<p style="text-align:center">Supplemental Material for:</p>

<p style="text-align:center">Pre-exposure Prophylaxis (PrEP) Strategies for African American Women</p>

<p style="text-align:center">Affected by Mass Incarceration: A Modeling Study</p>

Joëlla W. ADAMS, Ph.D.[1], Maria R. KHAN, Ph.D.[2], Sarah E. BESSEY, M.S.,[1] Samuel R. FRIEDMAN, Ph.D.[3], James M. MCMAHON, Ph.D.[4], Mark N. LURIE, Ph.D.[1], Sandro GALEA, M.D.[5], Brandon D.L. MARSHALL, Ph.D.[1*]

[1] Brown University School of Public Health, Providence, Rhode Island, United States of America

[2] Division of Comparative Effectiveness and Decision Science, Department of Population Health, New York University, New York City, New York, United States of America

[3] National Development and Research Institutes, New York City, New York, United States of America

[4] University of Rochester School of Nursing, Rochester, New York, United States of America

[5] Boston University School of Public Health, Boston, Massachusetts, United States of America

<p style="text-align:center">This Supplemental Digital Content includes additional information regarding the structure, parameterization, and results for the agent-based model. While not implemented formally or in full, the model description follows elements of the ODD (Overview, Design concepts, Details) protocol for describing individual- and agent-based models.[1, 2]</p>

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Study Purpose

The Treatment of Infection and Transmission in Agent-Based Networks (TITAN) model was developed to simulate HIV transmission dynamics within a mature epidemic setting. The TITAN model has previously been used to estimate the effect of combination intervention strategies in preventing HIV transmission, the impact of acute HIV infection on HIV transmission among people who inject drugs, and to detail HIV transmission dynamics within networks of injection drug use.[3-7] The model simulates HIV transmission, the natural history of HIV disease, as well as HIV screening and treatment. This analysis simulated the movement of men in and out of prison or jail to understand the complex dynamics between incarceration and HIV acquisition in women. This version of the model has been previously used to estimate the impact of mass incarceration on HIV acquisition among African American women and to evaluate interventions for HIV-infected African American men with a history of incarceration.[8] The objective of the present analysis was to identify which PrEP prescription strategies best offer protection to African American women living within an urban setting heavily impacted by mass incarceration

Agent Entities, State Variables, and Scales

Agent Population

The model consisted of agents representing individuals within the African American population of Philadelphia, Pennsylvania aged 18 years or older. As our study objective focused on heterosexual HIV transmission, our study population consisted of heterosexual women, heterosexual men, and men who have sex with men and women (MSMW). The 2010 U.S. Census reported that there were 267,998 African American women and 203,776 African American men living in Philadelphia aged 18 or older. The Philadelphia Department of Public Health estimated that there are 14,023 African American MSM in Philadelphia. Therefore, we subtracted 14,023 from the 2010 Census male population for a final heterosexual or MSMW male population of 189,753. The final target population of 457,751 was 41.4% male and 58.5% female. The model allowed for death and the entry of new agents to achieve an open population in steady state.

State Variables

Agents were stratified in two fundamental ways: sex (male vs. female) and injection drug use status (person who injects drugs (PWID) vs. non-PWID). Agents had both fixed and dynamic attributes (see **S1 Table**). Fixed attributes, including sex and sexual partner preference, did not vary over time within the model.

For this analysis, female agents could only engage in sexual relationships with male agents while male agents could engage in sexual relationships either with female agents (i.e., heterosexual) or with agents of both sexes (i.e., bisexual or men who have sex with men and women (MSMW)). Dyer et al. analyzed nationally representative data and found that 83 of 1,423 African American male respondents or 5.8% reported a history of sex with both men and women.[9] Therefore, 6% of male agents within our model were classified as MSMW and had twice the HIV incidence and prevalence rate compared to men who had sex with women exclusively.[10] We did not include male agents who exclusively have sexual relationships with other men (i.e., MSM) or female agents who exclusively have sexual relationships with other women as the focus of this study was on HIV acquisition via heterosexual HIV transmission.

Agents were classified as a PWID if they had engaged in injection activity within the past month, otherwise the agent was considered a non-PWID. This classification could change over time (i.e. an agent ceased or began to inject). For PWID agents, PWID-specific parameters always superseded the other sex-specific parameters where there was non-congruence. For example, monthly mortality estimates for PWID agents are much higher than for non-PWID male agents, and thus a male PWID will be assigned the PWID value for mortality. The probability of being assigned a given set of characteristics was determined based on Philadelphia HIV surveillance data (**S1 Table**). The Philadelphia Department of Public Health estimated in 2017 that 1.73% of the African American population were current injectors or PWID.[11] Therefore, 1.73% of African American women and 1.73% of African American men were classified as PWID at model initiation.

Dynamic attributes that could change over time included HIV serostatus, HIV diagnosis status, adherence to highly active antiretroviral therapy (HAART), AIDS status, pre-exposure prophylaxis (PrEP) status, PWID status, and incarceration status. Each agent was classified as either HIV-infected or HIV-uninfected. HIV-infected agents were either diagnosed or not, were on HAART or not, and, if on treatment, had an adherence level to HAART (0-29%, 30-49%, 50-69%, 70-89%, ≥90%) and AIDS-status (yes/no), dependent on HIV care engagement. HIV disease progression and treatment are described in more detail in the subsection titled "HIV Disease Progression and Treatment". Agents could be prescribed PrEP, described in more detail in the subsection titled "Pre-exposure Prophylaxis (PrEP)". Agents could be persons with current injection drug use (PWID) or non-PWID. Parameters related to injection drug use are described in more detail in the subsection titled "Injection Drug Use". All male agents could be classified by incarceration status as: a) never incarcerated, b) currently incarcerated, or c) having a history of incarceration. For the purposes of this analysis, female agents were not eligible to experience incarceration within the model. Details on the parameterization of incarceration and partner incarceration are further described within the subsection titled "Incarceration".

S1 Table. Fixed and time variant state variables of agents.

State Variable	Fixed	Time Variant	Data Source
Sex	X		2000 U.S. Census
Sexual Partner Type	X		Lieb *et al.*[12], Dyer *et al.*[9]
PWID Status		X	AACO
HIV Serostatus		X	AACO
HIV Diagnosis Status		X	Marks *et al.*[13]
HAART Adherence		X	AACO
AIDS Status		X	AACO
PrEP Status		X	assumed
Incarceration Status		X	Goldkamp *et al.*[14], PCS[15], Mauer *et al.*[16]

Abbreviations: PWID- person who injects drugs, AACO- AIDS Activities Coordinating Office within the Philadelphia Department of Public Health; HAART- highly active antiretroviral therapy; PCS- Philadelphia Commission on Sentencing

Time Scale

      Within the model, one time step represented one month and simulations were run for 168 months or 14 years. The model was calibrated using data on African American men and women living in Philadelphia from 2011-2015 and then used to project ten years into the future (i.e., 2015-2025). The first four years (i.e., start of 2011-end of 2014) were used as a "run-in" period. Outcome measures are reported as averages for the last 120 months (i.e., 10 years) of the model runs.

Process Overview and Sequence

The total workflow for the model is diagrammed in **S1 Fig**. Additional details are provided below.

Design

At each time step *t*, agents updated their state variables based on pre-programmed rules and interacted with other agents and the environment (i.e., prison/jail versus community). The sequence of workflow for the model was as follows: agents entered the partnering algorithm, agents interacted with other agents (i.e., sexual and injecting contact) within which HIV transmission could occur, state variables related to HIV and high-risk behavior were updated, male agents entered or exited correctional facility, state variables related to incarceration were updated, HIV-undiagnosed agents were eligible for HIV testing and to initiate PrEP, HIV-diagnosed agents were eligible to receive ART, all agents were eligible for death/replacement.

At each time step, all male agents not currently incarcerated were eligible to enter jail or prison. All actively incarcerated male agents at the beginning of the time step were eligible to be released from jail or prison if their sentence length had been served. Parameterization of incarceration rates and related risk behaviors are described in the subsection titled "Incarceration". While incarcerated, male agents were not eligible to interact with other agents (i.e., no sexual contact or sharing of injection needles or works could occur).

At model initialization and at each time step thereafter, a network was constructed such that each index agent *i* interacted (i.e., has sex with or injects with) *j* others in the agent population, where *j* is greater than or equal to zero. Agents connected to other agents via a sexual partnership could either be classified as being within a casual (<1 month relationship duration) or main (≥1 month duration) partnership within which unprotected or protected vaginal sexual intercourse could occur. Agents sharing an injecting relationship simulated an interaction where syringes or injecting equipment was shared. The value of *j* for each agent varied per time step, and was specified by a random variable sampled from a probability distribution function. During transitions between time-steps, agents stochastically formed relationship connections. Upon relationship formation, the relationship was given a fixed duration drawn from a distribution. With each time step, the duration was subtracted until the relationship expired, in which the edge or connection between the two agents was broken and the relationship dissolved. The empirical sources to inform these distributions and more detailed information on partnership rates are discussed in the "Sexual Risk Behaviors" subsection.

