

FLUID DYNAMICS AND THERMODYNAMICS NUMERICAL MODELLING  
OF SELF-HEALING FIBRE REINFORCED LAMINATED COMPOSITES

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*To my family*

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## ABSTRACT

Inspired by the bleeding mechanism in living organisms to heal injury for survival, such capability has been integrated into a damaged laminate composite for autonomous internal repairing to extend its service life. The main healing mechanisms include infiltration of healing liquid into the crack plane, resulted from the breaching of pre-embedded vessels, which is triggered by a damage event. The later polymerization of the healant serves to restore the strength of the crack plane and hence inhibits further crack growth. The best healing performance is generally governed by both infiltration and polymerization rates of healing liquid at the crack tip. In ensuring assessment of these rates without excessive computational burden but free from the companion numerical stability-consistency-accuracy issues, in-house hydrodynamic and thermodynamic models based on the weak form Galerkin finite element (FE) method have been developed in this study. To simulate the micro-scale isothermal hydrodynamics of the Newtonian liquid, one-dimensional (1D) incompressible Stokes equations have been solved using the penalty function method. Computational matters, such as the feasible penalty parameter ( $\gamma_p$ ) for multiple flow geometries of single straight micro-channel, are discussed and numerically addressed. Meanwhile, the polymerization mechanics of healing liquid in a straight crack channel is obtained by solving the heat conduction formulation coupled with the phenomenological Arrhenius's rate equation and Crank-Nicolson time scheme. It is observed that the iterative Uzawa's technique, which employs forcing term correction in terms of the previous velocity solution, coupled with another forcing term correction in terms of the previous divergence of velocity solution is capable of eliminating the instability of axial pressure distribution and inconsistency of the conventional penalty model setting. Additionally, implementing termination criterion by equalizing the order of both maximum elemental divergence of velocity ( $EDV_{\max}$ ) and penalty parameter ensures stability, consistency, and accuracy of solution for  $1 \times 10^1 \leq \gamma_p \leq 1 \times 10^{11}$ . Adopting similar termination technique for the Crank-Nicolson predictor-corrector time integration scheme with the penalty formulation, the proposed model is capable of capturing the flow front motion in micro-channel by electing the temporal mesh size ( $\Delta t$ ) from a function of hydraulic diameter ( $D_h$ ) and spatial mesh size ( $\Delta x$ ). Parametric study for temperature and cure degree evolution by varying pre-exponential factor ( $\tilde{A}$ ), activation energy ( $\tilde{E}$ ),  $\tilde{n}$ -th order of reaction, and ultimate enthalpy of cure ( $\tilde{H}$ ) has been performed thoroughly where an optimal coupling between  $\tilde{A}$  and  $\tilde{E}$  is identified as the dominating factor in achieving the most favored repairing behavior. While the order of reaction imparts less significance in the evaluation, it is observed that polymeric healant with a higher numerical value of  $\tilde{H}$  is not beneficial either. The principal contribution of the present study includes the construction of a series of FE Eulerian frameworks that are reliable, without excessive computational burden, in assessing key diffusive mechanistic variables of extrinsic self-healing mechanisms in achieving optimal strength recovery of straight crack geometry in polymeric materials.

## ABSTRAK

Diilhamkan oleh mekanisme pendarahan dalam organisma hidup demi menyembuhkan kecederaan untuk kesinambungan hidup, keupayaan ini telah disepadukan ke dalam komposit lamina yang rosak untuk pembaikan dalaman autonomi demi pemanjangan hayat perkhidmatannya. Mekanisme penyembuhan utama termasuk penyusupan cecair penyembuh ke dalam pelan retak hasil daripada kebocoran saluran pra-tanam, yang dicitus oleh peristiwa kerosakan. Pempolimeran penyembuh seterusnya berfungsi untuk memulihkan kekuatan kawasan retak dan menghalang pertumbuhan retak. Prestasi penyembuhan terbaik biasanya dikawal oleh kedua-dua kadar penyusupan dan pempolimeran cecair penyembuh di hujung retak. Untuk menilai kekadaran ini tanpa beban komputeran yang berlebihan, tetapi bebas daripada masalah sambilan kestabilan-konsistensi-ketepatan, model hidrodinamik dan termodinamik bina-diri berdasarkan kaedah unsur terhingga (FE) Galerkin bentuk lemah telah dibangunkan di dalam kajian ini. Untuk simulasi hidrodinamik cecair Newtonian sesuhu berskala mikro, persamaan Stokes tak mampat satu dimensi (1D) telah diselesaikan dengan kaedah fungsi penalti. Isu komputeran, seperti kesesuaian parameter penalti ( $\gamma_p$ ) dengan pelbagai geometri aliran untuk saluran mikro lurus tunggal, telah dibincang dan ditangani secara berangka. Sementara itu, mekanik pempolimeran cecair penyembuh dalam saluran retak lurus telah diperolehi dengan menyelesaikan formulasi aliran haba yang dipasangkan dengan persamaan kadar fenomenologi Arrhenius dan skim masa Crank-Nicolson. Teknik lelaran Uzawa yang menggunakan pembetulan terma daya dalam bentuk penyelesaian halaju sebelumnya, dipasangkan dengan pembetulan terma daya dalam bentuk perbezaan penyelesaian halaju sebelumnya, telah diperhatikan mampu menghapus ketidakstabilan taburan tekanan paksi dan kekurangan konsistensi oleh ketetapan model penalti konvensional. Selain itu, pelaksanaan kriteria penamatan dengan menyamakan peringkat kedua-dua perbezaan halaju unsur maksimum dan parameter penalti mampu memastikan kestabilan, konsistensi, dan ketepatan penyelesaian untuk  $1 \times 10^1 \leq \gamma_p \leq 1 \times 10^{11}$ . Dengan teknik penamatan yang sama untuk skim integrasi masa peramal-pembetul Crank-Nicolson dengan formulasi penalti, model yang dicadang mampu menentukan pergerakan hadapan aliran dalam saluran-mikro dengan memilih saiz unsur tempoh ( $\Delta t$ ) daripada fungsi diameter hidraulik ( $D_h$ ) dan saiz unsur ruangan ( $\Delta x$ ). Kajian parametrik terhadap evolusi suhu dan tahap pengawetan dengan mengubah faktor pra-eksponen ( $\tilde{A}$ ), tenaga pengaktifan ( $\tilde{E}$ ), tindakbalas peringkat ke- $\tilde{n}$ , dan entalpi muktamad untuk awetan ( $\tilde{H}$ ) telah dijalankan dengan teliti di mana gandingan optima antara  $\tilde{A}$  dan  $\tilde{E}$  telah dikenalpasti sebagai faktor dominasi dalam mencapai kelakuan pembaikan terbaik. Walaupun peringkat reaksi kurang memberi implikasi dalam penilaian, penyembuh polimer dengan nilai  $\tilde{H}$  yang lebih tinggi juga diperhatikan tidak berfaedah. Sumbangan utama daripada kajian ini termasuk binaan satu siri rangka kerja FE Eulerian yang mantap, kurang beban komputeran, dalam menilai pembolehkan mekanistik sebaran utama untuk mekanisme penyembuhan diri ekstrinsik demi mencapai pemulihan kekuatan optima bagi geometri retak lurus bahan polimer.

