

model and the conventional model becomes smaller and smaller. At a fixed value of α , the ratio η/η' decreases as $\phi_{i,1}$ increases. For example, for $\alpha = 0.1$ and $\phi_{i,1} = 10.0$, this ratio becomes 0.32, while the same ratio is 0.6 for $\phi_{i,1} = 4.0$.

In conclusion, one can say that the prediction of the effectiveness factors from the conventional methods would give overestimated values, especially for small α .

The approach described here can also be applied to nonisothermal systems (Örs, 1977) and for other pellet geometries.

NOTATION

C_a	= concentration of reactant A in the macropores
C_i	= concentration of reactant A in the micropores
C_o	= external surface concentration of reactant A
D_a	= effective macropore diffusion coefficient
D_i	= effective micropore diffusion coefficient
k_r	= surface reaction rate constant
R	= radial coordinate for the pellet
R_o	= radius of the pellet
r	= radial coordinate for the particle
r_o	= radius of the particle
S	= surface area per unit mass of the catalyst

Greek Letters

α	= defined by Equation (9)
ϵ_a	= macropore porosity
η	= effectiveness factor
η'	= effectiveness factor of bidisperse pellet considering it as a monodisperse one
ζ	= dimensionless radial coordinate for the pellet, R/R_o
ρ_p	= $\rho_p'(1 - \epsilon_a)$ = pellet density
ρ_p'	= particle density
$\phi_{i,n}$	= Thiele modulus for an n^{th} order reaction

ψ_a	= dimensionless concentration in the macropores, C_a/C_o
ψ_i	= dimensionless concentration in the micropores, C_i/C_o
ξ	= dimensionless radial coordinate for the particle, r/r_o

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Collocation Solution of Creeping Newtonian Flow Through Sinusoidal Tubes

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Laminar flow through periodically constricted tubes is usually employed as a modeling device in the study of transfer processes in porous media (Payatakes, Tien and Turian, 1973a, 1974a, b; Slattery, 1974; Oh and Slattery, 1976; Sheffield and Metzner, 1976; Stegermeier, 1976; Payatakes, Brown and Tien, 1977; Payatakes and Neira, 1977; Fedkiw and Newman, 1977; Payatakes, Flumerfelt, and Ng, 1977).

The problem of laminar Newtonian flow through periodically constricted tubes was solved by Payatakes, Tien and Turian (1973b) with a finite-difference method of the stream function-vorticity type. This method has two substantial advantages. First, it applies to tubes of arbitrary

shape (allowing for wall discontinuities such as cusps, etc.) so long as the wall radius is a single-valued function of the axial coordinate. Second, it retains the non-linear inertial terms of the equation of motion, which are shown to become important at relatively low values of the Reynolds number (say, larger than 1 to 30). On the other hand, the finite difference method suffers from the disadvantages of 1) requiring large memory to achieve satisfactory accuracy, and 2) rendering the solution in matrix form, namely only on the network nodes. Stream function, velocity and pressure values at off-node points have to be calculated with two-dimensional interpolation techniques.

Hence, there are great incentives to develop analytical approximate solutions for this type of problem.

Dodson, Townsend and Walters (1971) developed

perturbation solutions of flow of Newtonian and non-Newtonian (using the Oldroyd model) fluids through sinusoidal tubes. Perturbation solutions of Newtonian flow through periodically constricted tubes, including the non-linear inertial effects, have been obtained by Chow and Soda (1972), and Lessen and Huang (1976). These works are of considerable interest, especially because they incorporate non-linear effects, but they are valid only for relatively small amplitude to wavelength ratios (say, less than 0.1). Perturbation solutions have already been used to study heat and mass transfer in tubes with geometry of varying cross-section (Chow and Soda, 1973a, 1973b).

Collocation solutions, on the other hand, can be used with geometries where the amplitude to wavelength ratio is large (see also Fedkiw and Newman, 1977). Such a collocation solution for creeping Newtonian flow through sinusoidal tubes is given below and is used to develop a chart that relates the dimensionless pressure drop to the geometrical parameters over a wide range of values of the latter.