Initialization

At model initialization (i.e., at time *t*=0 of a simulation run), there were 110,000 agents, roughly a quarter of our target population of 457,751. Runs were made with a quarter of the target population due to computing constraints. State variables were set stochastically from probability functions and allowed to vary among simulations. Initial values were based on the published literature and HIV surveillance data from the city of Philadelphia. The model was initialized with an HIV prevalence of 1.6% for women based on 2011 HIV surveillance data for African American women living in Philadelphia. According to this same HIV surveillance report, 3.8% of African American men living in Philadelphia are living with HIV. However, this estimate includes MSM who have a higher overall HIV prevalence compared to heterosexual men. Since MSM were not explicitly modeled in this study, we prioritized ensuring that the simulated HIV incidence and prevalence among African American women reflected data from HIV surveillance, and calibrated male rates to reflect these trends. PWID agents had an HIV prevalence of 15% for both men and women based on HIV surveillance data for African American PWID in Philadelphia.[11]

Surveillance data on the proportion of individuals living with HIV with lab results indicating viral suppression and CD4 lab results indicating AIDS were used to parameterize the proportion of HIV-diagnosed individuals on HAART and AIDS prevalence. At model initialization, the proportion of agents assigned to incarceration was based on previously published estimates and described in greater detail within the subsection titled "Incarceration". Initial conditions are presented are presented in **S2 Table.**

S2 Table. **Initial model conditions representing start of year 2011.**

Variable	Base estimate				Data Source
	Male Agents	*Male PWID^a*	*Female Agents*	*Female PWID^a*	
Community size *(%)*	41.4%	1.73%	58.5%	1.73%	Calculated, U.S. Census 2010, Lieb *et al*.[12], AACO
HIV prevalence (%)	3.9%[b]	15%	1.6%	15%	Calculated, AACO
Proportion of HIV-infected individuals with HIV diagnosis	90%		90%		AACO
Proportion of HIV-diagnosed individuals on HAART (%)	45%		51%		Assumed/calibrated, AACO
AIDS prevalence	67%		57%		Calculated, AACO
Proportion incarcerated (%)	2.74%	Varied [c]	n/a	n/a	Estimated, Goldkamp *et al*.[14]

[a] PWID agents are a subset of the gender (male or female) agent class. Parameters are equivalent to that of the male or female agent class unless specifically noted.
[b] HIV surveillance data reported HIV prevalence for African American men including MSM.
[c] PWID agents had an annual probability of being incarcerated of 42.8% based on the Philadelphia NHBS-IDU 2015 survey.[17] This was not a race-specific estimate. The exact starting proportion varied slightly but was based on this probability.

HIV Care Engagement

Following the partnering algorithm, HIV-diagnosed agents were eligible to receive highly active antiretroviral therapy (HAART) and HIV-undiagnosed agents were eligible to undergo HIV testing. HIV-infected agents on HAART also had specific probability of discontinuation of care, which corresponds to ceasing HAART and experiencing viral rebound. The probability of receiving HAART was calibrated to historical trends in rates of viral suppression observed in Philadelphia from 2011-2015 using HIV surveillance data.

Agents initiating HAART were assigned an adherence value, A, in the time step following initiation. HIV surveillance data from AACO on the percentage of individuals living with HIV who are virally suppressed was used to parameterize the proportion of individuals who achieved ≥90% adherence (A ≥90%) to HAART. Agents that did not achieve ≥90% adherence were assigned to one of four other adherence quartiles (0-29%, 30-49%, 50-69%, 70-89%) with equal probability. We assumed that adherence was constant while an agent was on therapy. We also note that, in this model, we did not account for type of HAART regimen or the development of virologic resistance; as such, the effect of adherence on virologic suppression and subsequent risk of transmission represent mean values observed in the treated population, and do not account for an increased risk of transmission due to the development of virologic resistance. HIV transmission risk by HAART adherence level is discussed in detail within the section titled "HIV Transmission".

All agents who were not previously diagnosed with HIV were eligible to undergo HIV testing. The probability of HIV testing was determined using a probability function that resulted in an average of 3.43% of male agents and 3.93% of female agents without a known HIV diagnosis being tested monthly. This was held constant throughout the model runs. PWID agents had an increased likelihood of HIV testing and an average of 5.29% of PWID agents without a known HIV diagnosis were tested monthly.[17] HIV testing parameterization was specific to Philadelphia and was drawn from NHBS data.[17, 18] In addition to the assumption that the likelihood of HIV testing was constant over time, we also assumed that HIV testing had 100% sensitivity and specificity. Based on AACO surveillance data estimates for 2014-2016, our model assumed that 90% of individuals living with HIV were diagnosed.[11]

The discontinuation of HAART was parameterized using several national estimates. African Americans and women have been shown to have particularly high hazards of HAART discontinuation.[19, 20] In a longitudinal study of 753 men and women living with HIV (50% African American), Robison et al. estimated that 61% (n=298/492) of women and 59% (n=534/913) of African Americans discontinued HAART within twelve months of initiation.[19] Another longitudinal study of women living with HIV within the Women's Interagency HIV Study estimated that 25% of women discontinued HAART for at least six months during the study's five year follow-up. Within our model, HIV-diagnosed male agents on HAART had a 42% probability of discontinuing HAART per year while female agents on HAART had a 52% probability per year.[19, 20] PWID agents did not have a separate rate of HAART discontinuation due to lack of available of data to inform this parameter. Agents who discontinued therapy at time step j re-initiated care at any time $t > j$ at the same rate as those who are newly diagnosed. Parameter estimates related to HIV screening and treatment are presented in **S3 Table**.

S3 Table. Parameter estimates related to HIV screening and treatment.

Variable	Base estimate				Data Source
	Male Agents	*Male PWID[a]*	*Female Agents*	*Female PWID[a]*	
HIV testing (monthly %)	3.43%	5.29%	3.93%	5.29%	NHBS[17, 18]
Proportion of HIV-infected agents with HIV diagnosis	90%		90%		AACO
Proportion of HIV-diagnosed agents on HAART	Increases over time				AACO
Discontinuation of HAART (% per year)	42%		52%		Robison *et al.*[19], Adieh-Grant *et al.*[20]

[a] PWID agents are a subset of the gender (male or female) agent class. Parameters are equivalent to that of the male or female agent class unless specifically noted.

HIV Disease Progression and Mortality

A detailed description of HIV disease progression within the TITAN model has been published previously.[3] Following acute HIV infection, which lasts for 3 monthly time steps, based on previous data [21], HIV-infected agents with latent stage infection progressed to AIDS at a rate dependent on treatment enrollment status and adherence.[22-24] This approach assured that there was a large variation in time-to-AIDS for the HIV-infected agent population, but also has a notable limitation in that all agents may progress to AIDS with equal probability at each point following acute infection, meaning that a very small portion may progress to AIDS sooner than population-level estimate and clinical case-studies suggest.[25] However, these instances of early progression are very rare. The probability of progression to AIDS for each adherence category is listed in **S4 Table**.

S4 Table. Parameters and data sources for HIV disease progression and mortality.

Variable	Base Estimate			Source
	Male Agents	*Female Agents*	*PWID Agents*	
Progression to AIDS (annual probability)[a]				Egger *et al.*[22], Moss *et al.*[23], Porter *et al.*[24]
Not on ART		0.005		
0% – 29% adherent to ART		0.005		
30% – 49% adherent to ART		0.0039		
50% – 69% adherent to ART		0.0032		
70% – 89% adherent to ART		0.0025		
≥90% adherent to ART		0.0008		
All-Cause Mortality Rate (per 1,000 person-years)				
Among HIV negative agents	7.31	3.77	21.7	NCHS[26], Mathers *et al.*[27]
Among HIV positive agents, not on ART	16.5	16.5	65.1	Estimated: Siddiqi *et al.*[28], Mathers *et al.*[27]
Among HIV positive agents, on ART	7.31	3.77	43.4	NCHS[26], Siddiqi *et al.*[28], Lappalainen *et al.*[29]
Among Agents diagnosed with AIDS	33	33	65.1	Estimated: Siddiqi *et al.*[28], Mathers *et al.*[27]

Abbreviations: HIV – human immunodeficiency virus; HAART –highly active antiretroviral therapy, NCHS – National Center for Health Statistics.
[a] HIV surveillance data used to estimate the proportion of agents achieve ≥90% of adherence upon initiating HAART (the remaining proportion are assigned to four other quartiles [0% - 29%, 30% - 49%, 50% - 69%, 70% - 89%] with equal probability)

There was a baseline probability of all-cause mortality for each agent class, as well as an increased probability of all-cause mortality for HIV-infected agents, based on their AIDS status and HAART adherence. All-cause mortality for HIV-uninfected agents was calculated using age standardized mortality rates reported from the National Center for Health Statistics (CDC WONDER Online Database) for African American men and women aged 15-64 averaged from 2005 to 2014.[26] HIV-infected agents on HAART were assumed to have the same average mortality rate as HIV-uninfected agents based on the published literature.[30] Mortality rates for African-American men and women living with HIV not on HAART and diagnosed with AIDS were estimated based on a national study.[28] Mortality rates for PWID agents were derived from a recent systematic review and national data.[27, 29] The model did not directly estimate mortality as a result of HIV infection or AIDS, but rather assigned unique values for all-cause mortality based on disease and treatment status.

