A Supplementary Information

A.1 The invasion of a CMS mutation without considering pollen limitation (Model 1)

Let Y be a dominant nuclear female-sterility mutation. Let c be the cytotype carrying the male-sterility mutation and n be the male-fertile cytotype. The frequency of each genotype is denoted as follows:

- $f^t_{\mathrm{XX,n}}$: frequency of hermaphrodites at generation t.
- $f^t_{\mathrm{XY,n}}$: frequency of males at generation t.
- $f^t_{\mathrm{XX,c}}$: frequency of females at generation t.
- $f^t_{\mathrm{XY,c}}$: frequency of males carrying the CMS mutation at generation t.

A.1.1 Invasion of a CMS mutation into a hermaphroditic population

In the case of females invading a hermaphroditic population, we only need to account for the frequency of these two genotypes. We have

$$f^t_{\mathrm{XX,n}} + f^t_{\mathrm{XX,c}} = 1$$

The change in the female frequency at the beginning determines the fate of the population. Let $r^t_{\mathrm{XX,c}}, r^t_{\mathrm{XX,n}}$ be the growth rate of the female and hermaphrodite frequencies in the population at time t, respectively. We then have $r^t_{\mathrm{XX,c}} = f^{t+1}_{\mathrm{XX,c}}/f^t_{\mathrm{XX,c}} - 1$, $r^t_{\mathrm{XX,n}} = f^{t+1}_{\mathrm{XX,n}}/f^t_{\mathrm{XX,n}} - 1$.

From the recurrence equation for the female frequency, we can calculate its growth rate $r^t_{\mathrm{XX,c}}$ as follows:

$$\begin{aligned}
f^{t+1}_{\mathrm{XX,c}} &= \frac{f^t_{XX} g}{f^t_{\mathrm{XX,n}}(1-s) + f^t_{\mathrm{XX,n}} s(1-d) + f^t_{\mathrm{XX,c}} g} \\
&= \frac{f^t_{\mathrm{XX,c}} g}{f^t_{\mathrm{XX,n}}(1-s+s-sd) + f^t_{\mathrm{XX,c}} g} \\
&= \frac{f^t_{\mathrm{XX,c}} g}{(1-f^t_{\mathrm{XX,c}})(1-sd) + f^t_{\mathrm{XX,c}} g} \\
\Leftrightarrow \frac{f^{t+1}_{\mathrm{XX,c}} - f^t_{\mathrm{XX,c}}}{f^t_{\mathrm{XX,c}}} &= \frac{g}{(1-f^t_{\mathrm{XX,c}})(1-sd) + f^t_{\mathrm{XX,c}} g} - 1 \\
r^t_{\mathrm{XX,c}} &= \frac{g}{(1-f^t_{\mathrm{XX,c}})(1-sd) + f^t_{\mathrm{XX,c}} g} - 1
\end{aligned}$$

The growth rate for the female frequency at time $t = 0$, $r^0_{\mathrm{XX,c}}$ at the minimum value of 0 is the threshold to determine whether CMS can invade and be fixed.

We can further elaborate this threshold as follows:

$$\begin{aligned}
0 &= r^0_{\mathrm{XX,c}} \\
\Leftrightarrow 1 &= \frac{g}{(1-f^0_{\mathrm{XX,c}})(1-sd)+f^0_{\mathrm{XX,c}}g} \\
\Leftrightarrow g &= (1-f^0_{\mathrm{XX,c}})(1-sd)+f^0_{\mathrm{XX,c}}g \\
\Leftrightarrow g(1-f^0_{\mathrm{XX,c}}) &= (1-f^0_{\mathrm{XX,c}})(1-sd) \\
\Leftrightarrow g &= 1-sd \qquad \text{(A1)}
\end{aligned}$$

