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Analytical Simulation of Micro Vascular Networks

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ABSTRACT

In present paper, our elaboration is employing mass equilibrium and fluid mechanics theories in order to come up with a novel model to calculate the healing time of a polymer with unique physical parameters. There have already been a small number of mathematical models of self-healing. Therefore, in this work, we try to formulate the problem, using mass conservation and fluid mechanics principles to reach a formulation which relates pressure, potential functions and other physical parameters to initial time of microcapsule fracture and final time of healing completion. In fact, the significance of this paper, unlike the numerical investigations of previous ones is that it gives a model presenting an analytical simulation which is applicable to design a micro vascular network.

KEYWORDS: Self-healing material, Self-healing phenomenon, Microcapsule, Micro-vascular network modeling, Composite material.

1. INTRODUCTION

Self-healing materials are a category of smart materials that have the structural ability to repair damage caused by mechanical usage over time. The inspiration comes from biological systems, which have the ability to heal after being wounded. In the first stages the cracks and other types of damage on a micro scale level has been shown to change thermal, electrical, and acoustical properties, and eventually contributes to whole scale failure of the material. Usually, cracks are mended by hand, which is difficult because cracks are often hard to detect. A material (polymers, ceramics, etc.) that can intrinsically correct damage caused by normal usage could lower production costs of a number of different industrial processes through longer part lifetime, reduction of inefficiency over time caused by degradation, as well as prevent costs incurred by material failure[1]. For a material to be defined as self-healing, it is necessary that the healing process occurs without human intervention. Some examples that include healing polymers that are not "self-healing" polymers. When a wound is made in our body, it starts working astonishingly to heal it and we can obviously see how the self-healing process goes on. Historically, by simulating the human body models, researchers have provided scientific methods to improve the characteristics of self-healing phenomenon.

First interest in self-healing material came in 1970 in order to include self-healing characteristics in research space crafts like Shuttle, in order for the material in the rockets to be able to heal themselves. In 2001, a polymer was made in micro scale in which the self healing material spread in case the capsule fractured. In the same year, researchers made in vitro paint-self-healers.

The first group of self-healing materials are included inside the hollow fibers of the diameter 30-100 μm and a porosity of 65% which are commonly used in the fabrication of laminates. The hollow fibers may contain resin systems which give off paint in the event of paint fracture. On the account of external damaging factors, the microcapsules first resist the disruption of mechanical structure, which could be viewed by X-ray analysis[6].

Second group of Self-Healing Materials consist of a vascular network. A vascular network can be made within a "sandwich" structure containing the self-healing material. After fracture, the cavity system lets the healers inside the damaged structure to rearrange the mechanic structure. Like blood circulation system, the vascular network may be filled with the healer materials [6].

This work aims at providing a mathematical model to make a logical relationship for the healing process using momentum, mass conservation, single phase fluid and Darcy equation.

PROBLEM DESCRIPTION

In this section we will introduce the problem and solving procedure. Considering a theoretical analysis is the main core of present paper. In first stage, describing materials and methods of solving is contemplated to create a clue in readers mind.

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The self-healing materials comprise of 3 parts:

1. General Material (GM): consist of everything used in the final product.
2. Capsulated Bubbles: consist of materials which do not blend with HA, and survive through reactions.
3. Healing Element: a solvent or catalyst around the healing material which react with GM. When a fracture is made, several bubbles containing solvent or catalyst would blow, making the GM flow to fill and amend the fracture. The healing material is pumped constantly in this system so that it can survive infinitely [3].

Now our elaboration is to introduce micro capsules. The microcapsules are an important factor of self-healing material and should be designed carefully. The main problems dealing with these microcapsules that we should be careful about them are as following;

1. The capsulation process should be compatible with the self-healing material [1].
2. The microcapsule walls should be rigid enough in order to retain their adherence properties. So, they are healed by polymer matrix which guarantees the blow up of the capsules when the composite is damaged. A microcapsule network can be seen in Fig.1, [2].
3. Composite Capsulated Healing Material: these composite materials come together by a binder. This healer contains a fluid called DCPD, which capsulate the small bubbles emitted by composites. There are 100-200 bubbles per square inch. Using the catalyst radinium, the monomer DCPD starts making polymerization loops by the Grubbs catalyst base. This polymerization is indicated in Figs. 2[5, 8].