HIV Transmission

To model HIV transmission, we simulated the monthly number of unprotected (i.e., condomless) sexual and shared injection acts between pairs of connected, serodiscordant agents. We did not simulate male-to-male sexual behavior as this analysis focused on heterosexual HIV transmission. To account for the higher HIV incidence and prevalence among MSMW, we implemented a spontaneous source of HIV infection for MSMW that resulted in this population having approximately double the HIV prevalence and incidence of exclusively heterosexual men.[10]

For modeled relationships, the following was implemented: at every time step, the number of sex and injection acts for each agent was drawn from a Poisson distribution. We assumed that HIV-diagnosed agents were 50% less likely to engage in unprotected intercourse with their partners, based on prior literature.[31] We did not model changes in injection risk behaviors related to HIV diagnosis for HIV-diagnosed PWID agents based on data from a systematic review assessing changes in injection-related risk behavior following initiation of antiretroviral therapy.[32] We assumed that undiagnosed, HIV-infected agents engaged in sexual and injection risk behavior at the same probability as HIV negative individuals.

If a pair of serodiscordant agents engaged in sexual or injecting risk behavior, the model implemented a stochastic algorithm to determine whether HIV transmission occurred. To calculate the probability of HIV transmission to an uninfected partner, we used the per-act probabilities (β_a) shown in **S5 Table**, based on previously published estimates.[33, 34] We did not model unprotected anal intercourse between agents.

The probabilities listed in **S5 Table** represent the average risk of transmission during an unprotected vaginal sexual intercourse event or shared needles or works injecting event during chronic stage HIV infection. To account for higher viral load and an increased risk of transmission during acute phase infection, we multiplied these probabilities by a factor of 4.3 during the first three time steps following seroconversion, which represents the average increase in transmission risk during acute HIV infection.[35, 36]

In order to calculate the overall transmission risk per partnership per time step, β_p, we employed a Binomial process model,[37] i.e.:

$$\beta_p \sim Bin(n, \beta_a) = \frac{\beta_p!}{(\beta_p - n)!\, n!} \beta_a{}^{\beta_p}(1 - \beta_a)^{n-\beta_p}, \qquad \beta_p \epsilon \{1, \cdots, n\}$$

where β_a is the per-act transmission probability. These probabilities were also dependent on the HIV treatment status and adherence pattern of the HIV-infected partner. We modeled the relationship between HAART adherence and the suppression of viral replication implicitly, such that, for each adherence value (A), we assigned a different value for per-contact risk of HIV transmission $\beta_{a,A}$. As shown in **S5 Table**, higher values of HAART adherence reduced the per-event probability of HIV transmission. ART adherence levels ≥90% were a proxy for viral suppression as the probability of HIV transmission decreased to 0.0001 per unprotected vaginal sex act. These values have been estimated from previously conducted studies investigating the relationship between adherence and viral load,[38] as well as the effect of viral suppression on HIV transmission.[34]

S5 Table. Parameters and data sources for HIV transmission.

| Variable	Base Estimate		Source
	Male Agents	*Female Agents*	
HIV transmission risk per unprotected vaginal sex act (chronic phase) by adherence to HAART level			Gray *et al.*[33], Quinn *et al.*[34]
Not on HAART	0.0010		
0-29% adherent	0.0010		
30-49% adherent	0.0008		
50-69% adherent	0.0004		
70-89% adherent	0.0002		
≥90% adherent	0.0001		
HIV transmission risk per needle or works injection sharing act (chronic phase) by adherence to HAART level			Kaplan *et al.*[39], Baggaley *et al.*[40], Hudgens *et al.*[41]
Not on HAART	0.0070		
0-29% adherent	0.0070		
30-49% adherent	0.0056		
50-69% adherent	0.0028		
70-89% adherent	0.0014		
≥90% adherent	0.0002		
Increase in infectivity during acute stage infection	4.3		Bellan *et al.*[36], Wawer *et al.*[35]
Early phase duration (months)	3		Bellan *et al.*[36], Wawer *et al.*[35]

Sexual Risk Behaviors

Probability functions were approximated by the authors based on available data from surveys of sexual partnerships. The majority of these values were extrapolated from studies with published National HIV Behavioral Surveillance (NHBS) data and calibrated to fit the model's monthly time-steps.[18] To be included within the NHBS HET survey, participants had to be between 18 and 60 years of age, report vaginal or anal sex with an opposite sex partner in the 12 months before interview, report their gender either as male or female, and have been recruited from a poverty area or a U.S. Census tract where at least 20% of the residents live below the poverty threshold, and meet the definition of "low socioeconomic status (SES)", defined as having completed no more than a high school education or having a household income at or below the U.S. Department of Health and Human Services poverty guidelines.[18] For our model parameters, we used NHBS data for African Americans living in Philadelphia. Therefore, this definition overlaps closely with our modeled population (i.e., over the age of 18, heterosexual African American men and women). In a recent report, the Pew Charitable Trust used U.S. Census Bureau data to calculate that 88% of African Americans in Philadelphia live in a census tract where >20% of residents live below the poverty threshold.[42] While we are not able to exactly replicate the low SES definition, 31% of the total African American population of Philadelphia lives below the poverty threshold and 49% of all Philadelphia residents (including all races and ethnicities) have no more than a high school education.[42] Therefore, we feel that it is realistic to use the estimates from the NHBS-HET cycle for our modeled population.

In the NHBS survey, the median number of sexual partners per year and interquartile range (IQR) reported for African American men and women in 2013 was 3 (IQR: 1, 7) partners for men and 2 (IQR: 1,4) partners for women.[43] Parameters for PWID agents was based on national or Philadelphia-specific NHBS data for heterosexual African American injection drug users in 2015.[17]

These estimates were used to define a series of Poisson distributions. Upon agent creation, each agent has a "desired" target number of partners per year pulled from the Poisson distribution relevant to their category (i.e., male/female, PWID/non-PWID, high-risk/not high-risk.). Once a year, the agent's target number of partners for that given year is determined by drawing from a standard normal distribution with a mean centered at that "desired" target number. Therefore, we have two sources of stochastic variation in the number of partners. Notably, this target number of partners is not guaranteed to be satisfied through partnerships in the model at every time step. The agent may have more or less partners than the target. In addition, the target number is inclusive of partnerships that exist at the start of the year. Partner turnover and relationship duration were both tools for calibrating trends in HIV incidence. Implementing the partner numbers reported within the NHBS survey for non-PWID agents led to unrealistically high partner turnover. Therefore, the number of partners was calibrated and is more conservative than the number reported within the NHBS survey. On average, a male agent has slightly less than one current partner and gains a new partner every 1.5 years. Female agents have a slightly lower number of current and new partners.

Male to male sexual relationships were not explicitly modeled; however, 6% of male agents were classified as MSMW. Based on a meta-analysis by Friedman et al, MSMW agents had twice the HIV incidence and prevalence rate of the male agents who exclusively had sexual relationships with female agents.[10] Through modeling an increased risk of HIV for MSMW, we introducing potential "bridging" of the risk of HIV sexual transmission related to MSM-behavior to heterosexual women.[9, 10]

Assortative mixing is the increased likelihood of a relationship forming between individuals with similar probabilities for an outcome.[44] In this analysis, assortative mixing refers to agents being more likely to share a sexual relationship with an agent at a similar level of HIV-risk. Assortative mixing based on racial or ethnic background as well as sociodemographic attributes such as education level or substance use have been explored as potential drivers of HIV racial disparities.[44, 45] Since our agent population is racially homogenous (i.e., all African American), 100% assortative mixing based on race is implemented by default. However, other factors may determine assortative mixing, including stressful life experiences or discrimination.[46, 47] A network analysis based in Bushwick, Brooklyn found that nearly a quarter (23%) of persons reporting a partner with a history of incarceration had 2+ partners with incarceration history.[48] Therefore, we implement assortative mixing related to involvement with the criminal justice system within sexual networks in our model. Male agents with a history of incarceration had a 30% probability of forming a sexual partnership with a female agent who had experienced partner incarceration and vice versa. The partnering algorithm is diagrammed in **S2 Fig**.

