Mathematical Modeling of New Phase Growth Due to Solute Diffusion

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Abstract

The growth of the stationary new phase formed from supersaturated liquid has significant role in many areas such as, the growth of bubbles in heavy oil and the growth of crystalline solid in hydrate engineering. The simplified governing equations for new phase growth in a solution has been formulated and solved for a single nucleate, assuming that mass transfer is the rate limiting step. This problem is of interest to heavy-oil solution gas drive and gas transportation. Applications to growth of hydrate as new phase in a hydrate-water slurry and bubble as new phase in heavy oil were shown. It can also be applied to the analysis of the growth of a stationary gas bubble as a result of mass transfer of one component from the liquid to the gas forming the bubble. The growth behavior of a single nucleate is needed in order to study population growth.

Governing Equations

The growth of the new phases formed in solutions has significant role in many areas such as, heavy oil reservoir (bubble growth) and hydrate engineering (hydrate particle). The formation and growth of new phases in a solution happens under the favorable thermodynamic conditions. In the case of bubbles and solid particles in fluids favorable thermodynamic conditions are specific pressure and temperature. The growth is a competition between kinetic, heat and diffusion limitations.

To be able to study the growth of the new phases formed in solutions analytically consider a stationary spherical gas, liquid or solid phase with an initial radius of δ which is growing in a solution phase of infinite extent due to the transfer of a solute from the solution phase to the gas, liquid or solid phase. Besides more simplifications of the problem is made by the following assumptions; (i) neither changes of density due to mass transfer in new phase, nor solution surrounding it; (ii) mass transfer, not chemical reaction or heat transfer control of new phase growth; (iii) restricting to 2-component (solute and solvent) systems at constant temperature and pressure, with no chemical reaction; (iv) no mass transfer other than ordinary diffusion with constant diffusivity coefficients; (v) equilibrium condition on the interface; (vi) no surface tension or body forces; and (vii) constant mass fraction of the new phase. The governing equations can be summarized as follow:

a) For solvent surrounding the new phase,

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 u) = 0 \qquad r > R(t) \tag{1}$$

b) For the solute surrounding the new phase,

$$\frac{\partial C}{\partial t} = D(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r}\frac{\partial C}{\partial r}) - u\frac{\partial C}{\partial r} \qquad r > R(t) \qquad (2)$$

c) For the solute in the new phase,

$$\frac{d}{dt}(\tfrac{4}{3}\pi R^3 m\rho_n) = 4\pi R^2 \{C(R,t)[\dot{R} - u(R)] + D\frac{\partial C(R,t)}{\partial r}\}$$

After simplification,

$$m\rho_n \dot{R} = C(R,t)[\dot{R} - u(R)] + D\frac{\partial C(R,t)}{\partial r} \qquad (3)$$

d) For the solvent in the new phase,

$$\frac{d}{dt}[\tfrac{4}{3}\pi R^3 \rho_h] = 4\pi R^2 \rho_L[\dot{R} - u(R)]$$

Or,

$$u(R) = \varepsilon \dot{R} , \qquad (4)$$

Where;

$$\varepsilon = 1 - \frac{\rho_n}{\rho}, \qquad \omega = 1 - \varepsilon \qquad (5)$$

Figure 1 shows the notation and the initial condition of the problem. The initial and boundary conditions can be written as;

I.C.:

$$R(0) = \delta \qquad (6)$$
$$C(r,0) = C_0 \qquad (7)$$

B.C.:

$$C(R,t) = C_e \qquad (8)$$
$$C(\infty,t) = C_0 \qquad (9)$$

The solution has been obtained following the Scriven's work by integrating equation (1) and using equation (4) to find,

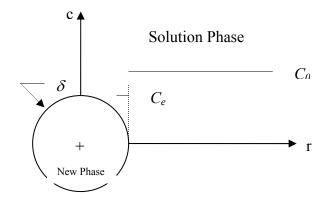$$u = \varepsilon \dot{R}\left(\frac{R}{r}\right)^2 \qquad (10)$$

Fig. 1. Initial condition for new phase growth

Replacing for u and $u(R)$, in (2) and (3) and using the method of combined variables to solve the obtained differential equation with the relevant boundary and initial conditions for the solute concentration at any time t and distance r:

$$\frac{C_0 - C}{C_0 - C_e} = \frac{\int\limits_{\frac{r}{2\sqrt{D(t+\alpha)}}}^{\infty} \upsilon^{-2} Exp(-\upsilon^2 - 2\varepsilon\beta^3\upsilon^{-1})d\upsilon}{\int\limits_{\beta}^{\infty} \upsilon^{-2} Exp(-\upsilon^2 - 2\varepsilon\beta^3\upsilon^{-1})d\upsilon} \tag{11}$$