Consider a sinusoidal tube with minimum diameter r_1 , maximum diameter r_2 , and wavelength h . Let $r_a = (r_1 + r_2)/2$ be the arithmetic mean of r_1 and r_2 , and $b = (r_2 - r_1)/(r_2 + r_1)$ the reduced amplitude. Consider cylindrical coordinates (r, z) with origin at a cross-section of diameter r_a . Letting $r_w(z)$ denote the wall radius and introducing dimensionless variables as follows,

$$r^* = \frac{r}{h}, \quad r_1^* = \frac{r_1}{h}, \quad r_2^* = \frac{r_2}{h}, \quad r_a^* = \frac{r_a}{h},$$

$$z^* = \frac{z}{h}, \quad r_w^* = \frac{r_w}{h} \quad (1)$$

we have

$$r_w^*(z^*) = r_a^* (1 + b \sin 2\pi z^*) \quad (2)$$

Let v_r and v_z be the radial and axial velocity components and v_r^* and v_z^* their dimensionless counterparts, defined by

$$v_r^* = \frac{v_r}{v_o}, \quad v_z^* = \frac{v_z}{v_o} \quad (3)$$

where v_o is the mean velocity at the most narrow cross section ($z^* = -1/4$). A dimensionless stream function is defined by

$$v_r^* = \frac{1}{r^*} \frac{\partial \psi^*}{\partial z^*}, \quad v_z^* = -\frac{1}{r^*} \frac{\partial \psi^*}{\partial r^*} \quad (4)$$

The domain of interest, $[0 \leq r^* \leq r_w^*(z^*); -1/4 \leq z^* \leq 1/4]$ is transformed into a rectangular one by introducing a new variable

$$\xi = \frac{r^*}{r_w^*(z^*)} \quad (5)$$

The transformation can be used rigorously only if the wall profile does not have discontinuities (e.g. cusps)—only then can the symmetry condition around the plane $z^* = 1/4$ be satisfied exactly. If the wall profile is merely piecewise continuous, then a considerably more elaborate transformation is required (Neira and Payatakes, 1978).

A collocation solution is given by

$$\psi^* \approx \psi_N^*(\xi, z^*) = \frac{1}{2} r_1^{*2} (1 - \xi)^2$$

$$+ \sum_{k=1}^N C_k \xi (1 - \xi)^{i+1} \cos \left[2\pi(j-1) \left(z^* + \frac{1}{4} \right) \right] \quad (6)$$

