CRACK MORPHOLOGY EVOLUTION DUE TO PYROLYSIS AND COMBUSTION IN SOLIDS

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ABSTRACT

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A model is presented for processes that couple thermal degradation to cracking, with a focus on crack formation and propagation during pyrolysis. As the pyrolysis front propagates into the sample, a charring layer is left behind which contains voids, fractures and defects. Cracks propagate to release tensile stresses accumulated when the sample is losing its mass. They can intersect each other, forming loops, which are isolated fragments, unable to provide structural support.

The pyrolysis cracking process is simulated using FEM (Finite Element Method). The FEM code is parallelized using MPI (Message Passing Interface) in order to accelerate and capture the damage on a meso scale. Various dimensionless groups characterizing the problem are determined. Parameter groups are varied to investigate their effects on the morphology of the crack patterns. The crack patterns obtained from the numerical simulations are quantified using image analysis algorithms and functions that were developed and implemented in MATLAB.

The crack patterns share similar morphological features with other patterns found in nature or in laboratories, such as the hierarchy of the cracking arrays of quenched plates, the polygonal mud cracks, the tree-like structures of river network, and leaf veins. The expression of the tree-like or loop-like behavior is dependent upon the choices of the parameters. In particular, as the ratio of tensile strength to Youngs modulus increases, the crack behavior shifts from intersecting toward branching. The behavior is also influenced by possible anisotropy in the thermal diffusivity: behaviors that range from cracks that spread out to cracks that cluster together. Furthermore, other quantities, such as crack spacing, crack length, crack propagation rate, loop directions, junction angles and their distributions, crack initiation time, as well as their dependence on material properties, are computed as well, which provides additional understanding of the governing mechanisms.

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CHAPTER 1

INTRODUCTION AND BACKGROUND

This study investigates the interactions between combustion and the change of morphology during burning of solids. The study has its origin partly in military applications such as crack development in burning propellants and composite polymer vehicle parts. It is motivated by the cracking pattern on the charred XGnP residue samples that were tested using the cone calorimeter facility in the MSU ERC Combustion Laboratory. In daily life, such behavior is found in burned wood logs. We propose a model for the process that involves combustion, pyrolysis and cracking, with focus on the mechanisms of crack formation and propagation during pyrolysis. Numerical simulations followed by quantification of crack morphologies reveal fundamental principles of the combustion cracking process.

In the literature, there are studies that address different aspects of the mutual interactions between the solid and gas phases during combustion. One of the first works of this kind is Parker's model for wood pyrolysis [1]. Assuming the charring solids takes a trapezoided shape when cracked, Parker derived a system of governing equations for energy and mass balance. The Fire Dynamic Simulator (FDS) [3], a fluid dynamics based source code developed by NIST and VTT for the simulation of fire driven buoyant flow, can be used to simulate the burning of solid objects. In the FDS, solids can pyrolyze according to multiple simultaneous or serial Arrhenius chemical kinetics reactions. Then they can disappear or be removed from the computational domain when their density reaches a "burn away" limit. The FDS was also used to investigate the structural collapse of buildings, such as the modeling of World Trade Center fire event in 2001 [4]. Developed mainly for chemically reacting flow, the FDS has thermal and fluid submodels that have been validated. To enhance the submodel pyrolysis of the FDS, the source code Gpyro (A 3D Generalized Pyrolysis model) [5], [6] was developed by C. Lautenberger. Gpyro allows the solids to change its shape due to density reduction, by shrinking, which is the simplest form of mechanical deformation. Other works that consider small scale flames, such as [7], [8], [9], [10], couple flame spread with a moving charring, or melting, interface. In such moving pyrolysis interface models, the solids divide into two distinct zones: a char layer near the surface where solids fully degraded and a virgin zone deeper inside within solid, which pyrolysis/degradation has not yet influenced. Furthermore, in such a model, the transition from virgin material to char is taken to occur across an infinitesimally thin "sheet" or surface, which is the so-called pyrolysis front. The infinitesimally thin reaction front is an idealization of the actual process. In other flame spread or pyrolysis models [11], [12], the transition is taken to occur over a region of finite dimension, namely the pyrolysis length or the reaction zone thickness. Other studies investigate the relationship between char formation and flame spread, such as in the numerical simulation of pyrolysis and flame spread of a pine needles [13]. In all of these flame spread models there is no accounting for crack formation or surface deformation, two processes that are confirmed as discussed above for wood logs, by routine empirical observation.

Certain areas of research other than flame spread, [14] have theoretically investigated the propagation of cracks in convective burning of propellant using a cohesive zone model which related the gas pressure to the cohesive force ahead of the crack tips. In studies of spalling of concrete structure in fire [16], [17] the processes of water transport are coupled with heat transfer and the thermal expansion of the evaporating vapor, which is believed to cause concrete damage. Some studies have examined char shrinkage and fissure formation using the principle of energy minimization. For example [18] correlates the total crack length to the surface density and the shrinkage gradient. The study [19] calculates the surface elastic strain and the size of char blisters. In these studies, cracks are either assumed to exist prior to the heating process and remain unchanged, or they are altogether neglected. Among the models mentioned above, the ones that are considered in more greater detail in this thesis are: Parker's model of pyrolysis; FDS pyrolysis of solids and flaming of pyrolysis gases, shrinkage strain due to mass loss. Each model itself is not adequate to either capture the solid and gas-phase flame interactions nor do they include mechanisms for crack formation in pyrolysis. Here, an interdisciplinary model is proposed that ties together different processes in the two phases: heat transfer, pyrolysis, and elastic deformation and fracture. Fig. 1.1 shows the roadmap of the overall process, which is the combination of different submodels labeled as A, B, C, D, E, F. The interconnections between them are represented by arrows. The bold arrows represent strong coupling and the thin ones signify weak coupling. Among these six submodels, four belong to the solid phase: A (Heat transfer in Solid), B (Pyrolysis), C (Deformation and Stress Analysis) and D (Mechanical Damage) while the other two are for the gas phase: E (Momentum Heat and Mass Transfer in Gas Phase), F (Reacting Gas). Different categories relate to each other in the following ways: (A) provides the temperature distribution for rates of substance decomposition in (B). These chemical reactions (B) require energy (endothermic) to break the bonds which cause them to serve as a heat sink in the energy equation (A). The combustible gases are released, which may be ignited when they gain contact with the oxygen ambient at a sufficiently high temperature. These exothermic chemical reactions in the gas phase involve hundreds of reactants and they release thermal energy which can support the flame (F). (E), the equations that describe transportation of energy, species and momentum are solved, providing the distribution of species concentration and temperature in the gas phase. The solid substance can gradually lose its mass via pyrolysis, which serves to build up the tensile stress (C), which can fracture the sample when a certain stress threshold limit is exceeded (D). For flame retardancy, char formation without cracking is a desirable feature because it can serve as a low thermal conductivity barrier between the flame and the virgin material [20]. Cracks (D) modify the paths that hot in-depth gases use to escape from the solid matrix to the free stream (E). In particular, without fissures, hot pyrolysis gases at high pressure will be pushed back into virgin materials at lower pressure by pressure gradient

force. They may condense and later, when they are reheated, diffuse through the hot char layer to the surface where they can react with atmospheric oxygen [11]. However, the presence of cracks will create an instantaneous releasing pathway for those gases, which then enter the free stream. Similarly, cracks augment the oxygen pathway into the interior region of the decomposing solids. When char is exposed to oxygen, it can undergo an oxidation process which forms carbon dioxide and ash. Cracks also alter the stress distribution in the solid sample (C) by concentrating stresses and may even form loops which are the the isolated material fragments.



Figure 1.1: The roadmap to our study.

1.1 Combustion and Pyrolysis

The thermal process inside solids can be described by using the continuum heat conduction equation, with the heat source or sink terms from pyrolysis reactions (either exothermic or endothermic). This equation can be solved subject to various boundary conditions, which describe physical processes such as radiation from flames or an incident heat flux, as well as convection and radiation to the ambient gas. In a model that accounts for a pyrolysis front that separates the charred from the uncharred region, heat equations for the charred and the uncharred matrices can be solved separately due to the assumption that there is a transformation of thermal properties from the uncharred to charred substances. One additional condition is required for this type of thermal model: continuity of temperature at the interface. The distribution of temperature can be obtained using either numerical or analytical methods. While the analytical solution exists only for a restricted set of problems, such as those that possess self similar solutions or Fourier representations, numerical methods can be widely used and do not necessarily require the formal division of regions. Numerical models can range from solving very detailed systems of PDEs to generating integral solutions that include surface temperature, heat penetration and pyrolysis depth. In the later case, a temperature profile, usually linear or quadratic is assumed.

Concerning chemical reaction, all hydrocarbon substances decompose at rates that are accelerated at high temperature. Some polymers, like wax and PMMA, transform into liquids (i.e the melt) before evaporating into gaseous fuels. Others, such as wood, rubbers, bio wastes,... are broken down into combustible gases (tars) and solid residue (char) via multiple chemical reactions in a process termed "pyrolysis." In pre-modern times, pyrolysis was used to make charcoals from wood logs. Nowadays, pyrolysis is a major method for producing gas fuels, biogas, coke, activated carbon, etc and for reducing industrial waste. It has received much attention due to its importance in industrial applications. The simplest pyrolysis model neglects all chemical kinetics but includes a pyrolysis front defined by a limiting temperature [21]. This front, theoretically described by a line in 2D or a surface in 3D models, divides solids into charred and uncharred regions. According to this models, solids change its component over an infinitestimally thin front. More complex models are kinetically controlled. The reactions range between simplified singe step reaction models to multiple steps and reactants. Kinetics parameters for those models are extracted from TGA (Thermogravimetric analysis) experiments. Pyrolyzable materials, which have a char residue more than 5% of the original weighted, for example cellulosic, rubber, DGEBA, PET, PEI, PEEK, are categorized as charring substances. While others such as PMMA, POM, PLA, PP, HIPS, are non charring ones.

In a pyrolysis model of [11] that includes convective and radiative heat exchange with ambient, the process is divided into four different heating stages according to the changes in temperature, mass flux and char values. In particular, in the initial heating stage the temperature is constantly rising but has not reached a value where it can induce a pyrolysis chemical reaction. In this stage the mass flux released is negligibly small. In the second stage, mass flux is produced along with a char front that propagates into the interior region. In the third stage, the temperature equilibrates to a maximum limit value when there is a balance between heat flux from the flame and convective heat loss to the ambient. The mass flux attains its peak value in this stage, then it gradually decreases. The final stage is marked by a thick char layer that forms near the end of the process.

Among pyrolyzing polymers, wood is studied extensively because of its wide range of applications. Wood is structured from long chain hydrocarbon polymers, whose the primary component is cellulose. The other components are hemicellulose, lignin, magnan and xylan. Owing to its polymeric and composite nature, wood pyrolyzes in multiple steps into multiple products. Each of its components has its own bond breaking tendency. Generally speaking, the products from wood pyrolysis belong to one of the three categories: char/residue, gas (CO, CO_2 , H_2O) and tar (other volatiles than gas, rich in 1,6 anhydro compound [29]). Wood pyrolysis models are very numerous [23], [24], [25],

[26], [27], [28], varying from a model defined solely based on the pyrolysis temperature to models with chemical reactions that can further be classified into: one step-single reactions; one step-multiple reactions; multiple step-multiple reactions. Kinetic parameters for each reaction are attained by fitting TGA data into Arrhenius equations, which usually take the form:

$$\frac{\partial \rho}{\partial t} = -A(\rho - \rho_c)^n e^{-\frac{T_a}{T}},$$
(1.1)

where n is the order of reaction, A is the pre-exponential factor and T_a is an activation energy. For the one step-single reaction model: *virgin* wood \rightarrow volatiles + char, which is used in this thesis. The power (n = 1) produces a good fit with many experimental data. With n = 1, Eq. (1.1) reduces to Eq. (2.2) in chapter 1. More details about the pyrolysis parameters and pyrolysis models of wood are presented in Section 5.2.

The Parker model [1] considers the pyrolysis of wood as a process of endothermic chemical kinetics of its five components (water, cellulose, lignin, manan, xylan). Initially, thermal energy is provided by the incident heat flux to desorb the water and to decompose the other four components into volatiles (also called tars) and char which is assumed to have no weight, i.e, $\rho_c = 0$. Thus the mass loss rate for each species takes the following form:

$$\frac{\partial \rho}{\partial t} = -A\rho^n e^{-\frac{T_a}{T}}.$$
(1.2)

When total density reaches a critical value which is equivalent to ρ_c in (1.1), no mass flux is produced. The volatiles released are assumed to reside in the solid as they diffuse inward, eventually reaching the solid surface and entering the gas stream. When the surface mass flux is high enough to ignite and support a flame, the pyrolysis process becomes self sustaining by radiation from the flame at high temperature ($T_f = 1200^{\circ}C$) and thermal convection from the hot, flowing gas. Heat is removed from the solid surface by convection and by radiation by the cold ambient air at temperature T_{∞} . The total heat flux to the surface is given by

$$q'' = q_0 - q_h - q_r \tag{1.3}$$

in which q_0 is the incident heat flux, and q_h and q_r are the convective and radiative heat fluxes between the ambient and the flame. The effect of deformation is included in the char shrinkage term and by mass flow through fissures in char layer. The depth of the char layer is defined as the location where the solid density is 90% of its original value. The dependence of the thermo-physical and thermo-chemical properties on temperature and solid mass was taken by Parker from the literature. The measurement of the heat of combustion and kinetic parameters was done as part of that work. For numerical calculation, the solid was divided into parallel slices with moving boundaries so that no solid material crosses the boundaries. That boundary movement is characterized by a shrinkage factor variable that is a function of the char value. In summary, Parker's model includes both heat transfer and chemical kinetic models inside actively degrading, externally heated solids. The schematic representation of the model is shown in Fig. 1.2.

The pyrolysis of wood, like most other polymers, happens over a finite thickness layer, namely the reaction thickness region [11]. However, for some thermoplastics with very high activation energy, pyrolysis suddenly occurs when the temperature reaches a certain threshold value and the material instantaneously transforms to gas (gasification). The infinitesimally thin reaction zone can still be considered a good approximation for these kind of substances.

Pyropolis, Gpyro, ThermaKin are recently developed numerical codes that investigate aspects of pyrolysis such as phase transitions and mass diffusion. ThermaKin [30] solves the coupled heat and mass transfer of the released species in the solid phase during pyrolysis. Heat transfer mechanisms inside the solid include conductive, convective and radiative heat transfer handle up to thirty chemical reactions of first and second order. The governing equations in ThermaKin are the conservation of mass, energy and species with Arrhenius reaction rate for the chemical reactions. Developed for the simulation of



Figure 1.2: Parker model, showing the partially charred cells, the formation of fissures, and the various forms of heat transfer.

pyrolysis of fiber reinforced composites under conditions of standard fire tests, Pyropolis [31] captures the chemical kinetics of material constituents, solid heat transfer and Darcy's law for gas transfer inside solids. Pyropolis extracted its kinetic functions and their parameters from experimental data, i.e, it is an empirically based model.

The pyrolysis submodel in FDS [2], [3], which is one dimensional, is similar to ThermaKin, but it can be coupled to fluid phase models. FDS can extract kinetic parameters from TGA measurements. In FDS, the pyrolysis gases are released into a flow that can support combustion when the ambient oxygen concentration is sufficiently high enough to support the flame.

Char formation in pyrolysis is complicated, however little is known about its mechanisms. It is usually described and modeled as a competitive reaction with active cellulose in wood pyrolysis and is related to the residence time of hot volatiles. The formation of char is preferred over that of combustible gases and tar, at low temperature. The layer of char over top the surface of materials serves as a protective layer against flame, which makes some charring materials effectively fire retardant. Producing this char layer during burning is one goal in the artificial manufacture fire resistant materials. A recently developed model of char cracking by Li *et. al* relates shrinkage strain to thermal shock in pyrolysis ([18] and [19]) in which the thermal shock parameter is defined by [135] as

$$\phi_T = \frac{k\sigma_c(1-\nu)}{\gamma_t E} \tag{1.4}$$

Here γ_t is the thermal expansion coefficient, *E* is the Young's modulus, *k* is the thermal diffusivity, ν is Poisson's ratio and σ_c is the tensile strength of the material. To minimize thermal shock, beside choosing materials that have high ϕ_T , it is important to keep the temperature gradient low and to change the temperature slowly. Low temperature gradients can be obtained if the material has sufficiently high thermal diffusivity.

Baroudi *et. al* [32] treats char shrinkage as a thermoelastic buckling problem and they calculate the morphology of the char surface; Li *et. al* [33] correlate the level of the char shrinkage gradient to the heat flux and ambient pressure.

Park *et. al* in the study of wood pyrolysis [34], assert that wood splitting is caused by internal pressure, non uniform shrinkage, and structural weakness due to charring. The solid phase is then coupled to the gas phase via heat fluxes and mass fluxes at the interface. In pyrolysis without combustion models, such as the Parker model, the flame is represented by a flame heat flux term when the mass flux reaches a certain critical value. In solid fuel combustion models, the pyrolysis gases (pyrolysates or tars) are released into the flow, reacting with ambient oxygen and supporting the flame.

In general, a typical mathematical formulation of flame spreading over solid fuels has the following ingredients: heat transfer inside the solid (heat conduction); the finite rate chemical kinetics in the solid (Arrhenius law); mass transfer of species inside the solid (conservation of mass, Darcy's law); heat fluxes at the interface (convection, radiation); mass fluxes at the interface; finite rate chemical kinetics; heat transfer and species transfer; elliptical formulation of the flow fields in the gas phase [8], [9], [10], [12]. The FDS model: The FDS libraries can be either downloaded directly or compiled from source code files. The source code, written in both f90 and C^{++} programming languages, is available free of cost at *https* : //*github.com/firemodels/fds* at free of cost. Then it is compiled by Intel Fortran and C^{++} simultaneously, producing two separate libraries, FDS and Smokeview. The former serves the computational purposes and the latter serves as a graphic tool to visualize output quantities, such as geometry and the distribution of fluid flow, temperature and smoke particles. In this thesis the FDS library was run both in the serial mode and in the parallel mode at the MSU iCER parallel computing center and at the Linux cluster built from two personal laptop computers. Each laptop is a i3 dual core with two processors, yielding a total of four processors. MPI (Message Passing Interface) is used to communicate between the parallel processors. Fig. 1.3 shows the Linux cluster I built from two laptops to run FDS.



Figure 1.3: Linux cluster built from two personal laptops.

In summary, in none of the previous studies is there any modeling of the physical mechanisms that originate the cracking processes by thermally induced stress fields in the heated material. Therefore, understanding the mechanism of crack formation in pyrolyzing solids poses significant theoretical and computational challenges since there are currently no detailed predictive models for this mechanism. Furthermore, to date the observation of crack development in laboratory experiments has not been possible because of the high temperature of the solid sample, and the even higher temperature of the surface flame, which, along with the emission of pyrolysis gases and smoke, inhibits diagnostic measurements. In addition, the direct numerical simulation of cracks in the context of surface pyrolysis has not been carried out due to the absence of a comprehensive theory as well as the complexity stemming from the appearance of multiple cracks.

1.2 Cracks in drying and cooling

There has, been research on the related topic of shrinkage cracks, which may occur during drying. Concerning shrinkage cracks, models have been developed that describe how solids deform in response to driving forces such as high temperature in thermoelastic materials, moisture in the drying shrinkage of food pastes, pore pressure in drying colloidal gels, and species concentrations in crystals, see [35]. Similarly, stresses can be developed by the nonuniform shrinkage of a material subjected to external heating and subsequent thermal degradation (pyrolysis) and the associated induced mass loss. This hypothesis is supported by empirical observation and, more recently, by specific experiments that have sought correlations between cracking depth, heat penetration depth, and pyrolysis depth, see, e.g., [18].

Nature has provided examples of shrinkage cracks of which a sampling is discussed here. In geothermal science: crack columns in basalt cooling [38]; mud cracks in a wet rice field or in wet clay, [55], [56], [57], [65], mud peeling [58]; frozen solids under diurnal forcing [59], ice [61]; seasonal thermal contraction cracks in permafrost on Mars [60]; ground cracks [62]; drying soils [63], [75], saturated soil [64]. In biology: snake skin cracking patterns due to cell growth. These types of cracks are also generated in laboratories: parallel crack patterns in cold thermal shock ceramics [66], [67]; cracking of colloidal films [68], in drying suspensions [69], opal film in suspensions [70]; ring cracks in colloidal crystals of silica spheres on cover glass [71]; cracks in crystal decomposition; crack patterns in polymer crystallization [72] (rectangle, spiral, branching); splitting of food spaghetti [73], udon [74]; crack in concrete [76], hardened portland cement pastes [77] and in plastic cement [78]. In art: crack patterns on glaze ceramic or old paintings.

Chemical decomposition causes molar volume decrease . This is observed in the formation of cracks in crystal growth substances such as finely crystalline barium chloride dihydrate [79] and powdered potassium copper (II) chloride dihydrate [80]. In modeling, the reduction of the molecular equilibrium distance in quenching or chemical decomposition is represented by a proportionality between temperature difference or molar concentration and volumetric strain on the continuum scale. On the other hand, cracking of drying colloidal suspensions is driven by pore pressure thus the overall elastic stress is taken to be the sum of the mechanical stress and the pore suction. It is noted that the problems of quenching and directional drying of food are governed by the diffusion equations, such as the heat conduction and the crack length is found to scale with the square root of time, analogous to self similar variables that appear in general diffusive processes. In the problems of drying for colloidal solids, the pore pressure is related to pore size through Laplace's law and the evolution of crack length follows a power law.

In general practice, cracking in products should be avoided at all costs because it deteriorates the sample quality, thereby, malfunctioning the device. There are exceptions, for example the craze patterns in glaze ceramics, which is a desired aesthetic outcome.

These items listed below describes various shrinkage cracking mechanisms and the associated failure criteria for several kinds of materials found in many reference studies.

• Soil. Surface tension effects at air-water-soil contact (suction). *Horizontal stress at crack tip is more tensile than the tensile strength of the soil.* (*p* 266). *Rankine condition,*

[81].

- Thin films of colloidal silica. Pore pressure in fluid. *Cracks advance if tensile stress* exceeds σ_{go} , halt if it falls below σ_{stop} , [69].
- Colloidal in capillary tubes. Tensile stress σ₀ arising from contraction of the medium due to capillary pore pressure Eq. [1], page 3. *Minimizing the local strain energy density, by ratio between Griffith length and cell size, [82].*
- Backfill soil (silty clay) ground, excavated residual soil ground. Soil suction (pore air pressure, pore water pressure). *Net horizontal stress exceeds tensile strength of soil*, [62].
- Fine grained soil. Microscopic: variation in force acting between grains. Macroscopic: drying-induced strain. *Cohesive bond breaks irreversibly when normal force, tangential force, momentum of two discrete element exceeds an envelope; Eq. [3], [83].*
- Type 10 Portland cement with oxide composition. Water evaporation cause capillary stresses; C-S-H gel drying. *Shrinkage tensile stress exceeds a specified value*, [77].
- Concrete tensile strength. Free shrinkage of small elements of concrete cause by decrease of pore humidity as a function of humidity; Eq. [1]. *Tensile strength*, [84].
- Cementitious materials. Capillary pressure caused by curved water surface between particles. Plastic or capillary shrinkage, [78].
- Plain and fiber reinforced concrete. Shrinkage strain depends on moisture content; chemical shrinkage when volume of products is less than reactants. *Von Mises stress equal to the tensile strength*, [85].
- Concrete ring restrained by a steel ring. Stress due to restrained and differential moisture loss shrinkage. *Tensile stress exceeds critical value*, [86].

- Udon noodles (wheat flour and salt water) . Moisture loss. *Tensile stress exceeds critical value*, [74].
- Concrete. Chemical shrinkage, drying shrinkage. Rankine failure criterion, [87].
- Resin composite. Shrinkage due to polymerization. *Failure of bonding agents; micro-gap formation,* [88].
- Granular soils. Strain rate equals elastic strain rate plus metric change rate. Nonuniform particle size change generates self-equilibrated forces. *Crack initiates when strongest tensile contacts begin to fail,* [89].
- Starch and water mixture. Dessication. Contraction stresses exceed material strength,[38].
- Opal film made from suspension polystyrene sphere. Particle movement in solid is suppressed during wet to dry solid transition regime. [70].
- Basaltic lava flows. Stresses generated by thermal gradients. *First fracture appears when a maximum stress is exceeded. Hexagonal column of crack is formed by the energy minimization principle,* [90].
- Basalt. Purely tensile and anti plane shear during crack propagation. [91].
- Mud of clay particles. Pore pressure causes tensile stress, tensile stress gradient causes peeling cracks. *Crack peels in mode I and mode II of fracture mechanics*, [58].
- Spaghetti. Differential drying shrinkage. *Cracks are supposed to be caused by the stress values that exceed failure strength*, [73].
- (modeling). Saturated clay soil. Moisture loss. *Mode I stress intensity factor exceeds critical value (fracture toughness), [64].*
- (experiment and modeling). *Mode I stress intensity factor is larger than soils fracture toughness. Critical energy release rate is attained,* [92].

• (analytical). Colloidal. Shrinking colloidal is restrained by a rigid substrate. *J integral value or energy release rate is exceeded*, [93].

1.3 Physics base of fracture and damage

The literature of fracture has developed different theories about material failure. Among these are the phenomenal failure criterion; fracture mechanics; cohesive zone model and damage mechanics. According to the phenomenological failure theories, brittle and ductile materials behave differently in failure. In brittle materials, stretch increases linearly with stress until suddenly rupture occurs. On the other hand, ductile materials stretch linearly with applied load until a yield point after which stretch increases significantly without increase of applied load. Stresses are then redistributed as the sample deforms before actual failure occurs. Failure criteria are classified into different categories based on normal stress, shear stress, maximum principle stress, or maximum energy. Common phenomenological failure criteria and their contexts are listed below:

- the Tresca or maximum shear stress (brittle);
- the von Mises or maximum elastic distortional energy criterion (ductile);
- the Mohr-Coulomb failure criterion (cohesive-frictional solids);
- the Drucker-Prager (pressure-dependent solids);
- the Willam-Warnke (concrete);
- the Bresler-Pister (concrete);
- the Hankinson (orthotropic materials such as wood);
- the Hill yield criteria (anisotropic solids);
- the Tsai-Wu failure (anisotropic composites);

- the JohnsonHolmquist damage model (high-rate deformations of isotropic solids);
- the Hoek-Brown (rock masses);
- the Cam-Clay (for soils).

The maximum stress criteria (Rankine's theory) for brittle materials, also named the maximum stress theory, states that failure will occur if the maximum principle stress (σ_1, σ_2) reaches a critical tensile (σ_t) or compressive stress (σ_c) . This can be expressed mathematically as $-\sigma_c \leq \sigma_1, \sigma_2 \leq \sigma_t$. The maximum strain criterion (Saint Venant's theory), for brittle materials, states that when the maximum principle strain reaches a critical value, failure will occur:

 $\left|\frac{\sigma_1}{\sigma_c} - \nu \frac{\sigma_2}{|\sigma_t|}\right| = 1, \left|\frac{\sigma_2}{\sigma_c} - \nu \frac{\sigma_1}{|\sigma_t|}\right| = 1$, where ν is the Poisson's ratio.

The maximum shear stress (Tresca criteria), for ductile materials, is based on the yield stress which causes slippage of layers that are oriented 45⁰ degree to the normal stress. The Tresca criteria are summarized in table 1.1 below.

Both in tension	$\sigma_1 > 0, \sigma_2 > 0$	$\sigma_1, \sigma_2 < \sigma_t$
Both in compression	$\sigma_1 < 0, \sigma_2 < 0$	$\sigma_1, \sigma_2 > -\sigma_c$
σ_1 in tension, σ_2 in compression	$\sigma_1 > 0, \sigma_2 < 0$	$\frac{\sigma_1}{\sigma_t} + \frac{\sigma_2}{-\sigma_c} < 1$
σ_1 in compression, σ_2 in tension	$\sigma_1 < 0, \sigma_2 > 0$	$\frac{\sigma_1}{-\sigma_c} + \frac{\sigma_2}{\sigma_t} < 1$

Table 1.1: Tresca criteria

There is another type of failure theory for the yielding of ductile materials, which is based on the distortional strain energy, for example, the Von Mises criterion:

$$\sigma_1^2 - \sigma_1 \sigma_2 + \sigma_2^2 = \sigma_f^2 \tag{1.5}$$

or Coulomb- Mohr's theory:

$$\frac{\sigma_1}{\sigma_t} = 1, \frac{\sigma_2}{\sigma_t} = 1,$$
$$\frac{\sigma_1}{\sigma_t} = -1, \frac{\sigma_2}{\sigma_c} = -1,$$
$$\frac{\sigma_1}{\sigma_t} - \frac{\sigma_2}{\sigma_c} = + -1,$$

or the yield/failure criterion [37], for isotropic material, starting from the general polynomial expansion of the stress tensor, which has the form

$$L = \delta \sigma_{kk} + \zeta \sigma_{kk}^2 + \eta s_{ij} s_{ij} \tag{1.6}$$

where δ , ζ , η are the specified material constitutive parameters, s_{ij} is the deviatoric component of the stress σ_{ij} : $s_{ij} = \sigma_{ij} - \frac{\delta_{ij}}{3}\sigma_{kk}$. The elastic energy must be positive definite, which requires that $\delta = 0$. Thus, one form of *L*, which equal to elastic energy, is taken as

$$U = \frac{E}{2} \left(\beta \frac{\sigma_{kk}^2}{E} + \frac{3}{2} (1 - \beta) \frac{s_{ij} s_{ij}}{E} \frac{s_{ij}}{E} \right),$$
(1.7)

where

$$\beta = \frac{1 - 2\nu}{3} \tag{1.8}$$

and ν is Poisson's ratio.

Christensen assumes that homogeneous material does not fail under hydrostatic pressure but could fail under hydrostatic tension. This requires ζ in Eq. (1.6) to vanish, and the failure criterion according to Christensen is

$$\alpha \frac{\sigma_{kk}}{\kappa} + \frac{3}{2}(1+\alpha)\frac{s_{ij}s_{ij}}{\kappa^2} \le 1, \tag{1.9}$$

where $\kappa = |\sigma_c|$, which is the critical compressive stress and $\alpha = \frac{|\sigma_c|}{\sigma_t} - 1$ for a homogeneous material, for which:

$$0 \le \frac{\sigma_t}{|\sigma_c|} \le 1 \tag{1.10}$$

The ductile- brittle behavior is determined by the values of α :

$$\begin{split} \alpha < 1 : \frac{1}{2} &\leq \frac{\sigma_t}{|\sigma_c|} \leq 1 \\ \alpha = 1 : \frac{\sigma_t}{|\sigma_c|} = \frac{1}{2} \\ \alpha > 1 : 0 &\leq \frac{\sigma_t}{|\sigma_c|} \leq \frac{1}{2} \end{split} \qquad \qquad Ductile, \\ \text{Transition,} \\ \text{Brittle.} \end{split}$$

When $\alpha = 0$, Eq. (1.9) becomes $\frac{1}{2}s_{ij}s_{ij} \le \frac{\kappa^2}{3}$ which is the Mises criterion. When $\alpha \to \infty$, an extreme brittle condition, Eq. (1.9) becomes $\frac{1}{2}s_{ij}s_{ij} \le -\frac{\kappa\sigma_{kk}}{3}$. Those are the two extreme limits of α .