S2 Fig. Partnering algorithm.
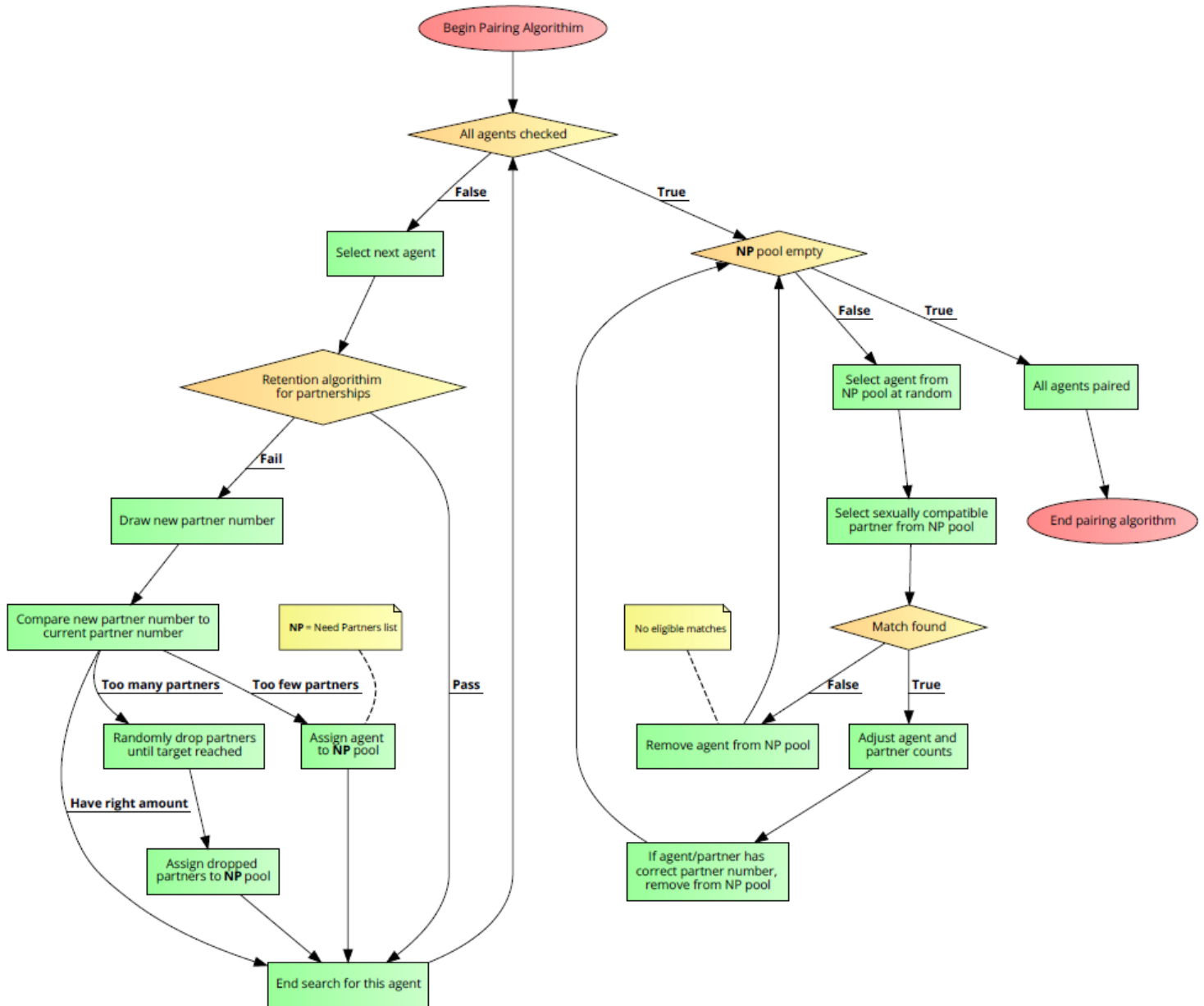
Agents who shared a sexual relationship in the network could engage in vaginal intercourse at each time step. To increase computational efficiency, only sexual activity between serodiscordant agents was simulated. Estimates for non-Hispanic African American men and women within the National Survey of Family Growth (NSFG), a national probability sample, was used to parameterize the mean and median number of times vaginal sexual intercourse was engaged in per time step.[49] The number of vaginal sex acts that a given dyad engaged in for a specific time step was determined stochastically using a Poisson-distributed estimate based on these parameters. Relationships (i.e., links) were either classified as main (lasting beyond one month or time step) or casual (lasting for only one month or time step). Relationship duration was informed by empiric data from the Seattle Sex Partner Survey.[50] The Seattle Sex Partner Survey interviewed 593 heterosexual men and women recruited from two sexually transmitted infection (STI) clinics for a longitudinal study from 1992 to 1995.[50] While a third of the sample was African American, race-specific estimates for the duration of relationships were not reported. Philadelphia-specific estimates for relationship duration and the mean and median number of vaginal sex acts were similarly not available. While the Seattle Sex Partner Survey was used as a starting point for parameterizing relationship duration, this survey likely includes more short-term relationships compared to the general population. Therefore, we calibrated relationship duration to approximate of partners per year reported by the NHBS-HET report for Philadelphia's African American population. The input distribution used for relationship duration is presented in **S6 Table**. At the initiation of every sexual relationship, the duration was pulled from this distribution.

The likelihood of unprotected vaginal intercourse was determined stochastically using a per-act probability based on empiric estimates from NHBS survey data.[43] We used national estimates from NHBS, which includes Philadelphia as one of the field sites, for

African American men and women interviewed in 2013. Within NHBS, men and women reported having unprotected sex 72% and 73% of the time with causal partners, and 89% and 92% of the time with main partners, respectively.[43] We averaged these probabilities within the model so that agents within casual relationships (defined as a relationship duration of less than one month or for only one time step) had a 72.5% probability of engaged in unprotected sex while agents within main relationships (defined as a relationship duration one month or more) had a 90.5% probability of engaging in unprotected sex. We followed the same procedure for creating the parameters for PWID agents based on national NHBS data for heterosexual African American injection drug users in 2015.[17] We assumed that that relationship duration, mean and median number of vaginal sex acts per month, and level of assortative mixing did not differ between PWID and non-PWID agents. Sexual behavior parameters and data sources are presented in **S6 Table**.

S6 Table. Parameter estimates for sexual behavior.

Variable	Base estimate				Data Source
	Male Agents	*Male PWID[a]*	*Female Agents*	*Female PWID[a]*	
Sexual partners over one year, median (IQR)	n/a	2 (1, 4)	n/a	3 (1, 15)	NHBS (national)[17]
Current partners at any one time point, mean (SD)	0.76 (1.04)	see above	0.72 (1.00)	see above	Calibrated
Cumulative new partners over 6 months, median (IQR)	0.30 (0.15-0.6)	see above	0.30 (0.08-0.53)	see above	Calibrated
Relationship duration	1-6 months (58.5%), 7-12 months (11.6%), 1-2 years (12.1%), 2-3 years (6%), 3-4 years (11.8%)				Calibrated
Mean number of vaginal sex acts per month (95% CI)	4.9 (4.3, 5.5)		4.9 (4.3, 5.6)		Leichliter *et al.*[49]
Median number of vaginal sex acts per month (95% CI)	2.5 (1.9, 3.0)		1.9 (1.5, 2.3)		Leichliter *et al.*[49]
Probability of unprotected sex with main partner (relationship duration ≥ 1 month)	90.5%	87%	90.5%	87%	Sionean *et al.*[43], NHBS (national)[17]
Probability of unprotected sex with casual partner (relationship duration <1 month)	72.5%	74.5%	72.5%	74.5%	Sionean *et al.*[43], NHBS (national)[17]
Assortative mixing	0.3		0.3		Estimated, Khan *et al.*[48]

Abbreviations: SD- standard deviation, IQR- interquartile range, CI- confidence interval

Injection Drug Use

Agents could initiate or cease injection drug use at any time step. PWID had a 0.2% chance of spontaneous drug use cessation, based on previous research, at which point they joined the non-PWID agent class.[51] The probability that an agent transitions to injection drug use (i.e., the PWID agent class) was calibrated to reflect the empirical PWID prevalence among African Americans in Philadelphia from 2015 HIV Surveillance data which was estimated to be 1.73% of the total population.[11]

Unless otherwise indicated, PWID agents retained the parameters of either male or female agents. Parameters that differed for PWID include: HIV incidence and prevalence, mortality rate, probability of incarceration, proportion of sex acts which are unprotected within main and casual relationships, median number of sex partners per year, and the probability of HIV testing based on previously published research on PWID within Philadelphia from NHBS or national studies. In addition, there were parameters related to injection risk behaviors and primarily parameterized using NHBS data from the IDU 2015 cycle in Philadelphia. These were gender- but not race-specific estimates due to limited sample size. Parameters related to injection drug use are presented in **S7 Table.**

S7 Table. Parameters related to injection drug use.