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## LIST OF ABBREVIATIONS

CG	–	Conjugate gradient
$CRE_t$	–	Change rate of energy with respect to time
$CRM_t$	–	Change rate of mass with respect to time
$CRMM_t$	–	Change rate of momentum with respect to time
CS	–	Control surface
CV	–	Control volume
DCB	–	Double cantilever beam
DCPD	–	Dicyclopentadiene
DD	–	Discrete divergence
DOF	–	Degree of freedom
EDV	–	Elemental divergence of velocity
$EDV_{max}$	–	Maximum elemental divergence of velocity
$EDV_{sum}$	–	Summation of elemental divergence of velocity
$EF_i$	–	External forces, $i = x, y, z$
ENB	–	Ethylidene-norbornene-based
FE	–	Finite element
GMRES	–	Generalized minimum residual
LBB	–	Ladyzhenskaya-Babuška-Brezzi
MR	–	Minimum residual
$NHF_i$	–	Net heat fluxes, $i = x, y, z$
$NMF_i$	–	Net mass fluxes, $i = x, y, z$
$NMMF_i$	–	Net momentum fluxes, $i = x, y, z$
$NRTE_i$	–	Net release of thermal energy, $i = x, y, z$
PE	–	Percentage of error
SD	–	Steepest descent
SPH	–	Smoothed particle hydrodynamics
PT	–	Progression time
TDCB	–	Tapered double cantilever beam

TEC	–	Truncation error coefficient
TEF <sub><i>i</i></sub>	–	Total external forces, $i = x, y, z$
TFT	–	Total filling time
TNMMF <sub><i>i</i></sub>	–	Total net momentum fluxes, $i = x, y, z$
1D, 2D, 3D	–	One-dimensional, two-dimensional, three-dimensional

## LIST OF SYMBOLS

$a$	–	Acceleration
$A$	–	Area
$\tilde{A}$	–	Pre-exponential factor
$c_a$	–	Acceleration parameter
$c_p$	–	Specific heat capacity
$C$	–	Convective transport matrix
$\hat{C}, \tilde{C}$	–	Proportionality constant
$D$	–	Channel diameter
$D_h$	–	Hydraulic diameter
$e$	–	Sequence number of elemental setting
$\hat{e}_x, \hat{e}_y, \hat{e}_z,$	–	Unit vectors
$\tilde{E}$	–	Activation energy
$f_x, f_y, F, F^*$	–	Force components
$g_x, g_y, g_z$	–	Gravitational components
$\tilde{G}$	–	Heat generation source
$h$	–	Number of spatial mesh size
$\tilde{H}$	–	Ultimate enthalpy of cure
$k_x, k_y, k_z$	–	Thermal conductivity
$\tilde{k}$	–	Reaction rate
$\hat{K}, K^*$	–	Fluid conductance matrix
$K_p$	–	Penalty matrix
$\tilde{K}$	–	Heat conductance matrix
$l, L$	–	Length
$\hat{M}, \tilde{M}$	–	Mass matrix
$M_p$	–	Consistent penalty matrix
$n$	–	Sequence number of iterative step
$\tilde{n}$	–	Order of cure reaction
$\hat{n}_x, \hat{n}_y, \hat{n}_z$	–	Unit normal vectors



$\hat{p}_e$	–	Elemental pressure correction
$P$	–	Pressure
$\hat{P}$	–	Global pressure correction
$q$	–	Elemental heat source
$Q$	–	Total heat transfer
$\hat{Q}$	–	Fluid diffusion matrix
$\tilde{Q}$	–	Heat generation matrix
$r$	–	Ramp rate
$R$	–	Universal gas constant
$Re$	–	Reynolds number
$t$	–	Time
$T$	–	Temperature
$u, v, \vec{v}, U, \hat{U}$	–	Velocity components
$\tilde{v}$	–	Predicted velocity
$V$	–	Volume
$w, w_h, w_p$	–	Weight functions
$\alpha$	–	Cure degree
$\Delta t$	–	Temporal mesh size
$\Delta x$	–	Spatial mesh size
$\Delta y, \Delta z$	–	Directional distance
$\epsilon$	–	Residual norm
$\gamma_p$	–	Penalty parameter
$\mu$	–	Viscosity
$\Omega$	–	Domain boundary
$\Phi, \phi$	–	Shape function
$\Psi, \psi$	–	Shape function
$\rho$	–	Density
$\sigma_{ij}$	–	Normal stress components, $i, j = x, y, z$
$\tau_{ij}$	–	Shear stress components, $i, j = x, y, z$
$\theta$	–	Order of generalized trapezoidal rule
$\Upsilon, v$	–	Shape function