There are other failure theories, for example: the theory based on fracture toughness, stress intensity factor and the strain energy release rate of fracture mechanics; the theory based on a damage variable of damage mechanics. Fracture mechanics was first developed by Griffith [123] to study crack propagation in glasses. In linear elastic fracture mechanics (LEFM), cracks surfaces are traction free, cracks grow when the stress intensity factor or strain energy release rate exceeds a certain limit to generate new free surface. In the cohesive zone of model fracture mechanics, the separation occurs over a region ahead of the crack tip and the potential crack surface is bound by a cohesive force.

Unlike LEFM, which assumes that failure only occurs at the crack tip, thus can only predict crack propagation, the cohesive zone model and damage mechanics are able to predict crack initiation. In the current problem, the charring solid develops voids and micro cracks when degrading before developing cracks, therefore the cohesive model or damage mechanics provide advantages and might be future work.

The analytical solution near crack tips for certain problems of LEFM can be derived using complex variable analysis. It is found that the stress field near tip of the crack σ is inversely proportional to the square root of the distance from crack tip r, as $K/(2\pi\sqrt{r})$. Here K is the stress intensity factor that depends on loading conditions, geometry, ect. Thus the stress is infinite at crack tip (where r = 0). The crack propagates when K reaches
a critical value, $K \ge K_c$. Using an energy balance approach, a certain quantity of energy, which can be calculated from the J integral, must be released for crack to propagate.

The continuum damage model (CDM), [124], [125], describes the evolution of damage along with stresses and strains by introducing the damage variable which may be either scalar or tensorial. The scalar damage variable D is defined as the limiting ratio of the total area that contain defects, cracks and the total area, as the latter approaches zero. The variable D ranges between 0 and 1: D = 0 corresponds to undamaged state, D = 1 to totally damaged state and 0 < D < 1 describes the partially damaged state. In numerical modeling, there are local approaches for crack propagation, such as the discrete crack increment approach which resolves the near crack tip fields. In these approaches, cracks extend when certain field quantities like stress, strain, energy ahead crack tip reach a limiting value. Crack propagation in the local CDM is characterized by the reduction of material stiffness. The crack zone is taken as the locus of points where D = 1. However, similar to other local approaches, the local CDM theory posses difficulties for numerical modeling, such as mesh dependence of the crack width and the accurate computation of the crack growth rate.

1.4 Modelling of cracks

Different theoretical or numerical approaches to cracking can classified as either continuum models, such as, fracture mechanics, damage mechanics, the Finite Element Method (FEM), the Extended Finite Element Method (XFEM), or discrete models including discrete elements, spring blocks, bundle spring block, electrical fuses, peridynamics or molecular dynamics. They can be also divided into local models (classical FEM, XFEM) which assumes that a material point only interacts with other points in a close neighborhood; or nonlocal models (peridynamics, molecular dynamics), [94] which have distance interactions with other material points. Compared to continuum methods such as FEM, discrete models require no remeshing and can handle a very high number of nodes since solving the linear algebraic system of equations is not required. On the other hand, FEM is a numerical method for solving PDEs for general materials, varying from elastic to viscoelastic to plastic, and uses higher order elements for better convergence toward potentially exact solutions.

The traditional FEM developed based on LEFM explicitly tracks cracks by nodes. It requires crack mesh alignment and thus continuous mesh refinement near the crack tip. The extended finite element method (XFEM) developed by Belytschko and Black [97], [98] enriches nodes in the neighborhood of a smooth crack using discontinuous Heaviside step functions and the asymptotic crack tip functions. XFEM has demonstrated mesh independence and thus re meshing is generally not required. The asymptotic crack tip functions are derived from theoretical fracture mechanics, given as

$$F_{1}(r,\theta) = \sqrt{rsin(\theta/2)}$$

$$F_{2}(r,\theta) = \sqrt{rcos(\theta/2)}$$

$$F_{3}(r,\theta) = \sqrt{rsin(\theta/2)sin\theta}$$

$$F_{4}(r,\theta) = \sqrt{rsin(\theta/2)sin\theta}$$
(1.11)

where (r, θ) is the local polar coordinate system at the crack tip. It is noted that the first function in (1.11) is discontinuous across the crack face. The numerical simulations of drying cracks in tree bark and two layer mud [110] produces realistic patterns which vary with parameters such as Young's modulus, layer thickness, rate of growth and shrinkage, threshold stress. [99] implemented the XFEM for the simulation of thermoelastic cracks. [100] presents a general structure of an object-oriented XFEM code and steps for extending an existing general purpose FEM code like Abaqus into a XFEM code with small modification. The modification is applied for: extended variable or degree of freedom per nodes, detecting elements cut by the cracks, enriched stiffness matrices, division of cut elements for numerical integration. The library OpenXFEM⁺⁺ written in C^{++} were developed by [100] and tested for various 2D crack problems.

Phase field model has become increasing popular with many applications and numerical codes for various problem, including fracture. In phase field model, the field is represented by a scalar field that varies continuously with locations. There are open phase field source codes such as MOOSE, FEniCS, OpenPhase, DUNE, FiPy, MICRESS, PACE 3D, (see [106], [107], [108], [109]). Some studies derived an FEM formula for the crack parameter and the displacement fields and implemented them in Abaqus using User subroutines, such as the work of [104]. A phase field model for poroelastic material is developed by [105]. More details about XFEM and phase field model of fracture are presented at the Appendix, Sections E and F.

The boundary element method (BEM) is also a numerical method that can be applied to model cracks. BEM resolves the unknown field on the boundary instead of the whole domain. One of the main drawbacks of BEM is that the fundamental solution of the partial differential equations must be known before as it will be used as the weight function.

The spring lattice model, first proposed by Kawai [111], discretizes the elastic domain with nodes connected by springs, [95], [96]. Each spring is characterized by a spring constant and a breaking threshold which is usually of Mohr-Coulomb type. Different types of lattice can be used in the model, usually square or hexagonal, which are either structured and randomly distributed or an unstructured mesh. In practice, an unstructured mesh like the Voronoi tessellation can avoid mesh biased when simulating cracks which is a problem when using square and hexagonal lattices. The degree of freedom in each node of the lattice, the displacements *u* and *v* can be extended to include another degree of freedom for rotation. To derive the spring constant of each lattice from the elastic parameters, the stored strain energy of the lattice cell $E_{cell} = \frac{1}{2} \sum_{j=1}^{N_b} F_j u_j$ is equated to that of the continuum material $E_{con} = \frac{1}{2} \int \sigma e d\Omega$. Here *F* is the spring force between two nodes in the lattice, N_b is the number of bonds in each lattice and *j* is the index of each spring. To

model the anisotropy, each spring constant is allowed to have different values depending on the spring orientation. There are various spring models, such as the Kirkwood model for isotropic materials, the Keating model for materials with negative Poisson's ratio, and the Wozniak "beam bending" approach for the spring lattice model. The criteria for crack initiation and propagation in spring models are usually simple, e.g, cracking occurs at locations where the spring breaks when certain threshold value is attained.

Discrete models have been applied and successfully generate realistic crack patterns in drying solids, such as the discrete element modeling of drying and cracking of soils [112]. In those models, the drying process is modeled by changing the spring natural length following the time exponent decaying rule.

There are other discrete methods, including molecular dynamics and peridynamics, both of which are nonlocal. While the former is on the nano scale, the latter can be both micro and meso scale, in which the size ranges near $1\mu m$. Similar to molecular dynamics, peridynamics is formulated without spatial differentials, thus it is able to simulate cracks which have discontinuities across their faces. The meso scale makes it less computationally expensive, which is an attractive feature. Peridynamics has been coupled with FEM for solving the thermal shock problem, such as [113], [114], [115], in which FEM was used for the heat transfer equations and peridynamics was used to model the thermal cracks. The bond force is incorporated with the thermal expansion or contraction. In [113], the coupling coefficient between thermal expansion and bond force is determined by equating two strain energy, in such way that the spring constant of the discrete spring model is found. Oterkus et al. [116] derived a peridynamics model for the fully coupled thermo mechanical problem based on conservation of energy and the free energy function of thermodynamics. Failure occurs when bond stretch exceeds a critical stretch value and that bond is broken and crack appears spontaneously. Omitting the effects of cracks on heat transfer in these studies of thermal shock is a common practice. Moreover, it is justifiable when the cracking direction is parallel to the heat flux direction.

CHAPTER 2

A MATHEMATICAL MODEL FOR THE PYROLYSIS CRACKING PROCESS

2.1 Governing equations in general coordinate system

Our mathematical model includes heat transfer in the solid, material breakdown (pyrolysis) under high temperature, elastic deformation, and crack formation in the solid material. Here, the gas phase provides, through the action of a hypothetical flame, the external heat flux for the solid phase which is the focus of our study. The temperature field $T(\vec{x}, t)$ in a general coordinate system is described by the heat conduction equation

$$\frac{\partial T}{\partial t} = \nabla . (\alpha \nabla T) \tag{2.1}$$

where α is the thermal diffusivity. The rate of pyrolysis is described by the following single step decomposition reaction

$$\frac{\partial \rho}{\partial t} = -A(\rho - \rho_c)e^{-T_a/T}.$$
(2.2)

Here *A* is the pre-exponential factor, T_a is the activation temperature and ρ_c is the lower bound of the solid density, or the char density. The stress tensor σ is related to the strain tensor ε by the standard linear elasticity relation (Hook's law):

$$\sigma = C : \varepsilon_m, \tag{2.3}$$

or equivalently

$$\varepsilon_m = S : \sigma, \tag{2.4}$$

where the subscript *m* stands for the mechanical component, and C and S are the fourth order stiffness and compliance tensors, respectively. The solid shrinks as it loses mass

during pyrolysis. The shrinkage is modeled by taking the shrinkage strain ε_v as being proportional to the amount of mass loss,

$$\varepsilon_v = \gamma(\rho - \rho_0) / \rho_0 I, \tag{2.5}$$

where γ is the coupling coefficient between mass loss and volumetric shrinkage. The overall strain ε is the sum of the mechanical strain ε_m caused by stresses and the shrinkage strain ε_v ,

$$\varepsilon = \varepsilon_m + \varepsilon_v. \tag{2.6}$$

Moreover, the total strain is related to displacements by the small deformation relation, which is given by

$$\varepsilon = \frac{1}{2} (\nabla \vec{u} + (\nabla \vec{u})^T), \qquad (2.7)$$

in which \vec{u} is the displacement vector. Stresses obey the quasi-steady state equilibrium equation which neglects the inertial term:

$$\nabla \sigma = 0. \tag{2.8}$$

It is assumed that cracks nucleate and grow whenever the maximum principal stress σ_p reaches a threshold value σ_c , which is taken here as a material constant. Thus cracking occurs at locations where

$$\sigma_p \ge \sigma_c. \tag{2.9}$$

Initial conditions are required for the temperature and density fields. The boundary conditions for the thermal and the stress problem can be either prescribed temperatures or displacements (Dirichlet), prescribed heat fluxes or traction (Neumann) or mixed (Robin) conditions, such as roller supports or convection at boundaries (especially the ones bordering the gas phase).

2.2 One problem in Cartesian coordinate system

Consider the main problem in a rectangular domain $\mathcal{B} = \{(x, y) | 0 < x < L, 0 < y < H\}$, which is enclosed by a boundary $\partial \mathcal{B} = \partial \mathcal{B}_1 \cup \partial \mathcal{B}_2 \cup \partial \mathcal{B}_3 \cup \partial \mathcal{B}_4$, In particular,

$$\partial \mathcal{B}_1 = \{(x, y) | x = 0, 0 \le y \le H\},\$$

$$\partial \mathcal{B}_2 = \{(x, y) | y = 0, 0 \le x \le L\},\$$

$$\partial \mathcal{B}_3 = \{(x, y) | x = L, 0 \le y \le H\},\$$

$$\partial \mathcal{B}_4 = \{(x, y) | y = H, 0 \le x \le L\}.$$

The heat conduction Eq. (2.1) in this coordinate system can be written as:

$$\frac{\partial T}{\partial t} = \alpha_x \frac{\partial^2 T}{\partial x^2} + \alpha_y \frac{\partial^2 T}{\partial y^2},\tag{2.10}$$

where α_x and α_y are the thermal diffusivities in the *x* and *y* directions, respectively, which are taken to be constants. The equation for the decomposition process is given by Eq. (2.2).

Because of the two-dimensional nature of the problem under consideration, the stress and strain tensors are taken to be of the form:

$$\varepsilon = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xx} & 0 \\ \varepsilon_{xy} & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{bmatrix}, \quad \sigma = \begin{bmatrix} \sigma_{xx} & \sigma_{xx} & 0 \\ \sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{bmatrix}. \quad (2.11)$$

Assuming an isotropic and homogeneous material, the stiffness tensor *C* is simplified and only dependent on two paramters. These are the Young's modulus, *E* and the Poisson's ratio, ν . The overall strain follows from Eq. (2.3), Eq. (2.6) and Eq. (2.5):

$$\varepsilon_{xx} = \frac{1}{E} \left(\sigma_{xx} - \nu \left(\sigma_{yy} + \sigma_{zz} \right) \right) + \gamma \frac{\rho - \rho_0}{\rho_0}, \qquad (2.12)$$

$$\varepsilon_{yy} = \frac{1}{E} \left(\sigma_{yy} - \nu \left(\sigma_{xx} + \sigma_{zz} \right) \right) + \gamma \frac{\rho - \rho_0}{\rho_0}, \tag{2.13}$$

$$\varepsilon_{zz} = \frac{1}{E} \left(\sigma_{zz} - \nu \left(\sigma_{xx} + \sigma_{yy} \right) \right) + \gamma \frac{\rho - \rho_0}{\rho_0}, \qquad (2.14)$$

$$\varepsilon_{xy} = \frac{1+\nu}{E} \sigma_{xy}.$$
(2.15)

One may consider two separate cases for analysis. The first case is the condition of plane strain in which $\varepsilon_{zz} = 0$. The second case is the condition of plane stress in which $\sigma_{zz} = 0$. For plane strain, it follows from the condition $\varepsilon_{zz} = 0$ and Eq. (2.14) that

$$\sigma_{zz} = \nu \left(\sigma_{xx} + \sigma_{yy} \right) - E \gamma \frac{\rho - \rho_0}{\rho_0}, \qquad (2.16)$$

and thus σ_{xx} , σ_{yy} are related to ε_{xx} , ε_{yy} via :

$$\sigma_{xx} = \frac{E}{1+\nu}\varepsilon_{xx} + \frac{E\nu}{(1+\nu)(1-2\nu)}\left(\varepsilon_{xx} + \varepsilon_{yy}\right) - \frac{E}{(1-2\nu)}\gamma\frac{\rho-\rho_0}{\rho_0},$$
 (2.17)

$$\sigma_{yy} = \frac{E}{1+\nu}\varepsilon_{yy} + \frac{E\nu}{(1+\nu)(1-2\nu)}\left(\varepsilon_{xx} + \varepsilon_{yy}\right) - \frac{E}{(1-2\nu)}\gamma\frac{\rho-\rho_0}{\rho_0}.$$
 (2.18)

For the plane stress condition, it follows from putting $\sigma_{zz} = 0$ in Eq. (2.12) to (2.14) that

$$\sigma_{xx} = \frac{E}{1+\nu} \varepsilon_{xx} + \frac{E\nu}{1-\nu^2} \left(\varepsilon_{xx} + \varepsilon_{yy} \right) - \frac{E}{(1-\nu)} \gamma \frac{\rho - \rho_0}{\rho_0}, \tag{2.19}$$

and

$$\sigma_{yy} = \frac{E}{1+\nu} \varepsilon_{yy} + \frac{E\nu}{1-\nu^2} \left(\varepsilon_{xx} + \varepsilon_{yy} \right) - \frac{E}{(1-\nu)} \gamma \frac{\rho - \rho_0}{\rho_0}.$$
 (2.20)

For both plane stress and plane strain, it follows immediately from Eq. (2.15) that :

$$\sigma_{xy} = \frac{E}{1+\nu} \varepsilon_{xy}.$$
(2.21)

The displacements in the horizontal and vertical directions are *u* and *v*, respectively, $\vec{u} = (u, v)$. The strains in the (x, y) plane are related to *u* and *v* by the standard relations, following Eq. (2.7):

$$\varepsilon_{xx} = \frac{\partial u}{\partial x}$$

$$\varepsilon_{yy} = \frac{\partial v}{\partial y}$$

$$\varepsilon_{xy} = \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)$$
(2.22)

The stress equations of equilibrium for both the plane strain and plane stress problems follow Eq. (2.8), which give

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} = 0, \qquad (2.23)$$

and

$$\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} = 0.$$
(2.24)

2.3 The Rectangular Sample

To illustrate this model, consider the following set of initial and boundary conditions as an example. Initially, the temperature field is uniform at the value T_0 :

$$t = 0: T = T_0. (2.25)$$

The thermal boundary conditions are taken to be the following: insulated at the lower surface $\partial \mathcal{B}_4$; upper surface $\partial \mathcal{B}_2$ is subjected to a heat flux q(x); the two lateral sides $\partial \mathcal{B}_1$ and $\partial \mathcal{B}_3$ are maintained at the initial temperature T_0 . These conditions read as

$$\partial \mathcal{B}_1: T = T_0, \tag{2.26}$$

$$\partial \mathcal{B}_2: \frac{\partial T}{\partial y} = 0, \tag{2.27}$$

$$\partial \mathcal{B}_3: T = T_0, \tag{2.28}$$

$$\partial \mathcal{B}_4: k_y \frac{\partial T}{\partial y} = q(x).$$
 (2.29)

In Eq. (2.29), the heat flux function is specified as a nonzero constant over the central region of the upper surface, viz,

$$q(x) = \begin{cases} 0 & \text{if } |x - \frac{L}{2}| > \frac{l}{2} \\ q_0 & \text{if } |x - \frac{L}{2}| \le \frac{l}{2}. \end{cases}$$
(2.30)

Here k_y is the thermal conductivity in the y direction and q_0 is the constant heat flux. For the pyrolysis problem (Eq. (2.2)), one initial condition is needed. Initially the material is taken to have uniform density ρ_0 . The boundary conditions for the stress problem are taken to be of the second and the third type:

$$\partial \mathcal{B}_{1}: \sigma_{xx} = 0, \sigma_{xy} = 0,$$

$$\partial \mathcal{B}_{2}: \sigma_{yy} = 0, \sigma_{xy} = 0,$$

$$\partial \mathcal{B}_{3}: \sigma_{xx} = 0, \sigma_{xy} = 0,$$

$$\partial \mathcal{B}_{4}: v = 0, \sigma_{xy} = 0,$$

(2.31)

which are equivalent to the roller condition on the lower surface \mathcal{B}_4 and the traction free conditions on the other surfaces \mathcal{B}_1 , \mathcal{B}_2 , \mathcal{B}_3 . The boundary conditions discussed above for the problems are illustrated in Fig. 2.1.

For the plane problem, two of the principal stresses occur in the (x, y) plane



Figure 2.1: Boundary conditions. Upper surface: heat flux, stress free. Lateral sides: fixed temperature, stress free. Lower surface: insulated, roller.

$$\sigma_1 = \frac{\sigma_{xx} + \sigma_{yy}}{2} + \sqrt{\left(\frac{\sigma_{xx} - \sigma_{yy}}{2}\right)^2 + \sigma_{xy}^2},\tag{2.32}$$

$$\sigma_2 = \frac{\sigma_{xx} + \sigma_{yy}}{2} - \sqrt{\left(\frac{\sigma_{xx} - \sigma_{yy}}{2}\right)^2 + \sigma_{xy}^2}.$$
(2.33)

The remaining principal stress, which is nonzero only in the plane strain case, is the stress normal to the (x, y) plane

$$\sigma_3 = \sigma_{zz}.\tag{2.34}$$

The maximum principal stress is then:

$$\sigma_p = max(\sigma_1, \sigma_2, \sigma_3) = max(\sigma_1, \sigma_3).$$

CHAPTER 3

NUMERICAL RESULTS FOR THE PROBLEM ON A RECTANGULAR DOMAIN

3.1 A Finite Volume scheme

The purpose of this section is to develop the numerical stencils that discretize the governing equations, Eqs (2.23), (2.24), in which the relations of stresses to strains and strains to displacements are given by Eqs. (2.22), (2.19), (2.20), (2.21), which satisfy the set of boundary conditions in Section 2.3. The computational domain \mathcal{B} is meshed using a structured grid. Traditionally, Taylor's truncation can be utilized to derive such stencils, however, with material depletion, a different method must be used. Following [118], the numerical stencils are derived by requiring direct satisfaction of the equations within a sub volume in an integral sense. This is recognized as a weaker condition of the original partial different equations. Let $\mathcal{B} = \bigcup_{k=1}^{N} \omega_k$, in which ω_k , $(k = \overline{1, N})$ is the sub volume centered at the grid node and N is the total number of them nodes. Each local node P may be surrounded by some or all nodes of neighbor nodes N, S, E, W, NE, SE, NW, SW depending on the geometry and location of node P.

Consider a general form of the equations in which shrinkage strain and volumetric external force are present and can be incorporated into one term, namely f in the governing equation,

$$\frac{\partial \sigma_{ij}}{\partial x_i} + f_i = 0 \tag{3.1}$$

Here index notation has been used instead of x and y for the spatial directions. The boundary conditions can be more general compared with (2.31), for example, they may include a specified value of the nonzero normal stress. In this context, the standard plane

stress relations between strain and stress were used, giving

$$\sigma_{ij} = \frac{E}{1+\nu} \varepsilon_{ij} + \frac{E\nu}{1-\nu^2} (\varepsilon_{kk}) \,\delta_{ij},\tag{3.2}$$

while the small deformation relation (2.22) still remains. In its index notation form, this term is

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right).$$
(3.3)

Integrating Eq. (3.1) over each ω_k gives

$$\iint_{\omega_k} \left(\frac{\partial \sigma_{ij}}{\partial x_j} + f_i \right) dx dy = 0.$$
(3.4)

Eq. (3.4) can also be interpreted as the weak form in FEM, in which the weight functions are chosen as Heaviside step function. Applying Green's theorem, Eq. (3.4) becomes

$$\int_{\partial \omega_k} \sigma_{ij} n_j ds = \iint_{\omega_k} f_i dx dy, \tag{3.5}$$

where *n* is the outward normal unit vector on the boundary. The stencils derived for each node depend on factors such as: the order of truncation error in the approximation of the spatial derivatives and the geometry of ω_k and the boundary conditions. For illustration purposes, consider the example of equi biaxial pulling and let ω_k be the domain indicated in Fig. 3.1, surrounding node P and having three neighboring nodes N, E and NE. Thus node P is the lower left corner of the computational domain. The four edges of the subvolume ω_k are $\gamma_1, \gamma_2, \gamma_3, \gamma_4$. In this case, the shear stress is zero and the normal stresses have the specified value σ_0 on the domain boundary $\partial \mathcal{B}$, and thus on segments γ_1, γ_4 .

For a uniform mesh of dimension *h*, the four edges all have equal length, which is $\frac{h}{2}$. On γ_1 : $\sigma_{xx} = \sigma_0$, $\sigma_{xy} = 0$; on γ_4 : $\sigma_{yy} = \sigma_0$, $\sigma_{xy} = 0$. The first component of Eq. (3.5) reads:

$$\int_{\partial \omega_k} \sigma_{1j} n_j dx dy = -\iint_{\omega_k} f_1 dx dy, \tag{3.6}$$



Figure 3.1: The sub volume at node P and its neighbor nodes.

in which the outward unit normal vectors of the four edges are: (-1,0), (0,1), (1,0), (0,-1), therefore. Eq. (3.6), using *x* and *y* notation, becomes

$$\int_{\gamma_1} \sigma_{xx} ds - \int_{\gamma_3} \sigma_{xx} ds + \int_{\gamma_2} \sigma_{xy} ds - \int_{\gamma_4} \sigma_{xy} ds = -\iint_{\omega_k} f_x dx dy.$$
(3.7)

On γ_3 , $\sigma_{xx} = \sigma_0$, $\sigma_{xy} = 0$ and on γ_4 , we have $\sigma_{xy} = 0$, $\sigma_{yy} = \sigma_0$. Substituting these expressions into Eq. (3.7) gives

$$\int_{\gamma_1} \sigma_{xx} ds + \int_{\gamma_2} \sigma_{xy} ds - \int_{\gamma_3} \sigma_0 ds - 0 = \frac{1}{4} h^2 \overline{f_x}, \tag{3.8}$$

where $\overline{f_x}$ is the volume averaged value of f_x . Similarly, the *y* component of the governing equation along with the boundary conditions gives

$$\int_{\gamma_1} \sigma_{xy} ds + \int_{\gamma_2} \sigma_{yy} ds - 0 - \sigma_0 \int_{\gamma_4} ds = \frac{1}{4} h^2 \overline{f_y}$$
(3.9)

From Eqs. (3.2) and (3.3), we obtain

$$\sigma_{xx} = \frac{E}{1 - \nu^2} \left(\frac{\partial u}{\partial x} + \nu \frac{\partial v}{\partial y} \right), \qquad (3.10)$$

$$\sigma_{yy} = \frac{E}{1 - \nu^2} \left(\frac{\partial v}{\partial y} + \nu \frac{\partial u}{\partial x} \right), \qquad (3.11)$$

$$\sigma_{xy} = \frac{E}{2(1+\nu)} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right).$$
(3.12)

Now we require an approximation for the displacement derivatives. The following first order approximations are used:

$$\int_{\gamma_1} \frac{\partial \phi}{\partial x} ds = \overline{\frac{\partial \phi}{\partial x}} |_{\gamma_1} \int_{\gamma_1} ds$$
$$= \left(\frac{3}{4} \frac{\phi - \phi}{h} + \frac{1}{4} \frac{\phi_{NE} - \phi}{h}\right) \frac{h}{2} + O(h), \tag{3.13}$$

and

$$\int_{\gamma_2} \frac{\partial \phi}{\partial y} ds = \overline{\frac{\partial \phi}{\partial y}} \Big|_{\gamma_2} \int_{\gamma_2} ds$$
$$= \left(\frac{3}{4} \frac{\phi - \phi}{h} + \frac{1}{4} \frac{\phi_{NE} - \phi}{h}\right) \frac{h}{2} + O(h). \tag{3.14}$$

Note that on γ_1 , ds = dy and the integral of $\frac{\partial \phi}{\partial y}$ is the true integrand which can be taken as

$$\int_{\gamma_1} \frac{\partial \phi}{\partial y} ds = \left(\frac{1}{4}(\phi + \phi + \phi_{NE} + \phi) - \frac{1}{2}(\phi + \phi)\right)\frac{h}{2} + O(h)$$
$$= \frac{1}{4}(\phi_{NE} + \phi - \phi - \phi) + O(h).$$
(3.15)

Similarly, on γ_2 , ds = -dx and

$$\int_{\gamma_2} \frac{\partial \phi}{\partial x} ds = \left(\frac{1}{4}(\phi + \phi + \phi_{NE} + \phi) - \frac{1}{2}(\phi + \phi)\right) + O(h)$$
$$= \frac{1}{4}(\phi + \phi_{NE} - \phi - \phi) + O(h).$$
(3.16)

Using the above approximations for the derivatives of displacements in Eqs. (3.8) and (3.9), two stencils for node P are

$$\frac{3}{8}(u_E - u_P) + \frac{1}{8}(u_{NE} - u_N) + \frac{\nu}{4}(v_N + v_{NE} - v_P - v_E)
+ \frac{3}{8}\left(\frac{1 - \nu}{2}\right)(u_N - u_P) + \frac{1 - \nu}{2}\frac{1}{8}(u_{NE} - u_E) + \frac{1}{4}\left(\frac{1 - \nu}{2}\right)(v_{NE} + v_E - v_N - v_P)
(3.17)
= \frac{1}{4}\overline{f_x}h^2 + g\frac{h}{2},$$

and

$$\frac{3}{8}(v_N - v_P) + \frac{1}{8}(v_{NE} - v_E) + \frac{\nu}{4}(u_{NE} + u_E - u_N - u_P) + \frac{3}{8}\left(\frac{1 - \nu}{2}\right)(v_E - v_P) + \frac{1}{8}\left(\frac{1 - \nu}{2}\right)(v_{NE} - v_N) + \frac{1}{4}\left(\frac{1 - \nu}{2}\right)(u_N + u_{NE} - u_P - u_E)$$
(3.18)

$$=\frac{1}{4}\overline{f_y}h^2+g\frac{h}{2},$$

where $g = \frac{1 - v^2}{E} \sigma_0$. In the case of unequal biaxial stresses, the values of σ_0 in the *g* expression in the first and second stencils should be replaced by the values of the pulling stresses in the *x* and *y* directions, σ_{0x} and σ_{0y} respectively.