Variable	Base estimate		Data Source
	Male PWID Agents	*Female PWID Agents*	
Receptive sharing of syringes, injecting equipment, or using a syringe to divide drugs (annual probability)	69%	63%	NHBS IDU-2015 Philadelphia
Median number of injection partners in past year with receptive syringe sharing (Q1, Q3)	2 (1, 3.5)	3 (1, 3)	NHBS IDU-2015 Philadelphia
Mean number of needle-sharing acts per day	4	4	Johnson *et al.*[52]
Probability of cessation of injection drug use per month	0.2%		Galai *et al.*[51]

Incarceration

Incarceration was implemented according to the following processes and parameters. We defined incarceration inclusively as being held in a prison or any other kind of detention facility for at least a month or longer. We were not able to account for short-term (i.e., <1 month) jail stays in this model. This definition is consistent with previously published agent-based modeling analyses of incarceration.[53, 54] As such, we assumed that the effect of incarceration on HIV treatment outcomes and agent behavioral processes does not vary across correctional environments. In other words, the parameter values reflect average incarceration experiences.

At model initialization, the proportion of agents assigned to incarceration was based on previously published estimates. In 2006, the Crime and Justice Research Center at Temple University submitted a report to the City of Philadelphia characterizing the demographic makeup of incarcerated individuals within the Philadelphia Department of Corrections.[14] At the end of November 2005, there were 8,541 individuals confined within the Philadelphia Prison system serving out sentences, awaiting bail or sentencing, detained on probation or parole violation, held on a bench warrant or held for another reason. We excluded 300 prisoners who were transferees from Delaware Country (n=8,241). Approximately 90% of inmates were men and 73% were African American, resulting in approximately 5,414 African American male prisoners. Using this count as the numerator and the U.S. Census 2000 count for the number of African American men over the age of 18 as the denominator (5,414/191,525), we estimated that between 2.7-2.8% of Philadelphia's African American male population was currently incarcerated at model initialization. This proportion was similar to other reported estimates (2.79% in 2005, 3.27% in 2010) for African American men from the state of Pennsylvania.[16, 55] PWID agents had an extremely high probability of incarceration (42.8% annual probability) based on Philadelphia's NHBS-IDU 2015 survey. This estimate was not race-specific. We implemented an HIV prevalence rate ratio of 5.0 comparing currently incarcerated men compared to non-incarcerated men based on national estimates.[56] This resulted in HIV-infected agents being more likely to experience incarceration throughout the study period compared to HIV-negative agents. For the *status quo* scenario, between 7.1 and 7.8% of the currently incarcerated population is HIV-infected, and this proportion generally remained stable over time. This proportion is higher than that observed in a rapid opt-out HIV testing study conducted in Philadelphia jails (estimating the HIV prevalence to be 3-4%); however, this study did not stratify by race, which may explain the difference between this estimate and the simulated prevalence in our model.[57]

A 2007 report from the Urban League of Philadelphia reported detailed information on sentence lengths and incarceration rates per 100,000 people for African American men in Philadelphia using 2006 data from the Philadelphia Commission on Sentencing.[15] Rates of incarceration and sentence lengths were reported by type of correctional facility (jail vs. prison) and recidivism status (first-time offender vs. prior incarceration). For example, the annual rate of incarceration in prison per 100,000 people for those with a prior record was 251 per 100,000 for African American men. These rates and sentence lengths were used to parameterize incarceration within the model and held constant through model runs (i.e., we modeled a constant rate of incarceration as race-specific rates and sentence lengths were not available for each year within the study period). Rather than using one summary rate of incarceration, we used four annual rates of incarceration: two rates specific to jail (for first-time offenders and those with a prior record) and two rates specific to prison (first-time offenders and those with a prior record). The duration of sentences was also derived from distributions specific to jail or prison. Sentence lengths did not differ by PWID-status or by recidivism status.

When an agent became incarcerated, we assumed that all sexual contact with other agents temporarily ceased. Thus, while an HIV-infected agent is incarcerated, HIV transmission cannot occur. Since our focus was on community HIV incidence, we did not model HIV transmission between incarcerated agents. Main relationships (≥1 month in duration) could be maintained during incarceration, but had a 50% probability of dissolving during incarceration, based on previous research that reported relationship dissolution percentages of 30% and 50%.[58, 59] If the relationship was maintained during incarceration, the number of vaginal sexual intercourse acts per month was set to 0 (i.e., sex during conjugal visits was not modeled). Based on previously published research on HIV testing within Philadelphia correctional facilities and a systematic review on the HIV care continuum, we assumed that 69% of agents were tested for HIV at intake throughout the study period.[57] During incarceration, 40% of men with diagnosed HIV were assumed to achieve viral suppression.[60] These parameters were held constant throughout the study period.

Within the model, incarceration was programmed to directly impact sexual risk behavior and HIV care engagement. These behaviors were parameterized using observational studies on the impact of incarceration and partner incarceration.[60-64] Women were only eligible to experience increased risk behavior if the incarcerated partner was a main partner (i.e., relationship ≥1 month). The average duration of risk behavior for women was either six months following a relationship's dissolution or throughout a partner's incarceration, whichever was applicable. Within this model, 30% of women with incarcerated partners initiated high-risk behavior

immediately upon the partner's incarceration. In addition, if a relationship dissolved during a partner's incarceration, a female agent had a 50% probability of entering the high-risk group. The remaining women maintained the same risk profile they had before a partner's incarceration. Limited information was available on the proportion of women with incarcerated partners who increase sexual risk behaviors or the average duration of high-risk behavior. For women, high-risk behavior related to partner incarceration consisted of increasing the cumulative number of new sexual partners over a six month period from a median of 0.30 (interquartile range [IQR]: 0.08, 0.53) to a median of 5.3 (5.1-5.5). This increase was informed by an observational study of women with recently incarcerated partners that reported an average of 3.25 (standard deviation=3.25) new partners by ten months.[61]

Women with an incarcerated partner in the past year are over twice as likely to have a current STI compared to women without a recently incarcerated partner.[65] STI prevalence is also higher among men with a recent incarceration compared to those without a history of incarceration.[48, 65, 66] A current STI increases the likelihood of HIV acquisition: ranging from a two-fold increase with bacterial vaginosis to a six-fold increase with *N. gonorrhoeae*.[67] Therefore, based on this literature, we doubled the likelihood of HIV transmission per unprotected vaginal sex act for high-risk individuals (men and women) to account for this increased likelihood of a current STI. This probability is also dependent on the HIV-infected agent's adherence to HAART. For example, if the HIV-infected agent is treatment-naive, the base estimate for HIV transmission risk per unprotected vaginal sex act is 0.001.[33, 34] This probability doubles to 0.002 for men and women impacted by incarceration or partner incarceration for the duration of the high-risk period.

High-risk behavior related to incarceration for male agents initiated upon release from prison or jail. Based on a set of studies published on Project START, an HIV-prevention program focused on reducing HIV/STI risk in young men following release from prison, the simulation modeled an increase in the cumulative number of new sexual partners over six months from a median of 0.30 (IQR: 0.15-0.60) to 5.2 (5.1-5.3). This increase was informed by PROJECT START studies which reported an average of 1.8 new partners per month.[63, 64] All male agents who were released from prison or jail underwent this high-risk period. HIV acquisition risk was also doubled in this period to reflect the increased likelihood of a current STI related to the post-release period. In addition, HIV-infected men were less likely to be retained in HIV care post-release.[68] A recent systematic review of U.S. data found that 40% percent of prisoners are on HAART while incarcerated, while only 21% remain on HAART after release.[60] In our model, we set the probability of initiating HAART (for agents newly diagnosed at entry) such that overall treatment coverage was 40% in the correctional environment. Agents already on HAART and those newly diagnosed at entry could discontinue therapy upon release. Specifically, in the model, the probability of discontinuing HAART after release was estimated to be $1 - 0.21/0.40 = 0.475$ by six months post-release.

Once an incarcerated agent served his sentence length, he was returned to the eligible pool of agents and sought to re-establish links with partner(s). First, the previously incarcerated agent re-formed links with partner(s) he had prior to incarceration. To do so, the simulation took a snapshot of the existing relationships at the time of incarceration and stored this information. In the next time step following release, the model compared the number of partners the formerly incarcerated agent's partner(s) had with the drawn value(s) for $j_{i,t}$. If the current number exceeded $j_{i,t}$, partnerships were dissolved at random until that number was obtained. If the formerly incarcerated agent was dropped from that partner's network, the formerly incarcerated agent became eligible to form new partnerships. Thus, agents returning to the "community" may either resume old relationships or establish new relationships.[69]

In summary, incarceration in the model directly affected sexual networks through the disruption of existing partnerships and acquisition of new ones, which been demonstrated in prior studies, and is thought to play an important role in perpetuating HIV transmission in communities with high rates of incarceration.[70-72]

Assortative mixing related to incarceration and partner incarceration resulted in the creation of higher-risk sexual networks. Increased rates of partner concurrency and relationship turnover emerged as result of these changed behaviors rather than as a result of programmed parameters. In addition, incarceration negatively impacted HIV care engagement for men living with HIV and both incarceration and partner incarceration increased the likelihood of HIV transmission and acquisition. Parameters and data sources related to incarceration are presented in **S8 Table**.

