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Modal Analysis of Convection with Axial Diffusion

The one-dimensional model for convection with diffusion and with a source term for mass or energy generation or interchange is analyzed for the eigenvalues and the corresponding spatial eigenmodes as a function of the Peclet number. It is shown how the modal analysis of the source case, when the source coefficients for heat exchange and chemical reaction are spatially independent, is directly related to the no source solution. Numerical examples of determining the source term coefficient are included. These solutions form a base to discuss dynamic characteristics and stability and to which solutions for spatially dependent coefficients can be compared.

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SCOPE

Eigenvalues and corresponding eigenfunctions arise naturally and are useful in connection with systems described by linear partial differential equations. They are useful in the solution of the equations with given initial conditions and in the determination of system stability, measurement, and control. Linear partial differential equations arise when small perturbations about some operating state are considered for a linear or nonlinear system. In this paper we obtain the eigenvalues and associated eigenfunctions for the one dimensional linearized model for convection with axial diffusion and with a source term for mass or energy generation or interchange subject to the widely used Wehner and Wilhelm (1956) boundary conditions.

$$\frac{1}{Pe}\frac{\partial \phi}{\partial x^2} - \frac{\partial \phi}{\partial x} + \sigma\phi = \frac{\partial \phi}{\partial t}$$

$$\phi_F(t) = \phi(0, t) - \frac{1}{Pe}\frac{\partial \phi}{\partial x}(0, t)$$

$$\frac{\partial \phi}{\partial x}(1, t) = 0$$

This model has wide applicability arising in connection

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with heat and mass transfer in tubes and is especially important when considering tubular reactors with axial mixing. Our solutions cover the case when the linearized source term coefficient σ is spatially independent.

CONCLUSIONS AND SIGNIFICANCE

The eigenvalues and eigenmodes for the one-dimensional equation for convection with axial mixing and a source term have been documented for the accepted Wehner & Wilhelm (1956) boundary conditions. The no source adiabatic case provides the basis for all solutions with a spatially independent source term coefficient. The spatially dependent eigenmode is independent of the value of the source term coefficient and depends only on the value of the Peclet number. The eigenvalue and time-dependent eigenmode is dependent on the source term coefficient in a simple additive way.

Examples are given of the numerical determination of source term coefficients for heat exchange, mass exchange, and for heat generation in a tubular chemical reactor. These examples indicate that the contribution to the source term coefficient due to heat generation in a reactor is likely to overshadow the contribution due to heat exchange at the walls.

In the limiting case as $Pe \rightarrow 0$ (perfect mixing), λ°_i approaches -1.0 (as it should, namely, the reciprocal of the nondimensional holding time for a continuous stirred tank) with all higher eigenvalues approaching negative infinity. In the extreme as $Pe \rightarrow \infty$ (no axial diffusion, that is, plug flow) then all the λ°_i approach negative infinity actually being asymptotic to $-\frac{Pe}{4}$.

Knowledge of the eigenvalues and modes is useful in the solution of the equation with given initial conditions and in the determination of system stability, measurement, and control. In fact, the solution to initial value problems for systems governed by Equations (1) and (3) is given by Equation (5), while system stability can be assessed by using Figure 1 and Equation (6) to determine if the sign of all the λ_i are negative. Equation (10) allows determination of the zero crossings of the spatial eigenmodes. This is shown to be very useful in locating measurement probes for systems with low Peclet numbers.

The linearized equation for one-dimensional convection with axial diffusion of a scalar, conserved quantity in dimensionless form is

$$\frac{1}{Pe}\frac{\partial^2\phi}{\partial x^2} - \frac{\partial\phi}{\partial x} + \sigma\phi = \frac{\partial\phi}{\partial t} \qquad (1)$$

[See, for example, Weston (1971)].

ϕ is the dimensionless perturbation from a steady state of an intensive variable associated with a conserved quantity. The term $\sigma\phi$ accounts for any source or sink within the fluid or exchange at the transverse boundary, the coefficient σ being a transfer or reactivity coefficient. The dimensionless group Pe, a Peclet number, expresses the ratio of characteristic convection to diffusion.