A.1.2 The invasion of CMS into an androdioecious population

For androdioecy to evolve, males need to produce more pollen than a certain threshold (Charlesworth and Charlesworth, 1978):

$$\alpha = \frac{2(1-sd)}{1-s} \qquad \text{(A2)}$$

A.1.3 Thresholds for CMS invasion and fixation

Let P^t_{X} be the fraction of pollen not carrying the female-sterility mutation at generation t. Let $r^t_{\mathrm{XX,c}}, r^t_{\mathrm{XX,n}}$ be the growth rate of the female and hermaphrodite frequencies in the population at time t, respectively, as defined in section A.1.1. At any time point after CMS invasion, we have

$$\begin{aligned}
f^{t+1}_{\mathrm{XX,n}} &= \frac{f^t_{\mathrm{XX,n}}(1-s)P^t_{\mathrm{X}} + f^t_{\mathrm{XX,n}}s(1-d)}{f^t_{\mathrm{XX,n}}(1-sd)+f^t_{\mathrm{XX,c}}g} \\
f^{t+1}_{\mathrm{XX,c}} &= \frac{f^t_{\mathrm{XX,c}}P^t_{\mathrm{X}}g}{f^t_{\mathrm{XX,n}}(1-sd)+f^t_{\mathrm{XX,c}}g} \\
\Rightarrow \frac{f^{t+1}_{\mathrm{XX,c}}}{f^{t+1}_{\mathrm{XX,n}}} &= \frac{f^t_{\mathrm{XX,c}}P^t_{\mathrm{X}}g}{f^t_{\mathrm{XX,n}}(1-s)P^t_{\mathrm{X}} + f^t_{\mathrm{XX,n}}s(1-d)} \\
\Leftrightarrow \frac{f^{t+1}_{\mathrm{XX,c}} \div f^t_{\mathrm{XX,c}}}{f^{t+1}_{\mathrm{XX,n}} \div f^t_{\mathrm{XX,n}}} &= \frac{P^t_{\mathrm{X}}g}{(1-s)P^t_{\mathrm{X}}+s(1-d)} \\
\Leftrightarrow \frac{r^t_{\mathrm{XX,c}}+1}{r^t_{\mathrm{XX,n}}+1} &= \frac{P^t_{\mathrm{X}}g}{(1-s)P^t_{\mathrm{X}}+s(1-d)} \\
\Leftrightarrow \frac{r^t_{\mathrm{XX,c}}-r^t_{\mathrm{XX,n}}}{r^t_{\mathrm{XX,n}}+1} &= \frac{g}{1-s+\frac{s(1-d)}{P^t_{\mathrm{X}}}} - 1 \qquad \text{(A3)}
\end{aligned}$$

Note that the growth rate of the hermaphrodite frequency is $r^t_{\mathrm{XX,n}} > -1$. The denominator on the left side of equation (A3) is always positive. Whether the difference in the growth rate of the female and hermaphrodite frequencies are positive or negative, therefore, only depends on the sign of the right side of equation (A3). More precisely, $r^t_{\mathrm{XX,c}} - r^t_{\mathrm{XX,n}} \geq 0$ when

$$\frac{g}{1 - s + \frac{s(1-d)}{P_{\mathrm{X}}^{t}}} \geq 1 \tag{A4}$$

For $s(1-d) > 0$, the left side of (A4) is monotonically increasing over P_{X}^{t}. The CMS invades when (A4) is satisfied with the specific value of P_{X}^{t} at the moment of invasion. For $P_{\mathrm{X}}^{t} = 1$, i.e., the value at the moment of CMS invasion into a hermaphroditic population, (A4) is then $g \geq 1 - sd$. The minimum female fitness g required for the CMS to successfully invade is $g = 1 - sd$, identical to equation (A1). For $P_{\mathrm{X}}^{t} = 0.5$, i.e., the value at the moment of CMS fixation, reformulating (A4) gives us the threshold of g for CMS fixation.

$$\begin{aligned}
1 &= \frac{0.5g}{(1-s)0.5 + s(1-d)} \\
\Leftrightarrow 0.5g &= (1-s)0.5 + s(1-d) \\
\Leftrightarrow g &= (1-s) + 2s(1-d) \\
\Leftrightarrow g &= 1 + s - 2sd
\end{aligned} \tag{A5}$$

P_{X} is largest at the beginning of the invasion. This is also the fraction of pollen not carrying the female-sterility mutation at the equilibrium of an androdioecious population.