## LIST OF APPENDICES

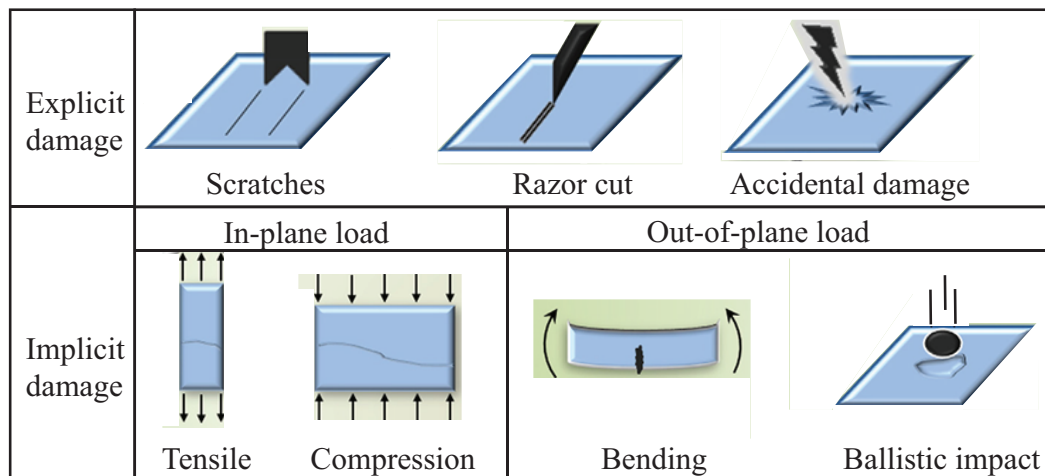
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# CHAPTER 1

## INTRODUCTION

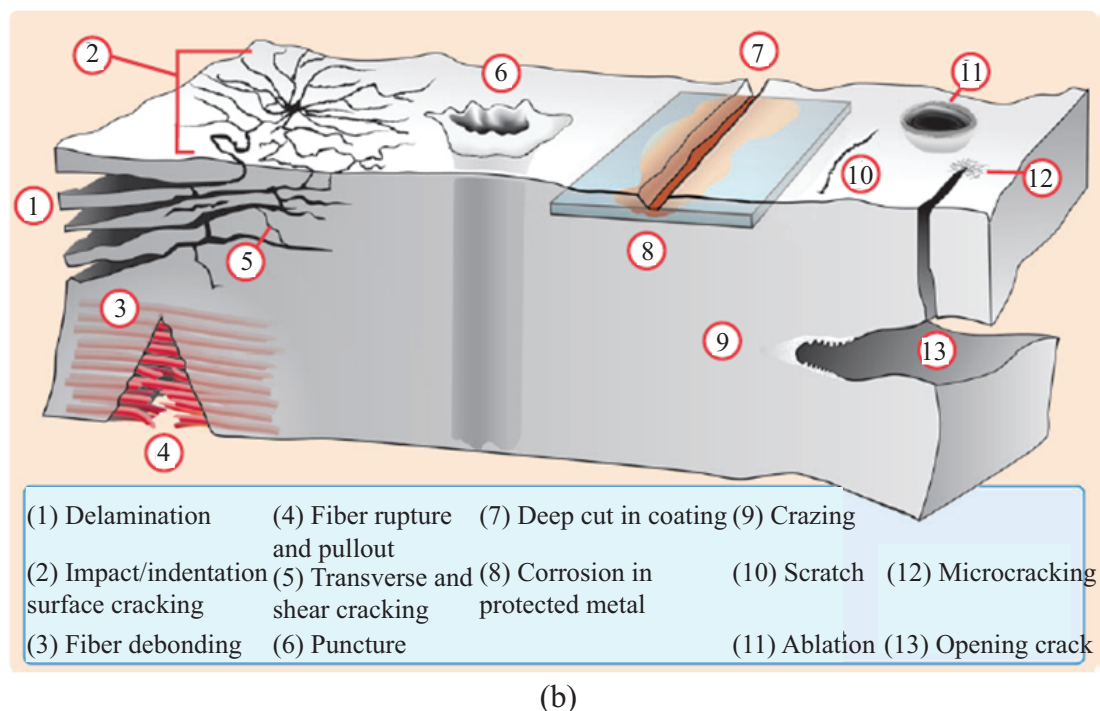
### 1.1 Background of the Study

Despite impressive functionality of polymeric materials in various engineering applications, from thin film to protective coat to fiber reinforced laminae to laminated composite, the material is vulnerable to numerous damage mechanisms (defined either as explicit or implicit damage) as schematically illustrated in Figure 1.1 (a). Typical implicit damage forms as depicted in Figure 1.1 (b) often induce the concerns of structural integrity (Zhang and Rong, 2011; Binder, 2013; Li and Meng, 2015) such as the transverse cracks and delamination that cross and lie between the plies of laminae, respectively. Of more relevance, the polymeric structures in structural application could lose partially the load carrying capability when subjected to these damage events that eventually cause catastrophic failure or fatigue once the cumulative damage intensity and/or severity exceeds the critical threshold.



