Int. J. Heat Mass Transfer. Vol. 17, pp. 1413–1416. Pergamon Press 1974. Printed in Great Britain

# HEAT AND MASS TRANSFER IN A POROUS WALL TUBULAR REACTOR

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(*Received* 8 *October* 1973 *and in revised form* 11 *January* 1974)

## NOMENCLATURE

$a$, radius of the tube;
$B$, $4h/\rho c_p u_o$, dimensionless;
$c_A$, concentration of $A$;
$c_{Ao}$, concentration of $A$ at inlet;
$c_E$, concentration of $A$ in material injected;
$c_{A_w}$, wall concentration of $A$, equals $c_A$ for plug flow;
$c_p$, average specific heat of reaction mixture;
$c_{p_E}$, average specific heat of material injected;
$C$, $c_A/c_{A_o}$;
$C_E$, $c_E/c_{A_o}$;
$E$, energy of activation;
$f_A$, the magnitude of the fraction of the inlet reactant flow rate that is depleted by the reaction in a reactor of given length;
$F_A$, flux of $A$ across tube wall, mols per unit area per unit time;
$h$, heat-transfer coefficient;
$H$, $2ak_o c^n_{A_o}(-\Delta H_R)/(u_o \rho c_p T_w)$, dimensionless;
$k$, rate constant (function of temperature) $= k_o \exp(-E/RT)$;
$k_o$, constant in Arrhenius equation, see above;
$K$, $2akc^{n-1}_{A_o}/u_o$ (isothermal case);
$\bar{K}$, $2ak_o c^{n-1}_{A_o}/u_o$;
$n$, order of reaction;
$-r_A$, rate of disappearance of $A$ by chemical reaction, mols per unit time per unit volume, equals $kc^n_A$;
$R$, gas constant;
$S$, $1-F_A/v_w c_{A_w}$;
$T$, temperature of reaction mixture;
$T_E$, uniform external temperature;
$T_{in}$, temperature at inlet of the reactor;
$u$, velocity at longitudinal position $z$;
$u_o$, velocity at inlet of the reactor;
$U$, $u/u_o$;
$v_w$, velocity at the wall;
$V$, $v_w/u_o$;
$z$, longitudinal position.

Greek symbols

$\alpha$, defined by equation (8);
$\beta$, defined by equation (T-10);
$\Delta H_R$, heat of reaction;
$\varepsilon$, $E/RT_w$, dimensionless;
$\theta$, $T/T_w$;
$\theta_E$, $T_E/T_w$;
$\lambda$, defined by equation (T-9);
$\xi$, $z/2a$;
$\rho$, average density of reaction mixture;
$\rho_E$, average density of material injected.

## INTRODUCTION

THE POROUS wall reactor is an object of current research interest. Very little has been published on the subject. A brief review of the literature may be found in a paper by Shah and Remmen [1]. The objectives of the present communication are:

(1) To extend the first order, isothermal, plug flow analysis of Shah and Remmen to reactions of order $n$.
(2) To establish a realistic basis for characterizing the performance of a porous wall reactor.
(3) To consider heat effects in a first order irreversible reaction with a view to studying the influence of wall permeation on "parametric sensitivity", (2).

## BASIC EQUATIONS

For the isothermal case, assuming constant fluid density and wall permeation velocity, the mass balances on reacting species A are:

(1) *Suction:*

$$\frac{\mathrm{d}}{\mathrm{d}\xi}(UC)+KC^n+4(1-S)VC=0 \tag{1}$$

$$U=1-4V\xi. \tag{2}$$

(2) *Injection:*

$$\frac{\mathrm{d}}{\mathrm{d}\xi}(UC)+KC^n-4VC_E=0 \tag{3}$$

$$U=1+4V\xi. \tag{4}$$

The analytical solutions to equations (1) and (3) subject to the boundary condition $C=1$ at $\xi=0$ are listed in Table 1. (Analytical solutions for the case of injection with $C_E \neq 0$ and $n \neq 1$, or 2 were not obtainable.)
For the non isothermal reactor the heat and mass balances for the case of injection may be expressed as follows:

$$\frac{\mathrm{d}C}{\mathrm{d}\xi}=\frac{4VC_E-\bar{K}C^n\exp\left(-\frac{\varepsilon}{\theta}\right)-4VC}{1+4V\xi} \tag{5}$$

$$\frac{\mathrm{d}\theta}{\mathrm{d}\xi}=\frac{HC^n\exp\left(-\frac{\varepsilon}{\theta}\right)-B(\theta-1)+4V(\theta_E-\theta)}{1+4V\xi} \tag{6}$$

$$C=1,\quad \theta=T_{\rm in}/T_{\rm wall}\quad \text{at}\quad \xi=0. \tag{7}$$

The starting equation is given by equation (7). In the derivation of the above equations the physical properties were assumed constant. Also $c_p/c_{pE}$ and $\rho/\rho_E$ are assumed to be unity. Analogous equations can be derived for the case of suction.