Let $f_{\mathrm{XX,n}}^{0}, f_{\mathrm{XY,n}}^{0}$ be the hermaphrodite and male frequencies, respectively, at the equilibrium of the androdioecious population. At time point 0, we have

$$\begin{aligned}
P_{\mathrm{X}}^{0} &= \frac{f_{\mathrm{XX,n}}^{0} + f_{\mathrm{XY,n}}^{0}\alpha 0.5}{f_{\mathrm{XX,n}}^{0} + f_{\mathrm{XY,n}}^{0}\alpha} \\
&= \frac{1 - f_{\mathrm{XY,n}}^{0}(0.5\alpha - 1)}{1 - f_{\mathrm{XY,n}}^{0}(\alpha - 1)}
\end{aligned}$$

As shown in previous work (Charlesworth and Charlesworth, 1978), the frequency of males at the equilibrium of the androdioecious population is

$$f_{\mathrm{XY,n}}^{0} = \frac{\alpha(1-s) - 2(1-sd)}{2(\alpha-1)(1-sd)}$$

The threshold for g so that CMS can invade an androdioecious population is

$$\begin{aligned}
1 &= \frac{g}{1 - s + \frac{s(1-d)}{P_{\mathrm{X}}^{0}}} \\
\Leftrightarrow g &= 1 - s + \frac{s(1-d)}{P_{\mathrm{X}}^{0}} \\
&= 1 - s + \frac{s(1-d)\left(1 - \frac{\alpha(1-s)-2(1-sd)}{2(\alpha-1)(1-sd)}(\alpha-1)\right)}{1 - \frac{\alpha(1-s)-2(1-sd)}{2(\alpha-1)(1-sd)}(0.5\alpha - 1)}
\end{aligned} \tag{A6}$$

A.1.4 Calculation of genotype frequencies at equilibrium

At equilibrium, the left side of inequality (A4) = 1. From this, we can calculate P_{X}^*, as well as the frequency of pollen carrying the female-sterility mutation P_{Y}^*, at the equilibrium.

$$\begin{aligned}
P_{\mathrm{X}}^* &= \frac{s(1-d)}{g+s-1} \\
P_{\mathrm{Y}}^* &= 1 - P_{\mathrm{X}}^* = \frac{g+sd-1}{g+s-1}
\end{aligned}$$

Let $f_{\mathrm{XY,n}}^*, f_{\mathrm{XX,n}}^*, f_{\mathrm{XY,c}}^*, f_{\mathrm{XX,c}}^*$ be the frequencies of males, hermaphrodites, males carrying the CMS, and females at equilibrium. Let e_{m} be the expression rate of CMS in males carrying them.

We can also calculate P_{Y}^* from the pollen production of each phenotype in the population.

$$P_{\mathrm{Y}}^* = \frac{0.5\alpha(f_{\mathrm{XY,n}}^* + f_{\mathrm{XY,c}}^*(1-e_{\mathrm{m}}))}{f_{\mathrm{XX,n}}^* + \alpha(f_{\mathrm{XY,n}}^* + f_{\mathrm{XY,c}}^*(1-e_{\mathrm{m}}))}$$

Let N_S^* be the total number of seeds in the population.

$$N_S^* = f_{\mathrm{XX,n}}^*(1-sd) + f_{\mathrm{XX,c}}^* g$$

We further have the recurrence equations evaluated at equilibrium.

$$\begin{aligned}
f_{\mathrm{XX,n}}^* &= \frac{f_{\mathrm{XX,n}}^*(1-s)P_{\mathrm{X}}^* + f_{\mathrm{XX,n}}^* s(1-d)}{N_S^*} \\
f_{\mathrm{XY,n}}^* &= \frac{f_{\mathrm{XX,n}}^*(1-s)P_{\mathrm{Y}}^*}{N_S^*} \\
f_{\mathrm{XX,c}}^* &= \frac{f_{\mathrm{XX,c}}^* g P_{\mathrm{X}}^*}{N_S^*} \\
f_{\mathrm{XY,c}}^* &= \frac{f_{\mathrm{XX,c}}^* g P_{\mathrm{Y}}^*}{N_S^*} \qquad \text{(A7)}
\end{aligned}$$