(a)

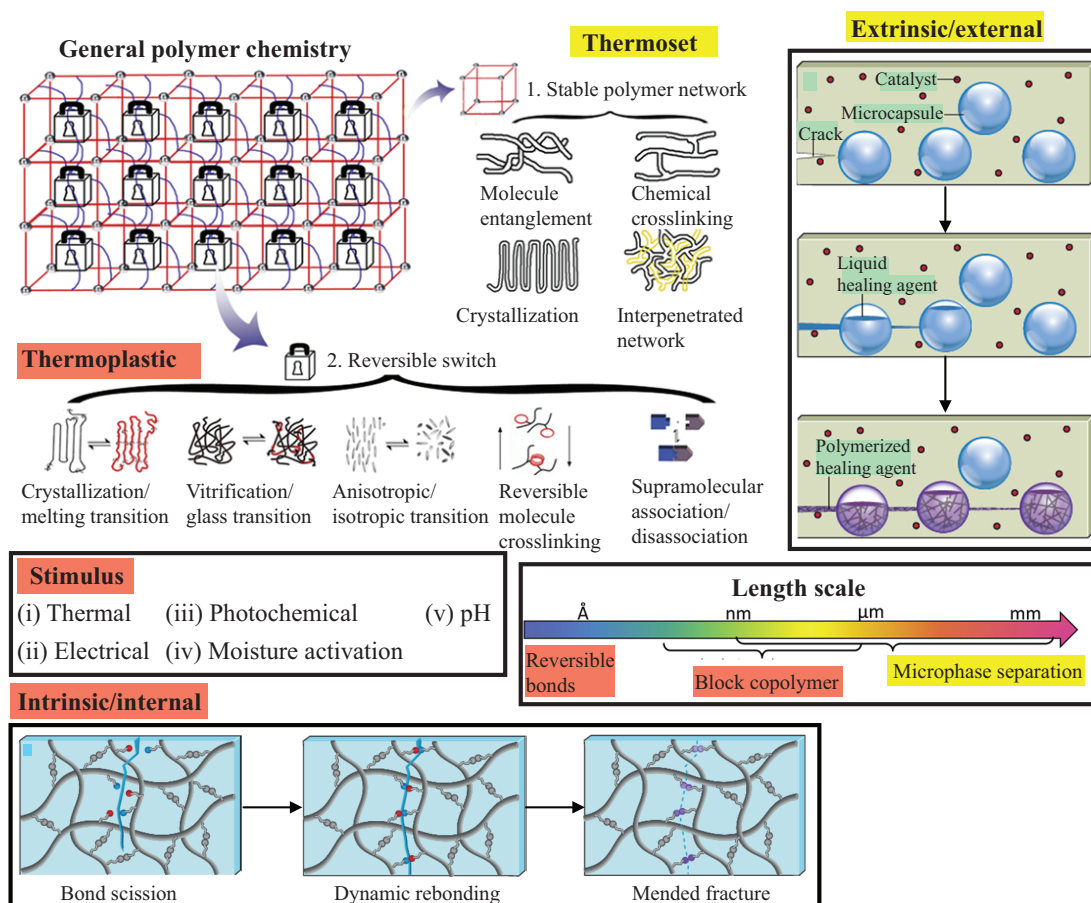
**Figure 1.1:** Typical (a) crack initiation (Zhang and Li, 2016) and (b) damage modes in polymeric materials (Blaiszik et al., 2010) (cont)



(b)

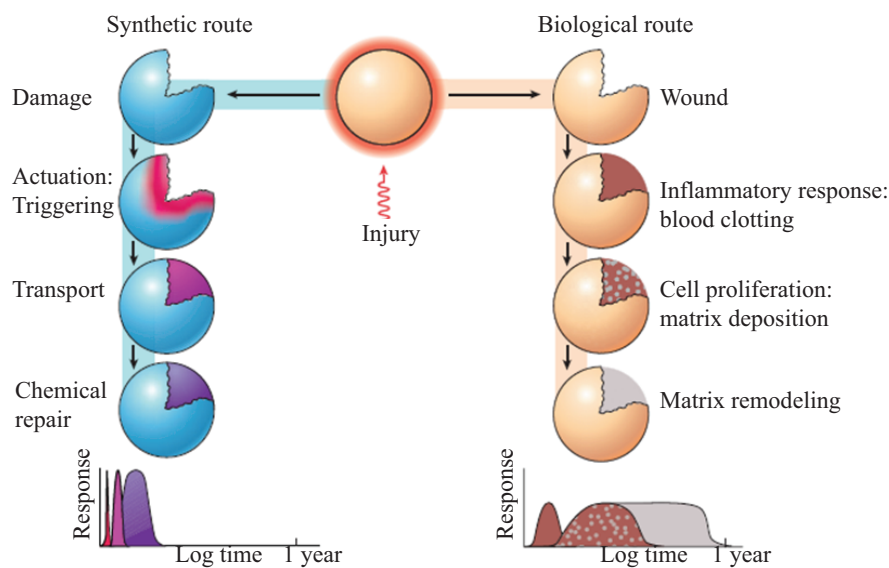
**Figure 1.1:** Typical (a) crack initiation (Zhang and Li, 2016) and (b) damage modes in polymeric materials (Blaiszik et al., 2010).

To counteract the degradation of the structural functionality of the material upon damage, the repairing measure shall initiate as early as possible to prohibit the increment of the level of severity. The complexity and hence efficiency of the maintenance scheme is often directly proportional to the intensity as well as severity of the damage events. Despite such awareness, the idea is often less likely implemented due to the difficulty in detecting these barely visible implicit damages. The detecting issue along with the tedious and costly outside-to-inside scratch repair works have motivated various innovative healing routes (Figure 1.2) for the polymeric materials. In general, the intrinsic/internal healing concept is applicable to the thermoplastic polymer due to its reversible switch of the broken crosslinking when subjected to certain stimulus. The extrinsic/external healing concept that generates a new volume of crosslinking is mostly characterized for the thermoset polymer due to its non-reversible network. Note that the implementation route and healing scale vary according to the repairing type achieved by the polymeric crosslinking (Zhang and Rong, 2011; Binder, 2013; Li and Meng, 2015). General details relevant to thermoplastic and thermoset polymeric materials have been highlighted with red and yellow color, respectively.