Table 1

Suction:

$$\alpha = \frac{1 - UC - 4V(1-S)\int_0^\xi C\,d\xi}{1 - 4V(1-S)\int_0^\xi C\,d\xi} \tag{T-1}$$

$n = 1,\ 0 \leqslant S \leqslant 1$:

$$C = (1-4V\xi)^{\frac{K}{4V} - S} \qquad \text{ref [3]} \tag{T-2}$$

$n \neq 1,\ S = 0$:

$$C = \left\{\ln\left[(1-4V\xi)^{\frac{(1-n)K}{4V}}\right] + 1\right\}^{\frac{1}{1-n}} \tag{T-3}$$

$n \neq 1,\ 0 < S \leqslant 1$:

$$C = \left[\frac{4VS}{K - (K - 4VS)(1-4V\xi)^{S(n-1)}}\right]^{\frac{1}{n-1}} \tag{T-4}$$

Injection:

$$\alpha = \frac{1 - UC + 4VC_E\xi}{1 + 4VC_E\xi} \tag{T-5}$$

$n = 1,\ C_E \geqslant 0$:

$$C = \frac{1}{\frac{K}{4V} + 1}\left[C_E + \left(\frac{K}{4V} + 1 - C_E\right)(1+4V\xi)^{-\left(\frac{K}{4V}+1\right)}\right] \tag{T-6}$$

$n \neq 1,\ C_E = 0$:

$$C = \left\{\frac{4V}{(K+4V)(1+4V\xi)^{n-1} - K}\right\}^{\frac{1}{n-1}} \tag{T-7}$$

$n = 2,\ C_E \neq 0$:

$$C = \frac{2V}{K}\left[\frac{(1+\beta)(1+4V\xi)^{-\beta} + \lambda(\beta - 1)}{\lambda - (1+4V\xi)^{-\beta}}\right] \tag{T-8}$$

where

$$\lambda = \frac{\frac{k}{2V} + 1 + \beta}{\frac{K}{2V} + 1 - \beta} \tag{T-9}$$

$$\beta = \sqrt{1 + KC_E/V} \tag{T-10}$$

## RESULTS AND DISCUSSION

Shah and Remmen [1] defined an index for the reactor performance, $f_A$, as "The magnitude of the fraction of the inlet reactant flow rate that is depleted by the reaction in a reactor of a given length". However, what is of interest is the magnitude of the fraction of the "net input" of the reactant converted in a reactor of a given length. In the case of injection of $A$, for example, the "net input" is the flow rate of $A$ at the inlet plus the flow rate of $A$ across the tube wall. Such a definition of reactor performance has, in fact, been used by Van de Vusse and Voetter [4]. For the case of suction of $A$ (and inerts) across the porous wall, "net input" of $A$ equals the inlet flow rate of $A$ minus the flow rate of $A$ across the wall, assuming that $A$ bled out of the reactor is recovered. For the case of suction or injection of inerts only, as well as for the case when the reactant bled out cannot be recovered, the "net input" of $A$ is just the inlet flow rate of $A$. The net conversion $\alpha$ is defined as follows:

$$\alpha = \frac{\int_0^z (-r_A)\pi a^2\,dz}{\text{"Net input" of } A}. \tag{8}$$

The pertinent equations for $\alpha$ may be found in Table 1. Equations (T-1) and (T-5) apply to both isothermal and non-isothermal cases.

*Isothermal case*

Figure 1 shows a plot of $\alpha$ vs $\xi$ for suction, injection, and the impervious wall case. In reference [1] it was stated that "in the case of suction the leaking of reactant through tube wall will obviously hurt the reactor performance. On the other hand, in the case of injection permeation of reactant through the tube wall will help in improving the performance of the reactor". These statements were based on $f_A$. However, on the basis of "net" conversion, $\alpha$, different conclusions may be reached (Fig. 1). For example, at a given $\xi$, $\alpha$ corresponding to injection of inerts is greater than that corresponding to injection of reactant. (Curves 5 and 6 in Fig. 1.) For curve 5, since there is no reactant permeation across the wall, $\alpha = f_A$. A plot of $f_A$ vs $\xi$ is also shown in Fig. 1; thus, on the basis of $f_A$, injection of reactant is more efficient compared with injection of inerts while on the basis of $\alpha$, the reverse is true. Also suction of $A$ (and inerts) is more efficient compared to suction of inerts alone (curves 1 and 2 in Fig. 1). From a design point of view $\alpha$ is a more realistic basis of reactor performance.

