ChemE 7510 – Mathematical Methods in Chemical Engineering

Partial Differential Equations - Finite Fourier Transform (FFT)

3) Solving PDE by FFT Method in Spherical Coordinates

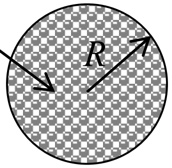
Basis functions: **Spherical Bessel functions** (trigonometric functions/r)

Modified spherical Bessel functions (hyperbolic functions/r)

Legendre's polynomials

Example: Transient diffusion in a sphere with 1st order reaction

Effective homogeneous reaction



Conservation equation of chemical species:

Fluid maintained at $c = c_\infty$

$$\frac{\partial c}{\partial t} = D\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c}{\partial r}\right) - kc$$

I.C. and B.C.s:

at $t = 0$, $c(r,0) = 0$

at $r = 0$, $c(0,t) = \text{finite, or } \frac{dc}{dr}(0,t) = 0$

at $r = R$, $c(R,t) = c_\infty$

Nondimensionalize with $\tilde{c} = \frac{c}{c_\infty};\ \eta = \frac{r}{R};\ \tau = \frac{t}{R^2/D}$

$$\boxed{\frac{\partial \tilde{c}}{\partial \tau} = \frac{1}{\eta^2}\frac{\partial}{\partial \eta}\left(\eta^2\frac{\partial \tilde{c}}{\partial \eta}\right) - \tilde{k}\tilde{c}}$$

at $\tau = 0$, $\tilde{c}(\eta,0) = 0$

at $\eta = 0$, $\tilde{c}(0,\tau) = \text{finite, or } \frac{d\tilde{c}}{d\eta}(0,\tau) = 0$

at $\eta = 1$, $\tilde{c}(1,\tau) = 1$

where $\tilde{k} = \frac{R^2/D}{1/k} = \frac{\text{diffusion time}}{\text{reaction time}} = Da_{II}$

i) steady diffusion in a sphere with 1st order reaction

$\tilde{c} = \tilde{c}(\eta)$

$$0 = \frac{1}{\eta^2}\frac{\partial}{\partial \eta}\left(\eta^2 \frac{\partial \tilde{c}}{\partial \eta}\right) - \tilde{k}\tilde{c}$$

at $\eta = 0$, $\tilde{c}(0) = \text{finite, or } \frac{d\tilde{c}}{d\eta}(0) = 0$

at $\eta = 1$, $\tilde{c}(1) = 1$

Modified spherical Bessel functions of order *n* satisfy ⇒ **Modified Bessel functions of order** $n + \frac{1}{2}$

$$\frac{d}{dx}\left(x^2 \frac{df}{dx}\right) - [m^2 x^2 + n(n+1)] f = 0$$

For $x = \eta$, $n = 0$, $f = \tilde{c}$, and $m = \sqrt{\tilde{k}}$

⇒ **Modified spherical Bessel functions of order 0** (hyperbolic functions/r)

$$\Rightarrow \quad \tilde{c}(\eta) = A\frac{\sinh(\sqrt{\tilde{k}}\eta)}{\eta} + B\frac{\cosh(\sqrt{\tilde{k}}\eta)}{\eta}$$

Applying B.C.s $\tilde{c}(0) = \text{finite}$ ⇒ $B = 0$

$$\tilde{c}(\eta) = A\frac{\sinh(\sqrt{\tilde{k}}\eta)}{\eta}$$

$$\tilde{c}(1) = A\sinh(\sqrt{\tilde{k}}) = 1 \quad \Rightarrow \quad A = \frac{1}{\sinh\sqrt{\tilde{k}}}$$

$$\boxed{\tilde{c}(\eta) = \frac{\sinh(\sqrt{\tilde{k}}\eta)}{\eta \sinh\sqrt{\tilde{k}}}}$$

Separation of Variables (SOV) for Homogeneous Equation of transient diffusion in spherical coord.

$$\frac{\partial \tilde{c}}{\partial \tau} = \frac{1}{\eta^2}\frac{\partial}{\partial \eta}\left(\eta^2 \frac{\partial \tilde{c}}{\partial \eta}\right)$$

with

at τ = 0, $\tilde{c}(\eta,0)=0$

at η = 0, $\tilde{c}(0,\tau)=\text{finite, or } \frac{d\tilde{c}}{d\eta}(0,\tau)=0$

at η = 1, $\tilde{c}(1,\tau)=1$

Assume $\tilde{c}(\eta,\tau)=\theta_n(\tau)\Phi(\eta)$ $\Longrightarrow$ $\frac{\theta_n'}{\theta_n} = \frac{1}{\eta^2\Phi}\frac{d}{d\eta}\left(\eta^2\frac{d\Phi}{d\eta}\right) = \text{const.} = -\lambda_n^2$

