ones that are input by the user through the interface.

b. load-lambda

Loads the hard-coded parameters (discussed in Table 2).

c. load-age-mix

Loads the hard-coded age-mixing matrix (Table 2).

d. create-population

By default, the population of agents is set to 10000, this however can be changed for any run. Minimum age of an agent in the population is 16 and maximum is 74. Each agent is randomly assigned an age sampled from a uniform distribution between 16 to 74 years of age. Sexual preference of each agent is based on the user inputs. The user of the model can select number of homosexuals and bi-sexual males and females in the population. We have calculated them from the NATSAL-3 dataset as mentioned in Table 2. The number of new sexual partners an agent takes each year is based on a probability distribution calculated from the NATSAL-3 survey data, explained already in the design concepts section. This probability distribution is based on the age, sex and sexual preference of the agent. All the agent specific parameters are set in this sub-sub-model. All other global parameters are set to values shown in Table 2. Each agent is initialised based on these global parameters, for example, an agent's sexual preference and ages are drawn from distribution described in Table 2.

e. initial-infection

This sub-sub-model picks up random high-risk agents (homosexual and bi-sexual men between 20-36 years of age) and sets their disease-status to "infected". The number of infected agents depend on the "initially_infected_MSM" parameter.

f. initial-relationships

This sub-model creates the sexual network. At the start of the simulation, there's 0.5 probability that each single agent will be in a relationship. This leads to a different number of turtles in long-term partnerships for each simulation (roughly around 75% each time).

g. initial-vaccination

Based on the type of vaccination_programme selected, this sub-model sets the vaccinated? parameter of some agents to TRUE.

Sub-models for each time-step/tick

1. Go-age

This sub-model increases age of each agent by 1 day. If an agent's age in days exceed 365, its age in years is increased by one and age in days is reset to 1. If an agent crosses 74 years of age, it dies and a new MSM aged 16 years is born.

a. Update-lambda

This sub-sub-model is implemented to update the "new-partners-per-year" attribute of the MSM agents if their age in years changes. Every time an agent's age is changed, its 'new-partners-per-year' attribute is resampled from a new Poisson distribution based on its current age.

2. Change-relationship-status

This is a sub-model where each agent changes its relationship status using some probability that is based on its age, sex and sexual preference. These probabilities are calculated using the ‘new-partners-per-year’ agent attribute and are explained in the previous section. For example, if an agent has attribute ‘new-partners-per-year’ set to 2, then the probability that an agent will find a new partner on the day will be:

$$P(\text{BreakupToday}) = 1 - e^{(-1 \times \frac{(2+0.1)}{365})}$$

We random draw a floating-point number between 0 and 1, and if its less than $P(\text{BreakupToday})$, the agent will break up with its current partner (if any) and find a new partner. To break up and agent from its current partner, the sub-sub-model breakup is called.

a. Breakup

A sub-sub-model to change the relationship status of an agent, i.e., remove long-term link.

3. Get-partners

In this sub model, the agents who are single find new partners. A potential list of partners is selected based on following criterion:

- Age-cohort of the agent: An agent can only mix with other agents from other cohorts based on probability from the age-mixing matrix.
- Sexual preference of the agent: Homosexual agents can only get a partner from the same sex. Bi-sexual agents can get partners from any sex.

Once a list of potential partners is ready, the agents can randomly select one partner from within that list.

The following are the sub-sub-models:

- a. Initiate-hetero-relationship.
Called for heterosexual agents. A list of potential partners is made which contains agents of the opposite sex. A single partner is selected from the list based on the agents age and a long-term link is added between the two.
- b. initiate-homo-relationship.
Called for homosexual agents. A list of potential partners is made which contains other agents who are of the same sex. A single partner is selected from the list based on the agents age and a long-term link is added between the two.
- c. initiate-bi-relationship.
Called for bi-sexual agents. Whether an agent finds a same-sex partner, or an opposite sex partner is based on a probability (bi_prob_same_sex). If a same-sex partner is sought, a list potential partners is made which contains other agents who fit the criterion.

4. Superspreader Event

Whether or not today will be a superspreader event depends on the “SuperSpreaderEventsPerYear” parameter. The superspreader events are equally spaced and occur on same days for each simulation. For example, if the “SuperSpreaderEventsPerYear” is equal to 30, there will be approximated 30 events in a year, each around 12 days apart.

A subset of agents attends the superspreader event. This subset composed 35 randomly selected high-risk agents (homosexual and bi-sexual men in age cohort 20-36 years).