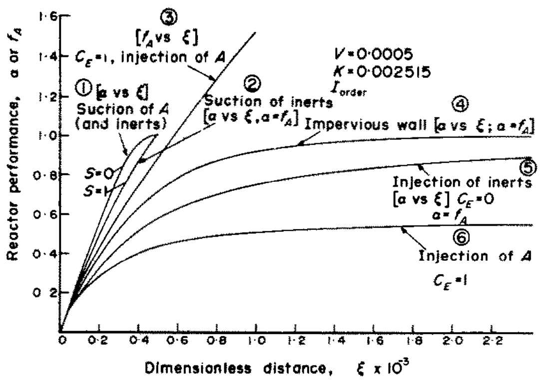


FIG. 1. Reactor performance vs dimensionless distance.

*Heat effects*

The values of the parameters were taken from reference [2]. $E = 22\,500$ cal., $[(-\Delta H_R)/\rho C_p] = 7300$(l.)(°C/g mol., $K_o = 3{\cdot}94 \times 10^{12}\,\text{min}^{-1}$, $C_{A_o} = 0{\cdot}02$ g mol/l., $[2h/a\rho C_p] = 0{\cdot}2\,\text{min}^{-1}$. $2a/u_o$ was chosen to be unity (min) so that an exact correspondence could be established with reference [2]. As in reference [2], the first order case, $n = 1$, was considered. The dimensionless parameters are: $\bar{K} = 3{\cdot}94 \times 10^{12}$, $B = 0{\cdot}2$. $\theta_E = 1$. The magnitudes of $H$ and $\varepsilon$ depend on $T_w$. For example, when $T_w = 340$°K, $\varepsilon = 33{\cdot}301364$ and $H = 1{\cdot}6918824 \times 10^{12}$. For all cases, $T_{in} = 340$°K. Equations (5) and (6) were solved simultaneously using the fourth order Range–Kutta scheme. Figure 2 shows the results ($\theta$ vs $\xi$) for $C_E = 0$ (injection of inert). Three values of $T_w$ are considered: 337·5, 340 and 342·5°K. $V = 0$ corresponds to the impervious wall reactor. It may be seen that a slight change in the wall temperature results in a substantial shift of the temperature profile. This has been referred to as "parametric sensitivity" [2]. It must be pointed out that the solution to the system of equations (5) and (6) is extremely sensitive to the term $\exp(-\varepsilon/\theta)$. The results for the impervious wall reactor ($V = 0$) differ from those reported in [2]. It is believed that this may be due to the fact that in reference [2], the solutions were found with the aid of an analog computer. In the present case, a digital computer (Univac Series 70/7) was used with double precision. With injection of inert into the system the temperature profiles flatten out considerably. However, from a design point of view, the temperature behavior should be considered along with "net" conversion. Figure 3 is such a plot. It may be seen that although the injection of inerts helps keep the temperature under control, the advantage is counteracted by the decrease in net conversion. Thus, both plots (Figs. 2 and 3) must be evaluated together in order to arrive at a reasonable basis for design. From a practical point of view the porous wall reactor is suitable for controlling exothermic reactions.

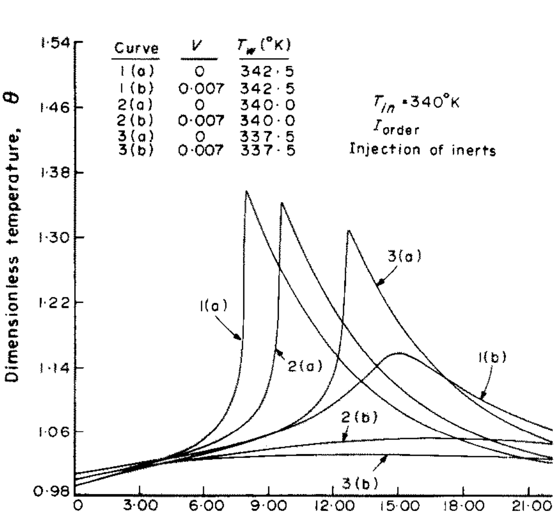


FIG. 2. Dimensionless temperature vs dimensionless distance.

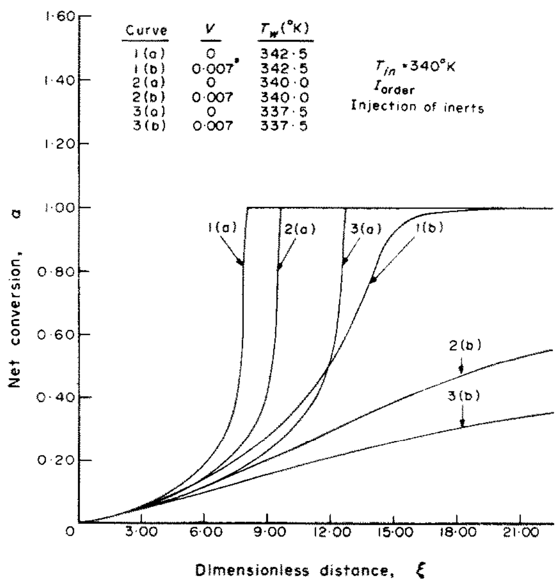


FIG. 3. Net conversion vs dimensionless distance.