After rearrangement, the stencils for the considered sub volume are:

$$\begin{cases} (0) \quad \left(-\frac{1}{8} + \frac{3}{8} \left(\frac{1-\nu}{2}\right)\right) \quad \left(\frac{1}{8} + \frac{1}{8} \left(\frac{1-\nu}{2}\right)\right) \\ (0) \quad \left(-\frac{3}{8} - \frac{3}{8} \left(\frac{1-\nu}{2}\right)\right) \quad \left(\frac{3}{8} - \frac{1}{8} \left(\frac{1-\nu}{2}\right)\right) \\ (0) \quad (0) \quad (0) \quad (0) \end{cases} + \begin{cases} (0) \quad \left(\frac{\nu}{4} - \frac{1}{4} \left(\frac{1-\nu}{2}\right)\right) \quad \left(\frac{\nu}{4} + \frac{1}{4} \left(\frac{1-\nu}{2}\right)\right) \\ (0) \quad \left(-\frac{\nu}{4} - \frac{1}{4} \left(\frac{1-\nu}{2}\right)\right) \quad \left(-\frac{\nu}{4} + \frac{1}{4} \left(\frac{1-\nu}{2}\right)\right) \\ (0) \quad (0) \quad (0) \quad (0) \end{cases} \end{cases} + \\ = \frac{1}{4}\overline{f_x}h^2 + \frac{1}{2}gh, \qquad (3.19)$$

$$\begin{cases} (0) \quad \left(-\frac{1}{4}\nu + \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) \quad \left(\frac{1}{4}\nu + \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) \\ (0) \quad \left(-\frac{1}{4}\nu - \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) \quad \left(\frac{1}{4}\nu - \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) \\ (0) \quad (0) \quad (0) \quad (0) \quad \\ \end{cases} + \begin{cases} (0) \quad \left(\frac{3}{8} - \frac{1}{8}\left(\frac{1-\nu}{2}\right)\right) \quad \left(\frac{1}{8} + \frac{1}{8}\left(\frac{1-\nu}{2}\right)\right) \\ (0) \quad \left(-\frac{3}{8} - \frac{3}{8}\left(\frac{1-\nu}{2}\right)\right) \quad \left(-\frac{1}{8} + \frac{3}{8}\left(\frac{1-\nu}{2}\right)\right) \\ (0) \quad (0) \quad SE(0) \end{cases} \\ = \frac{1}{4}\overline{fy}h^2 + \frac{1}{2}gh. \qquad (3.20)$$

Here the following convention is used to simplify the notation. The first matrices in Eqs. (3.19) and (3.20) contain the parameters associated with u, the second with v and the positions of the parameters in a matrix indicate the node. In particular:

$$\left\{\begin{array}{ccc}
NW & N & NE \\
W & P & E \\
SW & S & SE
\end{array}\right\}.$$
(3.21)

In a similar way, the stencils for the subvolume at the lower right corner of the sample which involve four local nodes P, N, W, NW, are

$$\begin{cases} \left(\frac{1}{8} + \frac{1}{8}\left(\frac{1-\nu}{2}\right)\right) & \left(-\frac{1}{8} + \frac{3}{8}\left(\frac{1-\nu}{2}\right)\right) & (0) \\ \left(\frac{3}{8} - \frac{1}{8}\left(\frac{1-\nu}{2}\right)\right) & \left(-\frac{3}{8} - \frac{3}{8}\left(\frac{1-\nu}{2}\right)\right) & (0) \\ (0) & (0) & (0) \end{cases} \\ + \begin{cases} \left(-\frac{\nu}{4} - \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & \left(-\frac{\nu}{4} + \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & (0) \\ \left(\frac{\nu}{4} - \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & \left(\frac{\nu}{4} + \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & (0) \\ (0) & (0) & (0) \end{cases} \\ = \frac{1}{4}\overline{f_x}h^2 - \frac{1}{2}gh, \qquad (3.22)$$

and

$$\begin{cases} \left(-\frac{1}{4}\nu - \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & \left(\frac{1}{4}\nu - \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & (0) \\ \left(-\frac{1}{4}\nu + \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & \left(\frac{1}{4}\nu + \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & (0) \\ (0) & (0) & (0) \end{cases} \\ + \begin{cases} \left(\frac{1}{8}\left(\frac{1-\nu}{2}\right) + \frac{1}{8}\right) & \left(-\frac{1}{8}\left(\frac{1-\nu}{2}\right) + \frac{3}{8}\right) & (0) \\ \left(\frac{3}{8}\left(\frac{1-\nu}{2}\right) - \frac{1}{8}\right) & \left(-\frac{3}{8}\left(\frac{1-\nu}{2}\right) - \frac{3}{8}\right) & (0) \\ (0) & (0) & (0) \end{cases} \\ = \frac{1}{4}\overline{f_y}h^2 + \frac{1}{2}gh. \end{cases}$$
(3.23)

For the upper right corner of the sample, the stencils are

$$\begin{cases} (0) & (0) & (0) \\ \left(\frac{3}{8} - \frac{1}{8}\left(\frac{1-\nu}{2}\right)\right) & \left(-\frac{3}{8} - \frac{3}{8}\left(\frac{1-\nu}{2}\right)\right) & (0) \\ \left(\frac{1}{8} + \frac{1}{8}\left(\frac{1-\nu}{2}\right)\right) & \left(-\frac{1}{8} + \frac{3}{8}\left(\frac{1-\nu}{2}\right)\right) & (0) \\ \end{cases}$$
$$+ \begin{cases} (0) & (0) & (0) \\ \left(-\frac{\nu}{4} + \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & \left(-\frac{\nu}{4} - \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & (0) \\ \left(\frac{\nu}{4} + \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & \left(\frac{\nu}{4} - \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & (0) \\ \end{cases}$$
$$= \frac{1}{4}\overline{f_x}h^2 - \frac{1}{2}gh, \qquad (3.24)$$

and

$$\begin{cases} (0) & (0) & (0) \\ \left(-\frac{1}{4}\left(\frac{1-\nu}{2}\right) + \frac{1}{4}\nu\right) & \left(-\frac{1}{4}\left(\frac{1-\nu}{2}\right) - \frac{1}{4}\nu\right) & (0) \\ \left(\frac{1}{4}\left(\frac{1-\nu}{2}\right) + \frac{1}{4}\nu\right) & \left(\frac{1}{4}\left(\frac{1-\nu}{2}\right) - \frac{1}{4}\nu\right) & (0) \end{cases} \\ + \begin{cases} (0) & (0) & (0) \\ \nu\left(\frac{3}{8}\left(\frac{1-\nu}{2}\right) - \frac{1}{8}\right) & \left(-\frac{1}{8}\left(\frac{1-\nu}{2}\right) + \frac{3}{8}\right) & (0) \\ \left(\frac{1}{8}\left(\frac{1-\nu}{2}\right) + \frac{1}{8}\right) & \left(-\frac{1}{8}\left(\frac{1-\nu}{2}\right) + \frac{3}{8}\right) & (0) \end{cases} \\ = \frac{1}{4}\overline{fy}h^2 - \frac{1}{2}gh. \end{cases}$$
(3.25)

For the upper left corner of the sample, the stencils are:

$$\begin{cases} (0) & (0) & (0) \\ (0) & \left(-\frac{3}{8} - \frac{3}{8}\left(\frac{1-\nu}{2}\right)\right) & \left(\frac{3}{8} - \frac{1}{8}\left(\frac{1-\nu}{2}\right)\right) \\ (0) & \left(-\frac{1}{8} + \frac{3}{8}\left(\frac{1-\nu}{2}\right)\right) & \left(\frac{1}{8} + \frac{1}{8}\left(\frac{1-\nu}{2}\right)\right) \\ (0) & \left(\frac{\nu}{4} - \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & \left(\frac{\nu}{4} - \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) \\ (0) & \left(-\frac{\nu}{4} + \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) & \left(-\frac{\nu}{4} - \frac{1}{4}\left(\frac{1-\nu}{2}\right)\right) \\ = \frac{1}{4}\overline{f_x}h^2 + \frac{1}{2}gh, \end{cases}$$
(3.26)

and

$$\begin{cases} (0) & (0) & (0) \\ (0) & \left(\frac{1}{4}\left(\frac{1-\nu}{2}\right) + \frac{1}{4}\nu\right) & \left(\frac{1}{4}\left(\frac{1-\nu}{2}\right) - \frac{1}{4}\nu\right) \\ (0) & \left(-\frac{1}{4}\left(\frac{1-\nu}{2}\right) + \frac{1}{4}\nu\right) & \left(-\frac{1}{4}\left(\frac{1-\nu}{2}\right) - \frac{1}{4}\nu\right) \end{cases} \\ + \begin{cases} (0) & (0) & (0) \\ (0) & \left(-\frac{3}{8}\left(\frac{1-\nu}{2}\right) - \frac{3}{8}\right) & \left(\frac{3}{8}\left(\frac{1-\nu}{2}\right) - \frac{1}{8}\right) \\ (0) & \left(-\frac{1}{8}\left(\frac{1-\nu}{2}\right) + \frac{3}{8}\right) & \left(\frac{1}{8}\left(\frac{1-\nu}{2}\right) + \frac{1}{8}\right) \end{cases} \\ = \frac{1}{4}\overline{f_y}h^2 - \frac{1}{2}gh. \end{cases}$$
(3.27)

To fully derive the stencils for all of the nodes in the grid, many different cases must be considered, each case corresponding to the way the material in the neighborhood of the node *P* is removed due to damage. Such detailed results are presented in the Appendix for interested readers. In the next section, the FEM will be discussed. The FEM reduces the work load of developing stencils for each node.

3.2 Finite Element implementation

The Finite Element method, due to its rigorous mathematical foundation, has been used extensively to produce some numerical solutions for some problems in solid mechanics and recently, in fluid mechanics. The isotropic triangular mesh is generated by the MATLAB function *mesh2d.m* which use the Delaunay algorithm to minimize the bandwidth. Both the initial boundary value heat transfer and the stress problems described in Sections 2.2 and 2.3 are numerically resolved using FEM. The formulation of the FEM for the latter is outlined. To simplify the notation in the FEM formulation of the stress balance equation, the Lame parameters are used instead of Young's modulus and Poisson's ratio and for plane stress condition, their relations are given by

$$\lambda' = \frac{E\nu}{1 - \nu^2},$$
$$\mu = \frac{E}{2(1 + \nu)}.$$

Thus the constitutive relations between stress and strain, Eqs. (2.19), (2.20), (2.21), can be written using index notation as

$$\sigma_{ij} = \lambda' (\varepsilon_{11} + \varepsilon_{22}) \delta_{ij} + 2\mu \varepsilon_{ij} + \sigma_0 \delta_{ij}, \qquad (3.28)$$

where

$$\sigma_0 = -\frac{\gamma}{(1-\nu)} \frac{\rho - \rho_0}{\rho_0},$$
(3.29)

and the relations related strain to displacement are given by Eqs .(2.22) or (3.3). In this work, the first order linear FEM on a triangular mesh is utilized. The linear triangular in reference coordinates (ξ , η) on which the integral of the weak form is performed are :

$$0 \le \xi \le 1,$$

$$0 \le \eta \le 1 - \xi,$$
 (3.30)

and the shape functions in this coordinate system are given by:

$$\varphi_{1}(\xi,\eta) = -\xi - \eta + 1,$$

 $\varphi_{2}(\xi,\eta) = \xi,$

 $\varphi_{3}(\xi,\eta) = \eta.$
(3.31)

These shape functions provide a linear transformation that transform the triangle in the domain (3.30) into a triangle ω_e with vertices $(x_k, y_k), k = 1, 2, 3$ in the material domain, which is given by

$$x = \sum_{k} x_{k} \varphi_{k}(\xi, \eta),$$

$$y = \sum_{k} y_{k} \varphi_{k}(\xi, \eta),$$
(3.32)

and an approximation of the displacements u and v by their nodal values, which are

unknown

$$u = \sum_{k} u_k \varphi_k(\xi, \eta),$$

$$v = \sum_{k} v_k \varphi_k(\xi, \eta).$$
(3.33)

The weak form of Eq. (3.28) can be obtained by multiplying the PDEs with weight functions and integrating them over the computational domain, \mathcal{B} . Using Galerkin's approach, these six independent 2D weight functions are chosen to be the shape functions in Eq. (3.31)

$$\begin{pmatrix} \varphi_1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \varphi_1 \end{pmatrix}, \begin{pmatrix} \varphi_2 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \varphi_2 \end{pmatrix}, \begin{pmatrix} 0 \\ \varphi_2 \end{pmatrix}, \begin{pmatrix} \varphi_3 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \varphi_3 \end{pmatrix}$$
(3.34)

The integral over each finite element ω_e is transformed into the integral over the local triangle (3.30) using (3.32) with the Jacobian of the transformation (3.32) given by

$$J(\xi,\eta) = \begin{vmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} \end{vmatrix}.$$

The FEM mesh used throughout these numerical simulations contains around N = 1e5 nodes. The thermal problem has one degree of freedom, dof = 1, which is the temperature per each node while the stress problem has two, dof = 2, which are u and v. Thus the total number of unknowns in each problem are of the order 1e5 and 2e5, which is a relatively large number compared to the capacity of a typical personal computer. Thus it is desirable to parallelize the code and ScaLAPACK library is used for that purpose. The global stiffness matrix G is assembled and stored in cyclic order by multiple processors operating in parallel. When an element is removed from the computational domain because its maximum principle stress reaches the threshold value, G is updated by the

processors that are involved in the element. Due to the piecewise shape functions, each node is only connected to its nearest neighbor, thus *G* is a banded matrix whose bandwidth depends on the node numbering technique. The system of linear algebraic equations is solved at each time step by the parallel LU factorization function of ScaLAPACK [119] while some steps, such as calculating the principle stresses for all elements, remain serial. ScaLAPACK is also called to write output to files in synchronous order.

3.3 Temperature and density fields

In Sections 3.3 and 3.4, the numerical simulations on the rectangular domain $L \times H = 5cm \times 2cm$ will be presented for one set of parameter values. The material properties used herein are in the characteristic range for a generic charring, rubber-like material. Representative values for the properties of such materials can be found in Refs. [120], [121] and [122]. The following numerical values are used for the thermal, pyrolysis and elastic parameters:

$$\lambda = 4.0 \times 10^{-7} \quad m^2 s^{-1}$$

$$q_0/k_y = 6.0 \times 10^5 \quad K/m$$

$$\rho_c/\rho_0 = 0.3$$

$$T_a = 9375 \quad K$$

$$A = e^{31.25} \quad s^{-1}$$

$$\nu = 0.45$$

$$\gamma = 1/3$$

$$T_0 = 300K$$

$$\sigma_c/E = 1/30.$$
(3.35)

All numerical results presented in this theis are produced by the FEM with linear

triangular mesh and mesh size h_e of approximately 0.01 *cm*. The temperature field is specified by the unsteady heat conduction Eq. (2.10) along with the initial and boundary conditions given by Eqs. (2.25), (2.26), (2.27), (2.28), (2.29), (2.30). For both problems, the time step is chosen to be 1 second, however the results are only written to output files at each certain time interval because of the limited storage ability. Here they are written out in every 50 *s*.

In this model, the heat flux condition (2.30) is applied from t = 0 through the whole simulation, which means the heat flux is continuously supplied and time independent. Moreover, there is no cooling mechanism such as convection or radiation carrying heat away from the surfaces, thus the temperature keeps rising with time until reaching equilibrium or steady state. The temperature attains its highest value at the center of the heat flux location. This can be seen from a sequence of temperature plots at 50, 1000, 6000 *s* in Fig. 3.2. The sample lower surface is insulated, $\frac{\partial T}{\partial y} = 0$, Eq. (2.27), so the temperature contour is vertically tangent to this surface. The two lateral sides are maintained at the initial temperature T_0 , Eq. (2.25). This is the lowest temperature value in the domain.

The distribution θ along the vertical middle line of the sample at t = 100, 1000, 2000, 3000, 4000, 5000, 6000 s can be seen from Fig. 3.3.

Initially, the mass loss rate is zero or negligibly small due to low temperature, thus the density is uniformly at its original value. After that, the sample pyrolyzes, beginning at the upper surface. A density of 99.95% of the original value is considered as the onset of pyrolysis. This happens at $t = 18 \ s$. The sample density always has its lowest value at the location of the highest temperature, the center of the heated region. The first char value is attained there, at approximately 116 *s*, see Fig. 3.4 (a). Before the lower insulated surface starts pyrolyzing at 4500 *s*, the char layer region grows radially because the heat flux is localized. The char region avoids the two cold walls because the low temperature



Figure 3.2: The dimensionless temperature $\theta = (T - T_0)/T_0$ at t = 50, 1000, 6000 *s* from top to bottom figures. The left and right sides are cold walls while lower wall is insulated. The sample is heated at the upper surface by a heat flux confined to the center region over the length l = 0.1L

in those regions produces a negligible mass loss rate in the Arrhenius Eq. (2.2).



Figure 3.3: The distribution of the dimensionless temperature θ along the vertical middle line of the sample where $\overline{x} = 0.5$ at different times as indicated in the legend, in which $\overline{x} = x/L$ and $\overline{y} = y/L$

The location furthest from the center of the heat flux that has char density $\overline{\rho} = 0.3$ is called the char front and the location where pyrolysis has not yet started that is closest to that center is termed the pyrolysis front. These fronts are curves in this 2D problem and can be seen from Fig. 3.5. Furthermore, the density gradient is appreciable only in a narrow region that separates the charred from the uncharred regions, or between the two fronts. Over this small distance, δ , the dimensionless density $\overline{\rho}$, defined as $\overline{\rho} = \rho/\rho_0$, drops from the uncharred value $\overline{\rho} = 1.0$ to charred value $\overline{\rho} = 0.3$ (dark blue color to white color in Fig. 3.5). In calculation, the value $\overline{\rho} = 0.99$ instead of $\overline{\rho} = 1.0$ is taken for tracking the pyrolysis front because of practical purpose. The magnitude of the density gradient may be approximated by $(\rho_0 - \rho_c)/\delta$, where δ assumes different values at different locations during the heating and pyrolyzing process.

The evolution of $\overline{\rho}$ and δ at the mid-vertical line of the sample is plotted in Fig. 3.6, where time *t* is rescaled with the characteristic heat conduction time, $t_{hc} = H^2/\alpha_y$. A more systematic justification for choosing this value will be given in Section 6. For the parameters used in this simulation, $t_{hc} = 1000 \ s$. At $t/t_{hc} = 2$, the char front is still far



Figure 3.4: Plots of $\overline{\rho}$ from left to right, top to bottom of the figure corresponds to t = 100, 300, 1000, 1500, 2000, 3000, 4500, 6000 *s*, respectively. The char region grows radially from the center of the heated region. Close to t=6000 s, char region reaches the insulated lower surface but avoids the cold side walls.



Figure 3.5: Char front and pyrolysis front are indicated by curved arcs. Their separation δ at one location is indicated by the \leftrightarrow .

from lower surface. Up to this time, the curve δ vs. t/t_{hc} is fitted well by the square root function $t^{1/2}$ so the density gradient decreases as $t^{-1/2}$. An analytical derivation of this result for a one dimensional pyrolysis model is presented in [11].



Figure 3.6: (a) The dimensionless density $\overline{\rho} = \rho/\rho_0$ at the mid-vertical line ($\overline{x} = 0.5$, where $\overline{x} = x/L$) at different times. It decreases from uncharred ($\overline{\rho} = 1.0$) to the char value ($\overline{\rho} = 0.3$) over the distance δ between the charred and uncharred regions. (b) The evolution of the locations that define $\rho = 0.3, 0.5, 1.0$ and δ . The δ vs. time curve fits well to a square root function.

Under the simplifying assumption that the sample shall never crack, one may calculate the upper limit σ_m that the maximum principle stress will attain over the course of any specified heating time. σ_m varies with parameter values except the cracking threshold σ_c . For the set of parameters used in this simulation, this limit value is $\sigma_m = 0.18666E$; when $\sigma_c > \sigma_m$, no cracks will form in the sample from heating. When $\sigma_c < \sigma_m$ and the sample fractures in response to the accessible maximum principle stress criterion, the sample material is depleted by the sequential removal of elements from the computational domain. As a direct consequence of the removal of elements, the stress field is correspondingly modified. It is generally concentrated (enhanced) near the crack tip (damaged element). Prior to cracking, the stress field in this case is qualitatively simple to understand. Fig. 3.7 shows the maximum principle stress σ_1 at t = 150, 1000, 3000 s when the sample does not crack. It can be seen that the location of high maximum principle stress, σ_1 , correlates with the location of the high density gradient. Furthermore, the maximum value of σ_1 decreases from the time 150 s to the end of the simulation.



Figure 3.7: Maximum principle stress σ_1 at times t = 150,1000,3000,5500 s when the sample tensile strength σ_c is higher than σ_m . In such a case the sample does not develop cracks.

3.4 General behavior of crack evolution and morphology

The previous section discussed the evolution of the temperature, density and stress fields without cracks for one set of parameters given by Eq. (3.35) except σ_c , in which the condition $\sigma_c > \sigma_m$ is the relevant assumption. In this section, the same density field is used for shrinkage strain in the stress problem but cracks are now allowed to develop by using value of σ_c that is smaller than σ_m as in Eq. (3.35). The general behavior for the evolution and morphology of the cracks will be discussed here. Fig. 3.8 shows the distribution of the maximum principle stress σ_1 and the evolution of cracks up to *t*=6000 *s* at several times as indicated in the figure.

Based on the evolution of temperature, density and crack morphology, the process can be divided into five stages. These stages are: (a) inert heating (b) pyrolysis, not charred and, first crack initiation, (c) slightly charred, initiation dominant, (d) half charred and fast propagation, (e) almost fully charred, decelerated propagation. In the first stage (a), the sample temperature rises but is too small to produce an appreciable mass flux of volatiles. This is the same as the first stage of [11]. The evidence for this stage is based on values of the surface density for which $\bar{\rho} = 0.9995$ which is attained at t = 18 s. The first



Figure 3.8: Maximum principle stress σ_1 . Plots from left to right, top to bottom correspond to *t*=75, 300, 1000, 1500, 2000, 3000, 4500, 6000 *s*, respectively. At the end of the second stage, *t*=75 *s*, the first crack initiates.

stage then is taken to evolve from t = 0 to t=18 s. The temperature distribution at t=18 s is seen in Fig. 3.9. Following this stage is stage (b), pyrolysis begins but the sample density is still well above the char value. The cracking threshold has not yet been attained by the maximum principle stress due to low density gradient. The density gradient eventually attains a sufficiently high magnitude for the first crack to nucleate at t=75 s, which marks the end of stage (b). At this time, the lowest density value is $\overline{\rho} = 0.8345$.

The third stage (c) is characterized by a density whose gradient decays as $t^{-1/2}$ and continues toward the next stage, as mentioned in the previous section. Cracks initiate from the heated surface and propagate radially outward. The density first attains the char value $\bar{\rho} = 0.3$ when $t = 116 \ s$, see Fig. 3.10. Eventually, initiation activity is dimin-



Figure 3.9: θ at the end of the first stage t = 18 s when $\overline{\rho} = 0.995$ at the middle of the heated region on the upper surface.

ished and replaced by crack elongation and branching, which indicates transition to the next stage (d). At the end of stage (d) the density at the lower surface also attains the char value. Crack initiation is no longer observed and the existing cracks propagate at a slower pace. These cracks now intersect each other, forming loops and network-like patterns. The specific times for each stage are the following: (a) from 0 *s* to 18 *s*, (b) from 19 *s* to 75 *s*, (c) from 76 *s* to 116 *s*, (d) from 117 *s* to about 4500 *s*, (e) from about 4500 *s* onward.



Figure 3.10: $\overline{\rho}$ at the end of the third stage t = 116 s when the upper surface starts charring.

Away from the two cold walls, the density gradient attains maximum magnitude during the stage (b) and then gradually decrease in strength over time as the char front moves from surface into the sample interior and δ grows. This is due largely to the diffusive nature of heat conduction. The maximum principle stress attained in the material also decreases, which explains why initiation happens first at the surface and then moves into the sample along with the region of high density gradient. Fig. 3.11 shows an example of this behavior. Later in the process, density gradient magnitude decreases and this reduces the maximum attainable principal stress, whereby few new cracks are able to form.



Figure 3.11: Maximum principle stress σ_1 at 300 *s* and 1000 *s*. Initiation sites indicated in the plots are at the sample interior where the local density gradient concentrates. Initiation activity stops at approximately 400 *s*.

The overall trend of propagation is directional, following the char front from the surface to the unburned region. Cracks develop radially and perpendicular to, and move in advance of, the char front. It is known that cracks advances in the direction obeying the principle of energy minimization and in the direction of maximum tangential stress [123]. The correlation between crack propagation and the density field is seen more easily by plotting the crack distribution over the density field, see Fig. 3.12. Here it is recalled that in this model, the evolution of density and temperature are not affected by the presence of cracks.

It can be seen from the plots for early times that the crack pattern exhibits a hierarchical behavior such that long and short branches alternate with each other during this stage.



Figure 3.12: Plots of $\overline{\rho}$ in sample along with cracking pattern at t= 75, 300, 1000, 1500, 2000, 3000, 4500, 6000 s. Cracking initiates at 75 s. At t = 100 s, cracks have already developed while the upper surface has not been charred yet. The pyrolysis front, followed by the char front, is always behind the longest cracks. At a later time, around 4500 s, the lower surface starts to pyrolyze; crack spacing in the middle region near the lower surface gets larger. This is also the location where δ is large and the density gradient is small. Cracks advance in directions that are perpendicular to the pyrolysis front.

This elegant pattern is similar to the distinctive periodic doubling pattern recognized in quenching and cold shock experiments by [67] in rectangular or in [126] circular sample. This hierarchy is more apparent in stage (c) or the early of stage (d) partly because the cracks have not yet intersected with each other (as they do in late stage (d)), as seen in Fig. 3.13. Unlike cracking arrays in quenched plates which initiate at the same time and form the periodic doubling patterns by closing every other crack, the cracks in this simulation can initiate at different times and most continue to propagate through the end of the simulation unless they intersect with one another.



Figure 3.13: The hierarchical structure of the crack pattern. The maximum principle stress field σ_1 at 3000 *s*. The long (indicated by $l \rightarrow$) and the short (s \rightarrow) branches alternate each other.

For most of the time, the maximum principal stress σ_1 at crack tip is larger than the critical cracking value σ_c , thus crack tips will actively propagate. Crack initiation, which happens during stage (c) and in early stage (d) is less favored than crack propagation. As a consequence, cracks usually comprise many well developed branches instead of short and isolated fissures.

Earlier cracks modify the stress field around newly emerged cracks and vice versa. From the sequences of crack images, it is observed that when one crack propagates, the crack in its neighborhood ceases moving temporarily during which time the tensile stresses around its tip increase before it once again continues in its forward motion. This may be described as a mutual unloading behavior, with the cracks relieving total energy in the vicinity of their neighboring cracks in an alternating, periodic manner. This explains also why these cracks propagate in a discrete rather than in a continuous manner.

After the initiation and propagation period, at the end of stage (d), the shorter branches eventually join the longer ones which already have curved ahead. The joining of two branches forms a loop which is an isolated fragment. Furthermore, these loops have shapes of polygons that are elongated toward the uncharred region. Analysis of the loop pattern is provided in chapter 4. Cracks tend to intersect the existing cracks or a free surface at a right angle. This tendency is explained by using the principle of maximum stress release and crack propagation, as proposed by Lachenbruch (1962) [127]. In contrast to crack intersection that joins two cracks is the process of crack branching, which occurs either by kinking (a sharp turn that can raise the stress) or bifurcation (splitting of the crack tips). For examples of junctions, see Fig. 3.14, in which three intersections at right angles are marked by the letter T in red. Moreover, in Fig. 3.15 for the crack pattern at 700 *s*, one crack tip is just about to split. At 1200 *s*, it becomes two active branches. The triple junction angles formed by three segments: one "mother" crack and its two "children" branches, deviates from $(120^o, 120^o, 120^o)$. This fact reflects the anisotropic nature of the driving field. Fig. 3.16 show examples of the nucleation at the kink of a child crack. These types of junctions are discussed in a study about junction formation in desiccation cracking [55].



Figure 3.14: Maximum principle stress σ_1 at 6000 *s*. Two crack intersections at right angle are marked by the letter T in red.

It is worthwide to note that while the temperature field (Fig. 3.2), density field (Fig. 3.4) and stress field without cracks (Fig. 3.7) are symmetric about the mid vertical line $\bar{x} = 0.5$, the crack patterns and thus stress fields with cracks (Fig. 3.8) are not. The breaking of symmetry is caused by unsymmetry of the triangular mesh when elements are removed. However, the crack patterns on the left and right parts of the sample are statistically similar. This issue is discussed a little further in the appendix, section C. Moreover, it can be seen from the appendix section D, that further refinement of mesh does not lead to statis-



Figure 3.15: Maximum principle stress σ_1 at 700 *s* and 1200 *s*. The crack tip indicated starts splitting at t = 700 s. At 1200 *s*, it has split into two branches.

tically different crack patterns. Thus the current mesh used is sufficiently fine to resolve details of crack evolution.

In summary, the crack pattern evolves through different characteristic stages of crack formation and propagation, these being stages (c), (d) and (e) of the overall process. In addition, each stage is characterized by a dominant physical mechanism. In particular, the crack patterns are generated through the action of two competing mechanisms of crack evolution, namely branching and joining. In the broader context of physically induced pattern formation, the former (branching) characterizes the development of a hierarchical network, which is typically caused by the transport of macroscopic quantities, such as water, or cell fluids in a water-channel system, leaf veins, blood veins, or tree branches, electrical flux, thermal energy, etc. The latter (joining) generates a network due to the coalescence of branches and is typically governed by a principle of energy minimization, as found in mud cracks, glazes, etc. Whereas the first mechanism is directional and drives the crack pattern in the early stages of these simulations, the other is isotropic and dominant in the later stages. In this work, the "veins" and pathways for the first mechanism


Figure 3.16: Maximum principle stress σ_1 at 3800, 4000, 4500 *s*. Junctions formed either by the nucleation of a child crack or by kinking are indicated with red arrows.

(branching) are created by the stress field in conjunction with the application of the maximum principle stress criterion in the material and are not, as in the processes mentioned above, pre-arranged either biologically or materially.

CHAPTER 4

MORPHOLOGICAL ANALYSIS AND QUANTIFICATION OF CRACK MORPHOLOGY

A variety of methods has been used for detecting cracks, such as methods of optical or ultrasonic, imaging. The macro crack image can be captured by a camera whereas electrical resistance tomography (ERT) and scanning electron microscopy (SEM) are used for micro size cracks. Imaging is usually followed by image analysis for further quantification. In this chapter, some fundamental concepts of mathematical morphology and image analysis related to analyzing cracking patterns are presented, followed by their applications to the patterns that are generated in this study.

In the FEM triangular mesh, when the averaged principal stress of an element exceeds a threshold value, the element is removed from the computational domain. This change is permanent. The history of the removal process is stored in a crack pattern variable Cby assigning the value of the variable at the removed element location equal to the time step at which it was removed. From this variable, the crack pattern at each time step is constructed. In particular, extracting the crack pattern at time $t = t_c$ from C requires searching all locations at which C attains values less than t_c . The set of these points forms the crack pattern at t_c . This way of storing also facilitates keeping track of crack orders, which can be used for assigning segment ranks (as discussed later).

