TABLE 2. EXPERIMENTAL GAS COMPOSITIONS

| Mole % | $CH_4$ | A | B | C | D |
|---|---|---|---|---|---|
| $CH_4$ | 99.7 | 79.4 | 64.5 | 43.1 | 21.7 |
| $H_2$ | 0.0 | 20.2 | 35.1 | 56.5 | 78.0 |
| $N_2$ | 0.2 | 0.3 | 0.3 | 0.2 | 0.2 |
| Others | 0.1 | 0.1 | 0.1 | 0.2 | 0.1 |

mole, and the density $\rho$ is gram mole per cubic centimeters. When all possible errors are considered, the Z values are probably accurate to ±0.10%.

The parameters $B$ are given in Table 1. Note that the values of $B$ coefficients are given for numerical precision, and the calculated Z should be rounded. The experimental gas compositions are given in Table 2. The maximum experimental pressure is also listed in Table 1; extrapolation to higher pressures is questionable. The $-129°C$ isotherms were not reanalyzed because there were too few points along these isotherms to justify the analytical method being used.

The values for methane are included in Table 1; however, the authors recommend that the equation of state by Vennix and Kobayashi (1969) be used for more precise computations on methane.

These data should be useful for present day coal gasification studies.

## ACKNOWLEDGMENT

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# A Simple Method of Calculating Effectiveness Factors for Heterogeneous Catalytic Gas-Solid Reactions

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For many practical purposes the design of a catalytic reactor may have to be made with a lack of precise information on the physical and chemical properties of reactants and products. Under such circumstances use of an elaborate model to predict the catalyst effectiveness may not be warranted and a simpler approach should suffice. This note presents a simple method of general utility for calculating effectiveness factors. The method which gives very good agreement with more exact solutions is similar to that recently noted by Aris (Aris, 1975, Georgakis and Aris, 1975). That method, however, involves a graphical solution whereas the method proposed in this note, being confined to isothermal or near isothermal conditions, requires (in combination with the asymptotic approximation) only the solution of a simple algebraic equation to determine particle effectiveness for any particular value of the Thiele modulus.

Many catalytic chemical reactions can be represented by the Langmuir-Hinshelwood model which is described by the general expressions

$$r = \frac{(kC_s^n)\,C^n}{[1 + (KC_s)C]^m} \tag{1}$$

With the assumption of constant diffusivity, a mass balance for the reactant in a catalyst pellet yields

$$D_e \nabla^2 C = r(C) \tag{2}$$

Extending previous results published by Aris (1957), Knudsen et al (1966) showed that the correlations of effectiveness factor and Thiele modulus for a sphere, cylinder, and flat plate lie close together when the characteristic dimension in the Thiele modulus is defined as the ratio of the volume to the outside surface through which the reactant can diffuse. Therefore, a simplified analysis for a flat plate can be extended to catalyst pellets of dif-

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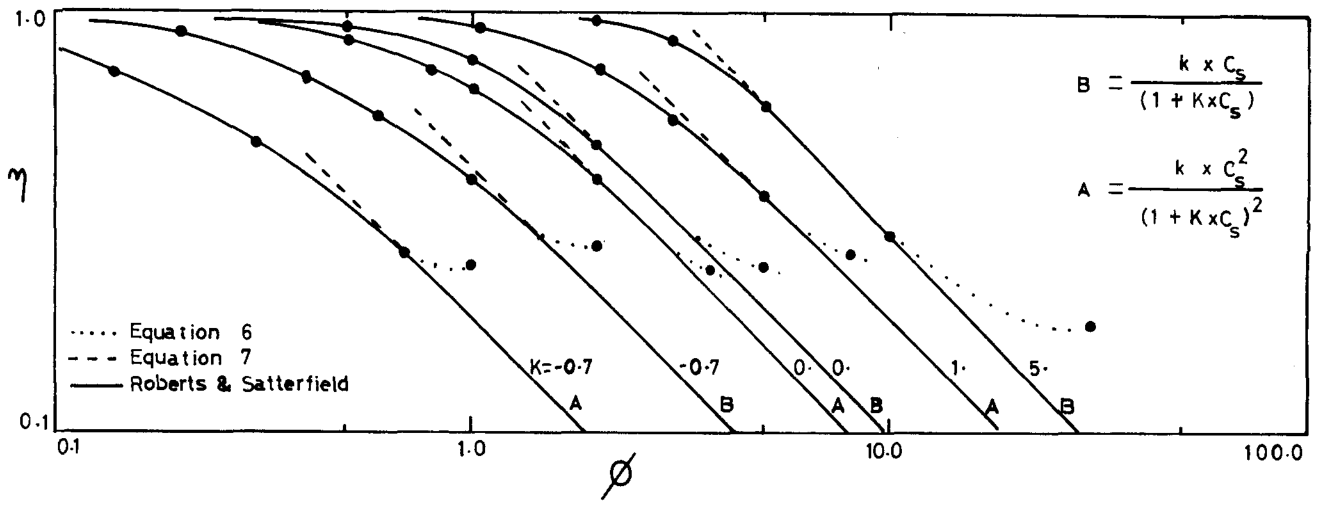