At equilibrium, the frequency of each phenotype is constant. From the equation of female frequency we have

$$
\begin{aligned}
N_S^* &= gP_{\mathrm{X}}^* \\
\Leftrightarrow f_{\mathrm{XX,n}}^*(1-sd) + f_{\mathrm{XX,c}}^* g &= gP_{\mathrm{X}}^* \\
\Leftrightarrow f_{\mathrm{XX,c}}^* &= \frac{gP_{\mathrm{X}}^* - f_{\mathrm{XX,n}}^*(1-sd)}{g} \\
&= P_{\mathrm{X}}^* - \frac{f_{\mathrm{XX,n}}^*(1-sd)}{g} \\
\Leftrightarrow f_{\mathrm{XY,c}}^* &= (P_{\mathrm{X}}^* - \frac{f_{\mathrm{XX,n}}^*(1-sd)}{g}) * \frac{P_{\mathrm{Y}}^*}{P_{\mathrm{X}}^*} \\
&= P_{\mathrm{Y}}^* - \frac{f_{\mathrm{XX,n}}^*(1-sd)(P_{\mathrm{Y}}^*)}{gP_{\mathrm{X}}^*} \\
\Leftrightarrow f_{\mathrm{XY,n}}^* &= \frac{f_{\mathrm{XX,n}}^*(1-s)P_{\mathrm{Y}}^*}{gP_{\mathrm{X}}^*} \\
\Leftrightarrow f_{\mathrm{XY,n}}^* + f_{\mathrm{XY,c}}^*(1-e_{\mathrm{m}}) &= \frac{f_{\mathrm{XX,n}}^*(1-s)P_{\mathrm{Y}}^*}{gP_{\mathrm{X}}^*} + (P_{\mathrm{Y}}^* - \frac{f_{\mathrm{XX,n}}^*(1-sd)(P_{\mathrm{Y}}^*)}{gP_{\mathrm{X}}^*})(1-e_{\mathrm{m}}) \\
&= P_{\mathrm{Y}}^*(\frac{f_{\mathrm{XX,n}}^*(1-s)}{gP_{\mathrm{X}}^*} + (1 - \frac{f_{\mathrm{XX,n}}^*(1-sd)}{gP_{\mathrm{X}}^*})(1-e_{\mathrm{m}})) \\
&= P_{\mathrm{Y}}^*(1-e_{\mathrm{m}} + f_{\mathrm{XX,n}}^*(\frac{1-s}{gP_{\mathrm{X}}^*} - \frac{(1-e_{\mathrm{m}})(1-sd)}{gP_{\mathrm{X}}^*})) \\
&= P_{\mathrm{Y}}^*(1-e_{\mathrm{m}} + f_{\mathrm{XX,n}}^*(\frac{1-s-(1-e_{\mathrm{m}})(1-sd)}{gP_{\mathrm{X}}^*}))
\end{aligned}
$$