Analysis of the crack patterns is performed on a rectangular grid of pixels $N_x \times N_y$, in which N_x is the number of pixels in the horizontal direction and N_y is in the vertical direction. Since the FEM mesh is triangular, it needs to be mapped onto the rectangular mesh. Let the integer N denote the ratio of dimensions between the rectangular mesh used for image analysis and the triangular FEM mesh. The centroid of each triangular element is calculated. When N equals unity, the pairs of centroid coordinates are rounded off to the nearest rectangular mesh grid points. In general, N > 1 and the centroid coordinates are rounded off.

nates are multiplied by *N* and then rounded off to the *N* nearest rectangular grid points. There are different types of pixel grids, usually four point or eight point connectivity matrix. In this work, the latter is used. Eight point connectivity considers that any local node is represented by a pair of integers $(i, j), 1 < i < N_x, 1 < j < N_y$ that is surrounded by eight neighbor nodes: (i + 1, j), (i - 1, j), (i, j + 1), (i, j - 1), (i + 1, j + 1), (i + 1, j - 1), (i - 1, j + 1), (i - 1, j - 1).

Morphological functions work on binary images which have only 0 (background) and 1 (foreground or object) pixels. If the cracking pattern is obtained from a colored picture, the image will be thresholded to a gray scale and then to a black and white image. Al-though not used directly in this work, there are some primary morphological functions (level 0) used to construct functions of higher levels in image analysis. Examples of such primary functions are the functions *erode*, *dilate*, *open*, *close* in which *dilate* adds surrounding pixels to object pixels and *erode* is the dilation of the background. The function *open* is *erode* followed by *dilate* while *close* is *dilate* followed by *erode*. These functions are centered by a structuring element which is a matrix containing 0 and 1 with a location indicating the pixel which it acts upon. These functions, along with the next higher level ones, can be found as built-in functions in MATLAB.

The first morphological function used in this work is *bwmorph.m* of *MATLAB* which belongs to level 1. After transforming from the triangular mesh to the rectangular mesh, the crack pattern is thinned to a one pixel thickness by *bwmorph.m* with the option "skeletonized." Besides "skeletonized", *bwmorph.m* makes other options available, such as finding branching points, ending points, leaving the outline of a shape, removing isolated pixels, thickening an image, ...etc. Nevertheless, for this work there is still a need for constructing additional functions which are considered at level 2.

4.1 Some image analysis concepts and algorithms

Assuming the crack pattern has a single pixel thickness, there are important concepts in quantifying our crack morphology that need to be defined. For any pixel in the black and white skeletonized image, the eight point connectivity matrix provides information about the total number of surrounding points and their positions relative to the point being considered. To eliminate the orientation dependence of the connectivity matrix on the coordinate system, the angular instead of the eight point connectivity matrix is used. Some auxiliary concepts required for this definition. The pixel rectangular grid is set of all pixels (i, j) in which $1 < i < N_x$, $1 < j < N_y$ with origin O, i = 1, j = 1. The horizontal axis vector \vec{Ox} points from left to right. Any two pixels specify a vector in which the counterclockwise directional angle α it makes with \vec{Ox} satisfies $0^o \leq \alpha \leq 360^o$. (Two directional angles have equal values if their difference divides as a multiple of 360°). The subscript O_x implies that vector \vec{Ox} forms one side of the angle. For each pixel (i, j), the set of all *n* vectors in which the vector heads are neighbors of (i, j) in the connectivity matrix and vector tail at the pixel considered is $(\vec{v_1}, \vec{v_2}, ..., \vec{v_n})$. This set divides the plane into *n* regions. The *n* vectors are arranged in ascending order, meaning $\alpha_{Ox}^1 < \alpha_{Ox}^2 < ... < \alpha_{Ox}^n$. The set of *n* angles formed by *n* vectors: $\alpha = \alpha_1, \alpha_2, ..., \alpha_{n-1}, \alpha_n$, satisfying the condition

$$\alpha_{j} = \alpha_{Ox}^{j+1} - \alpha_{Ox}^{j} i f j \neq n, \alpha_{n} = 360^{o} - \sum_{i=1}^{n-1} \alpha_{i},$$
(4.1)

is called the angular connectivity matrix.

As an example, consider the (foreground) pixel (i, j) in which its eight point connectivity matrix has two other (foreground) pixels (i, j + 1) and (i + 1, j + 1). In this case, n = 2and two vectors $\vec{v_1} = (0, 1)$, $\vec{v_2} = (1, 1)$ centered at (i,j) are formed, their two directional angles with Ox being $\alpha_{Ox}^1 = 90^\circ$ and $\alpha_{Ox}^2 = 45^\circ$. In ascending order, $\alpha_{Ox}'^1 = 45^\circ$ and $\alpha_{Ox}'^2 = 90^\circ$. Thus α at (i, j) is $(45^\circ, 315^\circ)$ according to Eq. (4.1). In general, since any pixel can have up to eight neighboring pixels in an eight point connectivity matrix, there is the possibility that α has eight elements, each being multiple of 45°. However, in a skeletonized image, this would not happen. Depending on the relative arrangement between pixels in skeletonized image, one pixel can be either: an end point, a junction between three or more segments or a middle point of a crack segment.

Knowing the relative position of any pixel in a skeletonized image pattern, the crack path from any crack tip or branch point to the nearest branch point or another tip can be stored in a variable by marking the coordinates of all the pixels lying on the path in a sequential order. This is termed a crack segment. A segment is an isolated crack if it connects two crack tips (end points). We will show later that this can also be found by using *bwboundaries MATLAB* function. A level 2 function is written to find crack segments in any network like pattern, not limited to the ones generated in this study. The algorithm for finding crack segments is presented below:

a) Find the set \mathcal{P} of all endpoints and junctions in a skeletonized image

b) For each point in \mathcal{P} , find the untraveled path to other nearest endpoint or junction, in a way a pencil traverses through all pixels without being lifted from the paper. Record this path as one segment. Mark the path as "traversed".

c) Repeat b) until there is no remaining untraveled path.

To aid in visualization, each segment is colored randomly by assigning *R*, *G*, *B* random values that vary between 0 and 225 to creat a random (*RGB*) triplet for each segment. The segment length can also be estimated. There are different methods of estimation. The simplest one approximates the total number of pixels in each segment to its length, regardless of the relative arrangement of the pixels. More precisely, the relative position between pixels, meaning the way pixels arrange in a segment should affect segment length. As shown in Fig. 4.1 a factor of $\sqrt{2}$ is used to correct the distance between two pixels indicated by the \longleftrightarrow .



Figure 4.1: Segment length illustration showing the need for the factor $\sqrt{2}$ for pixels joined at edges.

The angle formed by segments joining at a junction is also an important feature of network like image. There are various ways to calculate the angles formed at junctions. One way is to place a circle of small radius of order several pixels that centers at the junction and to find its intersections with crack segments as shown in Fig. 4.2. The angles of the arches centered at the junction and separated by the intersections will be the angles formed by segments. The other method for which a schematic picture is Fig. 4.3 used in this work provides more accurate values.



Figure 4.2: One method for finding the junction angle by using intersection points of the crack pattern with a circle.

The algorithm of the method sketched out by Fig. 4.3 is the following:

- a) At each junction, trace all of its surrounding segments.
- b) In each segment, for each pixel within vicinity r_s of the junction, calculate the angles



Figure 4.3: The same pixel pattern as Fig. 4.2 with a different method for finding the junction angles which average angles over different pixels.

made by Ox and the vector connecting it with the junction, α_{Ox}

c) For each segment, average over the angles calculated in step b).

d) Repeat step b) and c) for all segments sharing the junction.

e) Obtain all averaged angles of all of the segments made with the horizontal axis, sort in ascending order then convert them to angles formed between segments, similar to Eq. (4.1).

This algorithm is similar but not equivalent to calculating the angular connectivity matrix at the junction point, in which the eight point connectivity matrix is replaced by a circle of radius r_s . Because besides calculating the angle, this task requires keeping track of which segment a pixel belongs to. Since each segment can be tracked and its length can be calculated, the crack pattern now can be "thresholded" by trimming short branches. The trimmed crack pattern has only long branches remaining. This practice is helpful in some cases such as when calculating crack spacing between well defined crack segments. For patterns found in nature, such as the vein leaf or the polygonal mud or lava cracks, it is found that, initially the junctions occur right angles. Later, as the patterns evolve, the right angle junctions are relaxed into 120° junctions, [36], [90].

Fig. 4.4 is the skeletonized crack pattern at 6000 *s* in which each segment is colored and the total number of pixel comprising its length is displayed in random colors. In Fig. 4.4,

the same crack pattern is "cleaned up" by removing child branches which are less than a threshold value (two values eleven and five pixels are used to show the influence of the threshold value.



Figure 4.4: Skeletonized crack pattern at 6000 *s*. Each segment is colored randomly. The numbers placed in the middle of each segment represent the segment total number of pixels.



Figure 4.5: The same as Fig. 4.4 except that short branches less than five (left) and eleven (right) pixels are removed.

The number of loops, or their total area, is an important quantity that characterizes the damage degree of the materials. In image processing, there is an algorithms for labeling connected regions, named "grassfire" or "wave propagation" principle, based on the rule that a "swept out" or "burn away" pixel is never to be visited again, see Mathematical Morphology [200]. To identify loop in the crack pattern image, first of all, the MATLAB



Figure 4.6: Zoomed in section of Fig. 4.4 shows the values of the angles at each junction.

function *bwboundaries* (level 1) is called to identify loops and isolated cracks along with their exterior boundaries. Then another function is called to differentiate between a loop and an isolated crack. Its algorithm is the following:

(a) Pick a random point in the interior boundary of the object which might be either a loop (a region comprising of pixels 1) or an isolated crack (a segment comprising of pixels 1) as discussed above.

(b) Determine whether the random point is in contact with any background pixel (0 pixel). (c) If (b) is true, mark the object as not loop, exit. Otherwise, repeat (a) and (b) as long as no more than five random points have been tested. If more than five random points have been tested, mark the object as a loop then exit.

The total area in pixels of a looped or an isolated region is calculated by counting the total number of pixels that fill up the region after calling the MATLAB function *imfill* (level 1). In Fig. 4.7, each isolated crack branch is labeled as one region and colored in red. The boundaries of the closed regions are marked in blue and each branching crack (child) is marked in the cyan color. Child cracks start from a junction point of its mother crack as a result of bifurcation (splitting) or kinking, as mentioned in Section 3.4. In terms of image analysis, a child crack is a segment that connects an end point and the nearest junction pixel. In Fig. 4.8, the same crack pattern with Fig. 4.7 is plotted, in which the numbers

displayed at the centroid of each loop indicate the loop areas rescaled by the total sample area.



Figure 4.7: Skeletonized crack pattern at 6000 *s*. Numbers displayed at the lower right corner are total isolated branches, loops, child branches respectively.



Figure 4.8: Crack pattern with loops at 6000 *s* from Fig. 4.7. The area of each loop region is rescaled by the domain area and its value is displayed at the loop centroid.

Another morphological of importance in this study is the crack spacing. There are theoretical studies of crack spacing and penetration depth of shrinking slabs using the principle of energy minimization, [39], [40], which can explain the periodic doubling in system of parallel cracks. In [117], the spacing of thermal shock cracking arrays is used to inversely estimate the convective heat transfer coefficient. Crack spacing is interpreted differently depending on the morphologies of the patterns. For example, for the system of parallel cracks, like cracks in quenched sample, crack spacing is measured by finding the intersections of cracks with a straight line perpendicular to them. For an isotropic cracking network, such as a mud crack, or columnar cracks, the lines placed on the crack pattern must have random directions and the final result must be averaged over several different lines. In this study, in the case of a localized heat flux (small ratio of *l* to *L*), cracks propagate essentially radially. Thus it is natural to measure crack spacing at depth r_c using an arc of radius r_c placed in the crack pattern. The average arc angle $\overline{\gamma}$ across $r = r_c$ is taken as the arc angle divided by number of the arc intervals.

As an example, consider the third plot from the top, on the left, of Fig. 4.10 for the detailed steps of determining the average crack spacing at r = 0.5H. First, the skeletonized image of the crack pattern is "cleaned up" by removing all branches shorter than five pixels. Intersection points of the cracks with an arc radius $r_c = 0.5H$ are found by comparing two sets of branching points: (set A) is the set of branching points of the crack pattern alone, (set B) is the set of the branching points of the union of the crack pattern and the arc. Set B is found by the dilation then skeletonization of the union image. Because of the pixelated nature of the image, clustered spurious intersection points can be generated as shown in Fig. 4.9. Intersection pixels that are within a certain distance are reduced to one representative point. Here a four pixel distance is used as the criterion for grouping.

This results in total thirteen intersections points N = 13 as indicated in red numbers of Fig. 4.10 (bottom left), and their positions are all identified. However, for the current purpose of calculating average crack spacing, only the positions of the first and last points are needed. In particular, in this case, the locations of the 1st point is $(x_1, y_1) = (322, 63)$ and of the 13th one is $(x_N, y_N) = (678, 67)$. The location of arc center is $(x_c, y_c) = (500, 1)$. The arc angle γ is calculated from the following trigonometric relation



Figure 4.9: Spurious intersection points are grouped together.

$$\gamma = \arctan((x_c - x_1)/r_c) + \arctan((x_N - x_c)/r_c), \tag{4.2}$$

which yields $\gamma = 1.4573(rad)$. The average crack spacing is obtained by dividing the arch angle γ by the number of arc segments N - 1. The results here is 0.1214 *rad* or 21.85 °.

4.2 Morphological characterization of network-like patterns

Fracture patterns belong to a broader geometrical class, the network pattern, such as those of dendrite, Lichternberg tree, leaf veins, insect and bird nests, glaze, streams, rivers, streets, Internet, tree branches, mud cracks, soil cracks, etc. The study their morphologies can reveal the underlying physical and biological rules that generate these various patterns. They also have applications in pattern classification such as biological taxonomy. The available literature contains morphological studies based on topoplogical grapth theory, [48], such as the studies of river networks, [41], [42] and [43], bone structure [50], insect nests [49] and ant networks [47], [46].

The network patterns are included in a broader phenonmena, known as the Li patterns, such as water crystal, striation mark on animal shell, retiform cells of insect wings, ar-



Figure 4.10: Intersections of the "cleaned up" skeletonized crack pattern at 6000 *s* with an arc of radius $r_c/H=0.0317$, 0.1583, 0.2375, 0.3167, 0.4750, 0.6333, 0.7917, 0.9500, from left to right, top to bottom, respectively. Red numbers indicate intersection points.

rangement of cabbage leaves in section, Irish moss seaweed, reptilian skin formations, cloud like formations, spiral defects, angulated form in eroded shale ... The study of patterns found in nature and their dynamics, known as the Li pattern study, has been in existence from ancient time in Chinese philosophy. As quoted from George Steiner, (Life-lines) [201]:

"There is a haunting if deceptive modernity in the notion, so often celebrated by baroque poets and thinkers, that arteries and the branches of tree, the dancing motion of the microcosm and the solemn measures of the spheres, the marking on the back of the tortoise and the veined patterns on rocks, are all ciphers." Today, the morphological study of the patterns and their driven forces as well as the underlying mechanisms becomes increasing popular. The crack patterns in this study share both characteristics of the tree-like (leaf vein, Lichternberg, tree, fractal) and interconnected loop-like (street, neurite) patterns. The first type is directional and tends to form in systems with transportation such as that of fluid, nutrients, heat flux, electrical flux. The second type is isotropic, usually formed on a surface and follow directly the principal of energy minimization, [52], [51], [47]. They can be characterized using criterion such as crack rank [53], spacing, length, junction angle, number of sides/vertexes for each loop domain, loop domain direction, fractal numbers [54], etc. According to [54], the evolution of a physical or biological pattern often obeys the rule of local length mini-mization. Furthermore, in nature, the rank of cracks can be based on crack width because older cracks tend to be wider than newer ones.

The image analysis algorithm presented in this section can be applied to any pattern in general with necessary pre-treatment to enhance the contrast between background materials and cracks before converting them to black and white image. Some algorithms for calculating fractal (self similarity) quantities using image analysis will be outlined. The programming implementation on the algorithms has not been done in this thesis, but can be extended for future work. From [54], fractal lacunarity, the parameter characterizing the heterogeneity of a fractal image, is an important quantity that is discussed in this section. Assume an image of *M* total pixels is overlaid by boxes of size *L* (pixels). The number of boxes size *L* that are needed to cover the entire image N(L) is

$$N(L) = \sum_{m=1}^{K} \left(\frac{M}{m}\right) P(m,L), \qquad (4.3)$$

in which P(m, L) is the possibility that the box size L contains m pixels and K is the maximum number of image points that fall inside the box. For each pixel in the image, center it with a box of size L, then count the number of image pixels (pixel 1) that fall within the box, namely Φ . Then, building a histogram of Φ in the following way: P(m, L) is equal to

the number of times that Φ attains the value *m*, divided by total number of pixels centered by boxes which is also the total number of boxes considered. The variable log(N)/log(L)is defined as the fractal dimension, characterizing the space filling nature of the pattern. After obtaining the histogram of Φ , the fractal lacunarity parameter is given by

$$C(L) = \frac{\langle m^2 \rangle - \langle m \rangle^2}{\langle m \rangle^2},$$
(4.4)

which is the variance of the random variable Φ , where $\langle \rangle$ is the averaging operator, and $\langle m \rangle$ and $\langle m^2 \rangle$ are the average values of Φ and Φ^2 , in particular

$$< m > = \sum_{m=1}^{K} mP(m, L),$$
 (4.5)

and

$$< m^2 > = \sum_{m=1}^{K} m^2 P(m, L).$$
 (4.6)

Loops in a crack pattern are identified and quantified in term of their area and their total number in the previous section. In this section, more properties of loops as polygons will be discussed. Reference [129] presents the algorithm for finding number of vertices of a polygon which can be summarized as the following:

a) For each domain, specify its boundary.

b) Form a sequence of vectors with the same length in which the head of the next vector is the tail of the previous vector.

c) Calculate the angles formed by these vectors found in (b). The local maxima of these angles define the vertexes of the domain.

This parameter is useful for the quantification of patterns having many loop regions, such as mud cracks or glazes on ceramic. Fig. 4.11 is an illustration of the algorithm above, in which the arrows indicates the movement from one pixel to the next.



Figure 4.11: Schematic algorithm for finding vertex of a polygon. Each pair of arrows corresponds to a location of maximum angle change, which indicate vertexes.

Futhermore, each loop or isolated domain can be characterized by the following shape factors:

a) Area to perimeter squared ratio (circularity),

b) Aspect ratio (ratio of Feret's minimum length to maximum length),

c) Convexity (ratio between convex hull perimeter to actual perimeter),

d) Solidity (ratio between area of convex hull to the domain area),

e) Principal directions (eigenvectors), eigenvalues.

For example, following [129], the domain principal directions can be also based on the eigenvalues and eigenvectors of moment of inertia tensor *I* given by:

$$I = \begin{pmatrix} I_{xx} & I_{xy} \\ I_{xy} & I_{yy} \end{pmatrix},$$
(4.7)

in which:

$$I_{xx} = \iint_{\Omega} (x - x_c)^2 dx dy,$$

$$I_{yy} = \iint_{\Omega} (y - y_c)^2 dx dy,$$

$$I_{xy} = \iint_{\Omega} (y - y_c) (x - x_c) dx dy,$$

(4.8)

where (x_c, y_c) is the centroid of Ω . By using the summation rule of integration, Eq. (4.8)_{*a*},

in discrete form reads

$$I_{xx} = \sum_{i=1}^{N} (x_i - x_c)^2,$$

$$I_{yy} = \sum_{i=1}^{N} (y_i - y_c)^2,$$

$$I_{xy} = \sum_{i=1}^{N} (x_i - x_c)(y_i - y_c)^2,$$

Here *N* is the total number of pixels in the domain and (x_i, y_i) is the pixel's coordinate, $i = \overline{1, N}$. Moreover, the centroid is taken as: $x_c = \sum_{i=1}^{N} x_i/N$ and $y_c = \sum_{i=1}^{N} y_i/N$, which is coordinate averaging. The principal moments of inertia are eigenvalues of the inertia tensor, which are

$$I_1 = \frac{I_{xx} + I_{yy}}{2} + \sqrt{\frac{I_{xx} - I_{yy}^2}{2} + I_{xy}^2},$$
(4.9)

and

$$I_2 = \frac{I_{xx} + I_{yy}}{2} - \sqrt{\frac{I_{xx} - I_{yy}^2}{2} + I_{xy}^2}.$$
(4.10)

The corresponding principle direction θ_p satisfies the condition

$$\tan(2\theta_p) = \frac{2I_{xy}}{I_{xx} - I_{yy}}.$$
(4.11)

The ratio of largest to smallest eigenvalues is defined as the aspect ratio which characterizes the domain elongation. The shape factor based on the area ratio between the true object and the least circumscribed circle centered on the object center of gravity is used as a criterion to distinguishing voids from micro cracks, see [130]. Another way of identifying a region direction is presented in [138], in which an ellipse is fitted into the isolated region. The major and minor axes of the ellipse indicate region directions. Fig. 4.13 shows a loop that is inscribed by an ellipse.



Figure 4.12: Crack pattern with loops at 6000 *s* from Fig. 4.7. At the centroid of each loop region, there are two arrows indicating its inertial principle directions. Arrow lengths are rescaled by its principle moment of inertia: the ratio of two arrow lengths is the shape factor.



Figure 4.13: Inscribe a loop with an ellipse, as shown.

According to the theory of orientational ordering, the domain order parameter can be specified as

$$S_1 = \frac{\langle \cos^2(\theta) \rangle d - 1}{d - 1},\tag{4.12}$$

in which θ is the direction of the loop domains in a chosen coordinate system, *d* (equals two for 2D) is the spatial dimension and $\langle \rangle$ is the averaging operator. Loop like patterns can be quantified using other methods such as Fourier analysis. In this method, the crack density in one direction is calculated by summing all pixels (zero for background, one for

an image) in the other direction. Then this one dimensional density is transformed into a Fourier series.

The crack orientation and isotropy can also be characterized by the intersection counting method or oriented secant method, following [130]. A set of parallel equidistant lines titled at an angle θ with the Ox axis is placed into the crack pattern. The number of intersection points between the crack pattern and the lines $N_L(\theta)$ is a function of the angle θ as it varies between 0° and 180°. The degree of orientation ω is given as

$$\omega = \frac{N_{Lmax} - N_{Lmin}}{N_{Lmax} + \left(\frac{\pi}{2} - 1\right)},\tag{4.13}$$

thus satisfying $0 \le \omega \le 1$, where N_{Lmax} and N_{Lmin} are the maximum and minimum values of the function $N_L(\theta)$. If the crack pattern is isotropic, then $N_{Lmax} = N_{Lmin}$, whereby $\omega = 0$. If all cracks have the same direction, $N_{Lmin} = 0$, leaving $\omega = 1$.

In materials with randomly distributed cracks, the degree of damage can be characterized by the crack density. [139] derives the formulas for crack density from the damage variable which can be either scalar or tensorial. Reference [136] calculates this parameter from fracture energy and the J-integral for solid materials that may or may not have stress interaction with fluid. The results of [136] can be used for a system of randomly distributed slit cracks or abitrary convex shaped cracks. For the former type of cracks, crack density is found to be given by

$$d_c = \frac{8M < l >^2}{\pi^3},\tag{4.14}$$

where $\langle l \rangle$ is the mean crack length, $M = L_A/l$, $L_A = \pi N_L/2$ is the total crack length per unit area, and N_L is the number of cracks per unit length of the sample. For the latter one, it is equal to the average volume of micro voids per unit substance volume, which is

$$\epsilon = N < r_a^3 >, \tag{4.15}$$

where *N* is the number micro cracks per unit volume and r_a is the void radius. Reference [140] calculates the changes of material properties such as Young's modulus, shear modulus and Poisson's ratio for annealed and heavily cold-worked metals as a function of the crack density.

Related to crack density, crack width is another characteristic of cracking patterns often considered in examining concrete and soft substance on a substrate. Crack width has been found to be dependent on substrate friction [141], sample thickness [56], [142], material components and loading conditions. From the results of numerical simulations, the crack width can be constructed from the displacement field. In experimental practice, it can be taken as the ratio between crack area and its length in the skeletonized image.

In topological geometry, an interconnected pattern can be characterized by the Minkowski numbers. Reference [143] uses three Minkowski numbers to quantify the crack morphology in a drying soil, namely, M_0 , M_1 , M_2 , in which M_0 is the crack surface area, M_1 is the total crack length and M_2 is the Euler number. In image analysis practice, the M_0 value in pixel squared units is equivalent to the total number of black pixel before skeletonization. M_1 is the line integral along the crack path:

$$M_1 = \int_L ds, \tag{4.16}$$

which yields the crack length. As discussed in the previous section, Section 4.2, when neglecting the relative arrangement of pixels in a crack path, the line element *ds* equals one pixel. Therefore M_1 can be taken as the total number of black pixels in the image after skeletonizing. Otherwise, *ds* should be corrected by a $\sqrt{2}$ factor in the discrete form of the integral using summation rule. The last number is defined as:

$$M_2 = \int_L \frac{ds}{r} \tag{4.17}$$

where *r* is the radius of curvature along the crack path. Evaluating the above integral on a boundary gives 2π for a closed convex boundary (corresponding to an object) and

 -2π for a closed concave boundary (a loop or hole). Therefore M_2 equals the number of objects minus the number of loops and is used as a topological number that describes connectivity.

4.3 Quantification of crack morphology

In this section, the cracking patterns corresponding to one set of parameters that are produced in Section 3.4 are quantified using the image analysis algorithm presented in the previous sections. The morphology of the cracking pattern changes as time progresses through the five evolution stages as outlined earlier: (a) inert heating, not pyrolysis; (b) pyrolysis, crack initiation, not charred; (c) partially charred, mainly initiation, (d) crack elongation and fast propagation; (e) almost totally charred, slow propagation to stop. Among these stages, crack morphology is well defined in late stage (d) and early stage (e) and has little change as the simulation proceeds.

From a sequence of maximum principle stress plots, it can be seen that at the late stage (d), cracks formed previously are actively propagating and splitting and nucleation has not yet diminished. When each event, as propagation, splitting or nucleation happens, the number of cracks, crack tips and junctions changes. In elongation, the number of each kind remains the same. With initiation, one new crack is formed along with two crack tips. One of the tip remains inactive while the other propagates into the charring domain, forming a longer crack segment.

A junction, the common point between three crack segments, can be formed via different mechanisms. One is bifurcation, the splitting of one mother crack into two child cracks thereby turning the mother crack tip into a junction. Hence each type increases by one in number. A junction is also formed when a child crack springs off from its mother crack, usually at a kink point at which stresses are raised by the sharp turn. Another event that creates a new junction is crack intersection, the so called T-junction, because it occurs at a right angle. One intersection trades one tip for one junction, decreasing the total number

of crack tips while increasing the total number of junction by one for each.

In a skeletonized crack image, the end point and junction pixels are identified and counted at each time step, for example at 6000 *s* as seen in Fig. 4.14. The evolution of their total numbers are shown in Fig. 4.15. From the figure, it can be seen that, at the initiation stage (the third stage), the number of total crack tips (cross) increases at a faster rate compared with total junctions (dot) due to newly created cracks. Thus the difference between total number of crack tips and junctions increases at the third stage. It then remains constant during the evolution and propagation stages (the third and early fourth stages) because elongation activity predominates. After that, at the slow propagation and loop stage (late fourth and fifth stages), the difference decreases due to prevailing intersection.



Figure 4.14: Skeletonized crack pattern at 6000 *s*. Crack tips are marked by the letter e in blue and junctions are marked by the letter b in red. When one crack intersects another, its tip is replaced by an intersection point.

The statistics of segment length and junction angles are calculated for the well developed crack pattern of Section 3.4. 6000 *s* is chosen because at this time crack pattern has already evolved through all stages. The algorithms for calculating segment length and junction angle are discussed in the previous Section 4.1. They are applied for the whole frame, calculating the length of each segment and angles of each junction. Fig. 4.16 shows the probability distribution of segment length which is rescaled by the length of heated region *l*. As seen from the figure, the shorter segments have higher frequency of occurrence and



Figure 4.15: The evolution of total number of crack junctions, crack tips as well as their difference. The difference trends are increasing, remaining constant and decreasing from the third stage to the final stage.

vice versa. The PDF of the segment length show exponential decaying behavior which is a characteristic of fractal or self-similarity, see [131], [133], [134]. Moreover, in a numerical study of tectonic rupture [132], the distribution and fractal parameters of fracture length are determined by different phases and mechanisms of the faulting process, such as nucleation, growth and coalescence.



Figure 4.16: Probability distribution function of segment length corresponding to crack pattern at 6000 *s* in Fig. 4.4.

The probability distribution of the junction angles corresponding to the crack pattern at 6000 *s* is shown by Fig. 4.17. The junction angle has mean value $\mu_{\alpha} = 119.6803^{\circ}$ with standard deviation $\sigma_{\alpha} = 40.2904^{\circ}$. The slight deviation of μ_{α} from 120° implies that most of the junctions are triple. The angle of highest frequency is around this mean value (Y-junction) and the one of the second peak is in proximity to 90° (T-junction).



Figure 4.17: Probability distribution of junction angles corresponding to crack pattern at 6000s in Fig. 4.4

Some of very short segments are not true cracks, but are results from the process of thinning the image. Therefore the statistics of "cleaned up" crack pattern is also performed and compared to those of the original pattern above. Fig. 4.18 and 4.19 shows the distribution of segment length and junction angle corresponding to the thresholded crack pattern at 6000s in which segments of less than five pixels are removed. The density of the shorter segments decrease as a direct consequence of the trimming process.

In Fig. 4.20, the average crack spacing $\overline{\gamma}$ of the crack pattern in Section 3.4 at 6000 *s* as a function of crack depth r_c is plotted, in which r_c is normalized by the length of heated surface *l*. From the figure, it can be seen that the overall trend is a decrease in spacing except for $r_c > 3.5l$. On the other hand, crack intersection increases the spacing between



Figure 4.18: Probability distribution function of segment length corresponding to Fig. 4.5 when branches are thresholded.



Figure 4.19: Probability distribution of junction angles corresponding to Fig. 4.5 when branches are thresholded.

branches, resulting in local "jumps" of the curve. Closer to $r_c/l = 1$, crack spacing decreases exponentially due to branching and nucleation. From $r_c/l = 1$ to $r_c/l = 3.5$, crack spacing remains constant due to an apparent balance between branching and intersection . After that, branching diminishes and the average crack spacing grows.

