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SUBJECT: Gas Diffusion into a Bubble of Fixed Radius

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I STATEMENT OF PROBLEM

The problem for the diffusion of radiolytic gas into a bubble of fixed radius is solved. A constant source of radiolytic gas is assumed. The concentration of radiolytic gas at the bubble surface is related to the gas pressure within the bubble by Henry's constant.

II. MATHEMATICAL STATEMENT OF PROBLEM

The diffusion equation is

$$\frac{\partial c}{\partial t} = K \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial c}{\partial r}) + S \quad (1)$$

where

c = gas concentration
 K = diffusion constant
 S = constant source of radiolytic gas.

The boundary conditions on c are obtained from the following equations:

$$P = \frac{n}{V} K_B T \quad (\text{perfect gas law}) \quad (2)$$

where

η = number of gas molecules in a bubble

P = pressure

K_B = Boltzman constant

V = bubble volume

T = temperature

$$\frac{dh}{dt} = 4\pi R^2 K \left. \frac{\partial c}{\partial r} \right|_R \quad (3)$$

$$P = K_H c(R, t) \quad (\text{Henry's Law}) \quad (4)$$

with K_H = Henry's constant

Combining (2), (3), and (4), we obtain the boundary condition

$$\left. \frac{\partial c}{\partial t} (R, t) = \frac{3K_B T}{R} \frac{K}{K_H} \frac{\partial c}{\partial r} \right|_R \quad (5)$$

The initial conditions assumed are

$$P(t=0) = K_H C_0 \quad (6)$$

$$C(R, 0) = C_0 \quad (7)$$

III. SOLUTION OF PROBLEM

Introduce $u(r, t)$ defined by

$$C(r, t) = c_0 + St - \frac{u(r, t)}{r} \quad (8)$$

Equations (1), (5) and (7) become

$$\frac{\partial u}{\partial t} = K \frac{\partial^2 u}{\partial r^2} \quad (1')$$

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$$aRu(R,t) + \frac{\partial u}{\partial t}(R,t) = SR + aR^2 \frac{\partial u}{\partial r}(R,t) \quad (5)$$

where

$$a = \frac{3K_B T}{R^3} \frac{K}{K_H}$$

and

$$u(r,0) = 0 \quad (7')$$

The set of equations (1'), (5) and (7') can be solved by the Laplace transform technique:

Let
$$u(r,t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{pt} u(r,p) dp$$

Then (1'), (5) and (7') yield

$$pu(r,p) - u(r,0) = K \frac{\partial^2 u}{\partial r^2}(r,p) \quad (9)$$

$$aRu(R,p) + pu(R,p) = \frac{S}{p} + aR^2 \frac{\partial u}{\partial r}(R,p) \quad (10)$$

The solutions to (9) are

$$u(r,p) = A \pm (p) e^{\pm \sqrt{\frac{p}{K}} R} \quad (11)$$

and $A_+(p) = 0$ is necessary such that $u(r=\infty, t) = 0$.

Substitution of (11) into (10) yields

$$A_-(p) = \frac{(SR/p) e^{\sqrt{p/K} R}}{aR + p + aR^2 \sqrt{p/K}}$$

and

$$u(r,p) = \frac{SR}{p} \frac{e^{-q(r-R)}}{aR + p + aR^2 q} \quad (12)$$

$$q = \sqrt{p/K}$$

The inversion to obtain $u(r,t)$ is now carried out. Equation (2) can be rearranged to the form

$$u(r,p) = \frac{SR}{K} \frac{e^{-q(r-R)}}{p(q-q_+)(q-q_-)}$$

$$= \frac{SR}{K} \frac{1}{q_+ - q_-} \left[\frac{1}{p(q-q_+)} - \frac{1}{p(q-q_-)} \right] e^{-q(r-R)} \quad (13)$$

where

$$q_{\pm} = -\frac{aR^2}{2K} \pm 1 \sqrt{\frac{aR}{K} \left(1 - \frac{aR^3}{4K}\right)}, \quad \frac{aR^3}{4K} = \frac{3K_B T}{4K_H} < 1$$

The inversion is performed by Eq 14, p. 494 of Carslaw and Jaeger, Second Edition:

$$u(r,t) = \frac{SR}{K} \frac{1}{q_+ - q_-} 2i \operatorname{Im} \left[\frac{1}{q_+} e^{-q_+(r-R) + Ktq_+^2} \operatorname{erfc} \left\{ \frac{\frac{r-R}{2\sqrt{Kt}} - q_+\sqrt{Kt}}{1} \right\} - \frac{1}{q_+} \operatorname{erfc} \frac{r-R}{2\sqrt{Kt}} \right] \quad (14)$$

if it is recognized that

$$(\operatorname{erf} z)^* = \operatorname{erf}(z^*)$$

A useful form for $u(R,t)$ can be obtained by manipulation

$$u(R,t) = \frac{SR}{K} \left[\frac{1}{|q_+|^2} + \frac{2i}{q_+ - q_-} \operatorname{Im} \frac{e^{z^2} \operatorname{erfc} z}{q_+} \right] \quad (15)$$

with

$$z = -\sqrt{Kt}q_+ = -\sqrt{Kt}(q_R + iq_I) = x + iy \quad \begin{matrix} q_R < 0 \\ q_I < 0 \end{matrix} \quad (16)$$

The complimentary error function of complex argument is tabulated in Carslaw and Jaeger, p. 484 through the functions $u(x,y)$ and $v(x,y)$:

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$$\omega(iz) = e^{-z^2} \operatorname{erfc} z \quad (17)$$

$$\omega(z) = u(x,y) + iv(x,y)$$

A simple form for $u(R,t)$ is then

$$u(R,t) = \frac{SR}{K} \frac{1}{|q_+|^2} \left[1 + \frac{q_R}{q_I} v(-y,x) - u(-y,x) \right] \quad (18)$$

IV. Applicability of Solution to Inertial Pressure Calculations

In a reactor such as KEWB, the diffusion of radiolytic gas into a bubble tends to cause the gas pressure to increase. This pressure rise will occur if the diffusion is so rapid that the solution does not have time to expand away and thus relieve the gas pressure. These high pressure bubbles will compress the solution. The bubble pressures will drop and the (inertial) pressure in the solution will increase.

Although the bubble radius is not exactly constant, it is probably a good approximation to use the above solution to obtain the number of molecules per bubble

$$V(t) = \frac{V}{K_B T} P = \frac{V}{K_B T} K_M C(R,t) \quad (19)$$

Equation (1a) has been used by the author in calculating the inertial pressure in a model based on fission-nucleated bubbles.

The problem solved in this TDR should be compared with the bubble growth theory of H. P. Flatt⁽¹⁾. Flatt solves two cases: (1) the gas pressure is constant and thus the solution is assumed to expand sufficiently rapidly to alleviate any inertial pressures; (2) the pressure in the solution is a given function of time. The radius R is an unknown function for which one solves.

The present calculation considers a given radius and an unknown pressure. The present calculation thus complements the work of Flatt.

(1) H. P. Flatt, NAA-SR-3923, Transient Bubble Growth in a Homogeneous Reactor.