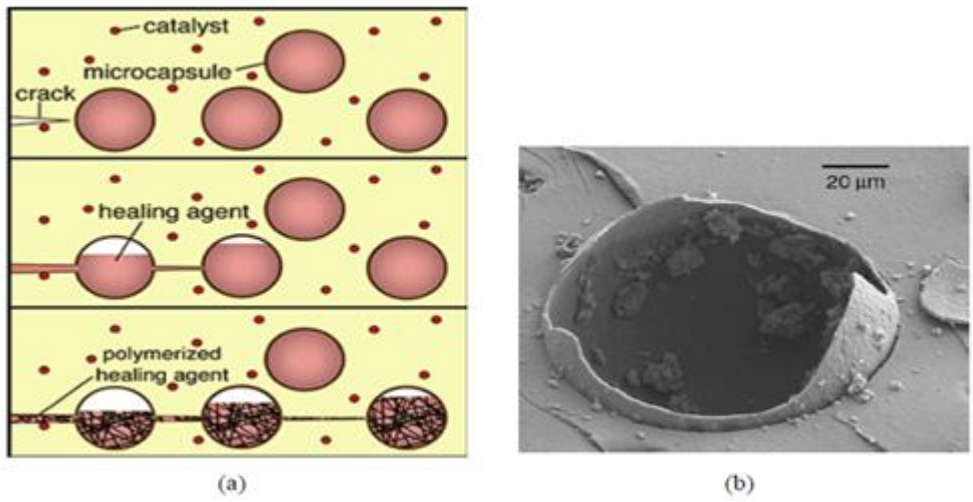

Figure 1: (a) Basic method of the microcapsule approach, (b) ESEM image showing ruptured microcapsule.

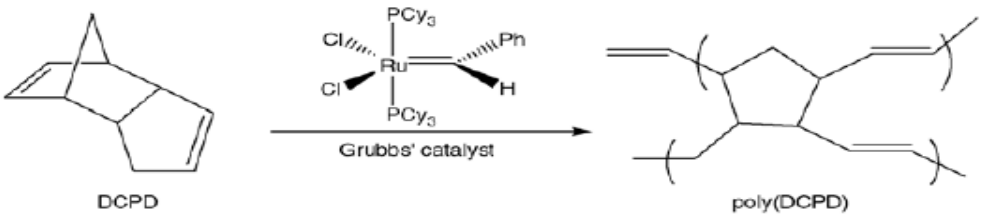

Figure 2: Effective steps of catalyst

RESULTS AND DISCUSSION

In this section, using the microcapsule fracture in micro vascular network, the mathematical model is investigated from the time of microcapsule fracture, t^n, to the time of healing completion,t^{n+1}. Our attempt is to provide a model that satisfies the logical relationships among self-healing parameters. We consider the behavior of capsulated material in micro-vascular network before and after the injection of self-healing material. Our

assumptions are based upon mass conservation, which describes the problem using integral analysis. The micro-vascular network used is as follows:
Mass Equilibrium: Considering the control volume presented in Fig. 3, we have:

$$m_1 - m_2 + m_s = m_a \quad (1)$$

Where:
m_1: Mass of the fluid entered into the block i before encapsulation and injection of self-healing material.
m_2: The mass provided after the capsule fracture and self-healing.
m_s: Mass of capsulated self-healing material (DCDP and other self-healers).
m_a: Extra mass saved or lost due to reaction in a define timescale.
The parameter *B* is defined as a function of pressure and temperature. Its value for a single phase fluid is:

$$B = \frac{\rho(s)}{\rho} \quad (2)$$

which indicates the ratio of the self-healing fluid density to the reference density (entire system).
During the solution process, we have to take some assumption. Although these assumptions might not meet real problems in nature, but to have a unique and more continent solution, taking them will help us to be closer to real problems in nature. Main assumptions concerning present problem are as following;

- The fluid is considered single phase.
- The Darcy equation is employed in order to relate the Debi and potential gradient.