The applicability of Equation (1) is extremely wide. For example, in a tube with heat transfer at the walls, ϕ can be taken as a perturbation in the dimensionless fluid temperature. In this case σ is a measure of the heat exchange rate transverse to the flow direction. Were the fluid in the tube to be reacting, σ would reflect the heat generation rate from the reaction. Obviously σ could be a combination of such terms. In the case of mass transfer ϕ would be a measure of species concentration and σ the mass transfer rate at the wall interface or the formation rate from the reaction taking place within the fluid. In an adiabatic tubular chemical reactor ϕ could represent a linear stoichiometric combination of concentration and temperature with σ equal to zero (Aris, 1969; Chiou, 1968). In a nonadiabatic tubular reactor, ϕ represents either temperature or species concentration, σ would be a measure of heat or mass generation and transfer, but the use of a single equation would then be just an approximation.

For the systems considered, the following boundary conditions of Wehner and Wilhelm (1956) are appropriate

$$\phi_F(t) = \phi(0,t) - \frac{1}{Pe}\frac{\partial\phi}{\partial x}(0,t) \qquad (2a)$$

$$\frac{\partial\phi}{\partial x}(1,t) = 0 \qquad (2b)$$

where ϕ_F represents the perturbation in feed condition about an operating steady state value while $\phi(0, t)$ describes ϕ just inside the entrance.

The characteristics of the system are put into evidence when the system is unforced, that is, in Equation (2), the perturbation in feed condition about its steady state value is zero and any nonzero perturbation in ϕ, are due to Equation (1) interior to the tube and not changes on or outside the transverse tube boundary. For this unforced autonomous case, the boundary conditions of Equation (2) become

$$\phi(0,t) - \frac{1}{Pe}\frac{\partial\phi}{\partial x}(0,t) = 0 \qquad (3a)$$

$$\frac{\partial\phi}{\partial x}(1,t) = 0 \qquad (3b)$$

Equation (1) subject to the boundary conditions of Equations (3) can be solved by the method of separation of variables to obtain

$$\phi(x,t) = \sum_{i=0}^{\infty} A_i e^{\lambda_i t}\psi_i(x) \qquad (4)$$

In Equation (4) the time-dependent eigenfunctions $e^{\lambda_i t}$ depend on the eigenvalues λ_i, and the $\psi_i(x)$ are the corresponding spatially dependent eigenmodes. The set of constants A_i are evaluated from a given initial condition $\phi(x, 0)$. For the autonomous system the eigenvalues and spatial eigenmodes are independent of the initial state of the system while the weighting coefficients A_i depend only on the initial state. Looked at in terms of eigenvalues and spatial eigenmodes, the system is said to be described from the viewpoint of modal analysis (Gould, 1969; Melcher, 1965). The eigenvalues immediately give information about system stability and dynamic characteristics. All the λ_i's must be negative for the system to be stable; the larger the magnitude of the λ_i, the faster is the transient response, etc.

EIGENVALUES AND EIGENFUNCTIONS OF EQUATION (1)

Carslaw and Jaeger (1959) show that by the transformation $\phi(x,t) = W(x,t)e^{\sigma t}$, Equation (1) and its boundary conditions transform to the identical mathematical form with dependent variable W but without any source term. It follows that

$$\phi(x,t) = \sum_{i=1}^{\infty} A_i e^{(\lambda_i^0+\sigma)t}\,\psi_i^0(x) \qquad (5)$$

where λ_i^0 ψ_i^0 are the eigenvalues and spatial eigenmodes for the case with no source term, that is, $\sigma = 0$. Explicitly, the relation between the eigenvalues for the source and no source cases is

$$\lambda_i = \lambda_i^0 + \sigma \qquad (6)$$

while

$$\psi_i(x) = \psi_i^0(x) \qquad (7)$$

Proceeding with the solution it is convenient to define the following variables:

$$\alpha = \frac{Pe}{2} \qquad (8)$$

$$\beta_i = \alpha\left[-\frac{4\lambda_i^0}{Pe} - 1\right]^{1/2} \qquad (9)$$

The solution for $\psi_i^0(x)$, the spatial eigenmode, is

$$\psi_i^0 = e^{\alpha x}\left[\frac{\beta_i}{\alpha}\cos\beta_i x + \sin\beta_i x\right] \qquad (10)$$

and the equation used to determine permissible eigenvalues λ_i^0 is

$$\tan\beta = -\frac{2\,\alpha\,\beta}{\alpha^2 - \beta^2} \qquad (11)$$

It can be shown that λ_i^0 must not only always be real but also always negative (Weinberger, 1965). Another important result is that the spatial eigenmodes are orthogonal with respect to the weighting function $Pe\,e^{-PeX}$, that is,

$$\int_0^1 Pe\,e^{-Pex}\,\psi_i(x)\psi_j(x)\,dx = 0 \quad i \neq j \qquad (12)$$

Equation (12) is true for Equation (1) even when σ is considered to be spatially dependent.

A plot of the first nine eigenvalues λ_i^0 is given in Figure

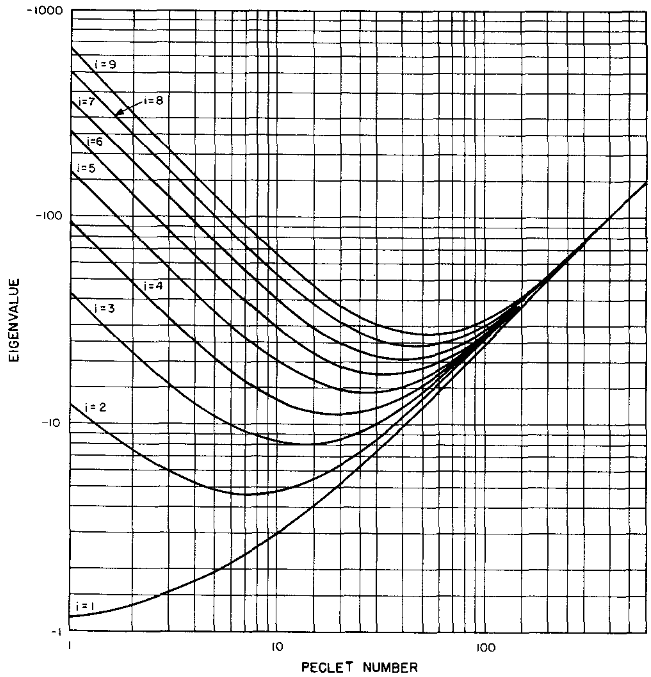

Fig. 1. Eigenvalues as a function of the Peclet number.

1 as a function of the Peclet number and Table 1 tabulates some of these. It should be noted that $\lambda_i^0 \to -1$ as $Pe \to 0$ (perfectly mixed open system and λ should be the negative reciprocal of the residence time) and λ_i^0 ($i > 1$) $\to -\infty$. Also, as Pe gets large (approaches a no mixing or plug flow condition) $\lambda_i^0 \to -\frac{Pe}{4}$ and approach negative infinity.

Equation (10) shows that all the spatial eigenmodes have the same exponential part $e^{\alpha x}$ for a given value of Pe and that each eigenmode varies only in the nature of the underlying sinusoid. Examples of a few eigenmodes for Pe = 5 are shown in Figure 2, while example of the underlying sinusoids for the same Peclet number are given in Figure 3. These underlying sinusoids are important for several reasons. First, the zeroes of the sinusoids are the zeroes of the spatial eigenmodes. Second, the factor e^{-Pex} in Equation (12) will exactly cancel the product of $e^{\alpha x}$ terms from Equation (10). The orthogonality condition of Equation (12) can then be viewed as the orthogonality of the underlying sinusoids.

THE SOURCE TERM

For systems without a source term, the source term coefficient σ is zero and λ_i and λ_i^0 are the same. Thus λ_i^0 is

TABLE 1. DEPENDENCE OF EIGENVALUES UPON PECLET NUMBER
(The first nine eigenvalues are given in the table for selected Peclet numbers).