On a super spreader event, all attending agents form short term sexual contact with each other.

5. Travel

Every few days, one of the susceptible high-risk agents (homosexual and bi-sexual men in age cohort 20-36 years) travel abroad and acquire Mpox. The frequency of this is based on the ImportedCasesPerYear parameter. If the ImportedCasesPerYear parameter is set to 30, this means that only each 12th day, a random high-risk MSM will travel. If the agent is susceptible and not protected against the vaccine, the agent will acquire Mpox.

6. SEIR

This sub-model performs the following actions:

- Exposure

This part contains the following sub-sub-routines:

a. set-disease-status

This function is called several times and based on the argument (input parameter), changes the agent's disease-status to "Infected", "Exposed" or "Recovered".

b. contract-disease-normal

The long-term sexual contact of the infected agent gets exposed to the disease. The probability that the long-term sexual partner will be exposed to the disease is based on the transmission probability and weekly contact rate. It is defined by the following equation:

$$P(S \rightarrow E_L) = TP \times WC = \frac{1}{8} * \frac{3}{7} = 0.0535$$

where TP is the transmission probability (assumed 1/8 in our study) and WC is the weekly contact rate (assumed 3/7 in our study).

c. contract-disease-through-party

The probability that the short-term sexual partner will acquire the disease ($P(S \rightarrow E_S)$) is based on the transmission probability only, weekly contact rate is not considered because it is assumed that the agents will always have a sexual encounter on the superspreader event.

$$P(S \rightarrow E_S) = TP = \frac{1}{8}$$

A random uniform number is drawn between 0 and 1. If the drawn number is less than $P(S \rightarrow E_L)$ or $P(S \rightarrow E_S)$, the partner(s) is exposed to the disease.

- Recovery

If the sick-period of the agent is over, the agents enter the "Recovered" state. Else, the days_sick counter is incremented by 1.

This part is implemented through the following sub-sub-model:

i. Stay_sick

This routine increments the `days_sick` counter of the agent. Until `days_sick` is equal to `sick_period`, the turtle will remain infectious (`disease-status = 3`). Once `stay_sick` is equal to the `sick_period`, the agent will enter “recovered” state.

- Infection

This part is implemented through the following sub-sub-model:

i. stay-exposed

Each agent remains in the “Exposed” state before becoming infectious or showing symptoms. If the exposed-period of the agent is over, the agent state is changed to “Infected”. Otherwise, the `days_exposed` counter is incremented by 1. A person can be infectious for up to four days before symptoms emerge (Ward et al. 2022). To achieve this, a random number is drawn from a uniform distribution $U(0, 4)$ and subtracted from the incubation period. Assume that `Inc` represents the incubation period for an exposed agent. $Inc - U(0, 4)$ represents the time an agent remains in the “Exposed” state without becoming infectious. This subtraction is only carried out when the incubation period for an agent is less than 6 days, otherwise the time in “Exposed” state can get very close to zero or even be negative.

Following are the sub-models run to simulate the infectious disease outbreak. Some sub-models are run every time but some are run only when certain conditions are met.

7. Go-age

This sub-model increases age of each agent by 1 day. If an agents age in days exceed 365, its age in years is increased by one and age in days is reset to 1. If an agent crosses 74 years of age, it dies and a new agent aged 16 years is born. Every time an agents age is changed, its ‘new-partners-per-year’ attribute is resampled from a new Poisson distribution based on its new age.

8. Change-relationship-status

This is a sub model where each agents changes its relationship status using some probability that is based on its age, sex and sexual preference. These probabilities are calculated using the new-partners-per-year agent attribute and are explained in the previous section. For example, if an agent has attribute ‘partners-per-year’ set to 2, then the probability that an agent will find a new partner on the day will be:

$$P(BreakupToday) = 1 - e^{(-1 \times \frac{(2+0.1)}{365})}$$

We random draw a floating-point number between 0 and 1, and if its less than $P(BreakupToday)$, the agent will break up with its current partner (if any) and find a new partner.

Get-partners is another sub-model. In this sub-model, agents who are single find new partners. A potential list of partners is selected based on following criterion:

- Age-cohort of the agent: An agent can only mix with other agents from other cohorts based on probability from the age-mixing matrix.

- Sex and sexual preference of the agent: Heterosexual agents can only get partner from the opposite sex. Homosexual agents can only get a partner from the same sex. Bi-sexual agents can get partners from any sex.

Once a list of potential partners is ready, the agents can randomly select one partner from within that list.

