GLOBAL SPECTRAL ANALYSIS FOR CONVECTION-DIFFUSION-REACTION EQUATION IN TWO-DIMENSIONS: EFFECTS OF NUMERICAL ANTI-DIFFUSION AND DISPERSION

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Abstract

A global spectral analysis of finite difference based numerical schemes for 2D convection-diffusion reaction equation is presented. Three important physical processes viz., convection, diffusion and reaction, are characterized in terms of the non-dimensional numerical parameters- CFL number N_c , Peclet number Pe and Damkohler number Da, in the spectral space. Analysis is performed for two space-time discretization schemes known for accuracy and robustness. The analysis shows the typical attribute of numerical schemes- convection speed, diffusion coefficient and reaction coefficient do not remain constant but are functions of the wavenumber. Property charts, which describe the accuracy and performance of the numerical scheme, are presented. An application of this analysis involving the receptivity of an incompressible flow is presented.

Keywords: Global spectral analysis, convection-diffusion-reaction equation.

Introduction:

Convection-diffusion-reaction (CDR) equation plays a central role in many disciplines of engineering, science and finances. This equation can be of relevance to acoustics [1], astrophysics [2], pattern formation and nonlinear dynamics as given in [3]. In the case of fluid dynamics, this equation has been used for the study of onset of convection with differentially heated fluid layer [4]; develop constitutive equations for (k_{k}) - turbulence models [5]. There are also applications towards heat transfer effects due to the dependence of coefficient of viscosity on temperature causing thermal convection [6], geothermal studies [7], formation of Rayleigh-Benard roll pattern [8]. A major impetus in studying the convection-diffusion-reaction equation is spatio-temporal patterns exhibited in mathematical biology [9]. The pioneering work of Turing on the chemical basis of morphogenesis [10] started the study of spatial pattern formations. Apart from this, this equation has been used in many ecological studies involving predator-prey dynamics in [11]. In combustion and reactive models, this equation is directly relevant as detailed chemical processes are represented by an equivalent system to track scalars [12].

In the present paper, a detailed global spectral analysis of numerical methods in the finite difference framework is reported for CDR equation. Two-dimensional (2D) CDR equation is analysed theoretically and property charts for two popular numerical methods are presented. An application of this analysis involving the receptivity of incompressible flow in a square lid driven cavity is also presented.

Spectral Analysis of Linear 2-D Convection-Diffusion-Reaction Equation:

We consider the 2D linear CDR equation as follows

$$\frac{\partial u}{\partial t} + c_x \frac{\partial u}{\partial x} + c_y \frac{\partial u}{\partial y} + su = \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \tag{1}$$

Here c_x , c_y , α and s are constants specifying the convection speed in *x*- and *y*-directions, coefficient of diffusion and coefficient of reaction, respectively.

Representing the unknown u(x,y,t), in the hybrid spectral plane [14] by

$$u(x,y,t) = \int \hat{U}(k_x,k_y,t)e^{i(k_xx+k_yy)}dk_xdk_y$$
⁽²⁾

and substituting this in Eq. (1) we obtain

$$\hat{U}(k_x, k_y, t) = \hat{F}(k_x, k_y) e^{-\alpha (k_x^2 + k_y^2)t} e^{-i(k_x c_x + k_y c_y)t} e^{-st}$$
(3)

To obtain the physical dispersion relation, the unknown is represented by the Fourier-Laplace transform given below.

$$u(x, y, t) = \int \int \int \bar{U}(k_x, k_y, \omega) e^{i(k_x x + k_y y - \omega t)} dk_x dk_y d\omega$$
(4)

which gives the physical dispersion relation as,

$$\omega = c_x k_x + c_y k_y - is - i\alpha (k_x^2 + k_y^2) \tag{5}$$

The complex phase speed can be obtained from this dispersion relation as,

$$c_{phys} = \frac{\omega}{\sqrt{k_x^2 + k_y^2}} = \frac{c_x k_x + c_y k_y - is - i\alpha (k_x^2 + k_y^2)}{\sqrt{k_x^2 + k_y^2}}$$
(6)

The physical group velocity components are defined as,

$$V_{gx} = \frac{\partial \omega}{\partial k_x} = c_x - 2i\alpha k_x \tag{7}$$

$$V_{gy} = \frac{\partial \omega}{\partial k_y} = c_y - 2i\alpha k_y \tag{8}$$

The physical amplification factor is obtained in terms of $N_c = \frac{c\Delta t}{h}$, $Pe = \frac{\alpha\Delta t}{h^2}$ and $Da = \frac{sh}{c}$ as,

$$G_{phys} = e^{-[Pe_x(k_xh_x)^2 + Pe_y(k_yh_y)^2]} e^{-i[N_{cx}k_xh_x + N_{cy}k_yh_y]} e^{-[N_cDa]}$$
(9)