**Fig. 1. Effectiveness factor as function of Thiele modulus for monomolecular and bimolecular reactions for selected values of parameter *K*.**

ferent shapes without much effort. Furthermore, Villadsen and Stewart (1967) presented a new technique of solving differential equations using orthogonal polynomials which yields

$$\nabla^2 C(i) = \sum_{j=1}^{N+1} B_{ij}\, C(j) \qquad (3)$$

where $B_{ij}$ are the collocation constants for the Laplacian and $N$ is the number of internal collocation points. When a single collocation point is used, the approximate solution is represented by a simple algebraic equation. The combination of both approximations, presented in the analysis which follows, leads to a very simple method of calculating effectiveness factors for any order of reaction expressed by equation (1).

The development is based upon a flat plate of catalyst and the approximate solution is obtained by a single point collocation ($N = 1$). In this case the combination of equations 2 and 3 reduces to

$$\frac{\phi^2}{2.5} \cdot \frac{\hat{C}^n}{(1 + KC_s\hat{C})^m} + \hat{C} - 1 = 0 \qquad (4)$$

where $c$ is the concentration of reactant at the single internal collocation point and the constant 2.5 is the value specified by Villadsen for a flat plate.

The effectiveness factor $\eta$, defined as the ratio of the rate of reaction for the whole catalyst divided by the rate at the surface conditions, can be calculated by orthogonal collocation through the expression (Villadsen, 1967)

$$\eta = \frac{(\lambda + 1)}{r(C = 1)} \Sigma\, w_i \cdot r(C_i) \qquad (5)$$

and again for a flat plate and one collocation point this simplifies to

$$\eta = 0.17\left[1 + \frac{0.83}{0.17} \cdot \hat{C}^n \cdot \left(\frac{1 + KC_s}{1 + KC_s\hat{C}}\right)^m\right] \qquad (6)$$

where $\hat{C}$ is the root in the interval 0 to 1 of Equation (4).

As the Thiele modulus increases the concentration gradient at the pellet surface increases and the concentration calculated by equation 4 becomes larger than its real value. This higher value yields in turn a larger effectiveness factor. For this region the asymptotic solution (Petersen 1965)

$$\eta = \frac{\sqrt{2}}{\phi}(1 + KC_s)^m \sqrt{\int_0^1 \frac{C^n}{(1 + KC_sC)^m}\, dC} \qquad (7)$$

may be used. This asymptotic approach however, gives higher values of the effectiveness factor for small values of Thiele modulus. Since the true effectiveness factor curve lies below the asymptote (7), the values calculated from equation (6) should be used only as long as they are less than those given by equation (7), which then becomes the more accurate approximation.

As an application of the method suggested in this note, a comparison is made in figure 1 between the results presented by Roberts and Satterfield for the monomolecular ($m = 1$) (1965) and bimolecular ($m = 2$) (1966) reaction mechanism and values calculated by the present method. As can be seen, the approximate values show very good agreement with the more exact solution for positive, zero and negative values of the equilibrium absorption parameter $K$ and thus cover a wide range of orders or reaction.

In conclusion, the method permits the calculation of effectiveness factors in a quick and simple way, without recourse to extensive and elaborate numerical methods, which would certainly require computing facilities and costly time consumption.