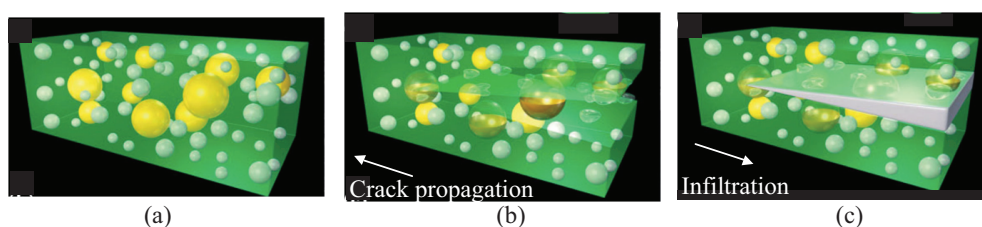
**Figure 1.2:** Innovative healing concepts corresponding to thermoplastic and thermoset polymers (Meng and Li, 2013; Yang et al., 2015; Patrick et al., 2016).

White et al. (2001) demonstrated the autonomous healing of the micro-scale damage in bulk polymer matrix by mimicking the simplified biological self-healing system as given in Figure 1.3. By autonomous, the system is meant to work without any human intervention. The trigger, either damage or wound in respective route, is responsible to initiate the transportation of the healant to the intended destination (e.g. blood delivery for the biological route). The subsequent response, mainly based on the chemical nature, is responsible for the repair of the damage/wound. Despite mimicking, the duration for the healing in synthetic system is much shorter than the biological system.



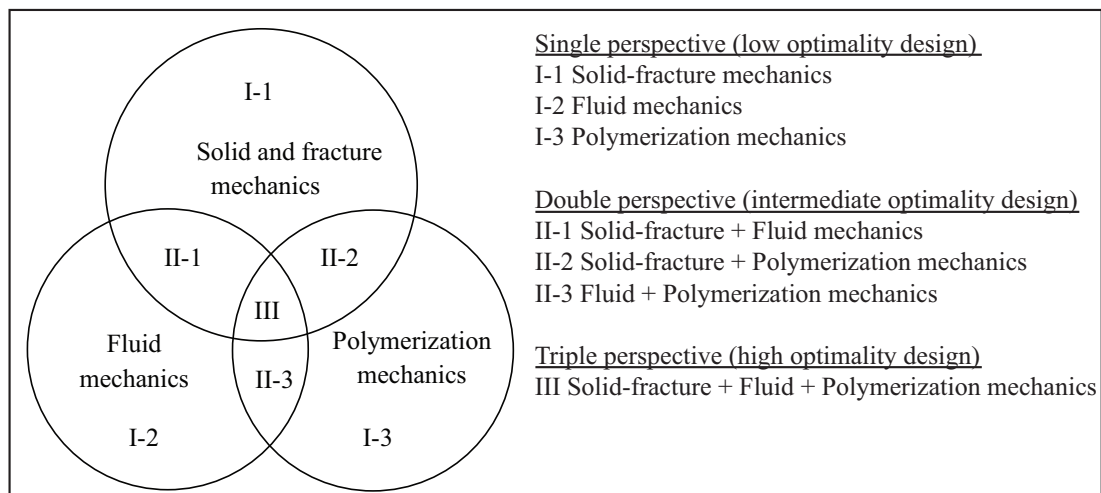
**Figure 1.3:** The conceptual synthetic system as inspired by the biological repairing route (Blaiszik et al., 2010).

The general key mechanisms of the external self-healing system by White et al. (2001) include the rupture of the container (i.e. encapsulated dicyclopentadiene and Grubb's catalyst) that triggers the flow and subsequent solidification of the healing chemical within the damage geometry (refer Figure 1.4 (b-c)) embedded in the bulk epoxy matrix. The term external is used since there is an embedment of an extra healing chemical-filled containers to the host material (Zwaag, 2007; Ghosh, 2009) to perform the autonomous healing functionality once it is damaged. The healing is mechanically triggered by the extending micro-crack that ruptures the embedded containers of the system, thereby attributing to the autonomous characteristic of the synthetic system.



**Figure 1.4:** Schematic of the (a) microcapsule system (b) typical crack propagation and (c) flow and subsequent solidification of healant in crack geometry (Murphy and Wudl, 2010).

The trigger, transport, and chemical repair in the practice of the external self-healing in polymeric materials are generally governed by solid, fluid, and polymerization mechanics along with multiple linear and/or nonlinear constitutive laws as proposed in the current thesis and presented in Figure 1.5. For optimal performance in healing, Zone III is the most desired but of the greatest complexity. This is because it overlaps all three chief mechanics (solid fracture, fluid, and polymerization), and therefore, the most realistic characterization of the healing behavior. When considered separately in a single field fashion (single perspective: Zones I-1, I-2, and I-3), optimality in healing is the lowest although they are of the least complexity in design. An intermediate level of optimality in design can be achieved by overlapping in consideration two of the three main mechanics as illustrated by the II-1, II-2, and II-3 Zones.



**Figure 1.5:** Typical consideration scopes and mechanics in extrinsic self-healing polymeric system.

For instance, there is no limitation on the incremental size of the containers within Zone I-2 consideration in order to maximize the pumping power on the healing liquid for the infiltration purpose. However, the container size is subjected to constraint if the consideration is arisen from Zone II-1. This is to align with the minimal detrimental loss strength of the specimen due to the containers embedment that is arisen from the consideration in Zone I-1. Various external self-healing trials have since been reported for different polymer matrices as well as their laminates (Hillewaere and Du Prez, 2015), adopting different containers (i.e. microcapsule, hollow fiber, vascular) and healing chemicals (mostly polymeric liquid), aiming at repairing different modes of micro-scale damage. The common goal of these works

remains in the search for the optimized synthetic system of the aforementioned variables in prolonging the service life of the man-made polymeric structures, preferably without human intervention.