As mentioned in Section 3.4, crack spacing correlates with the density gradient. In particular, close to the insulated lower surface where δ is large, the density gradient is small,



Figure 4.20: The average crack spacing as a function of normalized depth radius r_c/l when the crack pattern at 6000 *s* is thresholded using five pixels.

and the cracks are spaced more widely apart. The reverse applies to the other regions that are away from the lower surface. This echoes a finding of [38] made in a study of columnar cracks formed by temperature gradients in rocks. It is seen that the overall trend of the crack pattern is a decrease in spacing until $r_c > 3.5l$. In this figure, note that with intersection, the spacing still remains quite constant due to a balance between branching and intersection. Fewer branches can grow into the region $r_c > 3.5l$. Accordingly, the branching diminishes and the crack spacing grows.

CHAPTER 5

DIMENSIONLESS GROUPS AND MATERIAL PROPERTIES

5.1 Scaling Analysis

The purpose of this chapter is to find the dimensionless groups that could characterize the scaling of the plane stress initial boundary value problem in Section 2.2 and 2.3. The variables and their units in the problem are summarized in the table 5.1 below.

From the table, it can be seen that the heat conduction- pyrolysis- elasticity problem contains sixteen constants, in which the Poisson's ratio ν and the mass loss coefficient γ are dimensionless and the other fourteen have units composed from four basic units. Of these other fourteen, q_0 and k_y only appears as a ratio and so this leaves thirteen constants with units: $L, H, \alpha_x, \alpha_y, T_0, \frac{q_0}{k_y}, l, \rho_c, A, T_a, \rho_0, E, \sigma_c$. The four basic units can be taken as either length/ time/ temperature/ energy or length/ time/ temperature/ mass. By using the Buckingham Pi theorem, the thirteen preceding dimensional constants combine to form nine dimensionless Pi groups.

Materials could be divided into thermally thin or thermally thick depending on the ratio of heat penetration depth that is a function of heat flux, thermal diffusivity and material thickness. The heat penetration depth can be defined in terms of characteristic length for heat flux: $l_f = k_y T_0/q_0$. Thermally thick sample has the ratio l_f/H or $k_y T_0/(Hq_0)$ be a small value and vice versa, the value is large for thermally thin sample. For both thermally thin and thermally thick case, the ignition time, has been derived analytically in [144], which shows dependence on heat flux, thermal diffusivity, initial and ignition temperature. According to [144], when neglecting radiation heat loss, for thermally thick, the ignition time grows as q_0^{-2} while for thermally thin, it grows like q_0^{-1} .

The choice of the characteristic time of heat conduction as used in Section 3.3 is first more formally justified. For this purpose regard such a time t_{hc} as still to be determined.

Material constants		units 2D in terms of energy	units 2D in terms of mass	Equation of first appearance
L H	domain length domain width	length length	length length	
α_{x}	thermal diffusivity in x direction	length ² time	<u>length²</u> time	(2.10)
αy	thermal diffusivity in y direction	$\frac{length^2}{time}$	$\frac{length^2}{time}$	(2.10)
k _y	thermal conductivity	energy time×temperature	mass×length ² time ³ ×temperature	(2.29)
T_0 q_0 l ρ_c A T_a ρ_0 E ν γ σ_c	in y direction initial temperature heat flux parameter length of heated region limiting solid density pre exponent factor activation temperature initial solid density Young's modulus Poisson's ratio mass loss coefficient tensile strength	$temperature$ $energy$ $time \times length$ $length$ $length^4$ $time^{-1}$ $temperature$ $energy \times time^2$ $length^4$ $energy$ $length^4$ $energy$ $length^2$ $-$ $-$ $energy$ $length^2$	temperature $\frac{mass \times length}{time^3}$ length $\frac{mass}{length^2}$ time ⁻¹ temperature $\frac{mass}{length^2}$ $\frac{mass}{time^2}$	 (2.25) (2.30) (2.30) (2.2) (2.2) (2.2) (2.2) (2.12) (2.12) (2.12) (2.9)
Field variables		units in terms of energy	units in terms of mass	Equation of first appearance
Т	solid temperature	temperature	temperature	(2.10)
ρ	solid density	$\frac{energy \times time^2}{length^4}$	<u>mass</u> length ²	(2.2)
ε	strain tensor	_	_	(2.12)
σ	stress tensor	energy Tenoth2	<u>mass</u> time2	(2.12)
u	displacement	length	length	
V	displacement in the vertical direction	length	length	

Table 5.1: Variables and their units of the problem in Section 2.2 with initial and boundary conditions specified 2.3.

In addition, let $\tau = t/t_{hc}$, $\zeta = x/H$, $\eta = y/H$ (thus $0 < \zeta < L/H$, $0 < \eta < 1$) and $\theta = (T - T_0)/T_0$.

The dimensionless form of the energy equation Eq. (2.10) is

$$\frac{\partial\theta}{\partial\tau} = \frac{t_{hc}\alpha_y}{H^2} \left(\frac{\alpha_x}{\alpha_y} \frac{\partial^2\theta}{\partial\zeta^2} + \frac{\partial^2\theta}{\partial\eta^2} \right), \tag{5.1}$$

thus the time scale t_{hc} which characterizes Eq. (2.10) that naturally emerges is

$$t_{hc} = H^2 / \alpha_y, \tag{5.2}$$

whereupon Eq. (5.1) becomes

$$\frac{\partial\theta}{\partial\tau} = \left(\frac{\alpha_x}{\alpha_y}\frac{\partial^2\theta}{\partial\zeta^2} + \frac{\partial^2\theta}{\partial\eta^2}\right).$$
(5.3)

Note that t_{hc} as given by Eq. (5.2) coincides with that used in Section 3.3. The heat flux q_0 can also be used to characterize the heat flux time t_{flux} by using Eq. (2.29), (2.30). In particular, the dimensionless form of Eq. (2.29) using Eq. (2.30) is

$$\frac{\partial\theta}{\partial\eta} = \frac{q_0 H}{k_y T_0} \tag{5.4}$$

From Eq. (5.2), $H = \frac{t_{hc} \alpha_y}{H}$ and substituting this into Eq. (5.5) yields

$$\frac{\partial\theta}{\partial\eta} = \frac{q_0 t_{hc} \alpha_y}{H k_y T_0}.$$
(5.5)

which can be interpreted as the ratio of two characteristic times, one of them is t_{hc} and the other, using Eq. (2.30), can be defined as

$$t_{flux} = \frac{Hk_y T_0}{q_0 \alpha_y},\tag{5.6}$$

thus (5.5) becomes $\frac{\partial \theta}{\partial \eta} = \frac{t_{hc}}{t_{flux}}$ and t_{flux} defined by (5.6) characterizes the relation of thermal boundary condition (2.29) to the heat conduction equation Eq. (2.10). From Eq. (2.2), let $\overline{\rho} = \rho / \rho_0$, thus

$$\frac{\partial\overline{\rho}}{\partial\tau} = -t_{hc}A(\overline{\rho} - \overline{\rho_c})e^{-T_a/(T_0(\theta+1))},$$
(5.7)

which is equivalent to

$$\frac{\partial \overline{\rho}}{\partial \tau} = -t_{hc} A e^{-T_a/T_0} (\overline{\rho} - \overline{\rho_c}) e^{\frac{T_a}{T_0} \frac{\theta}{\theta + 1}}, \qquad (5.8)$$

thus the chemical reaction time scale that characterizes the pyrolysis reaction as described by Eq. (2.2) could be taken as: $t_{chem} = [Aexp(-T_a/T_0)]^{-1}$ and (5.9) becomes

$$\frac{\partial\overline{\rho}}{\partial\tau} = -\frac{t_{hc}}{t_{flux}}(\overline{\rho} - \overline{\rho_c})e^{\frac{T_a}{T_0}\frac{\theta}{\theta+1}},\tag{5.9}$$

Two Pi groups can be chosen as the length ratios, $\Pi_1 = H/L$ and $\Pi_2 = l/L$, which characterize the problem geometry. The third Pi group $\Pi_3 = \alpha_y/\alpha_x$ characterizes the anisotropy of the heat conduction problem, it can also be viewed as being derived from the dimensionless Eq. (5.3). Two other groups are chosen as the ratio of the two characteristic times: Π_4 equals t_{hc}/t_{flux} , or $q_0H/(k_yT_0)$ and Π_6 equals t_{hc}/t_{chem} or $H^2Ae^{\frac{-T_a}{T_0}}/\alpha_y$. Π_4 is also equal to l_f/H which can be used to distinguished thermally thick from thermally thin problem as mentioned above. The fifth group is chosen as the ratio of two temperatures $\Pi_5 = T_a/T_0$, along with Π_6 , relating the thermal and the pyrolysis processes. The seventh group is defined as the ratio of two densities $\Pi_7 = \rho_c/\rho_0$, defining the extent of pyrolysis.

The last two groups must contain Young's modulus *E* and tensile strength σ_c as they have not appeared in the seven groups from Π_1 to Π_7 yet. Both of the two parameters have the same unit *energy/length*². Let group Π_8 have *E*, thus Π_8 must also include one of the other parameters which have *energy* in their units, more specifically k_y , q_0 , ρ_c , ρ_0 . The same argument follows if one chooses *mass* instead of *energy* as the basic unit. Since Young's modulus is associated with stress (force per unit area) and density is an inertial term, their grouping is more reasonable. The ratio E/ρ_0 has unit $time^2/length^2$ which is relevant to some characteristic velocity. There are different ways to chose Π_8 that is a combination of E/ρ_0 , upon consideration that the pyrolysis problem provides direct input for the stress problem, Π_8 is chosen as $E/(\rho_0 (AH)^2)$.

Since both *E* and σ_c have the same unit, it is natural to let $\Pi_9 = \sigma_c/E$, the ratio of the cracking stress to the elastic modulus, as the final dimensionless group. Π_9 is a crack resistance parameter, when it is sufficiently large, no crack is able to form. The field of fracture mechanics often separates two distinct process, crack initiation and crack propagation. The theory of thermo elasticity suggests that materials having high tensile strength, thermal diffusivity, low Young's modulus and undergo slow thermal expansion [135] during heating can have better crack resistance. During cooling, most materials contract, or shrink, just as the pyrolyzing solid in this study contracts when it loses mass. Thus, the thermal contraction coefficient in cooling is analogous to the current mass loss coefficient because both serve as coefficients of the shrinkage stress.

Our problem, which is characterized by nine Pi groups, will employ characteristic units from the parameters H, t_{hc} , T_0 and ρ_0 (length, time, mass and temperature). From Eq. (5.3), Eq. (2.10) can be written as:

$$\partial\theta/\partial\tau = \left(\Pi_3\partial^2\theta/\partial\zeta^2 + \partial^2\theta/\partial\eta^2\right)$$
 (5.10)

The initial condition for the dimensionless temperature θ is $\theta = 0$, which is also the boundary condition at the two lateral sides, $\zeta = 0, L/H$. The boundary condition for θ on the insulated side ($\eta = 0$) is: $\partial \theta / \partial \eta = 0$, and on the heated side ($\eta = 1$), Eq. (2.29) and Eq. (2.30) give

/

$$\frac{\partial \theta}{\partial \eta} = \begin{cases} 0 & \text{if } |\zeta - \frac{1}{2\Pi_1}| > \frac{\Pi_2}{2\Pi_1} \\ \Pi_4 & \text{if } |\zeta - \frac{1}{2\Pi_1}| \le \frac{\Pi_2}{2\Pi_1}. \end{cases}$$
(5.11)

The pyrolysis equation Eq. (2.2) or (5.9) becomes

$$\partial \overline{\rho} / \partial \tau = -(\overline{\rho} - \Pi_7) \frac{1}{\Pi_6} e^{\Pi_5 \left(\frac{\theta}{1+\theta}\right)}.$$
(5.12)

Finally, the stresses are non-dimensionlized with respect to Young's modulus E using

$$E = (\Pi_8 / \Pi_6^2) \exp(2\Pi_5) [\rho_0 H^2 / t_{hc}^2],$$

viz. $\overline{\sigma_{xx}} = \sigma_{xx}/E, \overline{\sigma_{yy}} = \sigma_{yy}/E, \overline{\sigma_{xy}} = \sigma_{xy}/E, \overline{\sigma_{zz}} = \sigma_{zz}/E, \overline{\sigma_p} = \sigma_p/E$, where σ_p is the relevant principal stress.

When convective or radiative heat cooling is included in the model via the heat flux term in Eq. (2.29), there exists another temperature T_m which is the maximum temperature obtained since the incoming heat flux is balanced by heat loss terms. Then the Arrhenius equation could be rescaled in the following way, using different dimensionless temperature $\theta = (T - T_0)/(T_m - T_0)$ which varies between 0 and 1, Eq. (2.2) is rewritten as:

$$\frac{\partial \overline{\rho}}{\partial \tau} = (\overline{\rho} - \overline{\rho_c}) A t_0 e^{-\frac{T_a}{T_0}} e^{-T_a \left(\frac{1}{T} - \frac{1}{T_0}\right)}.$$
(5.13)

Consider the term $e^{-\frac{T_a}{T}}$ which can be rewritten as

$$e^{-\frac{T_{a}}{T}} = e^{-\frac{T_{a}}{T_{m}}} e^{-\left(\frac{T_{a}}{T} - \frac{T_{a}}{T_{m}}\right)}$$

= $e^{-\frac{T_{a}}{T_{m}}} e^{-T_{a}\left(\frac{T_{m} - T}{T_{m}T}\right)}$
= $e^{-\frac{T_{a}}{T_{m}}} e^{-\frac{T_{a}}{T_{m}}} \left(\frac{T_{m} - (T_{m} - T_{0})\theta - T_{0}}{T_{0} + (T_{m} - T_{0})\theta + T_{m} - T_{m}}\right)$
= $e^{-\frac{T_{a}}{T_{m}}} e^{-\frac{T_{a}}{T_{m}}} (T_{m} - T_{0}) \left(\frac{1 - \theta}{T_{m} - (T_{m} - T_{0})(1 - \theta)}\right)$
= $e^{-\frac{T_{a}}{T_{m}}} e^{-\frac{T_{a}}{T_{m}^{2}}} (T_{m} - T_{0}) \left(\frac{1 - \theta}{1 - \sigma(1 - \theta)}\right).$

in which the following dimensionless quantities are used: $\beta = \frac{T_a}{T_m^2}(T_m - T_0), \sigma = 1 - \frac{T_0}{T_m},$ $D^a = At_0 e^{-\frac{T_a}{T_m}}$, then the Arrhenius Eq. (2.2) written in dimensionless form is

$$\frac{\partial \overline{\rho}}{\partial \tau} = D^{a}(\overline{\rho} - \overline{\rho_{c}})exp\left(-\beta\left(\frac{1-\theta}{1-\sigma(1-\theta)}\right)\right),$$
(5.14)

as compared with (5.9).

Furthermore, in this problem, the stress balance is taken to be quasi steady, containing no inertia term. If inertial effect is taken into account, the stress balance in x direction with stress strain displacement relations following Equations (2.19), (2.19), (2.19) and (2.22) is:

$$\rho_0 \frac{\partial^2 u}{\partial t^2} = E\left(\frac{\partial^2 u}{\partial x^2} + s.t.s + \frac{\gamma}{1 - 2\nu} \frac{1}{\rho_0} \frac{\partial \rho}{\partial x}\right),\tag{5.15}$$

where *s.t.s* are some terms similar to $\frac{\partial^2 u}{\partial x^2}$, the second order spatial partial derivative of displacement, such as $\frac{\partial^2 u}{\partial y^2}$, $\frac{\partial^2 u}{\partial x \partial y}$, etc. The dimensionless form of (5.15) is

$$\frac{\partial^2 \overline{u}}{\partial \tau^2} = \frac{E t_{hc}^2}{\rho_0 H^2} \left(\frac{\partial^2 \overline{u}}{\partial \zeta^2} + s.t.s \right) + \frac{E t_{hc}^2}{\rho_0 H^2} \frac{\gamma}{1 - 2\nu} \frac{\partial \overline{\rho}}{\partial \zeta}.$$
(5.16)

where $\overline{u} = u/H$. Thus, in this case, Π_8 can be chosen as $\frac{Et_{hc}^2}{\rho_0 H^2}$ and another characteristic time that scales the wave propagation inside solid is taken as: $t_{wave} = \frac{\sqrt{\rho_0}H}{\sqrt{E}}$.

In summary, from this section, the eight dimensionless groups characterizing the thermalpyrolysis-mechanical problem are determined as the following

$$\Pi_{1} = \frac{H}{L}$$

$$\Pi_{2} = \frac{l}{L}$$

$$\Pi_{3} = \frac{\alpha_{y}}{\alpha_{x}}$$

$$\Pi_{4} = \frac{q_{0}H}{k_{y}T_{0}}$$

$$\Pi_{5} = \frac{T_{a}}{T_{0}}$$

$$\Pi_{6} = \frac{H^{2}Ae^{\frac{-T_{a}}{T_{0}}}}{\alpha_{y}}$$

$$\Pi_{7} = \frac{\rho_{c}}{\rho_{0}}$$

$$\Pi_{8} = \frac{E}{\rho_{0}(AH)^{2}}$$

$$\Pi_{9} = \frac{\sigma_{c}}{E}$$

$$(5.17)$$

5.2 Material Properties

This section will review the thermal and mechanical properties of four classes of important materials (cellulosic, thermoset, thermoplastic, XGnP) of special interest.

Cellulosic materials, which are studied extensively in literature, are important charring pyrolysis substance. Existing in nature, cellulose, along with other long chained natural polymers such hemicellulose, lignin, magnan, xylan, are found in wood. Since wood has long fiber arranged in a cylindrical structure, their thermal and mechanical properties of wood is orthotropic. The values of these quantities also vary depending on types of wood. The Youngs modulus *E* and Poissons ratio *v* of various kinds of wood species, taking into account its orthotropy, could be found in table 4.1 and 4.2 of [22] respectively. It is not uncommon to find properties for wood to be tabulated as if the wood is isotropic. In cylindrical coordinate, let *z* the fiber direction, *r* the radial direction and θ the tangential direction. Among six Poissons ratio, $v_{r\theta}$ often has highest value and $v_{z\theta}$ has lowest value. Wood typically has low thermal conductivity (less than $1Wm^{-1}1K^{-1}$), which makes it a good choice for thermal insulation.

[156] considers cellulose pyrolyzing via one single step reaction or multiple one step chemical reactions (cellulose to C_2H_4 , CH_4 , C_2H_6 , C_3H_6 , CH_3OH , CH_3CHO , H_2O , CO, CO_2 , etc) via Eq. (5.18) and provides kinetics parameters for each reaction which are tabulated in table II of [156]. Table 4 of [167] provides kinetics parameters for Alcell and Kraft lignin at different temperature ranges. The lignin pyrolysis model in [169] is similar to the model in [156] for cellulose, in which lignin decomposes into CO, CH_4 , CO_2 , C_2H_4 , C_2H_6 , H_2O , HCHO, H_2O + HCHO, C_3H_6 and char. Other models including [168] accumulate all volatiles ith into a single volatile term.

$$\frac{dV_i}{dt} = (V^{*,i} - V_i)A_i e^{-\frac{E_{a,i}}{RT}},$$
(5.18)

where V_i is volume of gas species i th, $V^{*,i}$ is the available volume of gas species i th, A_i and $E_{a,i}$ are frequency or pre-exponent factor and activation energy of the reaction for creation of gas species i th. When all gas species terms are accumulated into a single gas term, the kinetics parameters are equal to those of Eq. (2.2) for solid decomposition. From [160], the activation energy for the devolatilization of cellulose, hemicellulose, liginin are 236 *kcal/mole*, 100 *kcal/mole*, 46 *kcal/mole* respectively. Table 5.2 below summaries the study of cellulosic properties found in the literature.

Cellulosic materials			
[161] <i>birch</i> 0.307 to 0.513			
[161] <i>birch</i> 0.335 to 0.537			
[161] <i>birch</i> 0.291 to 0.37			
[161] <i>birch</i> 0.177 to 0.25			
[170] pine wood $0.166 + 0.396X^*$			
[169] milled wood lignin 14% ρ_0 , [160] hard wood, char yield 14 – 23%, soft			
wood, char yield $20-26\%$			
[162] white oak 842.0, base wood 461.0, [170] pine wood 590-640			
[146] fir 2.1×10^8 , [155] cellulose 1.7×10^4 , [23] cellulose 1.2×10^6 , [146]			
firwood 2.1 $ imes$ 10 8 ,			
[149] cellulose 0.019-0.14, [151] beechsawdust ($T \leq 600K$), 0.0053, [151]			
$T \ge 600K$, 2.3×10^4 , [151] cellulose 6.79×10^3 , [151] cellulose 6.79×10^9 ,			
[152] cellulose 3.9×10^{11} , [170] cellulose 0.7×10^5 , [153] lignin 1.2×10^8 ,			
[153] hemicellulose 1.45×10^9 , [154] wood 10^8			
[171] cellulose 6.8×10^9 , [168] lignin $78.3(160K - 680K)$, $1.5(410K - 680K)$			
1680K), [169] <i>milled wood lignin</i> 5650 or 10 ^{5.53}			
$\label{eq:constraint} \ensuremath{\left[163\right]}\ensuremath{\textit{lignin}}\ 1.65 \times 10^4 (280K-344K), 0.0933 (344K-435K), \ensuremath{\left[164\right]}\ensuremath{\textit{lignin}}\ 1.65 \times 10^4 (280K-344K), 0.0933 (344K-435K), \ensuremath{\left[164\right]}\ lignin$			
7.16 × 10 ¹⁰ (280K – 300K), [165] periodate lignin –(260K – 375K)			
[166] Aspen wood lignin 4.43×10^6			
[150] cellulose, in nitrogen 6.06×10^9 , $n = 0.46$, cellulose, in steam $1.67 \times$			
10^9 , $n = 0.51$, [170] hemicellulose 2×10^{10}			

Table 5.2: Literature study of cellulosic material properties.
[172] Pinus pinaster wood, seven components, first component 4.2 × 10⁶, second component 1.2 × 10¹¹, [172] Pinus pinaster bark, seven components, first component 3.3 × 10⁴, second component 2.2 × 10¹², [172] Chestnut tree wood, eight components, first component 1.9 × 10¹⁰, second component 3.0 × 10¹⁵, [172] Cellulose-Whatman filter paper 6.8 × 10¹²
[173] almond shell 1.37 × 10⁶, hazenut shell 1.34 × 10⁶, beech wood 8.09 × 10¹⁰

 $\begin{array}{ll} E_{a}(\frac{kJ}{mol}) & [155] \ cellulose \ 79.4, \ [23] \ cellulose \ 100.5, \ [146] \ firwood \ 101 + 142X, \\ & [149] \ cellulose \ 8.8-33.4, \ [151] \ beechsawdust \ (T \ \leq \ 600K), 18, \ [151] \ (T \ \geq \ 600K), 84, \ [151] \ cellulose \ 71, \ [151] \ cellulose \ 139, \ [152] \ cellulose \ 166.4, \ [170] \\ & cellulose \ 146, \ [153] \ lignin \ 141.3, \ [153] \ hemicellulose \ 123.7, \ [154] \ wood \ 125.4 \\ & [171] \ cellulose \ 33.4, \ \ [168] \ lignin \ 25.08(160K - \ 680K), \ 30.54(410K - \ 1680K), \ [169] \ milled \ wood \ lignin \ 81.2 \\ & [163] \ lignin \ \ 86.52(280K - \ 344K), \ \ 37.08(344K - \ 435K), \ \ [164] \ lignin \ 164] \ lignin \ 164 \ lignin \ 164$

143.3(280K – 300K), [165] periodate lignin 35.9 – 75.7(260K – 375K)

[166] Aspen wood lignin 57.5 – 168.92, [160] lignin 46

[150] cellulose, in nitrogen 153.13, n = 0.46, cellulose, in steam 143.09, n = 0.51, [160] cellulose 236

[160] hemicellulose 100, [174] hemicellulose 110, [170] hemicellulose 83

[172] Pinus pinaster wood, seven components, first component 83, second component 146, [172] Pinus pinaster bark, seven components, first component 52, second component 159, [172] Chestnut tree wood, eight components, first component 117, second component 188, [172] Cellulose-Whatman filter paper 167

[173] almond shell 92.82, hazenut shell 92.36, beech wood 123 ~ 150

$$\begin{split} t_{chem} \left(\frac{1}{A}e^{\frac{E_{a}}{RT_{0}}}\right) & [155] \ cellulose \ 3.93 \times 10^{9}, [23] \ cellulose \ 1.59 \times 10^{12}, \\ & [149] \ cellulose \ 1792.7 - 4.67 \times 10^{6}, [151] \ beechsawdust \ (T \leq 600K), 2.56 \times 10^{5}, \ (T \geq 600K), 1.83 \times 10^{10} \\ & [151] \ cellulose \ 3.39 \times 10^{8}, 2.34 \times 10^{14}, [152] \ cellulose \ 2.41 \times 10^{17} \\ & [153] \ lignin \ 3.34 \times 10^{16}, [153] \ hemicellulose \ 2.38 \times 10^{12} \\ & [154] \ wood \ 6.837 \times 10^{13}, [171] \ cellulose \ 9.6 \times 10^{-5} \\ & [168] \ lignin \ 297.3, [164] \ lignin \ 1.24 \times 10^{14} \\ & [166] \ Aspen \ wood \ lignin \ 2320.5 \end{split}$$

Beside cellulosic, other important materials are rubber, thermoset, thermoplastics, XGnP and its composites. Rubber is composed of elastomers which are elastic and have cross linked chains. It can be derived from natural rubber tree or from crude oil. Thermoset and thermoplastics are two kinds of plastic substances in which the first type re-

mains forever in solid state once it is cured [175]. xGnP is a carbon derived nanomaterial that is newly developed which has excellent physical properties, such as low weight, high stiffness and tensile strength, very high thermal conductivity, [182], [184], [185]. xGnP nano platelets, when arranged horizontally in materials exposed to flame, can dissipate heat to the lateral sides and serve as gas and thermal barrier between the heat flux and unburned substance. Their materials properties are all listed in the following tables, 5.3, 5.4, 5.5, 5.6.

Properties	Rubber					
$\alpha(\frac{m^2}{s})$	[177] $\frac{k}{\rho_0 c_p} = 4 \times 10^{-8}$, Figure 7 of [176] conductive natural rubber (4)					
	HAF/NR) B2C 0 – 50% at 70°C 10 × 10^{-8} – 18×10^{-8}					
$k(\frac{J}{mKs})$	[177] 0.11, [179], Figure 7 of [176] conductive natural rubber (40 HAF/NR)					
	<i>B2C</i> 0 – 50% <i>at</i> 70° <i>C</i> 2.1-4.5, <i>CNT/SBRBR</i> 0.08-0.13					
$\rho_c(\frac{kg}{m^3})$	[178] 400.0					
$\rho_0(\frac{kg}{m^3})$	[177] 1200.0, [179] (SBR) 956.0, [179] (NBR) 935.0					
	[179] (IIR) 925.0 , (CR) 1275, (NR) 914.0					
$T_a(K)$						
$A(\frac{1}{s})$	[177] 2×10^9 , [180](<i>nitrile</i>) 10^{12} , [181] (<i>tyre</i>) 10^{10}					
	Fluoroelastomers $5.2 imes 10^{18}$					
$E_a(\frac{kJ}{mol})$	[177] 76					
	[180] (nitrile) 101.0, [180] (neoprene) 96.3, [180] (natural) 113.0					
	[180] (EPDM) 92.0, [180] (PVC/nitrile) 105.0					
	Fluoroelastomers 210.8					
$t_{chem} \left(\frac{1}{A} e^{\frac{E_a}{2RT_0}} \right)$	[177] 0.00206, [180] (nitrile) 0.000621, Fluoroelastomers 0.368					
$t_{chem} \left(\frac{1}{A} e^{\frac{E_a}{RT_0}} \right)$	[177] 8555.06, [180] (nitrile) 385742.3, Fluoroelastomers 7.07×10^{17}					
E(GPa)	ethylene propylene rubber 1.21, rubber 0.01					
	natural rubber 1.2					
$\sigma_c(MPa)$	[180] (nitrile) 16.0, [180] (neoprene) 17.8, [180] (PVC/nitrile) 14.6					
	natural rubber 14.2					
ν	[177] 0.49					

Table 5.3: Properties parameters of rubber.

 $c_{p}(\frac{J}{kgK})$ [177] 2200.0, [179], Figure 7 of [176] conductive natural rubber (40 $HAF/NR) B2C \ 0 - 50\% \ at \ 70^{\circ}C \ 15000 - 35000$ $\Pi_{9}(\sigma_{c}/E)$ natural rubber 0.0118 $\Pi_{3}(\alpha_{x}/\alpha_{y})$ 1.0 (rubber is isotropic) $\Pi_{7}(\rho_{c}/\rho_{0})$ [177] tire pyrolyzed in inert environment 33 - 38% $\Pi_{8}H^{2}\left(\frac{E}{\rho_{0}A^{2}}\right)$ 2.5 × 10⁻¹⁶ - 10⁻²¹ $t_{hc}H^{-2}(\alpha_{y}^{-1})$ [177] 25 × 10⁶ $t_{flux}\frac{q_{0}}{HT_{0}}(k_{y}/\alpha_{y})$ [177] 2.75 × 10⁶

Properties	xGnP
$\alpha_T \times 10^{-6} (\frac{m^2}{s})$	[182] 15-as made 2.75, 15-annealed 3.28, 15-annealed, cold pressed 1.59, 1-as
	made 1.1, 1-anneled 1.39, 1-annealed, cold pressed 0.71

 $\alpha_{||} \times 10^{-6} (\frac{m^2}{s}) \quad [182] \text{ 15-as made 188 , 15-annealed 204, 15-annealed, cold pressed 215, 1-as made 17.2, 1-anneled 20.2, 1-annealed, cold pressed 24.5}$

$$k_T(\frac{J}{mKs})$$
 [182] 15-as made 1.43, 15-annealed 1.331, 15-annealed, cold pressed 1.28,
1-as made 0.56, 1-anneled 0.7, 1-annealed, cold pressed 0.65

$$k_{||}(\frac{J}{mKs})$$
 [182] 15-as made 98, 15-annealed 107, 15-annealed, cold pressed 178, 1-as made 8.66, 1-anneled 10.5, 1-annealed, cold pressed 22.6

$$t_{flux} \frac{q_0}{HT_0} (k_T/\alpha_T)$$
15-as made 52 × 10⁴, 15-annealed 40.5 × 10⁴, 15-annealed, cold pressed
80.5 × 10⁴, 1-as made 50.9 × 10⁴, 1-anneled 50.35 × 10⁴, 1-annealed, cold pressed 91.5 × 10⁴

 $\rho_{c}(\frac{kg}{m^{3}}) \rho_{0}(\frac{kg}{m^{3}}) \qquad [182] 15\text{-as made 730, 15-annealed 730, 15-annealed, cold pressed 115, 1-as}$ made 710, 1-anneled 710, 1-annealed, cold pressed 1300 $c_{p}(\frac{J}{kgK}) \qquad [182] 710.0$

Table 5.4: Material values of xGnP.