9. Superspreader Event

Whether or not today will be a superspreader event depends on the “Superspreadereventsperyear” parameter. The superspreader events are equally spaced and occur on same days for each simulation. For example, if there the “SuperSpreaderEventsPerYear” is equal to 30, there will be approximated 30 events in a year, each around 12 days apart.

A subset of agents attends the superspreader event. This subset composed 35 randomly selected MSM agents (whose sex is male and sexual preference is either homosexual or bi-sexual) and within age-cohorts 2 to 5 (20-36 years old).

On a super spreader event, all attending agents form short term sexual contact with each other.

10. Travel

Every few days, one of the susceptible agents who are MSM between 20-36 years of age travel and acquire Mpox. The frequency of this is based on the ImportedCasesPerYear parameter. If the ImportedCasesPerYear parameter is set to 30, this means that only each 12th day, a random agent is selected who is MSM and is within age-bracket 20-36 years old will travel. If the agent is susceptible and not protected against the vaccine, the agent will acquire Mpox.

11. SEIR

This submodel has the following sub-submodels:

a. Exposure

All agents who are infected pass on the infection to their long-term. The probability that the long-term sexual partner will be exposed to the disease is based on the transmission probability and weekly contact rate. It is defined by the following equation:

$$P(S \rightarrow E_L) = TP \times WC = \frac{1}{8} * \frac{3}{7} = 0.0535$$

$$P(S \rightarrow E_S) = TP = \frac{1}{8}$$

where TP is the transmission probability (assumed 1/8 in our study) and WC is the weekly contact rate (assumed 3/7 in our study). The probability that the short-term sexual partner will acquire the disease ($P(S \rightarrow E_S)$) is based on the transmission probability only, weekly contact rate is not considered because it is assumed that the agents will always have a sexual encounter on the superspreader event. A random uniform number is drawn between 0 and 1. If the drawn number is less than $P(S \rightarrow E_L)$ or $P(S \rightarrow E_S)$, the partner(s) is exposed to the disease.

b. Recovery

If the sick-period of the agent is over, the agents enter the “Recovered” state. Else, the days_sick counter is incremented by 1.

Stay_sick: this routine increments the days_sick counter of the agent. Until days_sick is equal to sick_period, the turtle will remain infectious (disease-status = 3). Once stay_sick is equal to the sick_period, the agent will enter “recovered” state.

c. Infection

Each agent remains in the “Exposed” state before becoming infectious or showing symptoms. If the exposed-period of the agent is over, the agent state is changed to “Infected”. Otherwise, the days_exposed counter is incremented by 1. A person can be infectious for up to four days before symptoms emerge (Ward et al. 2022). To achieve this, a random number is drawn from a uniform distribution $U(0, 4)$ and subtracted from the incubation period. Assume that Inc represents the incubation period for an exposed agent. $Inc - U(0, 4)$ represents the time period an agent remains in the “Exposed” state without becoming infectious. This subtraction is only carried out when the incubation period for an agent is less than 6 days, otherwise the time period in “Exposed” state can get very close to zero or even be negative.

Miscellaneous Sub-models

The following two sub-models are run at the end of the simulation

1. TimeVaryingR

Calculates the time-varying reproductive number R_t (retrospectively).

2. CalculateR

Calculates the effective reproductive number R_e .