On the other hand, we have

$$\begin{aligned}
P_{\mathrm{Y}}^{*} &= \frac{0.5\alpha(f_{\mathrm{XY,n}}^{*} + f_{\mathrm{XY,c}}^{*}(1-e_{\mathrm{m}}))}{f_{\mathrm{XX,n}}^{*} + \alpha(f_{\mathrm{XY,n}}^{*} + f_{\mathrm{XY,c}}^{*}(1-e_{\mathrm{m}}))} \\
\Leftrightarrow 1 - 2P_{\mathrm{Y}}^{*} &= \frac{f_{\mathrm{XX,n}}^{*}}{f_{\mathrm{XX,n}}^{*} + \alpha(f_{\mathrm{XY,n}}^{*} + f_{\mathrm{XY,c}}^{*}(1-e_{\mathrm{m}}))} \\
\Leftrightarrow \frac{1}{1-2P_{\mathrm{Y}}^{*}} &= 1 + \frac{\alpha(f_{\mathrm{XY,n}}^{*} + f_{\mathrm{XY,c}}^{*}(1-e_{\mathrm{m}}))}{f_{\mathrm{XX,n}}^{*}} \\
\Leftrightarrow \frac{2P_{\mathrm{Y}}^{*}f_{\mathrm{XX,n}}^{*}}{1-2P_{\mathrm{Y}}^{*}} &= \alpha(f_{\mathrm{XY,n}}^{*} + f_{\mathrm{XY,c}}^{*}(1-e_{\mathrm{m}})) \\
\Leftrightarrow \frac{2P_{\mathrm{Y}}^{*}f_{\mathrm{XX,n}}^{*}}{1-2P_{\mathrm{Y}}^{*}} &= \alpha P_{\mathrm{Y}}^{*}(1-e_{\mathrm{m}} + f_{\mathrm{XX,n}}^{*}(\frac{1-s-(1-e_{\mathrm{m}})(1-sd)}{gP_{\mathrm{X}}^{*}})) \\
\Leftrightarrow 2f_{\mathrm{XX,n}}^{*} &= \alpha(1-2P_{\mathrm{Y}}^{*})(1-e_{\mathrm{m}} + f_{\mathrm{XX,n}}^{*}(\frac{1-s-(1-e_{\mathrm{m}})(1-sd)}{gP_{\mathrm{X}}^{*}})) \\
\Leftrightarrow \alpha(1-2P_{\mathrm{Y}}^{*})(1-e_{\mathrm{m}}) &= f_{\mathrm{XX,n}}^{*}(2-\alpha(1-2P_{\mathrm{Y}}^{*})(\frac{1-s-(1-e_{\mathrm{m}})(1-sd)}{gP_{\mathrm{X}}^{*}})) \\
\Leftrightarrow f_{\mathrm{XX,n}}^{*} &= \frac{\alpha(1-2P_{\mathrm{Y}}^{*})(1-e_{\mathrm{m}})gP_{\mathrm{X}}^{*}}{2gP_{\mathrm{X}}^{*} - \alpha(1-2P_{\mathrm{Y}}^{*})(1-s-(1-e_{\mathrm{m}})(1-sd))} \\
\Leftrightarrow f_{\mathrm{XX,n}}^{*} &= \frac{\alpha(2P_{\mathrm{X}}^{*}-1)(1-e_{\mathrm{m}})gP_{\mathrm{X}}^{*}}{2gP_{\mathrm{X}}^{*} - \alpha(2P_{\mathrm{X}}^{*}-1)(1-s-(1-e_{\mathrm{m}})(1-sd))}
\end{aligned}$$

where $P_{\mathrm{X}}^{*} = \frac{s(1-d)}{g+s-1}$. $f_{\mathrm{XY,n}}^{*}, f_{\mathrm{XX,c}}^{*}, f_{\mathrm{XY,c}}^{*}$ can be calculated from $f_{\mathrm{XX,n}}^{*}$ following (A7). They depend only on $\alpha, s, d, g, e_{\mathrm{m}}$. The frequency of CMS is the sum of $f_{\mathrm{XX,c}}^{*}$ and $f_{\mathrm{XY,c}}^{*}$.

A.2 The effect of pollen limitation (Models 2 and 3)

We assume that pollen limitation occurs when the total pollen production is less a threshold pollen mount P, such that the proportion of fertilized outcrossed seeds decreases linearly from 1 to 0 with a decrease in pollen production to 0. Let L^t, P^t be the proportion of outcrossed seeds that is fertilized, and the total pollen production, respectively, at time t. $L^t = min\{1, \frac{P^t}{P}\}$.

For simulations and further calculation, we assume that pollen limitation occurs when pollen production falls below that of a hermaphroditic population. The pollen production of a hermaphroditic population is then $P = f_{\mathrm{XX,n}}^{*} * 1 = 1$ where $f_{\mathrm{XX,n}}^{*} = 1$. The proportion of outcrossed seeds that is fertilized at time t is then $L^t = min\{1, \frac{P^t}{P}\} = min\{1, P^t\}$.