Properties	xGnP composite		
E(GPa)	Figure 7 of [184] xGnP-1-PP nanocomposite 1.3 - 1.9, xGnP-15-PP		
	nanocomposite1.3-1.5, Figure 3 [185] xGnP/LLDPE nanocomposites 0.2-1.0		
	[186] monolayer graphene membrane 1000		
$\sigma_c(MPa)$	Figure 6 of [184] flexural strength <i>xGnP-1-PP nanocomposite</i> 40-51, <i>xGnP-</i>		
	15-PP nanocomposite 40-45, Figure 3 [185] xGnP/LLDPE nanocomposites		
	2-18		
	[186] monolayer graphene membrane 130000		
ν	[186] graphite in the basal plane 0.165		
$\Pi_9(\sigma_c/E)$	[184] xGnP-1-PP nanocomposite 0.0307-0.0268, xGnP-15-PP nanocomposite		
	0.0307-0.03, [185] xGnP/LLDPE nanocomposites 0.01-0.018		
	[186] monolayer graphene membrane 0.13		

Table 5.5: Material values of xGnP composites.

From the values of thermal conductivity, specific gravity and specific heat for different plastics in table 5.6, their thermal diffusivities are calculated, yielding relatively low values, which are of order $10^{-8} - 10^{-7}$. Below their glass transition temperature T_g , most plastics have tensile modulus of about 2*GPa* and tensile strength less than 35*MPa* at room temperature [187]. Thermosets and thermoplastics behaviors are different because of their different bond structures. Particularly, thermoplastics have both weak and strong bonds for which the weak ones break when the materials are heated while the strong ones are still remained. Thermosets have only strong bond which will break and the material decompose when subjected to high temperature. Thermoset materials have higher ratio of tensile strength σ_c vs tensile modulus *E* (in the range 0.01-0.03) when compared with thermoplastics ($10^{-4} - 3 \times 10^{-4}$).

Properties	Thermoset & Thermoplastics
α	from [187] polyurethane resin $4.927 \times 10^{-8} - 1.468 \times 10^{-7}$, urethane elas-
	tomer $2.94\times10^{-8}-1.60\times10^{-7}$, urethane rigid foam $6.69\times10^{-8}-1.53\times10^{-8}$
	$10^{-7}\text{, allyl resin } 6.18\times10^{-8}-7.02\times10^{-8}\text{, PMMA, commercial grade}$
	$1.153\times 10^{-7},~\text{PTFE}~8.52\times 10^{-8},~\text{Urea-fomaldehyde}$ alpha cellulose filler
	$1.13\times 10^{-7}-1.738\times 10^{-7}$, polypropylene 0.95×10^{-7} , polystyrene $1.11\times$
	10^{-7} , polymethyl methacrylate 1.18×10^{-7} , polyvinyl chloride 1.25×10^{-7} ,
	polyethylene terephthalate 1.43×10^{-7}
$k(\frac{J}{mKs})$	[188] uncured and cured thermoset polyesters 0.106-0.2092, polypropylene
	0.24
	[187] polyurethane resin 0.17-0.21, urethane elastomer 0.07-0.3, urethane
	rigid foam 0.06-0.12, allyl resin 0.199-0.21, PMMA, commercial grade 0.2,
	Urea-fomaldehyde alpha cellulose filler 0.285-0.409
	Table 5 of [187] selected plastics from 0.12 UP to 0.42 MF
$\rho_c(\frac{kg}{m^3})$	
$\rho_0(\frac{kg}{m^3})$	[189] benzoxazine epoxy copolymer 1200
111	[187] polyurethane resin 1100.0-1500.0, urethane elastomer 1100.0-1250.0,
	urethane rigid foam 560.0-640.0, allyl resin 1300-1400, PMMA, commercial
	grade 1180-1190, polyester resin 1100-1460, Urea-fomaldehyde alpha cellulose
	filler 1480-1500
$T_a(K)$	
$A(\frac{1}{s})$	[190] phenolic $4.48 imes 10^9$, nylon $1.85 imes 10^{13}$
	[171] Hydrogenated polystyrene 1.4×10^{14} , Poly-n-methylstyrene 7.2×10^{16} ,
	Poly- α -methylstyrene 8.3×10^{18}

Table 5.6: Material properties of thermosets and thermoplastics.

$$\begin{split} E_{a}(\frac{kJ}{mol}) & [190] \ phenolic 170.0, \ nylon 220.0 \\ & [171] \ Hydrogenated \ polystyrene \ 217, \ Poly-n-methylstyrene \ 246, \ Poly-a-methylstyrene \ 242 \\ &\sim 200 \\ t_{chem} \left(\frac{1}{A}e^{\frac{E_{d}}{RT_{0}}}\right) & [190] \ phenolic \ 8.9 \times 10^{19}, \ nylon \ 1.09 \times 10^{25}, \ [171] \ Hydrogenated \ polystyrene \\ 4.34 \times 10^{23}, \ Poly-n-methylstyrene \ 9.47 \times 10^{25}, \ Poly-a-methylstyrene \ 1.65 \times 10^{23} \\ &\sim 10^{20} \\ E(GPa) & [191] \ Acrylonitrile \ Butadiene \ Styrene \ 1.7-2.7, \ PBT \ 5-9, \ PA6 \ 5-9 \\ & [192] \ epoxy \ 2.0, \ composite \ epoxy \ graphene \ 3.1 \ at \ 300 \ K, \ epoxy \ 5.9, \ composite \ epoxy \ graphene \ 7.4 \ at \ 77 \ K, \ [193] \ 3.24 \\ & [189] \ benzoxazine \ epoxy \ 0 \ -50\% \ copolymer, \ flexural \ modulus \ 4.5-3.5 \\ & [187] \ glass \ fiber \ reinforce \ EP \ 175.0, \ alpha-cellulose \ filler, \ MF \ 9.0, \ PF \ 5.0-7.0, \ wood \ floor \ PF \ 6.0-8.0, \ glass \ fiber \ polyester \ 11.0-14.0 \\ & [194] \ Epoxy \ clay \ 0 \ -5\% \ nancomposite \ 2 \ -3, \ [195] \ glass \ fiber \ reinforced \ epoxy \ 3.2 \\ & Table \ 8 \ of \ [187] \ thermosets \ Phenolics \ 6.9-20.7, \ Unreinforced \ polyesters \ 2.83-3.45, \ Unreinforced \ epoxy \ 2.7-3.4, \ Reinforced \ polyesters \ 5.5-11.7 \\ & Table \ 8 \ of \ [187] \ thermosets \ Phenolics \ 6.9-20.7, \ Unreinforced \ polyesters \ 2.6, \ PSU \ 2.48, \ PPE \ 2.5, \ ABS \ 1.8-2.5, \ Nylon \ 6.26, \ Nylon \ 6/6, \ 159-3.79 \\ & Table \ 8 \ of \ [187] \ selected \ thermoplastics \ PEEK \ 1.1, \ Polycarbonate \ 2.3, \ PEI \ 3.0, \ PES \ 2.6, \ PSU \ 2.48, \ PPE \ 2.5, \ ABS \ 1.8-2.5, \ Nylon \ 6/2, \ Nylon \ 6/6, \ Nylon \ 6/6, \ Nylon \ 6/12, \ PC, \ PSU, \ PS, \ varying \ from \ 0.13 \ (pure \ Polypropylene, \ pure \ Nylon \ 6/6, \ Nylon \ 6/12, \ PC, \ PSU, \ PSV \ varying \ from \ 0.13 \ (pure \ Polypropylene, \ pure \ Nylon \ 6/6, \ Nylon \ 6/6$$

 $\sigma_{c}(MPa)$ [191] Acrylonitrile Butadiene Styrene 19.6-49.0, PBT 70-110, PA6 90-160, [189] benzoxazine epoxy 0 – 50% copolymer, flexural strength 125-165 [187] glass fiber reinforce EP 350.0, alpha-cellulose filler MF 50.0-90.0, PF 50.0-55.0, wood floor PF 45.0-60.0, glass fiber polyester 35.0-65.0, [194] Epoxy-clay 0 – 5%-nanocomposite 50 – 70, [195] glass fiber/epoxy at various strain rate 784.5-1198, [196] anhydride cured epoxy, the stress at brittle rupture 40.0

> Table 1 of [187] *LDPE* 10-12, *HDPE* 26-33, *LLDPE* 15-32, *PP or i-PP* 31-37, *TPX* 28, *PS or a-PS* 50, *s-PS* 41, *PMMA* 70, *PVC* 55, *PVF* 66-131, *PVDF* 48, *PCTFE* 30-39, *PTFE* 17-21, *PVOH* 83-152, *POM* 70, *PEO* 13-22, *nylon11* 38, *nylon12* 45, *nylon4/6* 100, *nylon6/6* 80, *nylon6/10* 55, *PC* 62, *PET* 72, *PBT* 52, *PEI* 105, *PAI* 152, *PI* 72-118, *PSU or PSF*, *PAS*, *PPS* 70, *PEK* 110 Table 8 of [187] thermosets *Aminos UF* 38-48, *Aminos MF* 48-55, *PUR* 24, *Unreinforced polyesters* 40-55, *Reinforced polyesters* 124-152, *Unreinforced epoxy* 42.7-82.7, *Unreinforced polyimide* 38.6

> Table 8 of [187] thermoplastics *Acetal* 60.7-68.9, *Polyamides* 80.7-94.5, *PEEK* 91.7, *Polycarbonate* 62-72.4, *PEI* 105, *PES* 84.1, *PSU* 70.3, *PPE* 53.8, *PPS* 65.5, *PPS* 40% glass 138, *PET* 62.1, *PET* 30% glass 150, *ABS* 32-45 Table 10 of [187] selected thermoplastics with glass filler 0 – 40%, including Styrene, SAN, ABS, PP, glass-coupled PP, PE, AC, Polyester, Nylon 6, Nylon 6/6, Nylon 6/12, PC, PSU, PPS at room temperature 32 (*Polypropylene*) to 214 (*Nylon* 6/6 40% glass fiber)

[196] anhydride cured epoxy $0.4(-50^{\circ}C), 0.41 - 0.42(T T_g) = -30^{\circ}C, 0.5(T > T_g)$

v

 $c_p(\frac{J}{k \circ K})$ [188] thermoset polyesters 1673-1882 [187] polyurethane resin 1300-2300, urethane elastomer 1700-1900, urethane rigid foam 1400, specific of polymers in general 1250-2510, polystyrene 1170, PMMA, commercial grade 1470, Urea-fomaldehyde alpha cellulose filler 1680 $\Pi_9(\sigma_c/E)$ [191] Acrylonitrile Butadiene Styrene 0.0115-0.0181, PBT 0.014-0.012, PA6 0.018-0.0177 from [194] Epoxy-clay 0 - 5%-nanocomposite 0.025 (pure epoxy)- 0.035 (epoxy-5% clay), from [195] glass fiber/epoxy at various strain rate 0.021 – 0.029 Table 10 of [187] selected thermoplastics with glass filler 0 - 40%, including Styrene, SAN, ABS, PP, glass-coupled PP, PE, AC, Polyester, Nylon 6, Nylon 6/6, Nylon 6/12, PC, PSU, PPS varying from 0.096 \times 10^{-3} (SAN 40% glass fiber) to 0.305×10^{-3} (Nylon 6/12) ~ 0.02 for thermosets, 0.0002 for thermoplastics 0.0 (plastics are considered non-charring materials)

 $\Pi_{7}(\rho_{c}/\rho_{0}) \qquad 0.0 \text{ (pl}$ $\Pi_{8}H^{2}\left(\frac{E}{\rho_{0}A^{2}}\right)$ $\frac{t_{hc}}{H^{2}}(\alpha^{-1}) \qquad \sim 10^{7}$ $t_{cl} = \frac{q_{0}}{P}(k/\alpha) \qquad \text{from}$

 $t_{flux} \frac{q_0}{HT_0}(k/\alpha)$ from [187] polyurethane resin 1430000-3450000, urethane elastomer 1870000-2375000, urethane rigid foam 784000-896000, PMMA, commercial grade 1734600-1749300, Urea-fomaldehyde alpha cellulose filler 2486400-2520000

 $\sim 2 \times 10^{6}$

 $t_{chem}\left(\frac{1}{A}e^{\frac{E_a}{2RT_0}}\right)$ [171] Hydrogenated polystyrene 55729.1, Poly-n-methylstyrene 36278.0, Poly- α -methylstyrene 141.1

$$t_{chem}\left(\frac{1}{A}e^{\frac{E_a}{RT_0}}
ight)$$
 [171] Hydrogenated polystyrene 4.34 × 10²³, Poly-n-methylstyrene 9.4758743 × 10²⁵, Poly- α -methylstyrene 1.6534333 × 10²³

Table IV in [171] contains kinetics parameters for various organic materials (ferulic acid, perylene tetracarboxylic acid anhydride, protocatechuic acid, naphthalene tetracarboxylic acid, mellitic acid, tartaric acid, polystyrene, teflon, polyethylene, hydrogenated polystyrene, poly-n-methylstyrene, poly-oc-methylstyrene, poly(methyl methacrylate), poly(methyl acrylate), cellulose).

From material properties in tables 5.2, 5.3, 5.4, 5.5, 5.6., the representative parameter values for each material are taken and tabulated in table 5.7. The last column contains material property values used in the numerical simulation of sections 3.3 and 3.4.

	Rubbers	Cellulosics	Thermosets	Thermoplastics	Original data
$\alpha(m^2/s)$	10^{-7}	$3 imes 10^{-7}$	10^{-7}		10^{-7}
k(J/mKs)	0.1	$0.3(z), 0.2(r\theta)$	0.3		
$ ho_c$	400.0 (kg)	$20\%\rho_0$	0.0	0.0	300.0
$\rho_0(kg)$	1000.0	700.0	1200.0	1200.0	1000.0
А	10^{10}	10 ⁸			e ^{31.25}
$E_a(kJ/mo$	<i>l</i>)100.0	150.0	220.0	220.0	77
E(GPa)	1.0	15.0	5.0	1.0	
$\sigma_c(MPa)$	14.0		80.0	100.0	0.024 E
ν	0.49		0.4	0.4	0.45
c _p	2000.0	1500.0			

Table 5.7: Representative material parameters.

CHAPTER 6

CASE STUDIES

In this chapter, I will investigate how various parameters affect the problem by varying each of them. The rectangular domain as in chapter 3 is considered. As mentioned in section , the problems consists of total fifteen parameters, which are L, H, α_x , α_y , T_0 , $\frac{q_0}{k_y}$, l, ρ_c , A, T_a , ρ_0 , σ_c , E, ν . Among these parameters, the seven following ones are varied α_x , α_y , $\frac{q_0}{k_y}$, l, A, T_a , σ_c . Only Section 6.1 is driven by the same thermal pyrolysis problem as Section 3.4 because only the tensile strength σ_c is varied. While in other sections, the thermal and pyrolysis problem are also changed by varying other parameters. The original value of each parameter which are listed in Eq. (3.35) will be denoted with the superscript ⁰ to be differentiated from its values that are varied.

6.1 The effect of the cracking threshold

It is apparent that material with lower tensile strength σ_c is more prone to cracking, as reflected in the thermal shock parameters $\phi_T = \frac{k\sigma_c(1-\nu)}{\gamma_t E}$ (Eq. (1.4)). This section investigates how σ_c scales with quantities of crack morphology such as crack spacing, crack initiation, total opening surface and loop quantity. It is expected that the reduction of tensile strength leads to earlier initiation, denser and more total cracking surface. In Fig. 6.1, the crack patterns and the maximum principle stress fields σ_1 at 3000s are plotted for the simulations using different σ_c , in which values are indicated in the figure caption. The crack patterns at t = 3000, 5000, 6000 s are also plotted on the background which is the density field for better visibility in Fig. 6.2, 6.3, 6.4. It can be seen from these figures that, for small σ_c/E , crack patterns have loop regions, while sample of larger σ_c/E forms well developed, tree-like branches.

Effect on crack initiation time.



Figure 6.1: Maximum principle stress σ_1 at $t = 3000 \ s$ corresponding to various values of tensile strength σ_c/E , which equal 0.024, 0.0333, 0.0467, 0.0600, 0.0667, 0.0867, 0.1000, 0.1133, 0.1267, 0.1333, 0.1600, 0.1733 from left to right, top to bottom, respectively.

The higher the tensile strength σ_c , the longer it takes for the sample to reach that value and thus to initiate the first crack. Fig. 6.5 left shows how the cracking initiation time t_i changes with tensile strength, in which σ_c is rescaled by σ_m thus the rescaled tensile strength σ_c/σ_m varies between 0 and 1. The right limit value 1 corresponds to material



Figure 6.2: Cracking pattern for various values of tensile strength σ_c at 3000 *s*. As σ_c gets larger, crack morphology shifts from loop-like toward well developed tree-like or branching behavior.

that will never crack. Thus, in principle, the curve should asymptote the vertical line $\sigma_c/\sigma_m = 1$. However, this behavior is not seen from Fig. 6.5 left, probably due to the finite size of the elements. For σ_c/σ_m that is less than 0.8, the t_i vs. σ_c/σ_m curve follows power law of time. The red line in Fig. 6.5 left is the best least square fit to the data. Part



Figure 6.3: Cracking pattern for various tensile strength at 5000 *s*. As σ_c gets larger, crack morphology shifts from loop-like toward well developed tree-like or branching behavior.

of the data in Fig. 6.5 left corresponding to $\sigma_c / \sigma_m < 0.8$ is replotted on a log-log scale in Fig. 6.5 right for better observation of the power behavior.

The effect on total crack length

Before any crack initiates in the sample, the sample is exposed to the incident heat flux



Figure 6.4: Cracking pattern for various tensile strength at 6000 *s*. As σ_c gets larger, crack morphology shifts from loop-like toward well developed tree-like or branching behavior.

through the heat flux length *l*. When cracks appear, they open up the sample interior. The total surface openned up due to cracking is characterized by the total crack length l_c . It is a very important link in the vicious cycle of the thermal degradation process. Fig. 6.6 plots the evolution of the sample total crack length l_c of various σ_c indicated in the legend box.



Figure 6.5: Left: Crack initiation time vs tensile strength. Left: Part of the right figure that corresponds to $\sigma_c / \sigma_m < 0.8$ plotted in a log-log scale.



Figure 6.6: Evolution of total crack length for various tensile strength.

It can be seen from the plot that, for most samples, the total crack length l_c in sample with lower σ_c is shorter, provided that the comparison across different samples is made at the same time. Each curve in Fig. 6.6 qualitatively consists of two parts: the nonlinear part near the ignition time Fig. 6.7 and the linear part with slopes β decreasing consistently with σ_c .

Fig. 6.8 (c) plots β against σ_c in a log-log scale. The nonlinear parts of the curves in Fig. 6.7 for most values of σ_c are fitted into the equation



Figure 6.7: Nonlinear part of the Fig. 6.6.

$$log(l_c/l) = alog(t - t_i) + b \tag{6.1}$$

as shown by Fig. 6.8 (b), which means l_c is power in time, for which values of *a* and *b* vs σ_c/σ_m are shown in Fig. 6.8 (d). Sample with σ_c/σ_m near unity is not fitted into the power Eq. (6.1).

The effect on crack spacing

As seen from Fig. 6.9, in general, crack spacing is larger in tougher materials. All curves in Fig. 6.9 have similar trend: a quick dropping followed by a constant value period and then a rising period. And jumps in spacing due to crack branching or intersecting is also larger because materials with larger tensile strength σ_c have fewer cracks, thus increasing or decreasing the number of cracks just by one may causes substantial change in the average spacing.

Moreover, tensile strength also affects crack segment length and junction angles. As σ_c increases, crack segments get longer, the number of right angle junctions decline due to



Figure 6.8: (a) Fig. 6.7 with time axis of each curve shifted by its initiation time t_i . (b) a, b are parameters of the curve fitting $log(l_c/l) = alog(t - t_i) + b$ in Eq. (6.1). (c) slope β of the linear parts vs. tensile strength σ_c/σ_m on a loglog scale. (d) values of a and b vs. σ_c/σ_m .



Figure 6.9: Average crack spacing $\overline{\gamma}$ vs depth r_c/l for various σ_c/E as indicated in the legend.

more branching than intersection. The probability distributions of segment length and junction angles for various σ_c values are plotted in Figs. 6.10 and 6.11.

The evolution of the total number of loops and its dependence on the the tensile strength



Figure 6.10: Probability distribution of segment length when the crack image is not thresholded (left) and thresholded (right). Different colors correspond to different values of σ_c/σ_m as indicated in the legend.



Figure 6.11: Probability distribution of junction angle when the crack image is not thresholded (left) and thresholded (right) for various values of the tensile strengh σ_c/σ_m as indicated in the legend.

can be seen from Fig. 6.12.

6.2 The effect of thermal diffusivities

As discussed previously in Section 3.4, cracks tend to propagate in the directions that are perpendicular to the char front. Thus the profile of crack network is decided by the shape of the char front, which is directly related to the anisotropy of the thermal diffusivities, i.e., the ratio of α_y and α_x or Π_3 group. Also, materials of higher thermal diffusivity



Figure 6.12: Number of loops changes with time for different values of σ_c / σ_m (left) and its dependence on σ_c / σ_m at t = 1000, 2000, 3000, 4000, 5000, 6000 s (right).

allow heat to diffuse more quickly, thus have lower thermal gradient as well as density gradient and stresses. Excellent materials with high thermal anisotropy are graphite and their derivatives such as xGnP graphene nanoplatelets. The in depth thermal diffusivity α_y facilitates heat penetrating into the sample, thus larger α_y increases cracking depth into the sample interior. On the other hand, the horizontal thermal diffusivity α_x facilitates crack propagation horizontally, reducing cracking depth.

The distribution of the dimensionless temperature θ along the vertical middle line of the sample at t = 100, 500, 1000, 1500, 2000, 2500, 3000 s can be seen from Fig. 3.3 for three cases of α_x . As α_x gets larger (Fig. 3.3 (c)), the temperature more quickly reaches the state of equilibria. Futhermore, the steady state value of temperature corresponding to higher α_x is smaller and vice versa.

The effects of α_{χ} on the density field is illustrated in Fig. 6.14.

The evolution of locations \overline{y} of the char front $\overline{\rho} = 0.3$ (solid), the pyrolysis front $\overline{\rho} = 0.99$ (dashed) and their difference δ (dotted) for three cases of α_x (equal 0.1, 1, 1 of the original value respectively) is indicated in Fig. 6.15. It can be seen that samples of lower α_x get



Figure 6.13: The distribution of the dimensionless temperature θ along the vertical middle line of the sample where $\bar{x} = 0.5$ at different times as indicated in the legend for three cases of α_x . Left: $\alpha_x = 0.1\alpha_x^0$. Middle: $\alpha_x = \alpha_x^0$. Right: $\alpha_x = 10\alpha_x^0$.



Figure 6.14: The effects of α_x on density fields, figures are taken at t = 3000 s. Left figure: $\alpha_x = 0.1 \alpha_x^0$, $\Pi_3 = 10 \Pi_3^0$. Right figure: $\alpha_x = 10 \alpha_x^0$, $\Pi_3 = 0.1 \Pi_3^0$.

in depth charred more quickly which implies the char front and the pyrolysis front reach the lower surface at a faster rate. The pyrolysis length δ for $\alpha_x = 0.1 \alpha_x^0$ has comparable value with the original case, but it quickly drops to near zero as the char front approaches the lower surface.

The cracking pattern and maximum principal stress σ_1 for three cases of α_x are shown by Fig. 6.20. The sample of lower α_x (Fig. 6.16 left) initiates the first crack at 56 *s* while the sample of higher α_y (Fig. 6.16 right) takes 385 *s* to nucleate the first one.

While α_x only affects Π_3 , α_y also affects the heat conduction characteristic time $t_{hc} = H^2/\alpha_y$, and thus the group $\Pi_6 = t_{hc}/t_{chem} = \frac{H^2 Aexp(-T_a/T_0)}{\alpha_y}$. The distributions of the dimensionless temperature θ along the vertical middle line of the sample at t = 100, 500, 1000, 1500, 2000, 2500, 3000 *s* are plotted in Fig. 6.17 for three cases of α_y . Similar to α_x , higher α_y (Fig. 6.17 (c)) also causes the temperature to more quickly reach the steady state. Futhermore, the steady state temperature corresponding to higher α_y is smaller and



Figure 6.15: The location of the char front where $\bar{\rho} = 0.3$ is indicated by the solid line. The location of the pyrolysis front where $\bar{\rho} = 0.99$ is indicated by the dashed line. The pyrolysis length δ is indicated by the dotted line.



Figure 6.16: Varying $\Pi_3 = \alpha_y / \alpha_x$ via changing α_x . Left figure: $\alpha_x = 0.1 \alpha_x^0$, $\Pi_3 = 10 \Pi_3^0$, cracks grow in depth. Right figure: $\alpha_x = 10 \alpha_x^0$, $\Pi_3 = 0.1 \Pi_3^0$, cracks spread horizontally.

more uniformly distributed along \overline{y} , thus the onset of pyrolysis and crack initiation are delayed. However, once cracks initiate, they will quickly evolve and reach the lower surface because the rate of in depth heat transfer and pyrolysis are higher for larger α_y .



Figure 6.17: The distribution of the dimensionless temperature θ along the vertical middle line of the sample where $\overline{x} = 0.5$ at different times as indicated in the legend for three cases of α_y . Left: $\alpha_y = 0.1 \alpha_y^0$. Middle: $\alpha_y = \alpha_y^0$. Right: $\alpha_y = 10 \alpha_y^0$.

The effects of α_y on the density field is illustrated in Fig. 6.18. It can be seen from these figures that the sample of higher α_y sample has thicker pyrolysis length δ and thus larger crack spacing.



Figure 6.18: Varying both $\Pi_3 = \alpha_y / \alpha_x$ and $\Pi_6 = H^2 Aexp(-T_a/T_0) / \alpha_y$ by varying α_y , Density field at t = 2350 s. Left figure: $\alpha_y = 0.1 \alpha_y^0$ leads to $\Pi_3 = 0.1 \Pi_3^0$, $\Pi_6 = 10 \Pi_6^0$. Right figure: $\alpha_y = 10 \alpha_y^0$ leads to $\Pi_3 = 10 \Pi_3^0$, $\Pi_6 = 0.1 \Pi_6^0$.

The evolution of locations \overline{y} of the char front $\overline{\rho} = 0.3$ (solid), the pyrolysis front $\overline{\rho} = 0.99$ (dashed) and their difference δ (dotted) for three cases of α_y (equal 0.1, 1, 1 of the original value respectively) is indicated in Fig. 6.19.



Figure 6.19: The location of the char front where $\bar{\rho} = 0.3$ is indicated by the solid line. The location of the pyrolysis front where $\bar{\rho} = 0.99$ is indicated by the dashed line. The pyrolysis length δ is indicated by the dotted line.

The cracking pattern and maximum principal stress σ_1 for three cases of α_y are shown by Fig. 6.20. The sample of lower α_y (Fig. 6.20 left) initiates the first crack at 9 *s* while the

sample of higher α_{y} (Fig. 6.20 right) takes 1090 *s* to nucleate the first one.



Figure 6.20: Varying both $\Pi_3 = \alpha_y / \alpha_x$ and $\Pi_6 = H^2 Aexp(-T_a/T_0) / \alpha_y$ by varying α_y , t = 2350 s. Left figure: $\alpha_y = 0.1\alpha_y^0$ leads to $\Pi_3 = 0.1\Pi_3^0$, $\Pi_6 = 10\Pi_6^0$, cracks grow horizontally. Right figure: $\alpha_y = 10\alpha_y^0$ leads to $\Pi_3 = 10\Pi_3^0$, $\Pi_6 = 0.1\Pi_6^0$, cracks grow in depth and there are fewer cracks.

Thus, from varying the thermal diffusivities α_x and α_y , it can be concluded that higher thermal diffusivity causes the temperature to reach the equilibria state more quickly at a lower value and also delays the pyrolysis as well as cracking process. However, once charring or cracking start, the processes evolve at a faster rate. Moreover, the ratio α_y/α_x or group Π_3 decides the isotropy of the char region: higher Π_3 causes elongation of the char region in the vertical direction and more loops formed in the final crack patterns.

6.3 The effect of heat flux strength

In this section, the problems of various heat flux strength q_0 are studied. Except q_0 , every other parameters remain the same as indicated by Eq. (3.35). As discussed in the previous section, Section 6, q_0 rescales with the depth of heat penetration l_f . Also here it is noted that changing the heat flux q_0 will affect the following dimensionless Pi group, namely $\Pi_4 = t_{hc}/t_{flux} = q_0 H/k_y T_0$ by changing the heat flux characteristic time $t_{flux} = \frac{HT_0k_y}{\alpha_y q_0}$. In addition, it can be derived analytically that, the dimensionless temperature θ scales linearly with q_0 .

The distributions of the dimensionless temperature θ along the vertical middle line of the sample at t = 100, 500, 1000, 1500, 2000, 2500, 3000 s are plotted in Fig. 6.21 for three cases of q_0 as indicated in the figure caption. The general trend as expected is higher heat

flux correspond to higher temperature and vice versa. Futhermore, θ is linearly proportional to q_0 .



Figure 6.21: The distribution of the dimensionless temperature θ along the vertical middle line of the sample where $\bar{x} = 0.5$ at different times as indicated in the legend for three cases of q_0 . Left figure: $q_0 = 0.1q_0^0$. Middle figure: $q_0 = q_0^0$. Right figure: $q_0 = 10q_0^0$. θ scales linearly with q_0 .

The effect of q_0 on the density field can be seen from Fig. 6.22.



Figure 6.22: Density field $\overline{\rho}$ at 3000s. Varying heat flux q_0 affects $\Pi_4 = q_0 H/(k_y T_0)$. Left figure: $q_0 = 0.5q_0^0$, $\Pi_4 = 0.5\Pi_4^0$. Right figure: $q_0 = 2q_0^0$, $\Pi_4 = 2\Pi_4^0$.

The evolution of locations \overline{y} of the char front $\overline{\rho} = 0.3$ (solid), the pyrolysis front $\overline{\rho} = 0.99$ (dashed) and their difference δ (dotted) for three cases of q_0 (equal 0.5, 1, 2.0 of the original value respectively) is indicated in Fig. 6.23. It can be seen from this figure that δ is not much affected by the change of q_0 when $t < 1.5t_{hc}$. However, the sample pyrolyzes more quickly when q_0 is raised.