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Appendix I – Parameters

age-mix-agg

[0.747831829	0.177305409	0.049992136	0.014708313	0.007019141		
	0.001151133	0.001095006	0.00041946	0.000476774	0	0	0
	0	0]				
[0.231047208	0.490546778	0.185653325	0.057908237	0.022356877		
	0.007148993	0.003917986	0.001317601	0	0.000102724	0	0
	0	0]				
[0.127933614	0.21435767	0.4001897	0.14443666	0.078122539		
	0.019691981	0.009961396	0.002309779	0.002996109	0	0	0
	0	0]				
[0.076001244	0.16038241	0.280802333	0.262387001	0.116114574		
	0.034741706	0.037985451	0.021671947	0.003505733	0.000852436		
	0.005555166	0	0	0]		
[0.040796399	0.122034949	0.156768675	0.249481921	0.192635573		
	0.106408415	0.071892102	0.038002785	0.011678285	0.003363232	0.00496565	
	0.001972014	0	0]			
[0.046525192	0.10283495	0.130889686	0.115870047	0.192866939		
	0.161486445	0.133942873	0.064003387	0.024135176	0.019019923		
	0.003787471	0.002642426	0	0.002660646]		
[0.006346823	0.019760219	0.03678893	0.064084986	0.117526889		
	0.210149343	0.247059086	0.173584578	0.07977703	0.023804868		
	0.016404244	0	0.002626774	0	0.002781639]	
[0.012645278	0.01132567	0.075765226	0.07082388	0.13859355		
	0.117767443	0.180830415	0.22852376	0.108886271	0.021504307	0.0333342	
	0	0	0]			
[0.026439486	0.042959568	0.036182116	0.03214682	0.046332086		
	0.071440982	0.208081498	0.20870304	0.193550598	0.086363269		
	0.027714186	0.020086352	0	0]		
[0	0	0	0.077041259	0.12508842	0.160885877	
	0.045030504	0.225861297	0.137573529	0.178896382	0.042103777		
	0.007518954	0	0]			
[0	0	0.061103034	0.050863023	0.032146605	0.063440383	
	0.188836193	0.055444896	0.164926323	0.070105275	0.172241693	0.09067874	
	0.021798034	0.028415801	0]			
[0	0	0	0.150701142	0.018506024	0.019569801	0.063931694
	0.058109094	0.211889124	0.16732933	0.087347778	0.125179978		
	0.097436034	0	0]			
[0.045594308	0	0.026424301	0.052848602	0	0	0.023079258
	0.023580197	0	0.081017046	0.0779076	0.351577669	0.27334111	
	0.024811683	0.026424301]				
[0	0	0	0.064995283	0	0.066197868	
	0.115064423	0	0	0.073991064	0.286523556	0.393227806	0
]
[0	0	0	0	0	0	0
	0.324660919	0.283416828	0.522563003]			

lambda-hetero

New Partners Per Year Poisson Means for Heterosexual Men and Women

```
[[1.5916      1.1664 ]
 [1.418       0.7995 ]
 [0.8445      0.4307 ]
 [0.6163      0.4064 ]
 [0.5411      0.2946 ]
 [0.3972      0.1787 ]
 [0.2796      0.226   ]
 [0.3053      0.1435 ]
 [0.3566      0.1818 ]
 [0.2299      0.1191 ]
 [0.2379      0.07    ]
 [0.2239      0.047   ]
 [0.1136      0.0361 ]
 [0.0645      0.0065 ]
 [0.0496      0.0339 ]]
```

lambda-homo

New Partners Per Year Poisson Means for Homosexual Men and Women

```
[[1.7  1.7   ]
 [1.3  0.75  ]
 [0.625 0.4286 ]
 [3     0     ]
 [7.3333 0     ]
 [4.6667 0     ]
 [4.5    0     ]
 [6.6667 0     ]
 [0      1     ]
 [0      0     ]
 [1.3333 0     ]
 [0      0     ]
 [0      0     ]
 [0      0     ]
 [5      0     ] ]
```

lambda-bi-same-sex

New Same-Sex Partners Per Year Poisson Means for Bi-sexual Men and Women

```
[[0.9375      0.4444 ]
 [1.5238      0.5679 ]
 [0.6522      0.1667 ]
 [2.9231      0.1789 ]
 [1.05        0.1167 ]
 [9.3636      0.3077 ]]
```

```
[0.2727      0.1212 ]
[1.375       0.2059 ]
[0.2143      0.0714 ]
[0.0588      0.2105 ]
[0.7368      0.1      ]
[0.5417      0        ]
[0          0]
[0.25      0]
[0          0]
]
```

lambda-bi-opp-sex

New Opposite-Sex Partners Per Year Poisson Means for Bi-sexual Men and Women

```
[
  [0.6250      1.4889]
  [0.9524      1.5926]
  [ 1.1304      0.7619]
  [0.3077      0.6526]
  [1.0500      0.5833]
  [0.8182      0.5000]
  [2.0000      4.9091]
  [0.5000      0.7647]
  [0.2143      0.2143]
  [0.2941      0.1053]
  [0.2632      0]
  [0.5417      0.1818]
  [0          0.4286]
  [0.1250      0]
  [0          0]
]
```

bi_prob_same_sex

Probability of Bi-sexual Men and Women Forming Sexual Partnership with Same-sex

```
[[ 0.6000  0.2299]
```

```
  [0.6154  0.2629]
  [0.3659  0.1795]
  [0.9048  0.2152]
  [0.5000  0.1667]
  [0.9196  0.3810]
  [0.1200  0.0241]
  [0.7333  0.2121]
  [0.5000  0.2500]
  [0.1667  0.6667]
  [0.7368  1.0000]
  [0.5000   0]
  [ 0.5     0]
  [0.6667  0.5]
  [0.5     0.5] ]
```