Assessment on the optimality of the mechanical performance of the specimen due to the embedment of external healing system, through initial damage loss and final heal recovery of specific variables, is readily achievable based on the solid-fracture mechanics (Zwaag, 2007; Ghosh, 2009; Zhang and Rong, 2011). Nevertheless, a core attention on the fluid flow and polymerization realms of this new evolving scientific practice remains lacking and hence worth to be further addressed. Specifically, the behavior arisen based on the fluid-polymerization mechanics needs to be attached to the much conventional solid-fracture-solid framework to enable a much in-depth mechanical assessment. Note that the extrinsic healing mechanisms itself is of both multi-physics (i.e. structural, fracture, fluid, polymerization, heat transfer) and multi-scales (i.e. micro-crack and macro-specimen) nature. Hence, neglecting fluid flow and polymerization perspective in assessment is less realistic while also preventing the healing performance to achieve to its full potential as readily presented and discussed in Figure 1.5.

Experimental evaluation of both fluid and polymerization mechanics poses considerable difficulty in execution since these events occur within a micro-scale crack domain that is often embedded in the macro-scale opaque geometry. Also, there is a need for a high-end equipment set to capture the effective capturing of the relevant details (e.g. physical, chemical and thermal) that are multi-dimensional spanning as well as highly dynamic for a lengthy period. Numerical evaluation of these mechanics, for instance, based on the finite element (FE) spatial discretization and finite difference temporal discretization, seems practically attractive since a much convenient construction of the virtual environment to that of experimental is possible to deal with the dynamic phenomenon with multi-physics, multi-scales, and multi-dimensional nature.

Nevertheless, the adoption of these popular numerical approaches in evaluating the fluid flow and polymerization behaviors often induces concerns in terms of the numerical stability, consistency, and accuracy (Bathe, 1996; Reddy and Gartling, 2010; Zienkiewicz et al., 2013, 2014). As a matter of fact, the feasibility of the approach as an alternative to that of experimental is generally dependent on the numerical performance generated from the virtual framework constructed. The added advantage of the numerical assessment compared to the experimental framework, if numerous



parametric studies are to be performed on the search of the optimal external healing system, includes the labour-cost-time saving. Yet, it is less persuasive if the employed numerical framework lacks of stability, consistency, and accuracy. Hence, the in-depth discussion on the framework of numerical assessing these extrinsic self-healing mechanism is vital and of great potential to constitute one of the main research streams within the realm of self-healing man-made polymeric materials.

## 1.2 Problem Statement

The virtual framework, self-developed rather than relying on adjusting the features in any readily available commercialized software, targeting on the micro-scale fluid and polymerization mechanics that are relevant to the extrinsic self-healing polymeric system is worth to be explored considering no relevant work is reported in the literature thus far. Specifically, the framework should survive necessitated numerical verifications before further assessment can be conducted tailoring for the synthetic system design.

On one hand, the penalty finite element formulation for incompressible Stokes approximation is an ideal computational tool for simplistic fluid flow simulation (Zhou, 2012; Reddy and Gartling, 2010; Zienkiewicz et al., 2014). On the other hand, the basic energy flow is governed by the Fourier's law where relevant disturbance on the heat equilibrium due to the curing phenomenon, say involving polymeric liquid, could be simplistically represented by coupling phenomenological-based approach to the finite element formulation (Zhou, 2012; Reddy and Gartling, 2010; Zienkiewicz et al., 2013). Despite popularity of both formulations within the computational realm, a firm and unified set of guidelines in tackling the companion numerical issues (e.g. stability, consistency, and accuracy) when employing the weak form Galerkin finite element method as the base numerical framework remains under-developed (Bathe, 1996; Reddy and Gartling, 2010; Zienkiewicz et al., 2013, 2014) and hence a research gap worthy of special consideration in the present study.

To achieve the best repairing effect, the search of the optimal chemistry often begins with the fastest possible cure rate. Nevertheless, such chemistry is often accompanied by the relative extreme exothermic peak that is detrimental to the formation of the adhesive repair due to the induced residual stresses/distortions (Zhang and Rong, 2011; Zhou, 2012; Binder, 2013). Such damage healing invokes

a non-favorable strength restoration and shall constitute as one of the core criterions under the scope of solid-polymerization consideration (i.e. Zone II-2 in Figure 1.5). Adherent to the limited awareness of this mutual contribution in the self-healing polymer literature, the development of an evaluator system targeted on capturing these inter-linked characteristics based on the weak form Galerkin finite element model is lacking and worth to be explored.