with

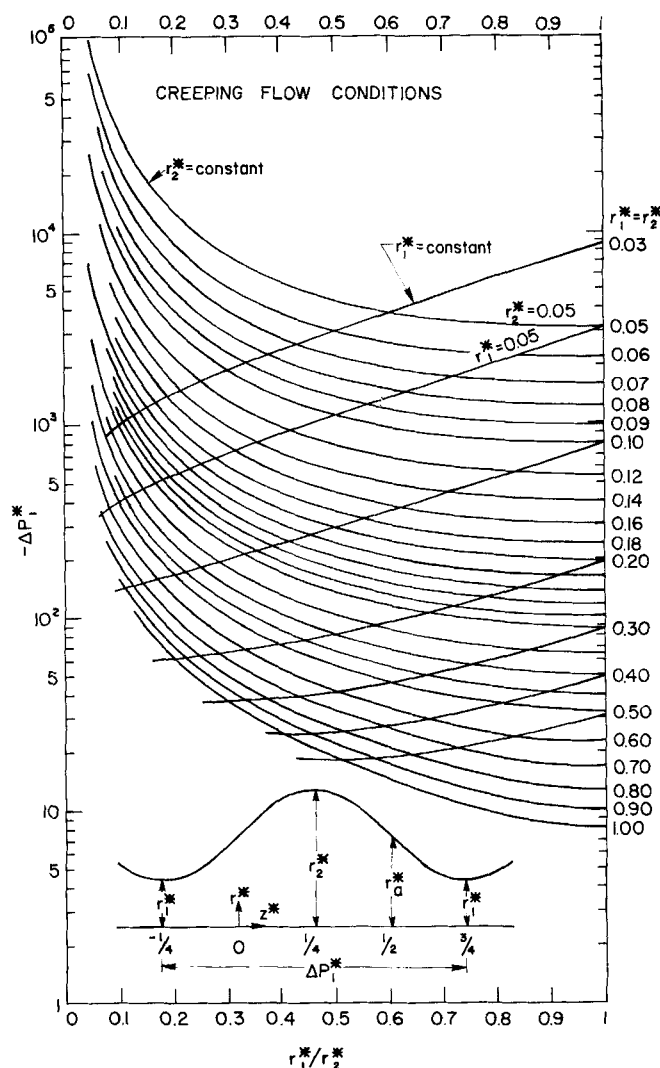


Fig. 1. Plot of values of $-\Delta P_1^*$ versus r_1^*/r_2^* with r_2^* as the parameter. A number of lines with constant r_1^* are also shown.

$$\left. \begin{aligned} i &= 1, \dots, n_r; & j &= 1, \dots, n_z \\ k &= (j-1)n_r + i; & N &= n_r n_z \end{aligned} \right\} \quad (7)$$

where n_r and n_z are the numbers of collocation points in the ξ and z directions, respectively, and N is the total number of collocation points.

It is easy to verify that the expression given by Equation (6) satisfies all boundary conditions, namely, no-slip on the wall, axial symmetry, periodicity and symmetry around the planes $z^* = \pm 1/4$.

The expansion coefficients are determined by setting the residuals at the interior collocation points to zero and solving the resulting linear system of N equations for the N unknowns. It was found that a good choice of collocation points is afforded by

$$\left. \begin{aligned} \{\xi_i; i = 1, \dots, n_r\} &= \text{roots of } P_{n_r}^{(0,0)}(\xi) \\ z_j^* &= \frac{\left(j - \frac{1}{4}\right)}{2n_z} - \frac{1}{4} \quad \text{for } j = 1, \dots, n_z \end{aligned} \right\} \quad (8)$$

where $P_n^{(\alpha,\beta)}(\xi)$ is the Jacobi polynomial of degree n and with parameters α and β . The axial coordinates of the collocation points, z_j^* , are the zeroes of the first omitted cosine function of the trial expansion (Mehler quadrature points).

TABLE 1. VALUES OF C_k FOR SINUSOIDAL TUBES OF VARIOUS GEOMETRIES; $n_r = n_z = \sqrt{N}$
WAS USED IN ALL CASES CONSIDERED HERE

r_1^*/r_2^* k	$r_2^* = 0.05$			
	0.2	0.4	0.6	0.8
1	-0.77868×10^{-6}	-0.17637×10^{-5}	-0.17725×10^{-5}	-0.79040×10^{-6}
2	-0.11961×10^{-7}	-0.13326×10^{-7}	-0.31321×10^{-8}	0.14705×10^{-8}
3	-0.12808×10^{-9}	0.33170×10^{-10}	0.44332×10^{-9}	0.57699×10^{-9}
4	0.39203×10^{-8}	0.13759×10^{-5}	0.23631×10^{-5}	0.23655×10^{-5}
5	0.10073×10^{-7}	0.18818×10^{-7}	0.11299×10^{-7}	-0.21370×10^{-8}
6	0.12487×10^{-9}	0.67820×10^{-10}	0.80408×10^{-10}	0.44776×10^{-9}
7	0.50931×10^{-6}	0.11609×10^{-5}	0.11713×10^{-5}	0.52332×10^{-6}
8	0.85593×10^{-8}	0.28698×10^{-8}	-0.10879×10^{-7}	-0.91300×10^{-8}
9	0.20560×10^{-9}	0.19097×10^{-10}	0.18881×10^{-10}	-0.23264×10^{-9}