Darcy equation:

$$u_x = \frac{q(x)}{A(x)} = -\beta c \frac{K(x)}{\mu} \frac{d\phi}{dx} \quad (3)$$

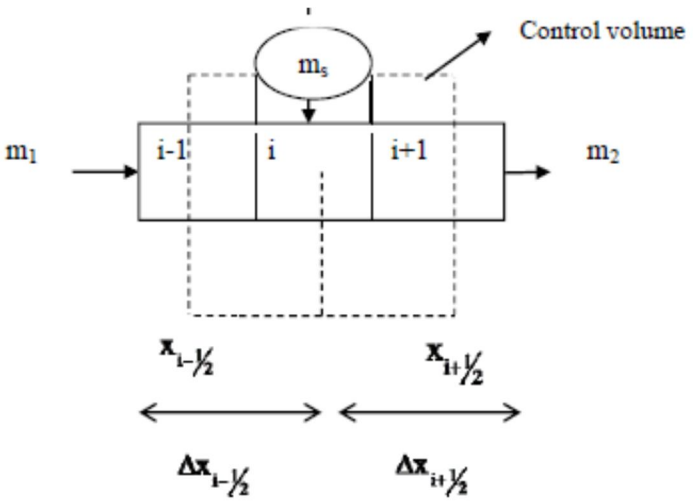

Figure 3: Control volume of a blocked micro vascular network.

The Darcy equation is used for single phase, dull-flow media; and with the no-slip condition, it is employed for incompressible fluids. In this equation, *k*, *β* and *c* are permeability, potential and porosity factor, respectively. Fig. 3 shows the block *i* and its surrounding blocks *(i+1)* and *(i-1)* in *x* direction. Each time, the block *i* moves through the block *i+1* and *i+1* level in $x_{i-1/2}$ with the mass flow rate $W_{x_{i-1/2}}$, and leaves the block *i+1* in $x_{i+1/2}$ with the mass flow rate $W_{x_{i+1/2}}$. Besides, the fluid enters block *i* by a well with the mass Debi, $\varphi_{mi.}$
We take the mass produced in reaction with healing material as m_r. So, the mass equilibrium (considering Fig.3) will be:

$$m_{si} + m_1\Big|_{x_{i-1/2}} - m_2\Big|_{x_{i+1/2}} = m_{ai} \quad (4)$$

Now, to take account for the time in healing equations, we employ Debi rates instead of masses. In this case we use the terms $W_{x_{i+1/2}}$, $W_{x_{i-1/2}}$ and M_{mi}.

$$m_1\Big|_{x_{i-1/2}} = \int_{t^n}^{t^{n+1}} w_x\Big|_{x - i/2} dt \quad (5)$$

$$m_2\Big|_{x_{i+1/2}} = \int_{t^n}^{t^{n+1}} w_x\Big|_{x_{i+1/2}} dt \quad (6)$$

$$m_{si} = \int_{t^n}^{t^{n+1}} M_{mi} dt \quad (7)$$

Substituting these relations in mass equilibrium equation, we get:

$$\int_{t^n}^{t^{n+1}} w\Big|_{x_{i-1/2}} dt - \int_{t^n}^{t^{n+1}} w\Big|_{x_{i+1/2}} dt + \int_{t^n}^{t^{n+1}} M_{mi} dt = m_{ai} \quad (8)$$

The accumulated mass based on volume with m_r is defined as:

$$\mathrm{m_{ai}} = \mathrm{v_{bi}}(\mathrm{m_{ri}^{n+1}} - \mathrm{m_{ri}^{m}})_{\mathrm{i}} \quad (9)$$

The reason we include m_r is to use volume in the relationships. $\xi \dot{m}x$ is the mass flux which is,

$$\xi \dot{m}x = W_x = \dot{m}_x A_x$$

In which,

$$\overset{\circ}{m}_x = \rho u_x \quad (10)$$

The accumulated fluid mass per unit volume in terms of porosity and fluid density parameters in micro-vascular network is defined as the following:

$$m_r = \xi\rho \quad (11)$$

The mass produced due to healing reaction in terms of resource volume Debi and fluid density is:

$$M_{mi} = \rho M \quad (12)$$

Substituting the relations regarding the main equilibrium, we have:

$$\int_{t^n}^{t^{n+1}} (\overset{\circ}{m}_x A_x)\Big|_{x - i/2} dt - \int_{t^n}^{t^{n+1}} (\overset{\circ}{m}_x A_x)\Big|_{x + i/2} dt + \int_{t^n}^{t^{n+1}} M_{mi} dt = v_{bi}(m_{ri}^{n+1} - m_{ri}^{n-1})_i \Rightarrow \int_{t^n}^{t^{n+1}} (\rho u_x A_x)\Big|_{x_{i-1/2}}$$

$$\Rightarrow -\int_{t^n}^{t^{n+1}} (\rho u_x A_x)_{x_{i+1/2}} dt + \int_{t^n}^{t^{n+1}} (\rho M)_i dt = v_{bi}(\xi p)_i^{n+1} - (\xi p)_i^n)_i \quad (13)$$