### **1.3 Objectives of the Study**

The examination of the fluid and polymerization mechanics as well as the search of the optimal strength recovery system through respective numerical setting, preferably in a stable and concise environment but yet at an affordable computational framework, is highly desirable considering the inherent multi-physics and multi-scales nature of the external self-healing practice. It is the aim of the present study to accomplish such efforts through the self-developed in-house MATLAB algorithms, the objectives of which include:

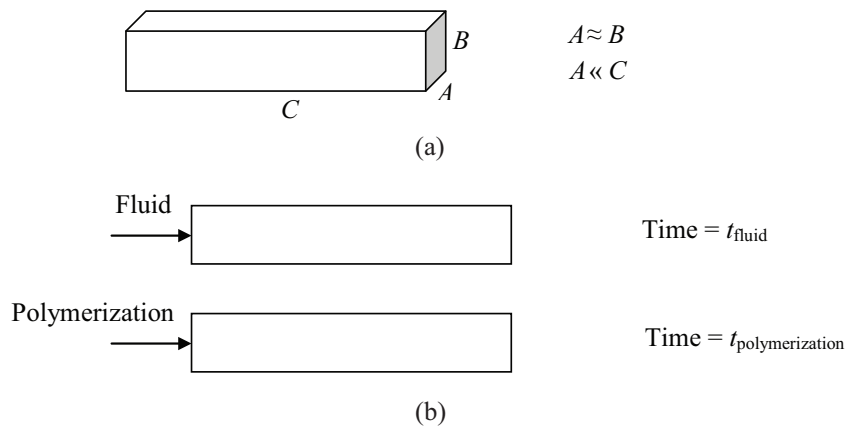
- (A) To formulate a discrete Stokes model in micro-scaled fluid setting by coupling the weak form Galerkin finite element method and penalty function method.
- (B) To determine the suitable numerical techniques and associated optimal parameters for the efficient use of model from Objective (A) in both steady and transient simulations.
- (C) To formulate a phenomenological-based polymerization model that couples to the heat conduction analysis by using the weak form Galerkin finite element method.
- (D) To determine the key kinetic parameters of the healing epoxy in fulfilling the polymerization optimality based on the model from Objective (C).

### **1.4 Scopes of the Study**

The multi-physics and multi-scales nature of the external self-healing practice in polymeric materials impose numerous potential scopes for study. The fracture mechanics is first excluded from consideration by limiting the present work to a readily formed crack geometry as schematically given in Figure 1.4 (b). Both fluid

and polymerization mechanics considered for the model are presumed to be bounded in a micro-scaled horizontal domain (refer Figure 1.4 (c)) as given in Figure 1.6 (a). Hence, the macro-scale undamaged portion is negligible.

Furthermore, the focus of relevant mechanics in 1D domain is adopted in the present study as presented in Figure 1.6 (b) due to the feasibility of dominantly unidirectional assumption (Reddy, 2006; Zienkiewicz et al., 2013) if the cross-sectional dimension (i.e.  $\mu\text{m}$  scale) is sufficiently small than that of length (i.e. mm scale). Moreover, the fluid and polymerization mechanics are considered separately in the present study to avoid the potential numerical complexity due to the multi-physics concern (Bathe, 1996; Reddy and Gartling, 2010). As a matter of fact, the time scale ( $t$ ) for fluid mechanics is often much shorter than that of the polymerization (refer response-time plot of synthetic system in Figure 1.3) due to the optimal infiltration rate requirement and hence the assumption of no obvious non-linearity overlapping concern among these mechanics is justified.



**Figure 1.6:** The domain of (a) presume crack geometry and (b) fluid flow and polymerization.

The scopes relevant to the hydrodynamics aspects in the present study include:

- (a) Flow nature
  - (i) Laminar flow.
  - (ii) Flow length  $< 20\text{mm}$ .
  - (iii) Micro-channel ( $10\mu\text{m} - 200\mu\text{m}$ ) (Kandlikar et al., 2005).

- (iv) Inlet velocity  $< 5\text{m/s}$ .
  - (v) Atmospheric outlet pressure.
  - (vi) Viscous incompressible Newtonian fluid.
- (b) Modeling framework
- (i) Stokes equations.
  - (ii) Velocity and pressure variables.
  - (iii) Weak form Galerkin finite element method.
  - (iv) Consistent penalty function method.
  - (v) Lagrangian shape functions (i.e. quadratic and linear).
  - (vi) Crank Nicolson predictor-corrector time integration scheme.

On the other hand, the scopes relevant to the thermodynamics as well as polymerization aspects in the present study are:

- (a) Heat transfer nature
- (i) Heat conduction.
  - (ii) Neumann inlet boundary (i.e. zero heat influx).
  - (iii) Dirichlet outlet boundary (i.e. constant temperature).
  - (iv) Phenomenological polymerization (Kessler and White, 2002; Zhou, 2012).
- (b) Modeling framework
- (i) Fourier's law.
  - (ii) Temperature and cure degree variables.
  - (iii) Weak form Galerkin finite element method.
  - (iv) Lagrangian shape function (i.e. linear).
  - (v) Crank-Nicolson time integration scheme.
  - (vi) Arrhenius's rate equation (Kessler and White, 2002; Zhou, 2012).

## 1.5 Significance of the Study

Two typical in-house weak form Galerkin finite element models targeted on capturing fluid dynamics and thermodynamics response are developed in the present study, respectively. Equipped with considerable numerical validation and verification, along with specific remedies to deal with the prompted underlying computational issues, these models are readily adopted to assess the infiltration and polymerization behaviors of the infilling polymeric liquid in single unidirectional crack geometry.

Besides, the output of these in-house models (e.g. velocity, pressure, evolution of both temperature as well as the cure degree) readily serves as the input parameters for both the structural and fracture module (refer Figure 1.5) in order to accomplish the core mechanics assessment of extrinsic self-healing mechanisms in polymeric materials. Specifically, the infilling behavior offers the details on the remaining crack portion that contribute nothing to structural strength and perhaps the next crack origin. On the other hand, the polymerization behavior (i.e. the axial cure degree along the unidirectional crack domain) offers the relevant information on the strength gain throughout the healed event to cater the next fracture.