Peclet number	$Pe = 1.0$	$Pe = 2$	$Pe = 5$	$Pe = 25$	$Pe = 50$	$Pe = 200$
λ_1^0	-1.17196×10^0	-1.35353×10^0	-1.94305×10^0	-6.54463×10^0	-1.26693×10^1	-5.01897×10^1
λ_2^0	-1.20219×10^1	-7.24618×10^0	-4.79945×10^0	-7.44229×10^0	-1.31787×10^1	-5.04269×10^1
λ_3^0	-4.17004×10^1	-2.21786×10^1	-1.09712×10^1	-8.97727×10^0	-1.40317×10^1	-5.07591×10^1
λ_4^0	-9.10636×10^1	-4.68847×10^1	-2.09257×10^1	-1.11899×10^1	-1.52339×10^1	-5.11862×10^1
λ_5^0	-1.60156×10^2	-8.14404×10^1	-3.47793×10^1	-1.41152×10^1	-1.67913×10^1	-5.17083×10^1
λ_6^0	-2.48985×10^2	-1.25859×10^2	-5.25629×10^1	-1.77791×10^1	-1.87104×10^1	-5.23255×10^1
λ_7^0	-3.57552×10^2	-1.80145×10^2	-7.42863×10^1	-2.21991×10^1	-2.09972×10^1	-5.30380×10^1
λ_8^0	-4.85858×10^2	-2.44300×10^2	-9.99537×10^1	-2.73866×10^1	-2.36569×10^1	-5.38457×10^1
λ_9^0	-6.33903×10^2	-3.18323×10^2	-1.29567×10^2	-3.33487×10^1	-2.66938×10^1	-5.47488×10^1

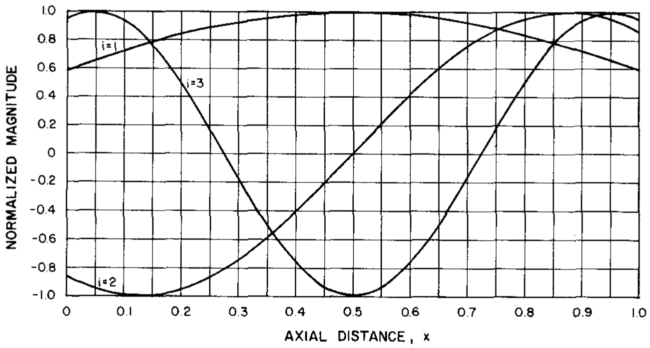

Fig. 2. Eigenmodes for $Pe = 5$, $\Psi_i(x)/\Psi_i(1)$.

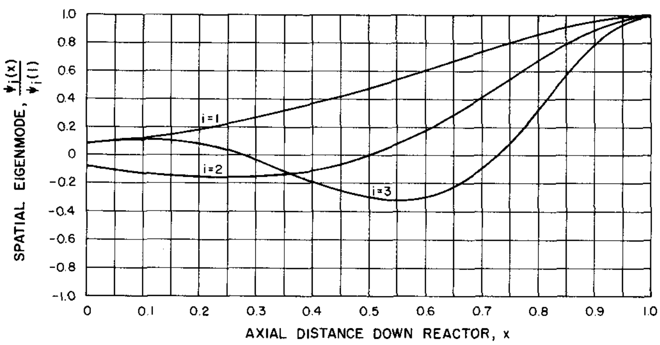

Fig. 3. Underlying sinusoids for $Pe = 5$.

to be associated with the no source, adiabatic case. For systems with source terms (for example, a heat exchanger or a chemical reactor), σ is nonzero and the value of λ_i is determined immediately from λ_i^0 using Equation (6).

Since all the λ_i^0 are real and negative, a negative value of σ makes the eigenvalues more negative. A positive value of σ has the opposite effect and, in fact, if a positive value of σ is larger than the absolute value of λ_1^0, the system is unstable. However, the spatial eigenmodes remain unchanged compared to those systems without a source term, that is, $\psi_i(x) = \psi_i^0(x)$. This occurs because the β_i determined by Equation (11) and used in Equation (10) are independent of σ as shown by Equations (8), (9), and (10). This agrees with the statement of Equation (7).

