A synchronized quorum of genetic clocks - Detailed model

$$\frac{d}{dt}AHL_{in} = k_1 LuxI + k_{in}AHL_{out} - (k_{out} + \lambda_1 + k_2)AHL_{in} - \gamma AiiA\frac{AHL_{in}}{t1 + AHL_{in}}$$
$$\frac{d}{dt}AHL_{out} = -(k_{in} + \lambda_2)AHL_{out} + k_{out}AHL_{in} + \frac{d^2}{dx^2}DAHL_{out}$$
$$\frac{d}{dt}LuxR : AHL = k_2 AHL_{in} - \lambda_3 LuxR : AHL$$
$$\frac{d}{dt}LuxI = \alpha_1 LuxR : AHL^2/(t_2^2 + LuxR : AHL^2) - \lambda_4 LuxI$$
$$\frac{d}{dt}AiiA = \alpha_2 LuxR : AHL^2/(t_2^2 + LuxR : AHL^2) - \lambda_5 AiiA$$

Parameters :

k_1 : production rate of internal AHL by LuxI
k_{in} : import rate of external AHL
k_{out} : export rate of internal AHL
λ_{1-5} : degradation rates
k_2 : AHL LuxR complex formation rate (assuming excess of LuxR)
γ : degradation of internal AHL by AiiA

Known parameters

$D \approx 2000\mu m$ per minutes
Period $=$ 50 to 80 minutes so effective half-lifes should be shorter

Simplifications

Neglected AHL:LuxR complex formation : AHL_{in} directly activates LuxI and AiiA
Neglected LuxI, AHL:LuxR, so AHL_{in} directly activates itself

Simplified model :

$\frac{d}{dt}AHL_{in} = \alpha_1 AHL_{in}^2/(t_2^2 + AHL_{in}^2) + k_{in}AHL_{out} - (k_{out} + \lambda_1 + k_2)AHL_{in} - \gamma AiiA\frac{AHL_{in}}{t1+AHL_{in}}$
$\frac{d}{dt}AiiA = \alpha_2 AHL_{in}^2/(t_2^2 + AHL_{in}^2) - \lambda_5 AiiA$
$\frac{d}{dt}AHL_{out} = -(k_{in} + \lambda_2)AHL_{out} + k_{out}AHL_{in} + \frac{d^2}{dx^2}DAHL_{out}$

Renaming variables :

$\frac{d}{dt}w = \alpha_1 w^2/(k_1^2 + w^2) - (\lambda_1 + k_{out})w - \gamma v\frac{w}{k_2+w} + k_{in}A$
$\frac{d}{dt}v = \alpha_2 w^2/(k_1^2 + w^2) - \lambda_2 v$
$\frac{d}{dt}A = k_{out}w - (\lambda_3 + k_{in})A + \frac{d^2}{dx^2}DA$

λ_1 is the export, degradation and complex formation of internal AHL
λ_3 is the import and degradation of external AHL
k_{in} is the import rate of external AHL

From the experiment it seems that the period is controled by the degradation rate of A (flow), so $1/\lambda_3$ should be quite big.

if $v \sim 1$ then $1/\gamma$ is the time it takes for v to degrade w $<$ 50 minutes, so let's take α_2 so that $v \sim 1$

Scaling the old model :

Target parameters value found by random sampling :

α_1 $[t^{-1}w]$	k_1 $[w]$	γ $[t^{-1}w\,v^{-1}]$	k_2 $[w]$	λ_1 $[t^{-1}]$	k_{out} $[t^{-1}]$	k_{in} $[t^{-1}]$	ϵ $[m^2t^{-1}]$	α_2 $[t^{-1}v]$	λ_2 $[t^{-1}]$	λ_3 $[t^{-1}]$	D $[m^2t^{-1}]$
3.9	0.9	0.29	0.6	1	1/22	0.14	1e-4	2.31	0.12	1/15	1666

Old model :

$\frac{d}{dt}w = 90w^2/(1^2 + w^2) - 5w - 400v\frac{w}{3+w} + A$
$\frac{d}{dt}v = 1w^2/(1^2 + w^2) - v$
$\frac{d}{dt}A = 4w - 0.5A + 4A_{xx}$

$t- > 8t$, $x- > 20x$

$\frac{d}{dt}w = 45/4w^2/(1^2 + w^2) - 5/8w - 50v\frac{w}{3+w} + 1/8A$
$\frac{d}{dt}v = 1/8w^2/(1^2 + w^2) - 1/8v$
$\frac{d}{dt}A = 1/2w - 1/16A + 1600A_{xx}$

w -> 1/3 w (change also scale of A), v->18*v :

$\frac{d}{dt}w = 15/4w^2/((1/3)^2 + w^2) - 5/8w - 25/27v\frac{w}{1+w} + 1/8A$
$\frac{d}{dt}v = 9/4w^2/((1/3)^2 + w^2) - 1/8v$
$\frac{d}{dt}A = 1/2w - 1/16A + 1600A_{xx}$

So $1/16 = (\lambda_3 + k_{in})$, $(\lambda_1 + k_{out}) = 5/8$, $k_{in} = 1/8$,$k_{out} = 1/2$

so $\lambda_3 = -1/16!$ and $\lambda_1 = 1/8$

Finaly we have :

α_1 $[t^{-1}w]$	k_1 $[w]$	γ $[t^{-1}w\,v^{-1}]$	k_2 $[w]$	λ_1 $[t^{-1}]$	k_{out} $[t^{-1}]$	k_{in} $[t^{-1}]$	ϵ $[m^2t^{-1}]$	α_2 $[t^{-1}v]$	λ_2 $[t^{-1}]$	λ_3 $[t^{-1}]$	D $[m^2t^{-1}]$
3.9	0.9	0.29	0.6	1	1/22	0.14	4	2.31	0.12	1/15	1600

α_1 $[t^{-1}w]$	k_1 $[w^2]$	γ $[t^{-1}w\,v^{-1}]$	k_2 $[w]$	λ_1 $[t^{-1}]$	k_{out} $[t^{-1}]$	k_{in} $[t^{-1}]$	ϵ $[m^2t^{-1}]$	α_2 $[t^{-1}v]$	λ_2 $[t^{-1}]$	λ_3 $[t^{-1}]$	D $[m^2t^{-1}]$
3.7	**0.33**	**0.92**	1	0.62	**1/2**	0.12	4	2.25	0.12	~**0**	1600
15/4	1/3	5/8	1	25/27	1/2	1/8	4	9/4	1/8	0	1600