r_1^*/r_2^* k	$r_2^* = 0.20$			
	0.2	0.4	0.6	0.8
1	-0.16630×10^{-3}	-0.40866×10^{-3}	-0.43817×10^{-3}	-0.20424×10^{-3}
2	-0.32444×10^{-4}	-0.42174×10^{-4}	-0.10925×10^{-4}	0.70315×10^{-5}
3	-0.54236×10^{-5}	-0.29629×10^{-5}	0.13797×10^{-5}	0.17592×10^{-6}
4	-0.11903×10^{-5}	0.33068×10^{-3}	0.58395×10^{-3}	0.59387×10^{-3}
5	0.91846×10^{-4}	0.61108×10^{-4}	0.40558×10^{-4}	-0.79149×10^{-5}
6	0.27275×10^{-4}	0.44730×10^{-5}	-0.21897×10^{-5}	-0.11246×10^{-5}
7	0.57219×10^{-5}	0.22352×10^{-3}	0.25725×10^{-3}	0.12439×10^{-3}
8	0.16052×10^{-5}	-0.52051×10^{-6}	-0.40228×10^{-4}	-0.35074×10^{-4}
9	0.86609×10^{-4}	0.41709×10^{-5}	0.18637×10^{-5}	0.26906×10^{-5}
10	0.19381×10^{-4}			
11	0.16720×10^{-5}			
12	0.10435×10^{-6}			
13	0.13273×10^{-4}			
14	-0.10917×10^{-4}			
15	-0.17588×10^{-5}			
16	-0.12497×10^{-5}			

r_1^*/r_2^* k	$r_2^* = 1.00$		
	0.4	0.6	0.8
1	-0.63317×10^{-1}	-0.11221	-0.10609
2	-0.66446×10^{-1}	-0.64912×10^{-1}	0.28340×10^{-1}
3	0.14139	-0.30983×10^{-1}	0.20916×10^{-1}
4	-0.37574	0.89592×10^{-1}	-0.10406×10^{-1}
5	0.22935	-0.29968×10^{-1}	0.20036
6	-0.30228×10^{-1}	0.11657	-0.12310×10^{-1}
7	0.46587×10^{-1}	0.11086	-0.73504×10^{-1}
8	0.81406×10^{-1}	0.11366	0.27541×10^{-1}
9	-0.21680	-0.18011	0.69118×10^{-1}
10	0.52916	0.51218×10^{-1}	-0.14489
11	-0.24466	0.74953×10^{-1}	0.89552×10^{-1}
12	0.13324×10^{-2}	-0.24700×10^{-1}	-0.16567×10^{-1}
13	0.27061×10^{-1}	-0.13534	0.26036×10^{-1}
14	-0.16114×10^{-1}	0.84806×10^{-1}	-0.91893×10^{-1}
15	0.12929	-0.67258×10^{-2}	0.10440
16	-0.98199×10^{-1}	0.38711×10^{-1}	-0.38579×10^{-1}
17	-0.13545	-0.84615×10^{-1}	
18	0.90072×10^{-1}	0.59664×10^{-2}	

(Continued on opposite page)

TABLE 1. (CONT'D.)