Generally, a thorough and representative mechanical assessment on the optimality of the healing performance in a single realistic crack geometry is readily achievable based on the output parameters generated by the in-house weak form Galerkin finite element models developed in the present study. Note that relevant work on this aspect remains lacking in the literature. Several companion benefits throughout the development of the in-house weak form Galerkin finite element models are highlighted herein:

- (a) The experience in numerical validating and verifying these models could be laid as the reference framework to develop much advanced infiltration and polymerization module corresponding to the much realistic crack phenomenon (i.e. 2D/3D spanning as well as multiple branches) and polymer chemistry.
- (b) The survival of the weak form Galerkin finite element fluid flow and heat transfer module from the computational issues encourages a unified numerical framework to be developed targeted on extrinsic self-healing mechanisms. Specifically, the transfer of the multi-physics variable under similar numerical method is convenient and favorable. Therefore, the effort contributed in the present study shall serve as a milestone for the upcoming research in this realm.

- (c) The benefit of coupling examination of multi-physics variable is demonstrated in the present study. Particularly, the unification of both temperature and cure degree evolution under a single evaluator is demonstrated to work ideally in assessing the solid-polymerization mechanics. Much representative and crucial examination in similar trend is expected shall the unified weak form Galerkin finite element framework is readily developed to assess the underlying multi-physics variables (i.e. stress, strains, velocity, pressure, temperature, cure degree, and etc.) embedded in the damage-transport-chemical repair of the extrinsic self-healing mechanisms in self-healing polymeric materials.

The relevant numerical difficulties, with respect to each independent aspect of diffusive fluid and energy flow, are demonstrated and solved within the limited scopes of the present study in the 1D domain. Specifically, two categories of discussion mainly on computational mechanics aspect are presented both theoretically and practically:

- (a) Effective use of penalty function method in solving both steady and transient incompressible Stokes equations
- (i) Demonstrate penalty parameter ( $\gamma_p$ )-spatial mesh ( $\Delta x$ ) relation in terms of numerical stability, consistency, and accuracy.
  - (ii) Demonstrate the role of elemental divergence of velocity (EDV) components corresponding to mass conservation in both iterative penalty setting and modified iterative penalty setting.
- (b) Demonstrate the problematic coupling of weak form Galerkin finite element spatial discretization and single-step finite difference temporal discretization in capturing the dynamic behaviors of diffusive fluid motion and diffusive energy transfer
- (i) Highlight on erroneous perspective that numerical stability, consistency, and accuracy is ensured as long as there is a sufficient mesh refinement (i.e. spatial, temporal, and both).
  - (ii) Establish the  $\Delta x$ -temporal mesh ( $\Delta t$ ) relation for efficient penalty fluid flow simulation

## 1.6 Outlines of the Thesis

This thesis comprises seven chapters. After the present introductory chapter, Section 2.1 focuses on the recent practical developments in self-healing polymeric materials, particularly those adopt external/extrinsic-based healing system. The key mechanics in the extrinsic self-healing mechanisms, namely fluid and polymerization, that are worth to be examined numerically are highlighted in Section 2.2. Relevant numerical issues and potential remedy, both steady and transient, if the FE Eulerian framework is adopted is then discussed in Section 2.3. The nature and scopes of the present study are then aligned with the main research issues stated throughout the previous discussions and listed in Section 2.4.

Section 3.1 and Section 3.2 present the main governing equations for the incompressible fluid flow and polymerization models in the present study, respectively. Generally, the weak form Galerkin formulations for both models along with their appropriate boundary conditions are given where the development ranging from the selection of shape functions to the assembly of the matrix system and later the solution procedure are discussed. Several expected findings from these models are highlighted in Section 3.3.

The pressure solutions in a straight micro-channel based on the FE incompressible fluid flow model are presented in Section 4.1. A beneficial remedy framework, based on the iterative penalty Galerkin FE setting, in terms of numerical stability and consistency is highlighted in Section 4.2. The optimal coupling between spatial mesh size and the penalty parameter for numerical accuracy is tested and a preliminary benchmark range is proposed in Section 4.3. A modified framework is later proposed in Section 4.4 due to the numerical deficiency of the benchmark range where the stability, consistency, and accuracy of the pressure solution based on the new framework are demonstrated. Several recommendations beneficial to the development of penalty Galerkin FE incompressible fluid flow model are summarized in Section 4.5.

The pressure solution resulted from the integration of the predictor-corrector temporal scheme to the penalty Galerkin FE model is presented in Section 5.1. The optimal coupling between the temporal mesh size and the penalty parameter is later tested in Section 5.2 for a wide range of the channel geometries and inflow conditions, most of which aligned to the extrinsic self-healing practice, where a parameter targeted for optimal stability, consistency, and accuracy of the pressure solutions is given.

Satisfactory performance of the parameter is later demonstrated for the flow front tracking in micro-channel along with the progression of the pressure distribution. The main guidelines beneficial to the development of transient penalty Galerkin FE incompressible fluid model are summarized in Section 5.3.

The steady heat conduction modeling with heat generation term is presented in Section 6.1 whereas extension of the framework aligned to the heat release due to the polymerization is given in Section 6.2. The heat generation and cure rates based on the polymerization kinetics adopted in Yuan et al. (2009) are evaluated in Section 6.3 where an useful relation between the temperature as well as cure evolution and the strength recovery performance of the self-healing specimen is proposed. Performance charts are generated in Section 6.4 from the parametric study adopting the key kinetic components of the epoxy healant where the main direction towards the optimal mechanical recovery is demonstrated. The beneficial search of the optimal mechanical performance based on the numerical framework is highlighted in Section 6.5.

Section 7.1 summarizes the main findings from the numerical solutions (e.g. velocity, pressure, temperature and cure degree) generated from the FE models in the present study where appropriate guidelines that ensure stability, consistency, and accuracy are listed. The postulated strength recovery, based on the numerical evaluation of both the temperature and cure degree evolution, as a simple tool beneficial to the optimal search of the self-healing polymer chemistry as presented in the present study is highlighted. Several recommendations aligning to the extrinsic self-healing practice in polymeric materials that are worth to be extended under the accomplishment of the scopes in the present study are also given.



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