Where β can be obtained from:

$$\phi(\varepsilon,\beta) = 2\beta^3 e^{\beta^2(1+2\epsilon)} \int\limits_{\beta}^{\infty} \upsilon^{-2} Exp(-\upsilon^2 - 2\varepsilon\beta^3\upsilon^{-1})d\upsilon = \gamma = \frac{C_0 - C_e}{m\rho_n - (1-\varepsilon)C_e} \tag{12}$$

The numerical solution to the above equation is given in literature (Scriven, 1959), therefore the growth radius of the new phase at any time t can be calculated from;

$$R = 2\beta\sqrt{D(t+\alpha)} \tag{13}$$

Where,

$$\alpha = \frac{\delta^2}{4D\beta^2} \tag{14}$$

The special cases where ϵ may be assumed approximately zero, simplifies equations (12) and (13), and the solutions for solute concentration and growth radius become;

$$C(r,t) = C_0 + \frac{R}{r}(C_e - C_0)erfc\left(\frac{r-R}{\sqrt{4Dt}}\right) \tag{15}$$

$$R = Bt^{\frac{1}{2}} + \delta \qquad (16)$$

Where;

$$B = \sqrt{\frac{D}{\pi}} \frac{C_0 - C_e}{m\rho_n - C_e} + \sqrt{\frac{D(C_0 - C_e)^2}{\pi(m\rho_n - C_e)^2} + \frac{2D(C_0 - C_e)}{(m\rho_n - C_e)}} \qquad (17)$$

Results

In order to see the behavior of the new phase growth, the solution of the obtained governing equations has been applied to the following situations;

1) Bubble growth in heavy oil solution gas drive
2) Carbon dioxide and methane hydrate particle growth in Gas Hydrate engineering, where ε is approximately zero and the accuracy of the approximate solution can be evaluated
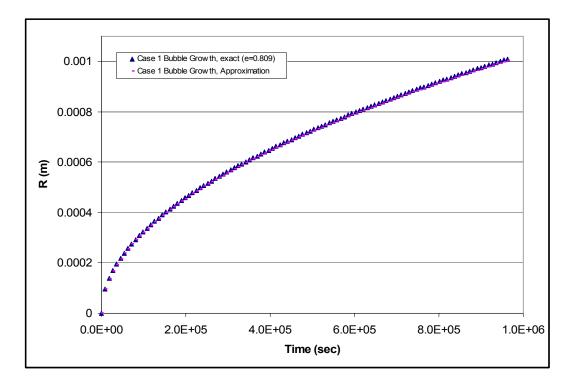

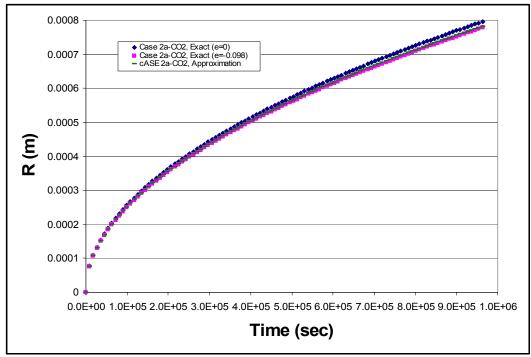**Fig. 2.** Growth of new phase particle for heavy oil solution gas derived

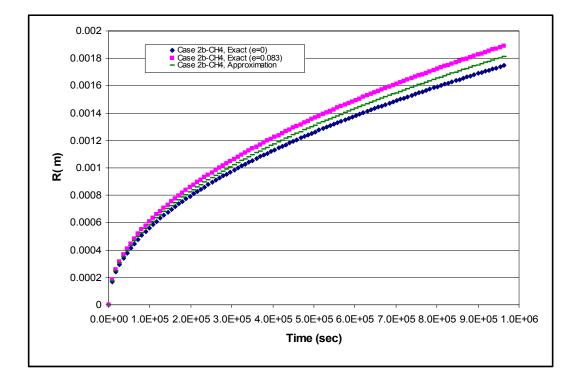**Fig. 3.** Growth of new phase particle for carbon dioxide gas hydrate

Fig. 4. Growth of new phase particle for methane gas hydrate
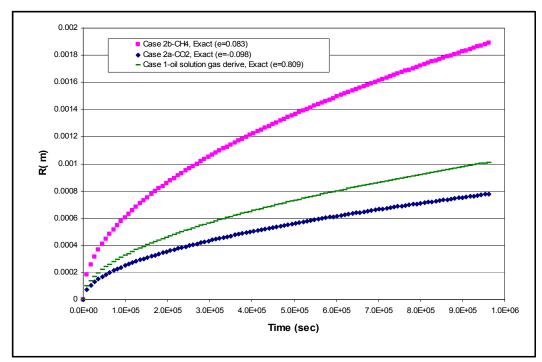
Fig. 5. Growth of new phase particle for heavy oil solution gas derive process, carbon dioxide, and methane gas hydrate