$r_2^* = 0.10$				
r_1^*/r_2^* k	0.2	0.4	0.6	0.8
1	-0.11969×10^{-4}	-0.27626×10^{-4}	-0.28159×10^{-4}	-0.12670×10^{-4}
2	-0.69239×10^{-6}	-0.80586×10^{-6}	-0.18351×10^{-6}	0.11187×10^{-6}
3	-0.40911×10^{-7}	-0.13981×10^{-7}	0.78257×10^{-8}	0.31777×10^{-8}
4	0.61450×10^{-5}	0.21739×10^{-4}	0.37548×10^{-4}	0.37708×10^{-4}
5	0.59719×10^{-6}	0.11492×10^{-5}	0.70685×10^{-6}	-0.12229×10^{-6}
6	0.32487×10^{-7}	0.20028×10^{-7}	-0.95572×10^{-8}	-0.36935×10^{-8}
7	0.73938×10^{-5}	0.17502×10^{-4}	0.18139×10^{-4}	0.82276×10^{-5}
8	0.45543×10^{-6}	0.13242×10^{-6}	-0.68368×10^{-6}	-0.59871×10^{-6}
9	0.47081×10^{-7}	0.22097×10^{-7}	0.93872×10^{-8}	0.11741×10^{-7}
$r_2 = 0.50$				
r_1^*/r_2^* k	0.2	0.4	0.6	0.8
1	-0.32825×10^{-2}	-0.10217×10^{-1}	-0.14148×10^{-1}	-0.80211×10^{-2}
2	-0.19393×10^{-2}	-0.38149×10^{-2}	-0.20287×10^{-2}	0.13713×10^{-2}
3	-0.22265×10^{-2}	-0.25288×10^{-2}	0.67552×10^{-3}	0.44426×10^{-4}
4	0.14941×10^{-2}	0.65195×10^{-3}	0.18506×10^{-3}	0.20220×10^{-1}
5	-0.16104×10^{-2}	0.87023×10^{-2}	0.18106×10^{-1}	-0.16429×10^{-2}
6	0.19173×10^{-2}	0.46879×10^{-2}	0.53169×10^{-2}	-0.55602×10^{-3}
7	0.15673×10^{-2}	0.41995×10^{-2}	-0.13674×10^{-3}	0.45739×10^{-2}
8	0.35106×10^{-2}	-0.55676×10^{-3}	-0.67360×10^{-3}	-0.54176×10^{-2}
9	-0.33913×10^{-2}	0.37449×10^{-2}	0.67418×10^{-2}	0.14874×10^{-2}
10	0.27816×10^{-2}	0.95936×10^{-3}	-0.30437×10^{-2}	
11	0.10652×10^{-2}	-0.10500×10^{-2}	-0.26079×10^{-2}	
12	0.85181×10^{-3}	-0.78183×10^{-3}	0.96080×10^{-3}	
13	-0.14847×10^{-2}	0.19358×10^{-2}	0.24784×10^{-2}	
14	0.27596×10^{-2}	-0.24266×10^{-2}	-0.51542×10^{-2}	
15	-0.13107×10^{-2}	0.51960×10^{-3}	0.31895×10^{-2}	
16	0.60259×10^{-3}	-0.14877×10^{-3}	-0.60864×10^{-3}	
17	0.83359×10^{-6}			
18	0.20677×10^{-4}			
19	-0.27584×10^{-3}			
20	-0.34088×10^{-3}			
21	0.25645×10^{-3}			
22	-0.44812×10^{-3}			
23	0.82504×10^{-3}			
24	-0.13697×10^{-2}			
25	0.73168×10^{-3}			
$r_2^* = 1.00$ (cont'd.)				
r_1^*/r_2^* k	0.4	0.6		
19	0.18609×10^{-1}	0.78186×10^{-1}		
20	-0.18500×10^{-3}	-0.38678×10^{-1}		
21	0.55320×10^{-1}	0.22044×10^{-1}		
22	-0.30262	-0.10581		
23	0.33062	0.18141		
24	-0.10336	-0.13363		
25	0.14970×10^{-1}	0.35971×10^{-1}		
26	-0.10724×10^{-1}			
27	-0.10371			
28	0.20009			
29	-0.12376			
30	0.23035×10^{-1}			
31	0.81080×10^{-2}			
32	-0.43562×10^{-1}			
33	0.82600×10^{-1}			
34	-0.68433×10^{-1}			
35	0.22788×10^{-1}			
36	-0.15075×10^{-2}			

Excellent convergence is attained in most cases with $N = 16$ collocation points, while $N = 9$ usually gives very good approximations. If r_1^*/r_2^* is very small (say,

less than 0.15) and r_2^* is rather large (say, larger than 0.75), 25 or more collocation points may be required.