Employing the volume coefficient $B = \frac{\rho_{sc}}{\rho}$ in the equation (13), and dividing both sides by ρ_{sc}, we get the following relation:

$$\int_{t^n}^{t^{n+1}} g_{x_{i-1/2}}(\phi_{i-1} - \phi_i)dt - \int_{t^n}^{t^{n+1}} g_{x_{i+1/2}}(\phi_{i+1} - \phi_i)dt + \int_{t^n}^{t^{n+1}} M_{sc}\, dt = v_{bi}\left((\frac{\xi}{B})_i^{n+1} - (\frac{\xi}{B})_i^n\right) \quad (14)$$

Depending on the above Darcy equation, we will get:

$$(u_x)\Big|_{x-i/2} = \beta_c \frac{(K_x)\Big|_{x_{i-1/2}}}{\mu_x\Big|_{x_{i-1/2}}}(\frac{\phi_{i-1} - \phi_i}{\Delta x_{i-1/2}}) \quad (15)$$

Where $K_{x_{i-1/2}}$ is related to the permeability between the blocks i and *i-1* and $\mu_{x_{i-1/2}}$ to the viscosity of the fluid accumulated in the blocks *i* and *i-1*:

$$(\mathrm{u_x})\Big|_{\mathrm{x_{i+1/2}}} = \beta_{\mathrm{c}} \frac{(\mathrm{K_x})\Big|_{\mathrm{x_{i+1/2}}}}{\mu_{\mathrm{x}}\Big|_{\mathrm{x_{i+1/2}}}}\left(\frac{\phi_{\mathrm{i}} - \phi_{\mathrm{i+1}}}{\Delta \mathrm{x_{i+1/2}}}\right)$$

The above equation will turn in to:

$$\int_{t^n}^{t^{n+1}} \left(g_{x_{i-1/2}}(\phi_{i-1} - \phi_i)\right)dt + \int_{t^n}^{t^{n+1}} g_{x_{i+1/2}}(\phi_{i+1} - \phi_i)dt + \int_{t^n}^{t^{n+1}} M_{sc}dt = v_{bi}\frac{d}{dp}\left(\frac{\xi}{B}\right)_i\left(p_i^{n+1} - p_i^n\right) \quad (16)$$

Where:

$$g_{x_{i+1/2}} = \frac{\beta_c(K_X)Ax}{\mu B \Delta x}\Big|_{x_{i+1/2}} \quad (17)$$

In terms of pressure, this equation may be written as:

$$\int_{t^n}^{t^{n+1}} \left(g_{x_{i-1/2}}(\phi_{i-1} - \phi_i)\right)dt + \int_{t^n}^{t^{n+1}} g_{x_{i+1/2}}(\phi_{i+1} - \phi_i)dt + \int_{t^n}^{t^{n+1}} M_{sc}dt = v_{bi}\frac{d}{dp}\left(\frac{\xi}{B}\right)_i\left(p_i^{n+1} - p_i^n\right) \quad (18)$$

Also, the potential functions can be changed to pressure functions;

$$\phi - \phi_0 = (\mathrm{p} - \mathrm{p}_0) - \partial(\mathrm{Z} - \mathrm{Z}_0) \quad (19)$$

The potential difference in the blocks I, i-1 and i+1 may be calculated as:

$$\begin{aligned}(\phi_{\mathrm{i-1}} - \phi_{\mathrm{i}}) &= (\mathrm{p_{i-1}} - \mathrm{p_i}) - \partial_{\mathrm{i-1/2}}(\mathrm{Z_{i-1}} - \mathrm{Z_i}) \\ \phi_{\mathrm{i+1}} - \phi_{\mathrm{i}} &= (\mathrm{p_{i+1}} - \mathrm{p_i}) - \partial_{\mathrm{i+1/2}}(\mathrm{Z_{i+1}} - \mathrm{Z_i})\end{aligned} \quad (20)$$