## NOTATION

$B_{ij}$ = collocation constant (Villadsen, 1967)
$C$ = dimensionless concentration
$C_s$ = concentration at pellet surface, gmol/cm$^3$
$\hat{C}$ = dimensionless concentration at the collocation point
$D_e$ = effective diffusivity, cm$^2$/s
$k$ = reaction rate constant, s$^{-1}$
$K$ = Langmuir adsorption constant, cm$^3$/gmol
$r$ = reaction rate, gmol/cm$^3$/s
$w_i$ = weight values (Villadsen, 1967)

### Greek Letters

$\phi$ = Thiele modulus defined as $L(kC_s^{n-1}/D)^{1/2}$
$\eta$ = effectiveness factor of catalyst pellet: (rate of reaction per pellet)/(rate at surface conditions)
$\lambda$ = geometry parameter (Villadsen, 1967)

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# Flow Through Permeable Beds Consisting of Layers of Different Size Spheres

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TABLE 1. HEIGHTS OF BED LAYERS, (MM)

| Bed | 3 mm spheres | 1 mm spheres | Total height |
|---|---|---|---|
| A | 27.9 | 111.8 | 139.7 |
| B | 55.9 | 83.8 | 139.7 |
| C | 83.8 | 55.9 | 139.7 |
| D | 111.8 | 27.9 | 139.7 |

This paper is concerned with the flow—pressure drop characteristics for non-Darcy flow in permeable beds consisting of two horizontal layers of different size spheres. To identify the extent of the interaction between the layers, the measured results are compared with those from a computational model which assumes that the constituent layers behave as if they are unrelated parallel flow paths. In the absence of alternative approaches, such a model would, in all likelihood, be employed to predict the characteristics of multilayer beds by making use of available information for single layer (that is, homogeneous) beds. Therefore, an experimental test of the computational model is of some practical relevance.

## EXPERIMENTS

The layered beds were contained in a test section having a 14 × 14 cm$^2$ cross section and a length of 35.6 cm. The lower and upper layers, respectively, consisted of 1 mm[*] and 3 mm spherical glass beads. Four layered beds were investigated, and the heights of the constituent layers are listed in Table 1. Experiments were also carried out for beds consisting exclusively of either 1 or 3 mm beads. These homogeneous bed experiments encompassed bed heights of 27.9, . . . and 139.7 mm.

The test section, made of Plexiglas, was instrumented with thirty pressure taps, fifteen in the top wall and fifteen in the bottom wall. The taps were spaced at 2.5 cm intervals along the spanwise center line of the respective wall. Packing of the spheres was accomplished by removal of the top wall. The packing process (see Bahrami, 1975) involved a succession of pourings and smoothings and, as a final stage, a tamping procedure.

The working fluid was water. It was supplied to the test section by means of a constant head tank. Adjustment of the water level in the tank permitted control of the rate of mass flow through the porous bed. Measurement of the mass flow was accomplished by the direct weighing method. The water temperature was maintained constant in the range 20°C ± 0.3° during the entire course of the experiments. Care was taken to remove air bubbles from the bed prior to the initiation of data collection. The pressure distributions were read from a manometer bank by a cathetometer capable of discriminating heights to within 0.05 mm.

## RESULTS AND DISCUSSION

The homogeneous bed experiments were performed first, and the measured flow—pressure drop data were examined with the aid of the Forchheimer relation, which is a nonlinear generalization of Darcy's law. For data analysis, a particularly convenient form of the Forchheimer law is

$$\frac{1}{\mu V}\left[-\frac{dp}{dx}\right]=\frac{1}{k}+\frac{c}{\sqrt{k}}\left(\frac{V}{\nu}\right) \qquad (1)$$

where $dp/dx$ is the streamwise pressure gradient. If data plotted on a graph of $(-dp/dx)/\mu V$ vs. $V/\nu$ yield a straight line relationship, then the Forchheimer relation is obeyed. Furthermore, the values of $c$ and $k$ can be deduced from the slope and the intercept of the straight line.

All of the homogeneous bed data were found to be well correlated by the Forchheimer relation (Bahrami, 1975). In round numbers, the respective permeabilities of the 1 and 3 mm beds were $0.7 \times 10^{-5}$ and $7 \times 10^{-5}$ cm$^2$. The $c$ values were in the range from 0.3 to 0.5.

For the layered beds, it may first be noted that for all the layer configurations and flow rates that were investigated, the pressure gradients measured along the top and bottom walls of the test section were within a fraction of a percent of each other. Furthermore, the $p$ vs. $x$ distributions were linear. Thus, the flows in the two layers were driven by a common and constant pressure gradient.

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[*] Nominal value; the beads were sifted between 16 and 20 mesh sieves having openings of 1 and 0.841 mm, respectively.