The velocity components are obtained readily from

$$v_r^* = \frac{1}{r^*} \left[\left(\frac{\partial \xi}{\partial z^*} \right)_{r^*} \left(\frac{\partial \psi^*}{\partial \xi} \right)_{z^*} + \left(\frac{\partial \psi^*}{\partial z^*} \right)_{\xi} \right],$$

$$v_z^* = -\frac{1}{r^* r_w^*} \left(\frac{\partial \psi^*}{\partial \xi} \right)_{z^*} \quad (9)$$

Values of C_k for various geometries are listed in Table 1. Let ΔP be the pressure drop along one segment of the tube.* A dimensionless pressure drop is defined by

$$\Delta P^* = \frac{\Delta P}{\rho v_o^2} \quad (10)$$

Under creeping flow conditions we have

$$\Delta P^* = \frac{\Delta P_1^* (r_1^*, r_2^*)}{N_{Re}}; \quad N_{Re} = \frac{h v_o}{\nu} \quad (11)$$

The quantity ΔP_1^* , calculated by integration of the viscous dissipation function (Neira and Payatakes, 1978), is plotted in Figure 1 versus r_1^*/r_2^* for various values of r_2^* . This plot and Equations (10) and (11) can be used to calculate pressure drop values under creeping flow conditions over a wide range to tube geometries.

The graph in Figure 1 and Equation (11) can also be used to plot the product $f_v(N_{Re})v$, where f_v is the friction factor, vs. r_1^* and r_2^* , or, equivalently, vs. $(r_2^* - r_1^*)$ and d_v^* . Here, d_v^* is the dimensionless volumetric diameter and is given by:

$$d_v^* = 2r_a^* \sqrt{1 + \frac{b^2}{2}} \quad (12)$$

Such results are in complete accord with the trends reported in Payatakes et al. (1973b, c).

The values of C_k in Table 1 and Equations (6) and (9) can be used to calculate the stream function and the velocity components for various tube geometries.

NOTATION

- $b = \frac{r_2 - r_1}{r_2 + r_1}$ = reduced amplitude
- C_k = collocation expansion coefficients
- d_v^* = dimensionless volumetric diameter
- $f_v = -\frac{d_v^{*5} \Delta P^*}{32 r_1^{*4}}$ = friction factor
- h = wavelength
- $N = n_r n_z$ = number of interior collocation points
- $N_{Re} = \frac{h v_o}{\nu}$ = Reynolds number
- $(N_{Re})_v = \frac{4 r_1^{*2}}{d_v^*} N_{Re}$ = Reynolds number based on the volumetric diameter
- n_r, n_z = number of radial and axial expansion functions (or collocation points)
- r, r^* = radial and dimensionless radial coordinates, respectively
- $r_a = \frac{r_1 + r_2}{2}$ = arithmetic mean radius
- r_a^* = dimensionless arithmetic mean radius, Equation (1)
- $r_w(z)$ = wall radius
- $r_w^*(z^*)$ = dimensionless wall radius, Equations (1) and (2)

- r_1, r_2 = minimum and maximum radii, respectively
- r_1^*, r_2^* = dimensionless minimum and maximum radii, Equation (1)
- v_r, v_z = radial and axial velocity components, respectively
- v_r^*, v_z^* = dimensionless radial and axial velocity components, Equation (3)
- v_o = mean velocity at a cross section of minimum radius
- z, z^* = axial and dimensionless axial coordinates, respectively

Greek Letters

- $\Delta P, \Delta P^*$ = pressure drop and dimensionless pressure drop along one tube segment, respectively
- ΔP_1^* = value of ΔP^* for $N_{Re} = 1$ (under the assumption of creeping flow)
- ν = kinematic viscosity
- ξ = new radial coordinate, Equation (5)
- ψ^* = dimensionless stream function, Equations (4) and (6)

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* Under creeping flow conditions the pressure at cross-sections of maximum and minimum diameter is independent of radial position.