Specific Numerical Examples of σ

Table 2 gives formulas for several physical cases where nonzero values of σ arise.

Example 1: Heat transfer to and from the wall

From Table 2

$$\sigma = -\frac{2hL}{r\,u\,C_p\,\rho} \qquad (13)$$

Some values for laboratory size equipment might be the following:

$L = 2.0$ m
$u = 0.5$ m/s
$\gamma = C_p\,\rho = 4.187 \times 10^6$ J/m$^3 \cdot$ K
$h = 4.187 \times 10^2$ J/m$^2 \cdot$ s $\cdot$ K
$r = .02$m

Substituting these values into Equation (13) we obtain

$\sigma = -.04$

Example 2: Energy generated by a chemical reaction

From Table 2, the approximation to σ is

$$\sigma = \frac{(-\Delta H)\,L}{u\,C_p\,\rho}\left(\frac{\partial R_v}{\partial T^*}\right)^0 \qquad (14)$$

For a second-order reaction

$$R_v = k_0\,C_1^*\,C_2^*\,e^{-E/RT^*} \qquad (15)$$

We obtain

$$\sigma = \frac{(-\Delta H)\,L}{u\,C_p\,\rho}\,R_v^0\left(\frac{E}{RT^{*2}}\right)^0 \qquad (16)$$

where the superscript ^{0} refers to operating steady state and σ varies with axial position in the reactor because of the variation of C_1^*, C_2^*, and T^*. To obtain an approximate but constant value for σ we take average values.

For example in the tubular reactor studied by Chiou (1968), a lower steady state occurred for system values as follows:

$L = 0.42$ m
$u = 0.03$ m/s
$\gamma = C_p\,\rho = 4.187 \times 10^6$ J/m$^3 \cdot$ K
$\Delta H = -5.799 \times 10^8$ J/kg mol (exothermic)
$k_0 = 1.380 \times 10^{11}$ m^3/kg mol $\cdot$ s
$E = 7.227 \times 10^7$ J/kg mol
$R = 8.3196 \times 10^3$ J/kg mol $\cdot$ K
$T^* = 290$ K, an average value
$C_1^* = 7.0 \times 10^{-1}$ kg mol/m^3, an average value
$C_2^* = 2.8$ kg mol/m^3, an average value

Using the above numbers,

$\sigma = +5.313$

Example 3: Diffusion from the wall of a tube

From Table 2

$$\sigma = \frac{-2\,k_M\,L}{r\,u\,C_T^*} \qquad (17)$$

TABLE 2. EVALUATION OF SOURCE COEFFICIENT $\sigma = \frac{L}{u\gamma}\left(\frac{\partial S^*}{\partial \phi^*}\right)^0$

Process	Description of source	S^*	γ	ϕ^*	σ
Heat transfer	energy transferred from fluid to wall/unit volume of system	$-\frac{2h}{r}(T^* - T^*w)$	$C_p\rho$ heat capacity/unit volume	T^*	$-\frac{2hL}{ruC_p\rho}$
Mass transfer	mass transferred from fluid to wall/unit volume of system	$-\frac{2k_M}{r}(Y^* - Y^*w)$	C_T^* total concentration	Y^*	$-\frac{2k_ML}{ruC_T^*}$
Heat evolved due to chemical reaction	energy evolved due to rate of reaction/unit volume, R_v	$(-\Delta H)R_v$	$C_p\rho$ heat capacity/unit volume	T^*	$+\frac{(-\Delta H)L}{uC_p\rho}\left(\frac{\partial R_v}{\partial T^*}\right)^0$

Typical values for a liquid system might be

$$L = 2.0 \text{ m}$$
$$u = 0.5 \text{ m/s}$$
$$\gamma = C_T^* = 5.5 \times 10^1 \text{ kg mol/m}^3$$
$$r = 0.02 \text{ m}$$
$$k_M = 1 \times 10^{-2} \text{ kg mol/m}^2 \cdot \text{s} \cdot \text{mol fr.}$$

hence

$$\sigma = -.07$$

IMPLICATIONS FOR CONTROL, MEASUREMENT, AND DESIGN

The eigenvalues λ_i and eigenmodes $\psi_i(x)$ documented in this paper are of use for the control of systems governed by Equation (1) and its boundary conditions. The first eigenvalue λ_1 immediately gives information on the stability of the system. To be stable λ_1 must be negative. The more negative is the first eigenvalue λ_1 the more stable is the system.