A.2.1 Pollen limitation with leftover hermaphroditic ovules aborted (Model 2)

Equation (A3), talking into account the effect of pollen limitation is

$$r^t_{\mathrm{XX,c}} - r^t_{\mathrm{XX,n}} \sim \frac{L^t g P^t_{\mathrm{X}}}{(1-s)L^t P^t_{\mathrm{X}} + s(1-d)}$$

$$r^t_{\mathrm{XX,c}} - r^t_{\mathrm{XX,n}} \sim \frac{g}{1-s+\frac{s(1-d)}{L^t P^t_{\mathrm{X}}}}$$

The condition for CMS fixation is then $g = 1 - s + \frac{s(1-d)}{L^t P^t_{\mathrm{X}}}$, with value L^t and P^t_{X} at the point of fixation, i.e., half of the population is males carrying CMS and the other half is females. The proportion of pollen not carrying the female-sterility mutation is then $P^t_{\mathrm{X}} = 0.5$. The total pollen production at this point is the total pollen production of males $P^t = 0.5\alpha(1-e_{\mathrm{m}})$ where 0.5 is the frequency of males in the population and $\alpha(1-e_{\mathrm{m}})$ is the pollen production of a male carrying CMS.

At transition to dioecy, we have

$$\begin{aligned} L^t P^t_{\mathrm{X}} &= min\{1, P^t\} \times P^t_{\mathrm{X}} \\ \Leftrightarrow L^t P^t_{\mathrm{X}} &= min\{1, \alpha(1-e_{\mathrm{m}})0.5\}0.5 \\ &= min\{0.5, 0.25\alpha(1-e_{\mathrm{m}})\} \end{aligned}$$

Inserting these expansion into inequality (A4), the threshold for CMS fixation under possible pollen limitation is

$$\begin{aligned} g &= 1 - s + \frac{s(1-d)}{min\{0.5, 0.25\alpha(1-e_{\mathrm{m}})\}} \\ g &= max\left\{1 + s - 2sd, 1 - s + \frac{s(1-d)}{0.25\alpha(1-e_{\mathrm{m}})}\right\} \\ \Leftrightarrow g &= max\left\{1 + s - 2sd, 1 - s + \frac{4s(1-d)}{\alpha(1-e_{\mathrm{m}})}\right\}, \end{aligned} \tag{A8}$$

where the left term of the right side is applied if there is more pollen in the population than the pollen limitation threshold, and the right term when it is less. The threshold for CMS fixation under pollen limitation is then

$$g = 1 - s + \frac{4s(1-d)}{\alpha(1-e_{\mathrm{m}})}$$

For general cases where the pollen limitation threshold is an arbitrary value P instead of value 1, $L^t P^t_{\mathrm{X}} = min\{1, P^t/P\}P^t_{\mathrm{X}}$ and the equation above becomes $g = 1 - s + \frac{4s(1-d)P}{\alpha(1-e_{\mathrm{m}})}$.

A.2.2 Pollen limitation where leftover hermaphroditic ovules can be reused for self-fertilization (Model 3)

Equation (A3), talking into account the effect of pollen limitation is

$$r^t_{\mathrm{XX,c}} - r^t_{\mathrm{XX,n}} \sim \frac{LgP^t_{\mathrm{X}}}{(1-s)LP^t_{\mathrm{X}} + s(1-d) + (1-s)(1-L)(1-d)}$$

When $P = 1$, similar to calculation in section A.2.1 the threshold for CMS fixation becomes

$$g = max\left\{1 + s - 2sd, (1-s)(2d-1) + \frac{4(1-d)}{\alpha(1-e_{\mathrm{m}})}\right\} \tag{A9}$$

For general cases where the pollen limitation threshold is an arbitrary value P, the threshold for CMS fixation under pollen limitation is $g = (1-s)(2d-1) + \frac{4(1-d)P}{\alpha(1-e_{\mathrm{m}})}$.