And finally, we get the following relation:

$$\int_{t^n}^{t^{n+1}} g_{x_{i-1/2}}\left[(p_{i-1} - p_i) - \partial_{i-1/2}(Z_{i-1} - Z_i)\right]dt + \int_{t^n}^{t^{n+1}} g_{x_{i+1/2}}\left[(p_{i+1} - p_i) - \partial_{i+1/2}(Z_{i+1} - Z_i)\right]dt + \int_{t^n}^{t^{n+1}} M_{sc}dt$$
$$= v_{bi}\frac{d}{dp}\left(\frac{\xi}{B}\right)_i\left(p_i^{n+1} - p_i\right) \quad (21)$$

With the foregoing equation, and knowing parameters such P_{i-1}-P_i, $g_{x_{i-1/2}}$ and ∂_i we can solve the equation (21); hence measure the time of the healing completion; i.e. in order to determine the healing time, it's sufficient to calculate the physical properties such as $\rho, k, \upsilon, \beta, pressure$, potential of *i*, *i+1*, and *i-1* and the amount of the heat transmitted to control volume. The model provided by Eq (21) is applicable to design of a micro vascular network.

CONCLUSION

Inspired by the natural self-healing characteristics that exist in living organisms, for example, the regenerative ability of humans to heal from cuts and broken bones, interest in self-healing materials is gaining more and more attention. Present paper addressed an important application of self-healing in composite materials. In this paper mass equilibrium and fluid mechanics theories were employed to create a novel model to calculate the healing time of a polymer with unique physical parameters. In this work, based on previous unsubstantial mathematical models like [9], we have tried to formulate the problem, using mass conservation and fluid mechanics principles to reach a formulation which relates pressure, potential functions and other physical parameters to initial time of microcapsule fracture and final time of healing completion. By doing so, we have provided a model presenting an analytical simulation which is applicable to design a micro vascular network. It is worthy to note that this study deserves further expansions via purporting more realized assumptions.

REFERENCES

1. Zang, M.Q. ,2008, "Self healing in polymers and polymer composites. Concepts, realization and outlook: A review". Polymer Letters 2 (4): 238–250. doi:10.3144/expresspolymlett.29
2. S. R. White, N. R. Sottos, P. H. Geubelle, J. S. Moore, M. R. Kessler, 2000“Autonomic healing of polymer composites”, Nature, 409, pp:794-797.
3. Richard P. Wool, 2008,“Self-healing materials: a review”, Soft Matter, 4,pp: 400-418.
4. M. Jonkers, Erik Schlangen, 2008,Development of a bacteria-based self healing concrete, Taylor Made Concrete Structures: New Solutions for our Society by Joost C. Walraven,978-0-415-47535-8.
5. Y. C. Yuan, T. Yin, M. Z. Rong, M. Q. Zhang, 2011,“Self healing in polymers and polymer composite: A review”, Polymer Letters, 5, 47–59.
6. S. TOOHEY, NANCY R. SOTTOS, JENNIFER A. LEWIS, 2007, “Self-healing materials with micro-vascular networks”, Nature Materials, 6, 581 – 585.
7. R. S. Trask, H R Williams and I P Bond, 2007,“Self-healing polymer composites: mimicking nature to enhance performance”,Bioinspiration&Biomimetics, doi:10.1088/1748-3182/2/1/P01.
8. S. van der Zwaag, N.H van Dijk, H.M Jonkers, S.D Mookhoek and W.G Sloof,2009,“Self-healing behavior in man-made engineering materials: bioinspired but taking into account their intrinsic character”, Philosophical Transactions of the Royal Society A, pp:1689-1704.
9. M. M. Yadollahi, M. AkifKaygusuz, R. Polat, R.Demirboga, RustemGul, M. Atashafrazeh, F.Goharkhaneh Asl, 2012 ,“Steel Fibers Effect in Strength Enhancement of Geopolymer Composite” Journal of Basic and Applied Scientific Research, 2(8).

List of Symbols

b	plate thickness
C_p	fluid heat capacity at constant pressure
h	Convective heat transfer coefficient
k_f	fluid thermal conductivity
k_s	solid plate thermal conductivity
q''	Heat flux
Re	Reynolds number based on plate length, $Re=\rho_f U_\infty L/\mu$
$\tilde{T}$	non-dimensional temperature defined in Eq. 4
T_∞	Free stream temperature
U_∞	Free stream velocity

Greek symbols

μ	fluid kinematic viscosity
ρ_f	fluid density