The corresponding numerical dispersion relation is given as,

$$\omega_{num} = \left(\sqrt{k_x^2 + k_y^2}\right)c_{num} - is_{num} - i\alpha_{num}(k_x^2 + k_y^2)$$
(10)

Noting that c_{num} , a_{num} and s_{num} do not remain constants, the numerical amplification factor can be represented as,

$$G_{num} = e^{-\alpha_{num}(k_x^2 + k_y^2)\Delta t} e^{-i\left(\sqrt{k_x^2 + k_y^2}\right)c_{num}\Delta t} e^{-s_{num}\Delta t}$$
(11)

Numerical phase shift per unit time step is given by,

$$tan(\beta_{num}) = -\left(\frac{(G_{num})_{Imag}}{(G_{num})_{Real}}\right)$$
(12)

where,

$$\beta_{num} = \left(\sqrt{k_x^2 + k_y^2}\right) c_{num} \Delta t$$

Therefore, the non-dimensional numerical phase speed is,

$$\frac{c_{num}}{c} = -\left\lfloor \frac{1}{N_{cx}(k_x h_x) + N_{cy}(k_y h_y)} \right\rfloor \tan^{-1} \left(\frac{(G_{num})_{Imag}}{(G_{num})_{Real}} \right)$$
(13)

$$\frac{(V_{gx})_{num}}{c_x} = \frac{1}{N_{cx}} \frac{d\beta_{num}}{d(k_x h_x)}$$
(14)

$$\frac{(V_{gy})_{num}}{c_y} = \frac{1}{N_{cy}} \frac{d\beta_{num}}{d(k_y h_y)}$$
(15)

The numerical reaction and diffusion coefficients are given as,

$$\frac{s_{num}}{s} = -\left(\frac{\ln|G_{num}|_{k=0}}{N_c Da}\right) \tag{16}$$

$$\frac{\alpha_{num}}{\alpha} = \frac{ln|G_{num}|_{k=0} - ln|G_{num}|}{[Pe_x(k_x h_x)^2 + Pe_y(k_y h_y)^2]}$$
(17)

Properties of 2D CDR Equation Obtained by GSA:

GSA is performed for two schemes (RK_4 -NCCD and RK_4 - $CD_2 - CD_2$) and the property charts are presented in this section. Here, NCCD scheme refers to a high accuracy combined compact difference scheme and the details of its stencil can be found in [15]. For the analyses reported here, the cell aspect ratio and the wave propagation angle have been prescribed as AR = 1 and $\theta = 60^\circ$, respectively. Also, the property charts are prepared in order to calibrate the present results with a case reported in [13] with very low convection speed ($c = 10^{-4}$) and the reaction coefficient of order one (s =1). This is done using a grid with thousand points in a unit domain covered with uniform spacing, so that $h_x = h_y = 10^{-3}$. Hence, this fixes the value of Da. Therefore, the present case of 2D CDR equation explores the parameter space dominated by reaction rate whereas convection plays a minor role.



FIGURE 1: CONTOURS OF G_{num} , $\frac{|G_{num}|}{|G_{phy}|}$, $\frac{\alpha_{num}}{\alpha}$ and $\frac{c_{num}}{c}$ FOR Da = 14.142, PLOTTED IN THE $(k_x h_x, k_y h_y)$ PLANE WITH Pe = 0.072 FOR RK_4 -NCCD SCHEME.



FIGURE 2: CONTOURS OF G_{num} , $\frac{|G_{num}|}{|G_{phy}|}$, $\frac{\alpha_{num}}{\alpha}$ and $\frac{c_{num}}{c}$ FOR Da = 14.142, PLOTTED IN THE (k_xh_x,k_yh_y) PLANE WITH Pe = 0.073 FOR RK_4 -NCCD SCHEME.



FIGURE 3: CONTOURS OF G_{num} , $\frac{|G_{num}|}{|G_{phy}|}$, $\frac{\alpha_{num}}{\alpha}$ AND $\frac{C_{num}}{c}$ FOR Da = 14.142, PLOTTED IN THE $(k_x h_x, k_y h_y)$ PLANE WITH Pe = 0.1725 FOR RK_4 - CD_2 - CD_2 SCHEME.



FIGURE 4: CONTOURS OF G_{num} , $\frac{|G_{num}|}{|G_{phy}|}$, $\frac{\alpha_{num}}{\alpha}$ AND $\frac{c_{num}}{c}$ FOR Da = 14.142, PLOTTED IN THE $(k_x h_x, k_y h_y)$ PLANE WITH

Pe = 0.1740 FOR RK_4 - CD_2 - CD_2 SCHEME

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