S8 Table. Parameters and data sources for the impact of incarceration or partner incarceration.

Variable	Base estimate			Data Source
	Male Agents	*PWID Male Agents*	*Female Agents*	
Proportion currently incarceration (%)	2.7-2.8%	See below	n/a	Calculated: Goldkamp *et al.*[14], Mauer *et al.*[16], Sakala *et al.*[55]
Annual probability of incarceration (%)	n/a	42.8%	n/a	NHBS IDU-2015 Philadelphia
HIV prevalence rate ratio for incarcerated vs. non-incarcerated men	5.0		n/a	Maruschak *et al.*[56]
Annual rate of incarceration in jail per 100,000 people for first-time offenders	100		n/a	PCS[15]
Annual rate of incarceration in jail per 100,000 people for those with a prior record	276		n/a	PCS[15]
Average length of minimum jail sentence (months)	8		n/a	PCS[15]
Average length of maximum jail sentence (months)	21.6		n/a	PCS[15]
Annual rate of incarceration in prison per 100,000 for first-time offenders	75		n/a	PCS[15]
Annual rate of incarceration in prison per 100,000 for those with a prior record	251		n/a	PCS[15]
Average length of minimum prison sentence (months)	45.6		n/a	PCS[15]

Average length of maximum jail sentence (months)	96	n/a	PCS[15]
HIV testing in correctional facility (probability upon intake)	69%	n/a	Beckwith et al.[57]
Percent of HIV-infected inmates on HAART while incarcerated	40%	n/a	Iroh et al.[60]
Percent of main relationships dissolving during incarceration	50%	n/a	Khan et al. 2011[58], Khan et al. 2018[59]
Current partners at start of high-risk period, mean (SD)	0.84 (1.2)	1.8 (1.5)	Calibrated
Cumulative new partners over 6 months, median (IQR)	5.2 (5.1-5.3)	5.3 (5.1-5.5)	Calibrated
Increase in HIV acquisition risk due to current STI	Doubled	Doubled	Rogers et al.[65], van de Wijgert et al.[67]
Percent of HIV-infected inmates maintained on HAART at six months post-release	21%	n/a	Iroh et al.[60]

Abbreviations: n/a- not applicable; PCS- Philadelphia Commission on Sentencing

ª All male agents released from prison or jail are high-risk for six months following release. 30% of women with a main partner who is incarcerated are high-risk immediately upon a partner's incarceration and 50% are high-risk if the relationship dissolves during a partner's incarceration.

Pre-exposure Prophylaxis (PrEP)

After a four year burn-in period, HIV-negative agents who meet certain eligibility criteria can initiate PrEP. The focus of the modeled PrEP strategies was on PrEP for women, although we included a scenario that prescribed PrEP to couples upon release (PrEP scenarios are described in detail within the "*Status Quo* and Intervention Scenarios" subsection).

Limited data are available reporting PrEP coverage levels, adherence, and retention specifically for heterosexual African American women in the United States. Exact estimates for the number of individuals on PrEP in Philadelphia are not available; however, reports from public health and community-based agencies suggest that PrEP is underutilized. Philadelphia FIGHT, the city's largest HIV/AIDS service organization, reported 250 active PrEP users as of September 2016.[73] In addition, while over 700 people have been referred to the Philadelphia Department of Public Health's free PrEP prescription program, only 170 have enrolled. Therefore, the *status quo* scenario does not include any prescription of PrEP by any agent to reflect the very low levels of use within this population.

We utilized published data from clinical trials of serodiscordant couples in Africa as well as smaller studies within the United States to parameterize the protection conferred by PrEP, PrEP adherence levels, and the probability of PrEP discontinuation. Large scale clinical trials based in Africa were used to parameterize the average reduction in HIV acquisition risk by the individual's adherence level (suboptimal vs. optimal adherence).[74-76] Once-daily Truvada efficacy was between 62-71%; however, a reduction of the relative risk of HIV infection of more than 85% was achieved among those with detectable tenofovir levels.[74] Within our model, 80% of agents on PrEP are assumed to be highly adherent (equivalent to 6-7 doses/week), and therefore, have a 94% reduction in relative risk of HIV acquisition. The remaining 20% of agents on PrEP fail to achieve high adherence, and therefore, only have a reduction of 59%. Adherence was based on data reported on female participants in a real-world study based in northern California.[77] Within this study, 13% of all participants had a PrEP adherence <80% based on pharmacy refill. The authors note that African Americans and women were less likely to have high adherence.[77] However, only twenty women were included in the final study. Another study based in the Bronx, New York provided PrEP for periconception or pregnant women. Half of the sixteen women who took PrEP had adherence challenges including side effects, social stressors, and difficulty adhering to a daily pill.[78]

Once an agent begins PrEP, they have a 15% probability of discontinuing per month. This results in agents being on PrEP for an average of six months. This discontinuation probability was informed by data on retention published by a study based out of Bronx sexual health clinic with a majority African American and Latina female patient population.[79] The authors reported that 61% of women prescribed PrEP were retained at three months and 38% at six months.[79] Parameters related to PrEP are summarized in **S9 Table**.

S9 Table. **Parameters and data sources for PrEP prescription for women within the United States.**

Variable	Estimate	Data Source
Efficacy of PrEP (percent reduction of the relative risk of HIV acquisition)	94% with high adherence 59% with suboptimal adherence	Baeten et al.[74], Thigpen et al.[75], Cottrell et al.[76]
Adherence to PrEP	80% high adherence (6-7 doses/week) 20% suboptimal adherence	Marcus et al.[77], Seidman et al.[78]
Probability of discontinuing PrEP per month	15%	Blackstock et al.[79]

Status Quo **and Intervention Scenarios**

        The model and parameters described above and summarized in S1-S9 Tables were used to generate the *status quo* model. Specifically, outputs from the *status quo* model represent HIV incidence and HIV prevalence estimates (per 100,000 persons) for Philadelphia from 2015-2025 as predicted by current trends and without the use of PrEP. In the accompanying manuscript, we describe the average HIV incidence and number of HIV transmissions for this 10-year period. Given the stochasticity inherent in these models, the *status quo* case was repeated 400 times with a quarter of the total population size (n=110,000) in order to obtain stable point estimates.

        For this analysis, we projected how HIV incidence would be impacted by hypothetical interventions by varying levels of PrEP coverage for men and women impacted by incarceration or partner incarceration or guided by CDC criteria. Specifically, the following targeting strategies were modelled:

1. **Recently Incarcerated Intervention:** Simulated an intervention in which women with a male partner entering a correctional facility initiate PrEP. PrEP initiation commences within one month of a partner's incarceration, independent of woman's high risk status.
2. **Recently Released Intervention:** Simulated an intervention in which women who are in an existing partnership with a male partner who leaves a correctional facility as well as women who initiate a relationship with a male partner who has left a correctional facility in the past six months initiate PrEP. PrEP initiation commences when the partner leaves the correctional facility (if an existing relationship) or when the relationship begins (if a new relationship).
3. **Couples-based PrEP Intervention:** Simulated an intervention in which couples (men and women, serodiscordant with an HIV-infected male partner or both HIV-negative) initiate PrEP when the male partner leaves a correctional facility.
4. **CDC Guideline Based Intervention:** Simulated an intervention in which women initiated PrEP if they began a relationship with a male partner who: a) has been diagnosed with HIV, b) is currently injecting drugs, or c) has sex with other men.

We varied the probability of PrEP initiation for eligible agents (criminal justice informed scenarios) or population coverage (for the CDC guideline scenario) to 10%, 30%, 60%, and 100%. For each of the scenarios, agents selected to initiate PrEP are randomly selected (i.e., selection was not based on sexual risk behaviors). PrEP adherence and retention levels did not systematically vary across scenarios within the main analyses.

Analyses based on the above three scenarios were run 400 times with ¼ population size (n=110,000).

Uncertainty Analyses

Uncertainty analyses were performed to evaluate the robustness of the model results to uncertainty in the input parameters. Specifically, we conducted uncertainty analyses decreasing adherence, varying retention on PrEP, and decreasing incarceration rates. These parameters are summarized in **S10 Table.** Each uncertainty analysis was run 100 times with ¼ the total population size (n=110,000).

S10 Table. Parameters varied within uncertainty analyses.