REFERENCES

1. Y. T. Shah and T. Remmen, Radial mass transfer effects in a porous wall tubular reactor, *Int. J. Heat Mass Transfer* **14**, 2109–2124 (1971).
2. O. Bilous and N. R. Amundson, Chemical reactor stability and sensitivity, *A.I.Ch.E. Jl* **2**, 117–126 (1956).
3. M. R. Doshi, R. Sankarasubramanian and W. N. Gill, A comment on "Radial mass transfer effects in a porous wall tubular reactor", *Int. J. Heat Mass Transfer* **16**, 525–526 (1973).
4. J. G. Van De Vusse and H. Voetter, Optimum pressure and concentration gradients in tubular reactors, *Chem. Engng Sci.* **14**, 90–98 (1961).


*Int. J. Heat Mass Transfer.* Vol. 17, pp. 1416–1418. Pergamon Press 1974. Printed in Great Britain

# EXTINCTION OF SPHERICAL DIFFUSION FLAMES: SPALDING'S APPROACH

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(*Received* 19 *October* 1973 *and in revised form* 29 *January* 1974)

### NOMENCLATURE

$B$, transfer number;
$b$, equation (7d);
$C$, stoichiometric mass of core species;
$D$, diffusion coefficient;
$G$, mass burning velocity through a stoichiometric mixture;
$I$, stoichiometric mass of species $i$;
$\dot{m}$, mass injection rate;
$p$, pressure;
$R$, volumetric consumption rate of injected fuel;
$r$, radial coordinate;
$t$, time;
$V$, mass of volatiles in solid fuel;
$v$, velocity component;
$Y$, mass fraction;
$\beta$, coupling function, equation (4b);
$\varepsilon$, flux fraction;
$\Lambda$, equation (7c);
$\nu$, stoichiometric parameter, equation (16b);
$\nu_s$, stoichiometric oxygen–fuel mass ratio;
$\xi$, dimensionless radial coordinate, equation (4a);
$\phi$, equation (4c);
$\rho$, density;
$\Psi$, dimensionless reaction rate;
$\dot{\omega}$, rate of species generation by chemical reaction.

Subscripts

$c$, core species;
$F$, fuel;
$i$, species $i$;
0, initial value;
O, oxygen;
$s$, solid;
$st$, stoichiometric;
$v$, volatiles;
$w$, wall condition;
$\infty$, condition at infinity.

Superscripts

$'''$, per unit volume;
$+$, dimensionless quantity.

### 1. INTRODUCTION

THE EXTINCTION problem of droplets has been studied in some detail [1–4] and an extinction criterion in a closed form for opposed jet diffusion flame was obtained by Spalding [5], using an approximate analytical technique. Del Notario *et al.* [6] investigated the extinction of spherical and premixed diffusion flames in air. This communication presents a closed form solution for the gas extinction of a spherical diffusion flame. It attempts to link the method of solution of an opposed jet diffusion flame as obtained by Spalding [5] with that of a spherical symmetric non-adiabatic diffusion flame.

### 2. GOVERNING EQUATIONS

Consider a porous sphere through which a mixture of fuel and inert gas is injected. The conservation equations are

Species: $$\rho v \frac{\mathrm{d}Y_i}{\mathrm{d}r} = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(\rho r^2 D \frac{\mathrm{d}Y_i}{\mathrm{d}r}\right) + \dot{\omega}_i''' \qquad (1)$$

Momentum: $$p = \text{constant} \qquad (2)$$

Overall Continuity: $$4\pi\rho v r^2 = \dot{m}. \qquad (3)$$

Let the Lewis number equal to unity.

$$\xi = \frac{\dot{m}}{4\pi\rho D r}, \qquad \beta_{ic} = \frac{Y_i}{I} - \frac{Y_c}{C} \qquad (4a, b)$$

and

$$\phi_{ic} = \frac{\beta_{ic} - \beta_{ic,\infty}}{\beta_{ic,w} - \beta_{ic,\infty}}. \qquad (4c)$$

From equations (1) and (4) for all $i \neq c$

$$\phi_{ic} = \frac{1 - \exp(-\xi)}{1 - \exp(-\xi_w)}. \qquad (5)$$