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A Critical Evaluation of the Semiimplicit Runge-Kutta Methods for Stiff Systems

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Frequently we encounter systems of ordinary differential equations in which there exists a large spread in the magnitude of the governing time constants. Conventional methods such as the explicit Runge-Kutta methods are known to be unsuitable for the integration of these so called stiff systems. Severe step length restrictions are imposed by the requirements for numerical stability, and thus a prohibitively large number of steps is often required.

A number of researchers have been actively seeking new techniques for the solution of such systems. Some of the more recent methods which have been given considerable attention are improved semiimplicit Runge-Kutta (SIRK) methods (Michelsen, 1976, 1977; Villadsen and Michelsen, 1978), an extension of the work of Caillaud and Padmanabhan (1971) to include a suitable step size adjustment procedure.

Their general formulation for $y' = f(y)$ is

$$k_i = (\underline{I} - ah\underline{J})^{-1} hf \left(y_n + \sum_{j=1}^{i-1} b_{ij}k_j \right) \quad i = 1, 2 \dots N$$

$$y_{n+1} = y_n + \sum_{i=1}^N R_i k_i$$

where

$$\underline{J} = (\partial f_i / \partial y_j)_{y_n}$$

N is the number of stages in the method. The constants a , b , and R are given by Michelsen (1977).

The Jacobian \underline{J} is evaluated once for each step, and the value of f at only one intermediate point is required. With LU decomposition of the matrix $(\underline{I} - ah\underline{J})$, the method requires only the solution of a set of linear equations equal in dimension to that of the system, with three different right-hand sides (for the third-order system). The solution process is then sequential in determining the k_i .

A full step-half step technique is used for step size adjustment. At each selected step size, the problem is first integrated by using the full step size. The same integration is then performed in two steps, each of length one half the original step. A refined solution vector, where the dominant $O(h^4)$ error term cancels, is found, and the next step size is proposed based on an empirical procedure. The step size is adjusted to keep the local truncation error below some specified value.

This method is known to have the property of absolute stability (the stability region associated with the formulation contains the open left half plane) and has been successfully applied by Michelsen (1976, 1977) to a number of stiff systems. However, in most of the published results, comparisons are made with the fourth-order explicit Runge-Kutta method only (constant step size). In all cases, the semiimplicit methods have been shown to be superior. Although no data were presented, Michelsen (1977) claims that the third-order method yielded identical results as Gear's method (1971) using about the same amount of computation time.

In this work, we attempt to evaluate critically the SIRK methods by a direct comparison of the third-order method (Villadsen and Michelsen, 1978) with the code developed by Hindmarsh (1974), possibly the best all-purpose, optimized, stiff package available. It is hoped that by direct comparison with an established package for stiff systems some insight can be gained into the potential of the SIRK methods.

NUMERICAL RESULTS

The systems used in the comparison represent a large spectrum of problem types: linear, nonlinear, problems with real and complex eigenvalues, large and small stiff systems, and problems with various degrees of stiffness. We have considered eighteen different problems and have selected six to present as representative examples, the general trend of results being comparable to the others.

Problem 1: nonlinear system of reaction rate equations, Robertson (1967):

$$y_1' = -0.04y_1 + 10^4 y_2 y_3 \quad \text{I.C. } y(0) = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$y_2' = 0.04y_1 - 10^4 y_2 y_3 - 3 \times 10^7 y_2^2$$

$$y_3' = 3 \times 10^7 y_2^2 \quad \text{Range} = (0, 10)$$

Problem 2: nonlinear example of Van der Pol's equation, Davis (1962):

$$y_1' = y_2 \quad \text{I.C. } y(0) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y_2' = 1000(1 - y_1^2)y_2 - y_1 \quad \text{Range} = (0, 2)$$

Problem 3: nonlinear chemistry example, Gear (1969):

$$y_1' = -0.013y_1 - 1000y_1 y_3 \quad \text{I.C. } y(0) = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$