Variable	Estimate		
	Lower Bound	*Upper Bound*	*Base*
Percent with optimal adherence to PrEP	0.50	n/a	0.80
Monthly probability of discontinuing PrEP	8%	30%	15%
Incarceration rates (reported in S8 Table)	-25%	-50%	100%

Uncertainty analyses decreasing the incarceration rate necessitated re-running the status quo scenario with a lower rate. Because agents with HIV were more likely to be in the community rather than correctional settings (where HIV transmission could not occur), the number of transmissions increased. The impact of decreasing incarceration rates on the percent of agents who experienced incarceration or partner incarceration over the ten-year period and the number of HIV transmissions within the scenarios are summarized in **S11 Table.**

S11 Table. Model output resulting from decreasing incarceration rates within uncertainty analyses.
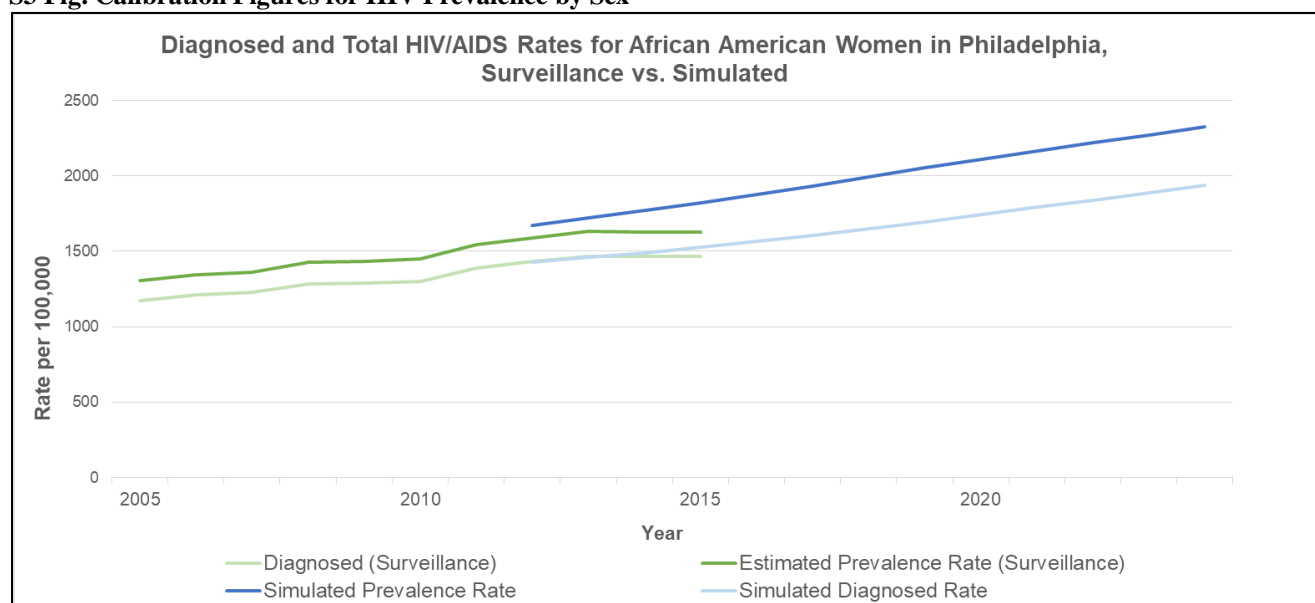
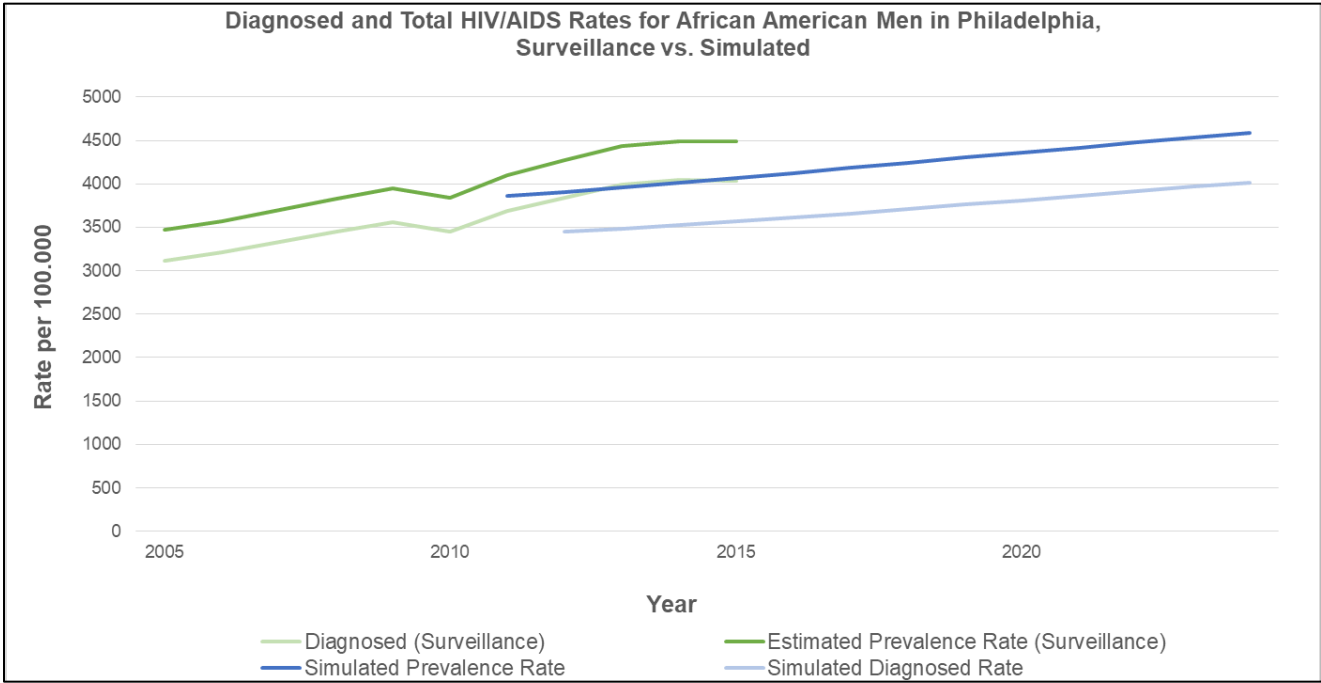| Model output	Analysis		
	Incarceration Rate 100% (Main)	*Incarceration Rate -25%*	*Incarceration Rate -50%*
Percent of total male population who experienced incarceration at the end of ten years	12.2%	9.4%	6.5%
Percent of HIV-infected male population who experienced incarceration at the end of ten years	35.2%	28.5%	19.8%
Percent of total female population who experienced partner incarceration at the end of ten years	2.9%	2.3%	1.7%
Total number of HIV transmissions in status quo (no PrEP for any agent)	2380 (2207-2559)	3766 (3314-4628)	4603 (3419-5981)
Averted HIV transmissions when prescribing PrEP for 30% of partners of **recently incarcerated** men, n (%)	54 (2%)	226 (5%)	373 (8%)
Averted HIV transmissions when prescribing PrEP for 30% of partners of **recently released** men, n (%)	496 (15%)	717 (19%)	969 (21%)
Averted HIV transmissions when prescribing PrEP for 30% of **couples** at release, n (%)	81 (2%)	235 (6%)	418 (9%)
Averted HIV transmissions when prescribing PrEP for 30% of women eligible according to **CDC** guidelines, n (%)	236 (7%)	396 (11%)	654 (14%)