The control of a system by modal analysis depends largely on the eigenvalues of the system. It is hoped that only a few eigenfunctions need be examined to reach an accurate approximation of the system. The fewer the number of significant eigenmodes, the simpler the analysis becomes. By examining Figure 1 in conjunction with Equations (5) and (6), it is clear only the first one or two eigenfunctions will be significant for low values of the Peclet number. However, as the Peclet number increases, the spread between the eigenvalues decreases to a point where many eigenfunctions will have to be considered for an accurate approximation and the usefulness of the approach decreases.

These same points are important in the measurement of system variables. By choosing a proper measurement point for low values of the Peclet number (signifying high diffusion rates), the variable can be considered almost a direct measurement of one eigenmode. For example, consider the second spatial eigenmode for $Pe = 5$ as shown in Figure 2. In this case, $\psi_2(x = 0.5)$ is zero (the node) and Table 1 shows that $\lambda_1 >> \lambda_i$ for $i \geq 3$. Then $e^{\lambda_1 t} \psi_1(x) >> e^{\lambda_i t} \psi_i(x)$ at the same axial point. Thus a measurement at the node of the second mode in systems of low Peclet number will give information directly about the first mode. Of course when all the eigenvalues begin to converge at high values of Peclet number, this point ceases to be so convenient.

For any change in σ there is a corresponding change in all the eigenvalues λ_i as shown by Equation (6). However, the spatial eigenmode does not change from the situation with $\sigma = 0$. Hence the solution to the measurement problem (what modes are important and where the measurement points should occur) for $\sigma = 0$ is the solution for the system at that Peclet number with any other value of σ.

In system design, σ may be modified to vary λ. However, the examples make it clear that the contribution of σ from even a lower steady state in a chemical reactor is about 2 orders of magnitude more important than the contribution from heat or mass exchange at the wall. This would make effective control of a reactor system by heat exchange through the walls a difficult proposition at best. Some improvement could be made in the heat exchange per unit volume by adding internal sources such as a heating coil. However, to effectively counteract the destabilizing effects of a source (one with a positive value for σ), it would probably be better to try to alter the operating steady state than to add another stabilizing source (one with a negative value for σ).

NOTATION

A = constant
a = area, m^2
C_p = heat capacity, J/K
C_T^* = total concentration, kg mol/m^3
C_i^* = concentration of ith reacting species, kg mol/m^3
E = activation energy
ΔH = heat of reaction
h = heat transfer coefficient, J/m^2 · s · K
i = integer index
k = mixing coefficient, m^2/s
k_0 = Arrenhius factor, m^3/kg mol · s
k_M = mass transfer rate, kg mol/m^2 · s
L = length, m
Pe = Peclet number, uL/k
R = gas constant, 8.3196 10^3 J/kg mol · K
R_v = reaction rate, kg mol/s · m^3
r = radius, m
S^* = volumetric generation rate, J/s · m^3
T^* = temperature, K
t = dimensionless time with respect to residence time L/u
u = velocity, m/s
V = volume, m^3
W = a transformation variable, $\phi(x, t)e^{-\sigma t}$
x = dimensionless distance with respect to L
Y = mole fraction of species
α = $Pe/2$
β = $(Pe/2) \cdot \left[\frac{-4\lambda^0}{Pe} - 1\right]^{1/2}$
γ = $C_p \cdot \rho$ or C_T^*
λ = eigenvalue
ρ = density, kg/m^3
σ = dimensionless source coefficient
ϕ = dimensionless scalar quantity, ϕ^*/ϕ_R^*
ψ = spatial eigenmode

Subscripts

F = feed quantity
R = reference value
W = wall

Superscript

0 = steady state values or eigensolutions with $\sigma = 0$
* = dimensional quantities

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