12.D.2. Boundary Conditions

Since (12.51-2) and (12.58-9) are $\boldsymbol{r}$-dependent, their solutions require the specification of the boundary conditions. We shall consider the following two types of boundary conditions.

Dirichlet: X & Y are held constant at the boundaries.

Neumann: $\hat{\boldsymbol{n}}\cdot\nabla_{\boldsymbol{r}} X$ & $\hat{\boldsymbol{n}}\cdot\nabla_{\boldsymbol{r}} Y$ are held constant at the boundaries.

where $\hat{\boldsymbol{n}}$ is the normal to the boundary.

For convenience, let the reaction chamber be rectangular with sides of lengths L_x, L_y & L_z.

Dirichlet Boundary Conditions

In the study of the stability of the spatially uniform steady state (12.55), we must set

$$X_{\text{bound}} = A \qquad\qquad Y_{\text{bound}} = \frac{B}{A}$$

to ensure that the state of no perturbations is (12.55).

Since

$$\delta x\Big|_{x=0} = \delta x\Big|_{x=L_x} = \delta x\Big|_{y=0} = \delta x\Big|_{y=L_y} = \delta x\Big|_{z=0} = \delta x\Big|_{z=L_z} = 0$$

and similarly for δy and δz, a single Fourier-Laplace component takes the form

$$\delta x(\boldsymbol{r}, t) = \tilde{x}(\boldsymbol{k}, \omega) \sin(k_x x) \sin(k_y y) \sin(k_z z)\, e^{\omega(\boldsymbol{k})\, t} \tag{12.60}$$

$$\delta y(\boldsymbol{r}, t) = \tilde{y}(\boldsymbol{k}, \omega) \sin(k_x x) \sin(k_y y) \sin(k_z z)\, e^{\omega(\boldsymbol{k})\, t} \tag{12.61}$$

where

$$k_j L_j = n_j \pi \qquad \text{with} \quad j = x, y, z \qquad \text{and} \quad n_j = 0, 1, 2, \ldots$$

$$\boldsymbol{k} = \sum_{j=x,y,z} k_j \hat{\boldsymbol{j}} = \frac{n_x \pi}{L_x}\hat{\boldsymbol{x}} + \frac{n_y \pi}{L_y}\hat{\boldsymbol{y}} + \frac{n_z \pi}{L_z}\hat{\boldsymbol{z}}$$

Note that the state $\boldsymbol{k} = 0$, with $n_x = n_y = n_z = 0$, is spatially uniform.

Neumann Boundary Conditions

In the study of the stability of the spatially uniform steady state (12.55), we must set

$$\hat{\boldsymbol{n}}\cdot\nabla_{\boldsymbol{r}} X = 0 \qquad\qquad \hat{\boldsymbol{n}}\cdot\nabla_{\boldsymbol{r}} Y = 0$$

which corresponds to no flow across the boundaries, to ensure that the state of no perturbations is (12.55).

Since

$$\frac{\partial}{\partial x}\delta x\Big|_{x=0} = \frac{\partial}{\partial x}\delta x\Big|_{x=L_x} = \frac{\partial}{\partial y}\delta x\Big|_{y=0} = \frac{\partial}{\partial y}\delta x\Big|_{y=L_y} = \frac{\partial}{\partial z}\delta x\Big|_{z=0} = \frac{\partial}{\partial z}\delta x\Big|_{z=L_y} = 0$$

and similarly for δy and δz, a single Fourier-Laplace component takes the form

$$\delta x(\boldsymbol{r}, t) = \tilde{x}(\boldsymbol{k}, \omega) \cos(k_x x) \cos(k_y y) \cos(k_z z)\, e^{\omega(\boldsymbol{k})\, t} \tag{12.62}$$

$$\delta y(\boldsymbol{r}, t) = \tilde{y}(\boldsymbol{k}, \omega) \cos(k_x x) \cos(k_y y) \cos(k_z z)\, e^{\omega(\boldsymbol{k})\, t} \tag{12.63}$$

where

$$k_j L_j = n_j \pi \qquad \text{with} \quad j = x, y, z \qquad \text{and} \quad n_j = 0, 1, 2, \ldots$$

Eigen-Equation

Since the partial differentiations in (12.58-9) are 1st order in time and 2nd order in space, substituting either (12.60-1) or (12.62-3) into (12.58-9) gives the same results

$$\omega \tilde{x} = \left(B - 1 - D_X k^2\right) \tilde{x} + A^2 \tilde{y}$$
$$\omega \tilde{y} = -B \tilde{x} - \left(A^2 + D_Y k^2\right) \tilde{y}$$

which takes the matrix form

$$\begin{pmatrix} \omega - B + 1 + D_X k^2 & -A^2 \\ B & \omega + A^2 + D_Y k^2 \end{pmatrix} \begin{pmatrix} \tilde{x} \\ \tilde{y} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{12.64}$$

or

$$\begin{pmatrix} \omega - C_1 & -A^2 \\ B & \omega + C_2 \end{pmatrix} \begin{pmatrix} \tilde{x} \\ \tilde{y} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{12.64a}$$

where

$$C_1 = B - 1 - D_X k^2 \qquad \text{and} \qquad C_2 = A^2 + D_Y k^2 \tag{12.66}$$

(12.64a) admits non-trivial solutions only if

$$\det \begin{vmatrix} \omega - C_1 & -A^2 \\ B & \omega + C_2 \end{vmatrix} = 0$$

i.e.

$$\omega^2 - (C_1 - C_2)\, \omega - C_1 C_2 + A^2 B = 0 \tag{12.65}$$

Solutions to (12.65) are

$$\omega_\pm = \frac{1}{2}\left[C_1 - C_2 \pm \sqrt{(C_1 - C_2)^2 + 4\left(C_1 C_2 - A^2 B\right)}\,\right]$$
$$= \frac{1}{2}\left[C_1 - C_2 \pm \sqrt{(C_1 + C_2)^2 - 4 A^2 B}\,\right] \tag{12.67}$$

Note that $\omega_\pm$ are the eigenvalues of the matrix $\begin{pmatrix} C_1 & A^2 \\ -B & -C_2 \end{pmatrix}$.