Model Calibration

      To calibrate the model, we employed an iterative indirect approach, following previously published recommendations.[80] First, the set of empirical behavioral and risk parameters were applied to the model agents, and preliminary outputs (e.g., HIV incidence among specific groups, agent class distributions) were assessed and compared to historic datasets.
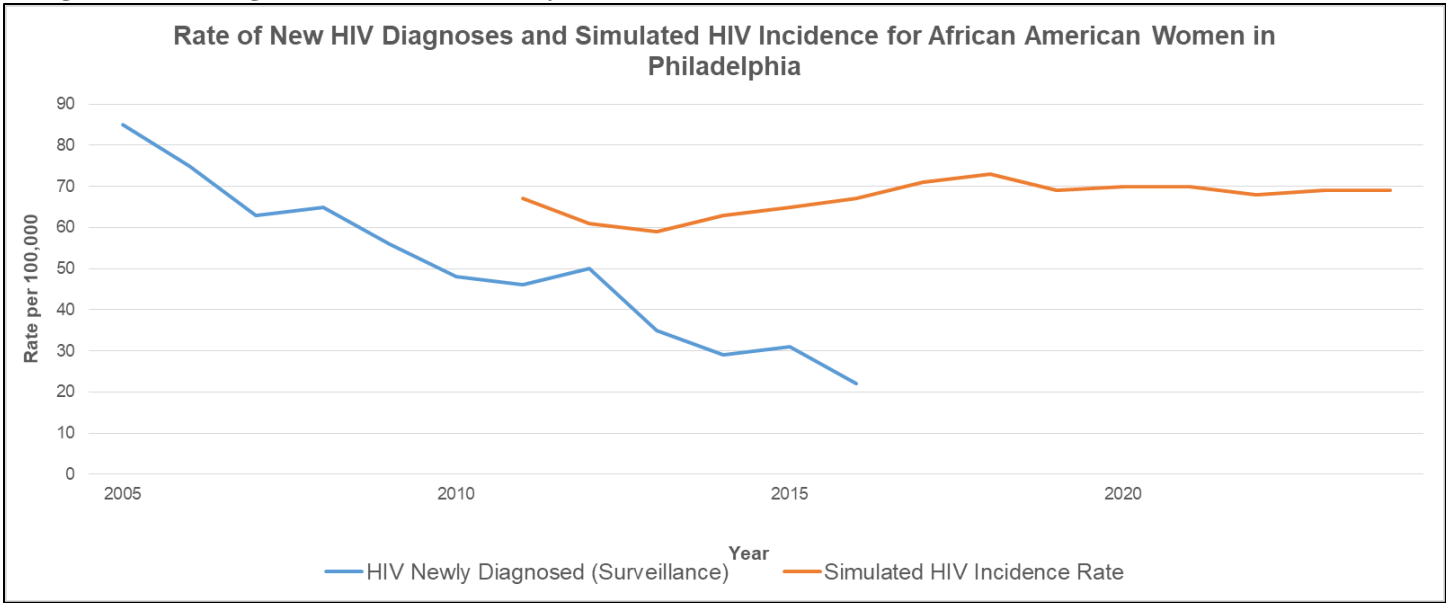
      S3 Fig compares HIV/AIDS prevalence and diagnosed HIV rates for African American men and women according to surveillance and that which was simulated by the model. We calibrated our model to prioritize trends in HIV prevalence for women. Simulated male diagnosis and prevalence rates (see **S3 Fig**) were lower than that reported by HIV surveillance due to inclusion of MSM within health department statistics. Using HIV surveillance data from 2012 and the 2010 U.S. Census, we estimate that approximately 2.5% of heterosexual African American men were living with HIV in 2012. The HIV prevalence rate at model initialization was 3.8% for African American men. However, male agents in the model include MSMW who had double the HIV incidence and prevalence rates of exclusively heterosexual men. Therefore, modeled prevalence rates are higher than these estimates for heterosexual men. Due to uncertainty of the percentage of prevalent HIV infections are among exclusively MSM vs. MSMW vs. exclusively heterosexual men, we prioritized ensuring HIV transmissions among women within our model reflected the numbers reported by surveillance reports. **S4 Fig** compares HIV incidence for African American men and women according to surveillance reports and simulated within the model. In 2015, 171 of 231 or 75% of the African American men newly diagnosed with HIV were MSM (https://www.phila.gov/documents/hiv-aids-data-and-research/). Therefore, HIV transmissions to male agents should represent approximately a quarter (25%) of that reported in HIV surveillance reports, which is indeed what is shown (see **S4 Fig**).
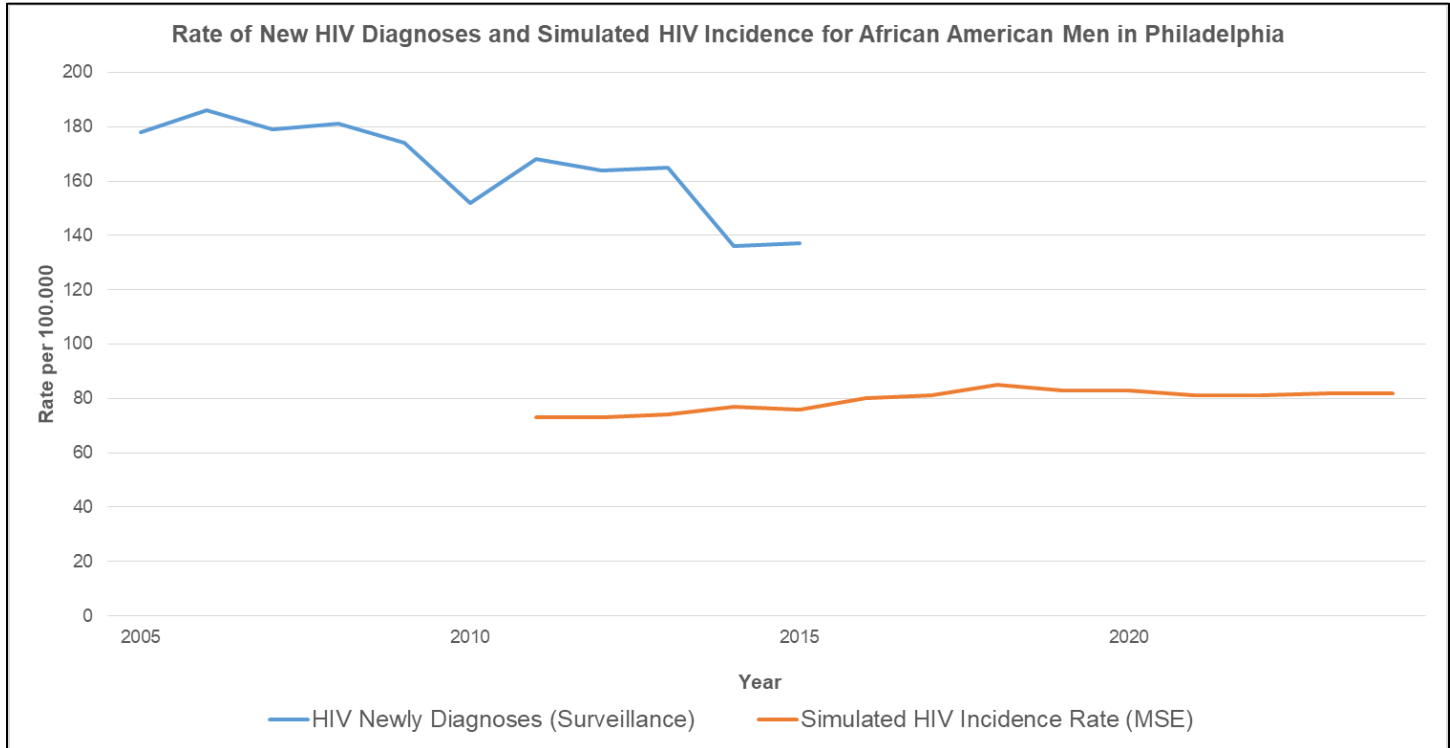
S3 Fig. Calibration Figures for HIV Prevalence by Sex

Diagnosed and Total HIV/AIDS Rates for African American Women in Philadelphia, Surveillance vs. Simulated

Diagnosed and Total HIV/AIDS Rates for African American Men in Philadelphia, Surveillance vs. Simulated

S4 Fig. Calibration Figures for HIV Incidence by Sex

Rate of New HIV Diagnoses and Simulated HIV Incidence for African American Women in Philadelphia

Rate of New HIV Diagnoses and Simulated HIV Incidence for African American Men in Philadelphia

Legend: — HIV Newly Diagnoses (Surveillance)   — Simulated HIV Incidence Rate (MSE)

Sweeping sensitivity analysis was performed to determine the model stability regarding key parameters, including the distribution of agent classes, HIV prevalence, HIV incidence, and incarceration prevalence over the simulation run time. These stress tests allowed us to measure qualitative and quantitative effects of core parameters, and through this we determined input variables that held the most significant changes in model outputs.

Model refinement was then conducted by adjusting key parameters for which there existed greater uncertainty in their values (e.g., frequency of condomless vaginal intercourse, monthly probability of HIV testing for specific agent classes) to minimize differences between model output and key historic information. Specifically, we focused on fitting the data to multiple outputs, including HIV incidence by agent class (e.g., gender), HIV prevalence by agent class, and HIV diagnosis rates per 100,000 population per year. We then ran a series of revised simulations and continued this process iteratively, until each set of model output approximated the historic data. Although this process does not necessarily guarantee model validity, it does permit the exclusion of parameter values that do not adequately reproduce the empiric data.[80] Well documented and previously published calibrated outputs for other variables of interest (e.g., HIV disease progression rates) remained unchanged.[81, 82]

Technical Details

The model was coded, tested, and calibrated in an open-source programming language (Python™ version 2.7.2). The simulation generated an agent matrix of 110,000 agents of varying classifications and substrata, which were managed by independent Python dictionaries. At each time step, information on the current agent state and each agent's partners were recorded, agents were assigned partners using the methods described above, and then interacted with each other along their network edges. All agents performed their acts simultaneously during a time step, requiring careful consideration to the order of operations and transition of states of each agent at this time. Agents then engaged in HIV treatment and were incarcerated, followed by a "die and replace" algorithm. This process was continued iteratively until the desired simulation time was met.

The program was run on a Beowulf supercomputing cluster consisting of multiple computer nodes and one head node, each with quad-core Intel™ CPUs and at least 8 GB of RAM. The *status quo* and counterfactual models were run for a duration of 168 time steps (14 years). The first 48 time steps (4 years) were omitted from final results to as this period was necessary in order to reach a steady-state and accurately reflect historical trends in empirical data for the status quo model. Results from the final 120 time steps (10 years) averaged over a total of 200 unique runs, each with a stochastically generated population following the parameters provided in S1-S10 Tables. Average runtime for a complete single iteration of the model was approximately 45 minutes.

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