1) Eigenfunction

η equation:

$$\frac{1}{\eta^2}\frac{d}{d\eta}\left(\eta^2\frac{d\Phi}{d\eta}\right)+\lambda_n^2\Phi=0$$

at η = 0, $\Phi_n(0)=\text{finite}$

at η = 1, $\Phi(1)=0$

Sturm-Liouville equation $\frac{1}{w(x)}\frac{d}{dx}\left(p(x)\frac{df}{dx}\right)-q(x)f=-\lambda^2 f$ **with** $w=\eta^2, p=\eta^2, \text{ and } q=0$

Spherical Bessel functions $\frac{1}{x^2}\frac{d}{dx}\left(x^2\frac{df}{dx}\right)+[m^2+\frac{n(n+1)}{x^2}]f=0$

For x = η, $n=0$, $f=\Phi$, and $m=\lambda$ (eigenvalue)

$\Longrightarrow$ **Spherical Bessel functions of order 0** (trigonometric functions/r)

$$\Longrightarrow \quad \Phi(\eta)=A\frac{\sin(\lambda_n\eta)}{\eta}+B\frac{\cos(\lambda_n\eta)}{\eta}$$

at η = 0, $\Phi_n(0)=\text{finite}$ $\Longrightarrow$ $B=0$

$$\Longrightarrow \quad \Phi(\eta)=A\frac{\sin(\lambda_n\eta)}{\eta}$$

2) Eigenvalues

at η = 1, $\Phi(1)=0$ $\Longrightarrow$ $\Phi(1)=A\sin\lambda_n$ $\Longrightarrow$ $\lambda_n=n\pi$ $\quad n=1,2,3\ldots$

To be determined by orthogonality

3) Coefficients

Orthogonality: $\int_0^1 \eta^2 \Phi_n(\eta)\Phi_m(\eta)d\eta = \int_0^1 \eta^2 A_n \frac{\sin(\lambda_n\eta)}{\eta} A_m \frac{\sin(\lambda_m\eta)}{\eta} d\eta = \left\langle \eta^2 A_n \frac{\sin(\lambda_n\eta)}{\eta}, A_m \frac{\sin(\lambda_m\eta)}{\eta} \right\rangle = \delta_{nm}$

$$= A_n^2 \int_0^1 \eta^2 \left\{ \frac{\sin(\lambda_n\eta)}{\eta} \right\}^2 d\eta = \frac{A_n^2}{2}$$

$$\Longrightarrow \quad A_n = \sqrt{2}$$

$$\boxed{\Phi(\eta) = \sqrt{2}\,\frac{\sin(\lambda_n\eta)}{\eta}} \qquad \lambda_n = n\pi \qquad n = 1, 2, 3 \ldots$$

Finite Fourier Transform (FFT)

1) Choose a basis function $\Phi(\eta) = \sqrt{2}\,\frac{\sin(\lambda_n\eta)}{\eta}$

$$\frac{1}{\eta^2}\frac{d}{d\eta}\left(\eta^2 \frac{d\Phi}{d\eta}\right) + \lambda_n^2 \Phi = 0$$

at $\eta = 0$, $\Phi_n(0) = \text{finite}$

at $\eta = 1$, $\Phi(1) = 0$

2) Expand solution in Fourier series $\theta(\eta,\tau) = \sum_{n=1}^{\infty} \theta_n(\tau)\Phi_n(\eta)$

To be determined

Define FFT $\langle \eta^2\Phi_n, \theta(\eta,\tau)\rangle = \int_0^1 \Phi_n \theta(\xi,\eta)\eta^2 d\eta = \sum_{m=1}^{\infty}\int_0^1 \Phi_n \theta_m(\tau)\Phi_m(\eta)\eta^2 d\eta = \theta_n(\tau)$

FFT of solution

Coeff.

3) FFT of PDE

$$\int_0^1 \Phi_n \left(\frac{\partial \tilde{c}}{\partial \tau} - \frac{1}{\eta^2}\frac{\partial}{\partial \eta}\left(\eta^2 \frac{\partial \tilde{c}}{\partial \eta}\right) - \tilde{k}\tilde{c} \right)\eta^2 d\eta = 0$$

$$\int_0^1 \Phi_n \frac{\partial \tilde{c}}{\partial \tau}\eta^2 d\eta = \frac{\partial}{\partial \tau}\int_0^1 \Phi_n \tilde{c}\eta^2 d\eta = \frac{\partial \theta_n}{\partial \tau}$$

$$-\int_0^1 \Phi_n \tilde{k}\tilde{c}\eta^2 d\eta = -\tilde{k}\int_0^1 \Phi_n \tilde{c}\eta^2 d\eta = -\tilde{k}\theta_n$$