The magnitude of q_0 affects the rate of pyrolysis and thus the rate of crack propagation but does not affect the crack spacing, as seen from Fig. 6.24, which shows the distributions of the maximum principal stresses σ_1 corresponding to three values of q_0 indicated



Figure 6.23: The location of the char front where $\overline{\rho} = 0.3$ is indicated by the solid line. The location of the pyrolysis front where $\overline{\rho} = 0.99$ is indicated by the dashed line. The pyrolysis length δ is indicated by the dotted line.

in the caption.



Figure 6.24: Maximum principle stress field at 3000*s*. Varying heat flux q_0 affects $\Pi_4 = q_0 H/(k_y T_0)$. Left figure: $q_0 = 0.5q_0^0$, $\Pi_4 = 0.5\Pi_4^0$. Right figure: $q_0 = 2q_0^0$, $\Pi_4 = 2\Pi_4^0$.

It is interesting to note about the similarity between the crack patterns in Fig. 6.24 (c) $(q_0 = 2q_0^0)$ at 3000*s* and Fig. 6.26 $(q_0 = q_0^0)$ at 6000 *s* (from Section 3.4); between the crack patterns in Fig. 6.24 upper $(q_0 = 0.5q_0^0)$ at 3000*s* and Fig. 6.27 $(q_0 = q_0^0)$ at 1500*s* (from Section 3.4), in term of crack depth and crack spacing.



Figure 6.25: The effect of q_0 on crack spacing.



Figure 6.26: Maximum principle stress (from Section 3.4) when $q_0 = q_0^0$ at 6000 *s*. Crack morphology in this figure is similar to that of Fig. 6.24 lower



Figure 6.27: Maximum principle stress (from Section 3.4) when $q_0 = q_0^0$ at 1500s. Crack morphology is similar to that of Fig. 6.24 upper.

6.4 The effect of heated region size

6.4.1 General observations

In this section, the only parameter that varies is the dimension l of the region over which heat flux is applied. The flame scale varies through only this parameter, indicating that this model can potentially be adapted to problems that span the range between very small flames (micro-flames) and very large flames. This parameter *l* influences the problem under the effect of the dimensionless Pi group Π_2 which is its ratio with the domain length $\Pi_2 = l/L$. The change of crack morphology corresponding to changing *l* is comparable to the nonlinear feedback: the more surfaces exposed to hot gases, the more quickly materials become char and more cracks develop.

The influence of *l* on the density field can be seen from Fig. 6.28, in which the left figure corresponds to l = 0.01L and the right figure corresponds to l = L. The middle figure corresponds to the standard case when l = 0.1L. In the upper figure, the activation energy is also raised 100 times higher than its standard value to accelerate the pyrolysis rate and induce crack. However, only a small crack is observed at $t = 6000 \ s$, see Fig. 6.29 right. Larger *l* causes larger area of the sample to be quickly pyrolyzed and charred.



Figure 6.28: Effects of varying the size of heated region *l* and thus $\Pi_2 = l/L$ on density field $\overline{\rho}$. Left figure: $\Pi_2 = 0.01$, $A = 100A^0$, t = 6000 s. Middle figure: $\Pi_2 = 1.0$, t = 3000 s. Right figure: $\Pi_2 = 0.1$, t = 3000 s



Figure 6.29: Effects of varying the size of heated region *l* on crack morphology. Left figure: $\Pi_2 = 0.01$, $A = 100A^0$, t = 6000 s. Middle figure: $\Pi_2 = 1.0$, t = 3000 s. Right figure: $\Pi_2.1$, t = 3000 s.

The rate of pyrolysis and the pyrolysis length δ for two cases of *l*, as indicated in the figure legend, is shown by Fig. 6.30.



Figure 6.30: The location of the char front where $\bar{\rho} = 0.3$ is indicated by the solid line. The location of the pyrolysis front where $\bar{\rho} = 0.99$ is indicated by the dashed line. The pyrolysis length δ is indicated by the dotted line.

6.4.2 The effect of varying σ_c when l = L

In this subsection, the various cases share the same temperature and density distributions as the only parameter that is varied is the tensile strength σ_c , similar to the analysis in Section 6.1, except here the whole upper surface is heated, i.e, l = L. The density fields at certain times indicated in the figure caption are plotted in Fig. 6.31.

When l = L, if the sample does not develop crack, the maximum possible value that the maximum principle stress σ_1 can attain is $\sigma_{m2} = 0.2E$, (compared with 0.18666*E* when l = 0.1L in Section 3.4). Fig. 6.32 shows the crack patterns and distribution of the maximum principle stress σ_1 at t = 3000 s for various values of σ_c as indicated in the figure caption.

In this case of uniformly heating on the upper surface, l = L, the crack spacing at certain depth is measured by placing a horizontal line into the crack pattern and counting the



Figure 6.31: Dimensionless density $\overline{\rho} = \rho/\rho_0$ at t = 50, 100, 500, 1000, 1200, 1350, 3000, 6000 *s* when l = L. Other parameter values are given by Eq. (3.35). At around t = 30 s, the upper surface starts to pyrolyze and at around 1350*s*, so does the lower surface.

intersection pixels. The crack spacing in this case has unit of length, instead of radian like in Section 3.4. Fig. 6.35 illustrates the procedure of measuring crack spacing at the depth of 0.5*H* in this case.

As seen from Fig. 6.35, the average crack spacing \bar{s} increases quite consistently with depth r_c , except for two lowest values of the tensile strength σ_c , in which \bar{s} shows fluctuation when r_c get closer to H (sample height.). The sudden jumps on each curve indicate bifurcation (jumping up) or joining (jumping down) of crack segments. Moreover, samples of higher σ_c have larger crack spacing and vice versa.



Figure 6.32: The crack patterns and distribution of the maximum principle stress σ_1 at t = 3000 s for $\sigma_c / E = 0.0240, 0.0333, 0.0467, 0.0600, 0.0667, 0.0867, 0.1000, 0.1733.$



Figure 6.33: Crack spacing is measured by placing a line into the crack pattern and counting intersection points. In this figure, the line is placed at depth 0.5*H*.

The time dependence of total crack length l_c for various σ_c is shown in Fig. 6.35. It can be seen from the figure that, each curve qualitatively consists of two parts: the nonlinear part when $t < 1.4t_{hc}$ and the linear part when $t > 1.4t_{hc}$. For the case l = L, around



Figure 6.34: The average crack spacing \overline{s} as a function of depth r_c for various values of σ_c as indicated in the legend.

 $t = 1.4t_{hc}$ is the time when the lower surface starts to become char as seen from Fig. 6.31. At this time, most of the sample has been charred. When $t > 1.4t_{hc}$, cracks slowly evolve, which is indicated by the small slopes of the linear parts. Besides, these slopes decrease with values of σ_c : sample with high σ_c almost develop no further cracks after this period.



Figure 6.35: The evolution of total crack length l_c for various values of σ_c as indicated in the legend when l = L. The total crack length is rescaled by the length l of the heated region, which is the sample width in this case.



Figure 6.36: Initiation time $t_i(s)$ changes with tensile strength σ_c when l = L, in which σ_c is rescaled by the maximum stress value of sample without cracks $\sigma_{m2} = 0.2E$.

6.5 The effect of activation energy

While the parameters that are varied in the previous sections, namely, the thermal diffusivities α_x , α_y , the heat flux q_0 , the size of the heated region *l* affect the problem by via the temperature, in these next two sections, the activation energy T_a and the pre-exponent factor *A* of the Arrhenius equation (2.2) are varied. Thus the temperature distribution remains the same as the standard cases. Only the density field and thus the cracking behavior are influenced. Since T_a appears inside the exponential term, it is only varied by 10% of its original value.

The evolution of locations \overline{y} of the char front $\overline{\rho} = 0.3$ (solid), the pyrolysis front $\overline{\rho} = 0.99$ (dashed) and their difference δ (dotted) for three cases of T_a (equal 0.9, 1, 1.1 of the original value respectively) is indicated in Fig. 6.38.

The activation temperature T_a affects the chemical characteristic time $t_{chem} = A^{-1}exp(T_a/T_0)$ and two Pi groups Π_5 and Π_6 which are defined in Section 6 as $\Pi_5 = T_a/T_0$ and $\Pi_6 = t_{hc}/t_{chem} = H^2 A e^{-T_a/T_0}/\alpha_y$ through the effect of Π_5 . Substances with higher activation


Figure 6.37: Varying activation temperature T_a affects $\Pi_5 = T_a/T_0$ and $\Pi_6 = H^2 A e^{-T_a/T_0}/\alpha_y$. Left: $\overline{\rho}$ plots. Right: σ_1 plots. Upper figure: $T_a = 0.9T_a^0$ leads to $\Pi_5 = 0.9\Pi_5^0$, $\Pi_6 = 23.336\Pi_6^0$. Lower figure: $T_a = 1.1T_a^0$ leads to $\Pi_5 = 1.1\Pi_5^0$, $\Pi_6 = 0.04285\Pi_6^0$.



Figure 6.38: The location of the char front where $\overline{\rho} = 0.3$ is indicated by the solid line. The location of the pyrolysis front where $\overline{\rho} = 0.99$ is indicated by the dashed line. The pyrolysis length δ is indicated by the dotted line.

temperature have larger chemical characteristic time and slower pyrolysis rate because higher amount of energy is required to start the reaction. The effect of T_a on crack spacing can be seen from Fig. 6.39.



Figure 6.39: The effect of T_a on crack spacing.

6.6 The effect of pre-exponent factor

The pre-exponent factor *A* has unit of time, it inversely scales with the characteristic time for pyrolysis reaction $t_{chem} = A^{-1}exp(T_a/T_0)$ and affects group $\Pi_6 = t_{hc}/t_{chem} = H^2Ae^{-T_a/T_0}/\alpha_y$. Effects of *A* on the crack pattern could be seen from Figs. 6.40 upper and 6.40 lower in which *A* is increased by a factor of ten in Fig. 6.40 upper and decreased by the same factor in Fig. 6.40 lower.

The evolution of locations \overline{y} of the char front $\overline{\rho} = 0.3$ (solid), the pyrolysis front $\overline{\rho} = 0.99$ (dashed) and their difference δ (dotted) for three cases of *A* (equal 0.1, 1, 10 of the original value respectively) is indicated in Fig. 6.41.

6.7 Morphological diagram

As mentioned previously, fracture patterns belongs to a broader topological class, the network pattern. They can be classified into several groups based on their morphologies. Tree like patterns are characterized by branching and bifurcation. They are typically



Figure 6.40: Varying $\Pi_6 = H^2 A e^{-T_a/T_0} / \alpha_y$ by varying A, t = 3000 s. Left: $\overline{\rho}$ plots. Right: σ_1 plots. Upper figures: $A = 10A^0$. $\Pi_6 = 10\Pi_6^0$. t = 3000 s. Lowers figure: $A = 0.1A^0$. $\Pi_6 = 0.1\Pi_6^0$. t = 3000 s.



Figure 6.41: The location of the char front where $\overline{\rho} = 0.3$ is indicated by the solid line. The location of the pyrolysis front where $\overline{\rho} = 0.99$ is indicated by the dashed line. The pyrolysis length δ is indicated by the dotted line. While higher value of *A* accelerates the pyrolysis, δ does not change drastically with *A*.

seen in systems in which directional transportation and delivery dominate, such as blood capillaries, tree branches, river network, leaf veins. The meaning of transportation could



Figure 6.42: The effect of *A* on crack spacing. When $A = 0.1A^0$, cracks evolve at a much slower pace and only make their way to half of the sample depth. The sudden jump of crack spacing in this case at $r_c/l = 1.5$ is caused by periodic doubling seen at early stage of crack evolution. The case $A = 10A^0$ produces similar morphology to the original case but the evolution happens at a faster rate.

be extended to heat transfer or directional charring in our problem. On the other hand, the polygonal or interconnected, loop like patterns are more direct consequences of the minimization principle, which is the minimization of total energy in fracture and of other quantities in other contexts. The driving fields of these patterns are isotropic, acting uniformly on a surface at an instant of time. Examples are mud crack, skin crack, ceramic glaze, craze.

As discussed in Chapter 4, the crack morphology can characterized in terms of quantities such as: fractal dimension, segment rank, crack spacing, crack length, number of loops, loop direction, junction angles. These quantities are affected by the values of parameter values. In particular, three parameters q_0 , A and T_a , affect the rate of heat transfer or pyrolysis and thus crack elongation, but do not have much influence on the crack morphology. They can be viewed as the parameters that scale the characteristic times of the problem. On the other hand, crack spacing is influenced by two groups $\Pi_9 = \sigma_c/E$ and $Pi_6 = \frac{H^2 Aexp(-T_a/T_0)}{\alpha_y}$. When the thermal diffusivity in one direction increases, temperature and density gradients in that direction get smaller while the pyrolysis length δ increases. This results in overall smaller stresses in the sample and larger crack spacing. If fracture resistance is understood as less and delayed damage, a pyrolysis cracking parameter can be taken as

$$\phi_P = \frac{\alpha_y exp(T_a/T_0)\sigma_c}{AE},\tag{6.2}$$

which is the ratio of Π_9 and Π_6 . Similar to the thermal shock parameter $\phi_T = \frac{k\sigma_c(1-\nu)}{\gamma_t E}$ (Eq. (1.4)) that characterizes damage in thermoelasticity, higher value of ϕ_P corresponds to materials that are more fracture resistant in this model.

Group Π_9 not only characterizes crack spacing, it also characterize the morphological shift from loop-like to tree-like behavior when its value gets larger. This behavior is also influence by the thermal anisotropy or Π_3 group: when $\Pi_3 = \alpha_y / \alpha_x$ is large, cracks cluster together near the central region of the sample, forming loop network. When Π_3 is small, cracks spreading out, forming tree like structure. The chart below Fig. 6.43 represents the competitive influences of these two groups Π_3 and Π_9 on the crack morphology in term of tree and loop behavior.



Figure 6.43: The competitive influence of $\Pi_3 = \alpha_y / \alpha_x$ and $\Pi_9 = \sigma_c / E$ on the morphology of the crack patterns. The horizontal axis is the tensile strength σ_c rescaled by its maximum value σ_m . The vertical axis is on the logarithm scale, $log_{10}(\alpha_x / \alpha_y)$ which is $-log_{10}(\Pi_3)$. Close to the origin where α_y / α_x is large and σ_c / E is small, the cracks tend to form loops. Away from the origin, they tend to develop branches, forming tree-like pattern.

CHAPTER 7

CRACKS ON A CIRCULAR DOMAIN

7.1 A radial heating problem

In the previous chapters, the problem is considered on a rectangular domain. On a circular domain with the assumption of axial symmetry, partial analytical solutions can be derived. It is "partial" because of the fact that, while there exists an analytical temperature and an analytical expression for stresses in terms of density, the Arrhenius equation which relates density to temperature, is not integrable. In particular, consider the following heating problem of a cylindrical rod:

Problem A A cylindrical rod of radius *R* and length *L*, initially at uniform temperature T_0 , is heated by an uniform heat flux per unit length q_0 from its center r = 0. The temperature *T* is governed by the heat conduction equation, Eq. (2.1) which, in cylindrical coordinate and under axis-symmetric condition, becomes

$$\frac{\partial T}{\partial t} = \frac{\alpha_r}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right), \tag{7.1}$$

where α_r is the thermal diffusivity in the radial direction. To solve the **problem A**, let consider a more general problem **Problem B**, in which its only difference with **problem A** is that the cylindrical rod is hollow. Let r_i be its inner radius and R its outer radius R. The Fourier's law that relates heat flux to temperature gradient provides the boundary condition at for **Problem B** at $r = r_0$ as

$$2\pi r_0 \left(k_r \frac{\partial T}{\partial r} \right) |_{r=r_i} = q_0, \tag{7.2}$$

where k_r is the thermal conductivity in the radial direction and q_0 is the heat release per unit length L. When $r_i = 0$, **Problem B** is identical to **Problem A**.

The analytical solution of the **Problem B** is obtained using the method of similar variable. From that, the analytical solution of the **Problem A** is obtained by taking limit $r_i \rightarrow 0$, which is

$$\frac{T(\eta) - T_0}{q_0 / (2\pi k_r)} = \int_{\eta}^{\infty} \frac{e^{-s^2}}{s} ds,$$
(7.3)

where $\eta = r/(2\sqrt{\alpha_r t})$ is the similarity variable. The density of the cylindrical rod follows from the Arrhenius relation, Eq. (2.2), which is

$$\frac{\partial \rho}{\partial t} = -A(\rho - \rho_0)e^{-\frac{T_a}{T}}.$$
(7.4)

in which ρ_0 is the initial rod density, T_a is the activation temperature and A is the preexponent factor. These parameters are the same as those from previous chapters. The stress balance equation in radial coordinate under axis symmetric condition is taken from Eq. (2.8) as

$$\frac{d\sigma_{rr}}{dr} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0, \tag{7.5}$$

and the total strain follow Equations (2.6), (2.4) for the axis symmetric problem and a general scalar shrinkage strain ε_0 :

$$\varepsilon_{rr} = \frac{\sigma_{rr} - \nu \sigma_{\theta\theta}}{E} + \varepsilon_0,$$

$$\varepsilon_{\theta\theta} = \frac{\sigma_{\theta\theta} - \nu \sigma_{rr}}{E} + \varepsilon_0.$$
(7.6)

The solution of the stress-strain problem (7.5) and (7.6) with traction-free boundary condition $\sigma_{rr}|_{r=R} = 0$, without cracking is given as

$$\sigma_{rr} = \frac{E}{R^2} \int_0^R \varepsilon_0(\zeta) \zeta d\zeta - \frac{E}{r^2} \int_0^r \varepsilon_0(\zeta) \zeta d\zeta,$$

$$\sigma_{\theta\theta} = -E\varepsilon_0 + \frac{E}{R^2} \int_0^R \varepsilon_0(\zeta) \zeta d\zeta + \frac{E}{r^2} \int_0^r \varepsilon_0(\zeta) \zeta d\zeta.$$
(7.7)

The detailed derivation of solution given Eq. (7.7) which corresponds to traction free condition at the outer radius and the other solution corresponding to pinned condition is given in Section 7.2. In our model, the shrinkage strain is taken as proportional to mass depletion $\varepsilon_0 = \gamma(\rho - \rho_0)$ as already given in Eq. (2.5). Thus the solution (7.7) becomes

$$\sigma_{rr} = \frac{\gamma E}{R^2} \int_0^R (\rho - \rho_0) \zeta d\zeta - \frac{\gamma E}{r^2} \int_0^r (\rho - \rho_0) \zeta d\zeta, \qquad (7.8)$$

for radial stress and

$$\sigma_{\theta\theta} = -\gamma E(\rho - \rho_0) + \frac{\gamma E}{R^2} \int_0^R (\rho - \rho_0) \zeta d\zeta + \frac{\gamma E}{r^2} \int_0^r (\rho - \rho_0) \zeta d\zeta.$$
(7.9)

for tangential stress. Since $\rho < \rho_0$, it can be proven that $\sigma_{rr} > 0$, $d\sigma_{rr}/dr < 0$ and $\sigma_{\theta\theta}(r = R) < 0$ if $d\rho/dr > 0$. Vice versa, $\sigma_{rr} < 0$, $d\sigma_{rr}/dr > 0$ and $\sigma_{\theta\theta}(r = R) > 0$ if $d\rho/dr < 0$. Physically, this implies that if the sample loses its mass from its center, the radial stress will be tensile and decreases with radius. In particular, using integration by parts the following integral by letting $\zeta d\zeta = d\left(\frac{1}{2}\zeta^2\right)$

$$\int_0^r (\rho - \rho_0) \zeta d\zeta = (\rho(r) - \rho_0) \frac{r^2}{2} - \int_0^r \frac{\zeta^2}{2} \frac{d\rho}{d\zeta} d\zeta,$$
(7.10)

when evaluated at r = R, giving

$$\int_0^R (\rho - \rho_0) \zeta d\zeta = (\rho(R) - \rho_0) \frac{R^2}{2} - \int_0^R \frac{\zeta^2}{2} \frac{d\rho}{d\zeta} d\zeta.$$
 (7.11)

Substituing two above relations into Eq. (7.9), estimating at r = R, yielding

$$\sigma_{\theta\theta}(r=R) = -\frac{2\gamma E}{R^2} \int_0^R \frac{d\rho}{d\zeta} \frac{\zeta^2}{2} d\zeta, \qquad (7.12)$$

which is negative as $\frac{d\rho}{dr} > 0$. Moreover, taking the limit as $r \to r_{\epsilon}$, where r_{ϵ} is very small, of the following quantity:

$$Lim_{r \to r_{\epsilon}} \left(\frac{1}{r^2} \int_0^r (\rho - \rho_0) \zeta d\zeta \right)$$

= $Lim_{r \to r_{\epsilon}} \frac{(\rho - \rho_0)r}{2r}$
= $(\rho(r_{\epsilon}) - \rho_0),$ (7.13)

(7.14)

then substituting the above expression and using(7.11) into Eq. (7.9) then evaluated at $r_{\epsilon} = 0$ gives the value of the tangential stress at the center as

$$\sigma_{\theta\theta}(r=0) = (\rho_{|}(r=R) - \rho_{|}(r=0)) - \frac{\gamma E}{R^2} \int_0^R \frac{d\rho}{dr} \frac{\zeta^2}{2} d\zeta,$$
(7.15)

which can be both positive or negative because in the RHS of (7.15), the first term is positive and the second term is negative for $\frac{d\rho}{dr} > 0$. From Eq. (7.8), taking the derivative of its second term

$$\frac{d}{dr}\left(\frac{\gamma E}{r^2}\int_0^r (\rho-\rho_0)\zeta d\zeta\right) = -\frac{2\gamma E}{r^3}\int_0^r (\rho-\rho_0)\zeta d\zeta + \frac{\gamma E}{r^2}(\rho-\rho_0)r, \qquad (7.16)$$

thus, the first derivative of radial stress is

$$\frac{d\sigma_{rr}}{dr} = -\frac{\gamma E}{r^3} \int_0^r \frac{d\rho}{d\zeta} \frac{\zeta^2}{2} d\zeta, \qquad (7.17)$$

which is always negative when $\frac{d\rho}{dr} > 0$. Note that the above expression can also be obtained from Eqs. (7.5), (7.8) and (7.9). Since $\sigma_{rr} = 0$ at r = R and $\frac{d\sigma_{rr}}{dr} < 0$, σ_{rr} always positive. Similarly, the first derivative of the tangential stress is

$$\frac{d\sigma_{\theta\theta}}{dr} = -\gamma E \frac{d\rho}{dr} + \frac{\gamma E}{r^3} \int_0^r \frac{d\rho}{d\zeta} \zeta^2 d\zeta, \qquad (7.18)$$

and the invariance of stress tensor

$$\sigma_{\theta\theta} + \sigma_{rr} = -\gamma E(\rho - \rho_0) + \frac{2\gamma E}{R^2} \int_0^R (\rho - \rho_0) \zeta d\zeta.$$
(7.19)

No conclusion can be made about the sign of expressions in Eq. (7.18) and Eq. (7.19) so tangential stress could be either tensile or compressive assuming the mass is lost from the center $\frac{d\rho}{dr} > 0$.

7.2 An analytical derivation for the radial stress

In this derivation, the shrinkage strain is taken as $\varepsilon(r)$ which is a general function of radius *r*. Starting from Eq. (2.7), the expressions of total strains for axial symmetry condition in cylindrical coordinates are

$$\varepsilon_{rr} = \frac{du}{dr}$$
$$\varepsilon_{\theta\theta} = \frac{u}{r}$$
(7.20)

Governing equation or stress balance is given by Eq. (7.5). Substituting Eq. (7.20) and (7.6) into the governing equation, Eq. (7.5) gives

$$\frac{d}{dr}\left(\frac{du}{dr} + \nu\frac{u}{r} - \frac{1+\nu}{r}\varepsilon_0\right) + (1-\nu)\left(\frac{du}{dr} - \frac{u}{r}\right) = 0.$$
(7.21)

Expanding the above expression to get the second order ordinary differential equation which is the Euler's equation

$$\frac{d^2u}{dr^2} + \frac{1}{r}\frac{du}{dr} - \frac{u}{r^2} = (1+\nu)\frac{d\varepsilon_0}{dr}.$$
(7.22)

The general solution of (7.22) can be obtained via using variable change: $r = r_0 e^t$ so $dr = r_0 e^t dt$ and $dt = e^{-t} r_0^{-1} dr = r^{-1} dr$, where r_0 is any characteristic length scale. Thus:

$$\frac{du}{dr} = \frac{du}{dt}\frac{dt}{dr} = e^{-t}r_0^{-1}\frac{du}{dt}$$
$$\frac{d^2u}{dr^2} = \frac{d}{dt}\left(e^{-t}r_0^{-1}\frac{du}{dt}\right)\frac{dt}{dr} = \left(\frac{d^2u}{dt^2} - \frac{du}{dt}\right)e^{-2t}r_0^{-2}$$

substituting these expressions back into (7.22) yields

$$(u_t'' - u_t' + u_t' - u)e^{-2t}r_0^{-2} = (1 + \nu)\frac{d\varepsilon_0}{dt}e^{-t}r_0^{-1}$$
(7.23)

or

$$(u'_t + u)' - (u'_t + u) = (1 + \nu)\frac{d\varepsilon_0}{dt}e^t r_0.$$
(7.24)

with $u'_t = \frac{du}{dt}$ and $u''_t = \frac{d^2u}{dt^2}$. Introduce the new dependent variable w(t)

$$w(t) = u'_t + u$$
 (7.25)

and substitute this into (7.23) after multiplying (7.23) with the integrating factor e^{-t}

$$(w(t)e^{-t})' = e^{-t}(1+\nu)\frac{d\varepsilon_0}{dt}e^t r_0$$
(7.26)

integrating both sides gives

$$w(t) = e^t (1+\nu) r_0 \left(\int_0^t \frac{d\varepsilon_0}{dt} dt + A \right), \qquad (7.27)$$

which can be written as

$$w(t) = e^{t}(1+\nu)r_{0}(\varepsilon_{0}+A)$$
(7.28)

where A is an integral constant which could be determined later from boundary conditions. u(t) can be solved from w(t)

$$(u(t)e^{t})' = w(t)e^{t} = e^{2t}(1+\nu)r_{0}(\varepsilon_{0}+A)$$

which gives

$$u(t) = e^{-t} \left(\int_0^t e^{2t} (1+\nu) r_0 \left(\varepsilon_0 + A\right) dt + B \right)$$

now changing back to normal variable *r* using the relation $e^{-t} = r_0 r^{-1}$

$$u(r) = r_0 r^{-1} \left(\int_0^r r^2 r_0^{-2} (1+\nu) r_0 \left(\varepsilon_0 + A\right) r^{-1} dr + B \right)$$

then the scaling length r_0 is cancelled out and the general solution u(r) is

$$u(r) = r^{-1} \left(\int_0^r r^2 (1+\nu) \left(\varepsilon_0 + A \right) r^{-1} dr + B \right)$$
(7.29)

here A, B are two constants of integration, in which B must vanish since u(r) is finite at r = 0. This gives

$$u(r) = r^{-1}(1+\nu) \left(\int_0^r \varepsilon_0(\zeta) \zeta d\zeta + A \frac{r^2}{2} \right),$$
(7.30)

A is found for two cases, the first one has traction free boundary condition which requires the radial stress σ_{rr} to vanish on the outer radius. From (7.30),

$$\frac{du}{dr} = -\frac{1+\nu}{r^2} \int_0^r \varepsilon_0(\zeta) \zeta d\zeta + (1+\nu)\varepsilon_0 + (1+\nu)\frac{A}{2}.$$
(7.31)

Substitute $\frac{du}{dr}$ and u(r) from (7.30) and (7.31) into the following expression for radial stress

$$\sigma_{rr} = \frac{E}{1 - \nu^2} \left(\frac{du}{dr} + \nu \frac{u}{r} \right) - \frac{E}{1 - \nu} \varepsilon_0, \tag{7.32}$$

which is obtained from (7.20) and (7.6), gives the following expression for radial stress

$$\sigma_{rr} = -\frac{E}{r^2} \int_0^r \varepsilon_0(\zeta) \zeta d\zeta + \frac{E(1+\nu)}{1-\nu} \frac{A}{2}.$$
(7.33)

The traction free condition at outer radius $\sigma_{rr}(r = R) = 0$ requires

$$-\frac{E}{R^2} \int_0^R \varepsilon_0(\zeta) \zeta d\zeta + \frac{E(1+\nu)}{1-\nu} \frac{A}{2} = 0$$
(7.34)

and thus:

$$A = \frac{2(1-\nu)}{(1+\nu)R^2} \int_0^R \varepsilon_0(\zeta) \zeta d\zeta$$
(7.35)

The parameter A is substituted back into the expression for displacement (7.30) and stress (7.33), giving

$$u(r) = (1+\nu) \left(\frac{1}{r} \int_0^r \varepsilon_0(\zeta) \zeta d\zeta + \frac{r}{R^2} \frac{(1-\nu)}{(1+\nu)} \int_0^R \varepsilon_0(\zeta) \zeta d\zeta\right)$$
(7.36)

$$\sigma_{rr} = \frac{E}{R^2} \int_0^R \varepsilon_0(\zeta) \zeta d\zeta - \frac{E}{r^2} \int_0^r \varepsilon_0(\zeta) \zeta d\zeta$$
(7.37)

and into the expression for the tangential stress, which is

$$\sigma_{\theta\theta} = \frac{E}{1 - \nu^2} \left(\frac{u}{r} + \nu \frac{du}{dr}\right) - \frac{E}{1 - \nu} \epsilon_0, \tag{7.38}$$

using (7.30) and (7.31), it becomes:

$$\sigma_{\theta\theta} = \frac{1}{r^2} \int_0^r \varepsilon_0(\zeta) d\zeta + \frac{E(1+\nu)^2}{(1-\nu^2)} \frac{A}{2} - E\varepsilon_0$$
(7.39)

Substituting A in (7.35) into the above expression gives

$$\sigma_{\theta\theta} = \frac{E}{r^2} \int_0^r \varepsilon_0(\zeta) d\zeta + \frac{E}{R^2} \int_0^R \varepsilon_0(\zeta) d\zeta - E\varepsilon_0$$
(7.40)

Three equations (7.36), (7.37), (7.40) are the analytical solutions for the axis symmetric shrinkage strain problem with traction free boundary condition.