Eigenvalue problem

$$\frac{1}{\eta^2}\frac{d}{d\eta}\left(\eta^2\frac{d\Phi}{d\eta}\right)+\lambda_n^2\Phi=0$$

at $\eta = 0$, $\Phi_n(0) = \text{finite}$

at $\eta = 1$, $\Phi(1) = 0$

$$\int_0^1 \Phi_n\left(\frac{1}{\eta^2}\frac{\partial}{\partial\eta}\left(\eta^2\frac{\partial\tilde{c}}{\partial\eta}\right)\right)\eta^2 d\eta=\Phi_n\eta^2\frac{\partial\tilde{c}}{\partial\eta}\bigg|_{\eta=0}^{\eta=1}-\int_0^1\frac{d\Phi_n}{d\eta}\left(\eta^2\frac{\partial\tilde{c}}{\partial\eta}\right)d\eta=\Phi_n(1)\frac{\partial\tilde{c}}{\partial\eta}(1,\tau)-\frac{d\Phi_n}{d\eta}\eta^2\tilde{c}\bigg|_{\eta=0}^{\eta=1}+\int_0^1\frac{d}{d\eta}\left(\eta^2\frac{d\Phi_n}{d\eta}\right)\tilde{c}\,d\eta$$

$$=-\frac{d\Phi_n(1)}{d\eta}\tilde{c}(1,\tau)+\int_0^1\frac{1}{\eta^2}\frac{d}{d\eta}\left(\eta\frac{d\Phi_n}{d\eta}\right)\tilde{c}\eta^2 d\eta$$

$$-\left(\lambda_n\sqrt{2}\frac{\cos(\lambda_n\eta)}{\eta}-\sqrt{2}\frac{\sin(\lambda_n\eta)}{\eta^2}\right)\bigg|_{\eta=1}$$

$$=-\lambda_n\sqrt{2}(-1)^n$$

$$=-\lambda_n^2\int_0^1\Phi_n\tilde{c}\eta^2 d\eta=-\lambda_n^2\theta_n(\tau)$$

$$\sqrt{2}\frac{\sin(\lambda_n\eta)}{\eta}\frac{1}{\eta}\bigg|_{\eta=1}=\Phi_n(1)\cdot 1=0$$

Due to non-homogeneous B.C.

Due to 1st order reaction

$$\Longrightarrow\quad \frac{d\theta_n(\tau)}{d\tau}+(\lambda_n^2+\tilde{k})\theta_n(\tau)=-\sqrt{2}\lambda_n(-1)^n$$

$$\Longrightarrow\quad \theta_n(\tau)=\theta_n^{(h)}+\theta_n^{(p)}=C_n e^{-(\lambda_n^2+\tilde{k})\tau}-\frac{\sqrt{2}\lambda_n(-1)^n}{\lambda_n^2+\tilde{k}}$$

4) FFT of I.C.

at $\tau = 0$, $\theta(\eta,0) = 0$

$$\Longrightarrow\quad \langle\Phi_n,\theta(\eta,0)\rangle=\int_0^1\Phi_n\theta(\xi,0)\eta^2 d\eta=\theta_n(0)=C_n-\frac{\sqrt{2}\lambda_n(-1)^n}{\lambda_n^2+\tilde{k}}=0\quad\Longrightarrow\quad C_n=\frac{\sqrt{2}\lambda_n(-1)^n}{\lambda_n^2+\tilde{k}}$$

$$\Longrightarrow\quad \theta_n(\tau)=-\frac{\sqrt{2}\lambda_n(-1)^n}{\lambda_n^2+\tilde{k}}[1-e^{-(\lambda_n^2+\tilde{k})\tau}]$$

$$\tilde{c}(\eta,\tau)=-2\sum_{n=1}^{\infty}\frac{\lambda_n(-1)^n}{\lambda_n^2+\tilde{k}}[1-e^{-(\lambda_n^2+\tilde{k})\tau}]\frac{\sin(\lambda_n\eta)}{\eta}=\underbrace{\frac{\sinh(\sqrt{\tilde{k}}\eta)}{\eta\sinh\sqrt{\tilde{k}}}}_{\tilde{c}_{steady}(\eta)}+\underbrace{2\sum_{n=1}^{\infty}\frac{\lambda_n(-1)^n}{\lambda_n^2+\tilde{k}}e^{-(\lambda_n^2+\tilde{k})\tau}\frac{\sin(\lambda_n\eta)}{\eta}}_{\tilde{c}_{transient}(\eta,\tau)}$$

$\lambda_n = n\pi$

$n = 1, 2, 3, \ldots$