Other boundary condition for the problem could be zero displacement (or pinned) at the outer radius u(r = R) = 0, then from (7.30)

$$A = -\frac{2}{R^2} \int_0^R \varepsilon_0(\zeta) \zeta d\zeta \tag{7.41}$$

subsequently, the expressions for displacement and stress are

$$u(r) = (1+\nu) \left(\frac{1}{r} \int_0^r \varepsilon_0(\zeta) \zeta d\zeta - \frac{r}{R^2} \int_0^R \varepsilon_0(\zeta) \zeta d\zeta\right),$$
(7.42)

and:

$$\sigma_{rr} = -\frac{E}{r^2} \int_0^r \varepsilon_0(\zeta) \zeta d\zeta - \frac{E(1+\nu)}{1-\nu} \frac{2}{R^2} \int_0^R \varepsilon_0(\zeta) \zeta d\zeta.$$
(7.43)

7.3 Numerical results without cracking

The analytical expressions of temperature and stresses Eqs. (7.3), (7.8) and (7.9) involve definite integrals, thus numerical integration must be ultilized. To simplify the integral in Eq. (7.3), define the dimensionless temperature θ as

$$\theta = \int_{\eta}^{\infty} \frac{e^{-s^2}}{s} ds, \qquad (7.44)$$

then using change of variable $u = \frac{1}{s}$, $\zeta = \frac{1}{\eta}$, and thus $du = -\frac{1}{s^2}ds$. Substituing into (7.44),

$$\theta = -\int_{\zeta}^{0} \frac{e^{-1/u^2}}{u} du,$$
(7.45)

or equivalently

$$\theta = \int_0^{\zeta} \frac{e^{-1/u^2}}{u} du,$$
(7.46)

where $\zeta = \frac{1}{\eta} = \frac{2\sqrt{\alpha_r t}}{r}$. Thus the new integration for does not involve the infinity limit and temperature can be expressed as:

$$T = T_0 + \frac{q_0}{2\pi k_r} \int_0^{2\sqrt{\alpha_r t}} \frac{e^{-1/u^2}}{u} du.$$
 (7.47)

The density is calculated from Eq. (7.4) once temperature distribution is known. Without cracking, stress fields can be given by Eqs. (7.8) and (7.9). Once cracking happens, those stress equations are no longer valid. In this section, the "semi" analytical solutions for temperature, density and stresses are discussed for one set of parameters as given below.

$$R = 2cm,$$

$$T_0 = 300 \quad K,$$

$$\alpha_r = 4 \times 10^{-7} \quad m^2 s^{-1},$$

$$\frac{q_0}{2\pi k_r} = 500 \quad K,$$

$$T_a = 12000 \quad K,$$

$$A = 10^8 \quad s^{-1},$$

$$\rho_0 = 1000 \quad kgm^{-3},$$

$$\rho_c = 300 \quad kgm^{-3},$$

$$\nu = 0.45,$$

$$\sigma_c / E = 0.012.$$

(7.48)

With these parameters, the distribution of the dimensionless temperature θ and density ρ are calculated using Eqs. Eqs. (7.3), 7.4 and plotted in Figs. 7.1 and 7.2, respectively. In these figures, the radial coordinate is rescaled by the sample radius *R*.

Then the density field can be used to calculate σ_{rr} and $\sigma_{\theta\theta}$ from Eqs. At the location near sample center where *r* is small, the approximation (7.13) can be used to evaluate stresses for a better accuracy. Their distribution at different times are shown by Figs. 7.3 and 7.4. It can be seen from these figures that, while σ_{rr} is always tensile, $\sigma_{\theta\theta}$ can be both tensile and compressive. In this problem, mass is losing from the center, $\sigma_{\theta\theta}$ is tensile near the center and compressive near the radius.



Figure 7.1: The distribution of the dimensionless temperature θ at different times from 1*s* to 600 *s* in radial heating condition.



Figure 7.2: The distribution of the dimensionless density $\overline{\rho}$ at different times from 1*s* to 600 *s* in radial heating condition.

7.4 Numerical results with cracking

Once cracks initiate, the analytical expressions for stresses are no longer valid. With the temperature and density fields given in Section 7.3 by numerical integration, the stress



Figure 7.3: The distribution of the radial stress σ_{rr} at different times from 1*s* to 600 *s* in radial heating condition.



Figure 7.4: The distribution of the tangential stress $\sigma_{\theta\theta}$ at different times from 1*s* to 600 *s* in radial heating condition.

field is resolved using FEM with isotropic triangular mesh of size 10^{-2} cm, the same as used in chapter 3. Fig. 7.5 shows one set of crack pattern corresponding to $\sigma_c/E = 0.0833$. Cracks initiate from the disk center where the heat flux is applied and spread outward. They tend to advance in the direction perpendicular to the char front.



Figure 7.5: The maximum principle stress σ_1 when $\sigma_c/E = 0.0833$ at t = 2, 10, 20, 40, 80, 100, 120, 160, 180, 200, 240, 280 s.

In Fig. 7.6, the same crack pattern in Fig. 7.5 is plotted on the background of the density field.

Fig. 7.7 compares the crack patterns of two values of $\sigma_c/E = 0.05$ (left) and 0.0833 (right). While both have comparable crack length, the one corresponding to lower value of σ_c/E produces crack pattern that has smaller spacing.



Figure 7.6: The evolution of the maximum principle stress σ_1 along with the cracking process when $\sigma_c/E = 0.0833 t = 2, 10, 20, 40, 80, 100, 120, 160, 180, 200, 240, 280 s$.



Figure 7.7: Maximum principle stress σ_1 (top) and density field $\overline{\rho}$ (bottom) when $\sigma_c/E=$ 0.05 (left) and 0.0833 (right) at t = 270 s

CHAPTER 8

CONCLUSIONS AND RECOMMENDATION FOR FUTURE WORK

A theoretical and numerical model is developed for crack development in solids that undergo thermo-chemical decomposition. It is proposed that material develop tensile stresses and fracture due to mass depletion. Important material parameters in this theory include thermal diffusivities, ratio of char to virgin material density, pre-exponential factor, activation temperature, ratio of cracking threshold to Young's modulus, Poisson's ratio and mass loss coefficient. Nine dimensionless parameter groups Π_1 through Π_9 that characterize the model are determined. The numerical simulation uses linear triangle FEM and implemented in FORTRAN programming language. Material damage is modelled by element extinction which introduces another characteristic length scale which is the mesh size. MPI (Message Passing Interface) is used to parallelize the code, thus making very fine mesh resolution possible. Mathematical morphology algorithms are developed and coded in MATLAB. They are used to analyze the crack morphologies produced and can be also applied to a broad range of network patterns. Furthermore, partial analytical solutions are derived for the circular domain under axis-symmetric condition along with numerical simulations of the crack. From the numerical simulations, it is found that there are groups that influence the morphology of the crack patterns while others just simply rescale the characteristic times . In particularly, the competitions between two groups Π_3 and Π_9 that characterize the thermal anisotropy and tensile strength of the material respectively, determine the loop-like or tree-like behavior of the crack pattern.

In this study, modeling of damage and thus crack propagation is done by deleting elements whose maximum principal stress exceeds a certain critical value. While this is a local approach to model cracks that have advantages of requiring no special treatment of cracks, it may cause mesh dependence (including both mesh size and mesh orientation) which is its main drawback. In this work, linear shape functions are used for displacements, thus its first spatial derivatives are constant over each element. So are the computed stress values. On the other hand, the theoretical stress field surrounding slit crack tips has very steep change. Thus the linearity of shape functions exaggerates the dependence of the stresses on the mesh size. Fortunately, thanks to MPI and the MSU High Performance Computer ICER, the mesh size used in this set of computations is very fine compared with sample size. This partially mitigates the issue of mesh size dependence.

Furthermore, unlike some numerical models such as the spring/ spring bundle network or crack band models that purposely impose statistical distribution on the spring strength or tensile strength [96], [206], we are not intended to introduce randomness into our model. However the somewhat random behavior of cracks is unavoidable because of its dependence on mesh orientation. Since the sequence of elements removed at the latter steps depends on the ones removed at the previous steps, randomness grows as crack develop. This causes crack morphology to be unsymmetrical about the middle vertical line of the sample despite of the symmetric boundary conditions. Moreover, in this study, crack morphology is analyzed from a statistical view point as it is quantified for various parameter values. The crack patterns on the left and right parts of the sample are statistically similar as seen from the appendix, section C. And despite change in mesh size, general behaviors of cracks, those determined by physical mechanisms, are unchanged as discussed in the appendix section D.

There are remedies to mesh dependence problem, among which is the nonlocal formular first developed by Bazant and Oh [94], for example the works [67] and [204], in which the stress is replaced by its weighted averaged value over a circle of some action radius *R*. The radius *R* is a function of tensile strength and fracture toughness. In this approach, damage happens at location ahead of crack tip where the weighted averaged stress exceeds its tensile strength. In local model to damage, mostly in the study of elastoplastic, there are remedies using some localization limiters. The foremost work of this type belongs to L'Hermite (1952), in which tensile strength or yield limit is proposed to be dependent on strain gradient, Floegl and Mang (1981), Schreyer and Chen (1984), Mang and Eberhardteiner (1986) strain gradient into yield function; Aifantis (1984), Bazant and Belytschko (1987) higher order strain gradient is included into strength definition. In Abaqus [205], it is done via scaling the strain with characteristic element size as discussed in Section 24.2.3 "Damage evolution and element removal for ductile metals". [204] reduces the tensile strength when larger finite element size is used while [203] suggests keeping the finite element size fixed in the regions around crack tips to avoid mesh dependence. [202] studies the influence of minimum element size on the determination of stress intensity factor. Willis [207] shows that one practice that can be used to reduce the the mesh dependence of FEM commercial codes is to adjust the fracture energy with chosen element size. According to the study of Guo *et. al.* [208], the chosen mesh size should be small enough compare with plastic zone length to capture the gradients around crack tips. When the mesh size is sufficiently fine, the zagged surface can represent micro defects.

Other than damage models, there are recently developed numerical approaches to cracks which are shown to be mesh independent. Such examples include damage mechanics, phase field model or XFEM which are applicable to various types of materials from elastic to viscoelastic and plastic. More details about the derivations of the XFEM and phase field model for the linear elastic fracture problem are found at the Appendix, Sections E and F. The problem can be extended to 3D which is much more computational expensive but is expected to be feasible with the use of parallel library such as MPI.

The model considered in this study the greatly simplified one from the general road map outlined earlier in the Introduction chapter. Thus there are great possibilities to expand it to obtain a more detailed descriptions of the related physical processes. For example, the solid material is not necessary only isotropic. Also large deformation approach can be used for materials exhibiting nonlinear elastic behavior. Moreover, thermal degradation turns solids into porous substances, thus poroelasticity model can be used. Current model assumes that material damage is induced by mass depletion stress which are tensile, a more general model can consider damage due to compressive stress. Moreover thermal and mechanical properties such as thermal diffusivities, mechanical strength, Young's modulus, etc...can change with temperature and density. In this model, cracks have no influence upon heat transfer inside solids. More detailed model can treat cracks as adiabatic which causes temperature jump across their surfaces using the discontinuous crack function of XFEM. The effects of mechanical boundary conditions or constraints can be considered, for example grip can be used instead of roller condition.

Current work has not yet model flame, the radiative and convective heat transfer provided by the flame is represented by a constant heat flux instead. Future work can include chemical reactions and transportation of energy and momentum of species in the gas phase to model ignition and flame spread. This requires solving set of chemically reactive convective diffusive flow equations in the gas phase. Reactants usually involve hundreds of species which are free radical and ions but can be simplified using mixture fraction formulation. The resulting PDE systems for species concentration and flow are highly nonlinear because they involve the exponential Arrhenius terms, convective terms and need to be solved by nonlinear numerical methods. Moving fluid exerts shear force on the solid upper surface. Furthermore, as outlined earlier in the Introduction chapter, there is a coupling between crack of solid phase and flame in gas phase. In particular, the existence of cracks allows flammable gaseous to be released directly into gas phase. High pressure also exerts an opening traction on crack surfaces. **APPENDICES**

APPENDIX A

AN ANALYTICAL SOLUTION UNDER SIMPLIFIED CONDITIONS.

The stress equilibrium equations, Eqs. (2.23), (2.24) can be written in terms of displacements u and v using Eq. (2.22), which relates the strain to the displacements and Eqs. (2.19), (2.20), (2.21), which relate stress to strain as

$$\frac{\partial^2 u}{\partial x^2} + \frac{1-\nu}{2} \frac{\partial^2 u}{\partial y^2} + \frac{1+\nu}{2} \frac{\partial^2 v}{\partial x \partial y} = \gamma \frac{1+\nu}{2\rho_0} \frac{\partial \rho}{\partial x'},$$
(A.1)

$$\frac{\partial^2 v}{\partial y^2} + \frac{1-\nu}{2} \frac{\partial^2 v}{\partial x^2} + \frac{1+\nu}{2} \frac{\partial^2 u}{\partial x \partial y} = \gamma \frac{1+\nu}{2\rho_0} \frac{\partial \rho}{\partial y}.$$
 (A.2)

In the special case when v = v(y), u = 0, Eq. (A.1) becomes $\frac{\partial \rho}{\partial x} = 0$ and Eq. (A.2) becomes

$$\frac{\partial^2 v}{\partial y^2} = \gamma \frac{1+\nu}{2\rho_0} \frac{\partial \rho}{\partial y'},\tag{A.3}$$

which is integrable. If the boundary conditions are appropriate, an analytical solution exist. With u = 0, v = v(y), the roller condition at y = 0 reduces to: y = 0 : v = 0, the traction free condition at y = H becomes

$$\frac{\partial v}{\partial y} = \gamma \frac{1+\nu}{2} \frac{\rho - \rho_0}{\rho_0}.$$
(A.4)

Now the question is, which 2D version of the boundary conditions for the left and right surfaces do not contradict with the assumption that u = 0, v = v(y). It turns out that this corresponds to roller conditions. Solving Eq. (A.3) subject to y = 0, v = 0 and Eq. (A.4) at y = H lead to the solution

$$v(y) = \gamma \frac{1+\nu}{2} \left(\frac{1}{\rho_0} \int_0^y \rho(\eta) d\eta - y \right)$$
(A.5)

provided that ρ is not dependent on the coordinate *x*.

APPENDIX B

NUMERICAL RESULTS FOR THE CASE $\sigma_c/E = 0.024$.

In the Section 3.4, the value $\sigma_c/E = 0.0333$ is used. This part presents the results for $\sigma_c/E = 0.024$ while other parameters are kept the same as those in Section 3.4. Fig. B.1 shows the distribution of the maximum principle stress σ_1 and the evolution of cracks up to $t = 6000 \ s$ at times indicated in the figure caption.

Based on the evolution of temperature, density and crack morphology, the process can be divided into four stages, which are: (a) inert heating (b) pyrolysis, not charred and, first crack initiation, (c) slightly charred, mainly initiation, (d) half charred and fast propagation, (e) almost charred, decelerated propagation. In the first stage (a), the sample temperature continues rising but is still too small to produce an appreciable mass flux. This is same as the first stage of [11]. The evidence for this stage is based on values of the surface density in which $\bar{\rho} = 0.9995$ happenning at t = 18 s is used. The first stage then is taken to evolve from t = 0 to t = 18 s. Following this stage, in stage (b), pyrolysis begins but the sample density is still well above the char value. The cracking threshold has not yet been attained by the maximum principle stress due to an insufficient density gradient. The density gradient eventually attains a sufficiently high value for the first crack to nucleate at t = 68 s, which marks the end of stage (b). At this time, the lowest density value is $\bar{\rho} = 0.8345$.

The third stage (c) is characterized by a density whose gradient decays as $t^{-1/2}$ and continue toward the next stage, as mentioned in the previous section. cracks initiate from the heated surface and propagate radially downward. The density first attains the char value $\bar{\rho} = 0.3$ when $t = 116 \ s$. Eventually, initiation activity is diminished and replaced by crack elongation and branching, which indicates transition to the next stage, stage (d) .At the end of stage (d) the density at the lower surface also attains the char value. Crack initiation is no longer observed and the existing cracks propagate at a slower pace. These



Figure B.1: Maximum principle stress σ_1 . Plots from left to right, top to bottom, correspond to t=50, 100, 300, 700, 1000, 1500, 2000, 2500, 3000, 4000, 4500, 5000, 5700, 6000 s, respectively

cracks now intersect each other, forming loops and network-like patterns. The specific times of each stage is the following: (a) from 0*s* to 18*s*, (b) from 19*s* to 68*s*, (c) from 68*s* to 116*s*, (d) from 117*s* to about 4500*s*, (e) from about 4500*s* onward.



Figure B.2: θ at the end of the first stage t = 18 s when $\overline{\rho} = 0.995$ at the middle of the heated region on the upper surface.

The correlation between crack propagation and the density field is seen more easily by plotting cracks over the density field, see Fig. B.3. It is noted that in this model, the evolution of density as well as temperature is not affected by crack presence.

It can be seen from plots for early times that the crack pattern exhibits hierarchical behavior such that long and short branches alternate with each other during this stage. This elegant pattern is similar to the distinctive periodic doubling pattern recognized in quenching or cold shock experiments by [67] in rectangle or in [126] circular sample. B.4 shows how crack patterns are affected by group Π_9 and Π_3



Figure B.3: Plots of $\overline{\rho}$ in sample with cracking pattern at *t*=100, 300, 1000, 2000, 3000, 4500, 5700, 6000 *s*. At *t* = 100 *s*, cracks have already developed while the upper surface has not been charred yet.



Figure B.4: Left: Loop behavior depends on $\Pi_9 = \sigma_c/E$. Right: Crack pattern change with $\Pi_3 = \alpha_y/\alpha_x$.

APPENDIX C

AVERAGE CRACK SPACING ON TWO HALVES OF THE SAMPLE

As mentioned in Section 3.4, the crack patterns on the left ($\bar{x} < 0.5$) and on the right ($\bar{x} > 0.5$) of the mid vertical line are not exactly the same in spite of symmetric boundary conditions. However, the two sides are statistically similar since the number of branches or average spacing on two sides are close. It can be seen from Fig. C.1 that compares the average spacing of the whole sample with the average spacing of cracks on the left side. Two samples of lower cracking threshold, $\sigma_c/E = 0.024$ (upper) and $\sigma_c/E = 0.033$ (lower), are chosen because they produce a higher number of cracks for better statistics.



Figure C.1: Average crack spacing of the whole sample and average crack spacing on the left half of the sample ($\bar{x} < 0.5$) for two cases of cracking threshold $\sigma_c/E = 0.024$ (upper) $\sigma_c/E = 0.033$ (lower).

APPENDIX D

CASE $\sigma_c / E = 0.033$ **USING DIFFERENT MESH SIZES**

In these sets of simulation, the mesh size is changed to examine its effects on crack morphology. In particular, finer mesh $h_e/2$ and coarser mesh $2h_e$ are used in this section, compared to the original mesh h_e used in the main part of the thesis.

Figure D.1 and D.3 shows the crack patterns at different times for $\sigma_c/E = 0.033$ using $2h_e$ and $h_e/2$ mesh, respectively. It can be seen by comparing three cases in Figures D.1 ($2h_e$), D.2 (h_e) and D.3 ($h_e/2$) that despite the difference in the local details, the general evolution behaviors related to inherent physical mechanisms remain unchanged. More specifically, cracks open up in the directions perpendicular to the pyrolysis front or contour level of density field and advance into char region; the intersections are made at an right angle; hierarchical patterns at early stage; cracks avoid cold walls.



Figure D.1: Maximum principal stress σ_1/E corresponding to $\sigma_c/E = 0.033$ at t = 100, 1000, 3000 and 5000 *s* from top to bottom, respectively. Mesh size $2h_e$ is used to produce this set of simulation.

The total number of crack branches or equivalently, the average crack spacing $\overline{\gamma}$ over three meshes $2h_e$, h_e and $h_e/2$ are compared by plotting them on the same figure as shown by Fig. D.4. It can be seen that the average crack spacing for all three meshes are comparable. Moreover, the crack patterns of the finer mesh ($h_e/2$) have less change than the



Figure D.2: Maximum principal stress σ_1/E corresponding to $\sigma_c/E = 0.033$ at t = 100, 1000, 3000 and 5000 *s*, from top to bottom, respectively. Mesh size h_e is used to produce this set of simulation. Note that this is the same crack pattern as shown by Fig. 3.8



Figure D.3: Maximum principal stress σ_1/E corresponding to $\sigma_c/E = 0.033$ at t = 100, 1000, 3000 and 5000 *s*, from top to bottom, respectively. The finite element size used to produce this set of cracks is $h_e/2$.

coarser mesh $(2h_e)$ when comparing with the original mesh (h_e) . The stress gradients on h_e and $h_e/2$ are resolved because the meshes are sufficiently fine. Stresses decays to the value zero away from crack tips over a distance of approximately ten finite elements in these two meshes. Thus while the mesh size cannot be chosen arbitrarily, and mesh dependency cannot be totally eliminated, the value h_e used here is sufficiently small so that finer reduction does not lead to significantly different crack patterns. Moreover, when using element removal, mesh size should be interpreted as an inherent length scale in this problem and should be chosen in range that is suitable to sample size and defect size.



Figure D.4: Average crack spacing using three meshes $2h_e$, h_e and $h_e/2$ for $\sigma_c/E = 0.033$

APPENDIX E

AN XFEM FORMULAR FOR THE THERMOELASTIC FRACTURE PROBLEM

The XFEM discretization presented in [99] for the thermoelastic problem can be applied directly to our study in which the shrinkage caused by temperature difference is replaced by shrinkage caused by mass depletion. Consider an elastic body in a domain Ω with crack Γ , subjected to an external body force \vec{X} and the following boundary conditions for displacements and stresses

$$u = \overline{u} \quad on \quad \Gamma_{u}$$

$$\sigma.n = \overline{t} \quad on \quad \Gamma_{t}$$

$$\sigma.n = 0 \quad on \quad \Gamma_{c}$$

(E.1)

Which are prescribed displacement on Γ_u , prescribed traction on Γ_t and traction free on Γ_c . The following equations of motion, equation of energy and constitutive equations are adapted from [99]

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j} + X_i \tag{E.2}$$

and

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial}{\partial x_i} \left(\frac{\partial T}{\partial x_i} \right) + R.$$
(E.3)

the general constitutive relations for the mass depletion or thermoelastic stress are taken as

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \lambda\varepsilon_{kk}\delta_{ij} + \beta\chi\delta_{ij} \tag{E.4}$$

where the coefficient β is taken tobe γ for mass depletion or $-\gamma_t(3\lambda + 2\mu)$ for thermoelastic problem and the function χ is $\overline{\rho} - 1$ or $T - T_0$ respectively. The boundary conditions
for the heat conduction problem are taken as prescribed heat flux q_0 on the boundary Γ_q .

The XFEM involves enriching the nodes surrounding cracks by the Heaviside functions and the crack tips functions given by Eq. (1.11). Each crack can be tracked by set of segments (or points, equivalently) that are not grid nodal points or by level set. This method can also be applied to multiple crack situations [98]. As a criterion for advancement of the direction of the crack tip, the angle θ can be based either on energy or stress field around crack tip. Crack advances in the direction that maximizes the rate of strain energy release, which is also the direction of maximum tangential stress. The displacements are approximated as:

$$\vec{u}(x,y) = \sum_{n \in N} N_n(x,y)\vec{a}_n + \sum_{n \in N_{cr}} N_N(x,y)[H(x,y) - H(x_n,y_n)]\vec{b}_n + \sum_{n \in N_{tip}} N_N(x,y) \sum_{m=1}^M [F_m(r,\theta) - F_m(r_n,\theta_n)]\vec{c}_{mn}$$
(E.5)

where *N* is the total number of nodes, $N_n(x, y)$ are usual shape functions (Lagrange type), $F_m(r, \theta), m = \overline{1, 4}$ are shape functions given by (1.11), $N_c r$ is the set of nodes whose support is cut by the crack and N_{tip} is the set of nodes surrounding the crack tip. In this study, temperature is taken to be discontinous across the crack face. Based on the analytical derivation of the asymptotic temperature solution near the crack tip, the temperature field is discretized as:

$$T(x,y) = \sum_{n \in N} N_n(x,y)a_n + \sum_{n \in N_{cr}} N_N(x,y)[H(x,y) - H(x_n,y_n)]b_n + \sum_{n \in N_{tip}} N_N(x,y)[F_1(r,\theta) - F_1(r_n,\theta_n)]c_n$$
(E.6)

The matrices obtained, including mass, stiffness and force matrices, derived by [99],

are similar to those using the FEM excepts there are parts involving the enriched functions ψ (including both Heaviside and crack tips functions).

$$\begin{bmatrix} C^{\theta} \end{bmatrix} = \begin{bmatrix} [C^{aa}] & [C^{ad}] \\ [C^{ad}] & [C^{dd}] \end{bmatrix}$$
(E.7)
$$\begin{bmatrix} K^{\theta} \end{bmatrix} = \begin{bmatrix} [K^{aa}] & [K^{ad}] \\ [K^{ad}] & [K^{dd}] \end{bmatrix}$$
(E.8)

$$F^{\theta} = \begin{bmatrix} (F^{a}) \\ (F^{d}) \end{bmatrix}$$
(E.9)

where the *ij* components of the matrices $[C^{aa}]$, $[C^{ad}]$, $[C^{dd}]$ are taken as

$$C_{ij}^{aa} = \int_{\Omega} N_i N_j d\Omega,$$

$$C_{ij}^{ad} = \int_{\Omega} N_i \Psi_j d\Omega,$$

$$C_{ij}^{dd} = \int_{\Omega} \Psi_i \Psi_j d\Omega.$$
(E.10)

and the components of the *K* matrices are

$$K_{ij}^{aa} = \int_{\Omega} \alpha \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) d\Omega,$$

$$K_{ij}^{ad} = \int_{\Omega} \alpha \left(\frac{\partial N_i}{\partial x} \frac{\partial \Psi_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial \Psi_j}{\partial y} \right) d\Omega,$$

$$K_{ij}^{dd} = \int_{\Omega} \alpha \left(\frac{\partial \Psi_i}{\partial x} \frac{\partial \Psi_j}{\partial x} + \frac{\partial \Psi_i}{\partial y} \frac{\partial \Psi_j}{\partial y} \right) d\Omega.$$

(E.11)

the *i* components of the forces for the thermal problem are

$$F_i^a = \int_{\Omega} N_i R d\Omega - \int_{\Gamma_q} N_i \overline{q_0} d\Gamma, \qquad (E.12)$$

and

$$F_i^d = \int_{\Omega} \Psi_i R d\Omega - \int_{\Gamma_q} \Psi_i \overline{q_0} d\Gamma.$$
(E.13)

For the elastic problem, let the vector of unknown be (u_i, v_i, d_i^u, d_i^v) , where u and v are the horizontal and vertical displacements, $(u, v)^T = \vec{a}, d_i^u, d_i^v$ are the x and y components of the enrichment degree of freedom \vec{d} that includes the Heaviside crack face parts \vec{b} and the stress function crack tip part \vec{c} . The matices of the elastic problem are the following

$$[M^{e}] = \begin{bmatrix} [M^{aa}] & [0] & [M^{ad}] & [0] \\ & [M^{aa}] & [0] & [M^{ad}] \\ & & [M^{dd}] & [0] \\ Sym. & & [M^{dd}] \end{bmatrix}$$
(E.14)
$$[K^{e}] = \begin{bmatrix} [K^{aa}_{xx}] & [K^{aa}_{xy}] & [K^{ad}_{xx}] & [K^{ad}_{xy}] \\ & & [K^{aa}_{yy}] & [K^{ad}_{yx}] & [K^{ad}_{yy}] \\ & & & [K^{dd}_{xx}] & [K^{dd}_{yy}] \end{bmatrix}$$
(E.15)
$$[K^{e}] = \begin{bmatrix} (F^{a}_{x}) \\ & (F^{a}_{y}) \\ & (F^{d}_{y}) \\ & (F^{d}_{y}) \end{bmatrix}$$
(E.16)

$$M_{ij}^{aa} = \int_{\Omega} \rho N_i N_j d\Omega$$

$$M_{ij}^{ab} = \int_{\Omega} \rho N_i \Phi_j d\Omega$$

$$M_{ij}^{bb} = \int_{\Omega} \rho \Phi_i \Phi_j d\Omega$$
(E.17)

$$\begin{split} K^{aa}_{xx,ij} &= \int_{\Omega} \left((2\mu + \lambda) \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \mu \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) d\Omega \\ K^{aa}_{xy,ij} &= \int_{\Omega} \left(\mu \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial x} + \lambda \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y} \right) d\Omega \\ K^{aa}_{yy,ij} &= \int_{\Omega} \left(\mu \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + (2\mu + \lambda) \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) d\Omega \\ K^{ab}_{xx,ij} &= \int_{\Omega} \left((2\mu + \lambda) \frac{\partial N_i}{\partial x} \frac{\partial \Phi_j}{\partial x} + \mu \frac{\partial N_i}{\partial y} \frac{\partial \Phi_j}{\partial y} \right) d\Omega \\ K^{ab}_{xy,ij} &= \int_{\Omega} \left(\mu \frac{\partial N_i}{\partial y} \frac{\partial \Phi_j}{\partial x} + \lambda \frac{\partial N_i}{\partial x} \frac{\partial \Phi_j}{\partial y} \right) d\Omega \\ K^{ab}_{yx,ij} &= \int_{\Omega} \left(\mu \frac{\partial N_i}{\partial x} \frac{\partial \Phi_j}{\partial y} + \lambda \frac{\partial N_i}{\partial x} \frac{\partial \Phi_j}{\partial y} \right) d\Omega \\ K^{ab}_{xx,ij} &= \int_{\Omega} \left((2\mu + \lambda) \frac{\partial \Phi_i}{\partial x} \frac{\partial \Phi_j}{\partial y} + \lambda \frac{\partial N_i}{\partial y} \frac{\partial \Phi_j}{\partial x} \right) d\Omega \\ K^{bb}_{xx,ij} &= \int_{\Omega} \left((2\mu + \lambda) \frac{\partial \Phi_i}{\partial x} \frac{\partial \Phi_j}{\partial x} + \mu \frac{\partial \Phi_i}{\partial y} \frac{\partial \Phi_j}{\partial y} \right) d\Omega \\ K^{bb}_{xy,ij} &= \int_{\Omega} \left(\mu \frac{\partial \Phi_i}{\partial y} \frac{\partial \Phi_j}{\partial x} + \lambda \frac{\partial \Phi_i}{\partial x} \frac{\partial \Phi_j}{\partial y} \right) d\Omega \\ K^{bb}_{yy,ij} &= \int_{\Omega} \left(\mu \frac{\partial \Phi_i}{\partial x} \frac{\partial \Phi_j}{\partial x} + (2\mu + \lambda) \frac{\partial \Phi_i}{\partial y} \frac{\partial \Phi_j}{\partial y} \right) d\Omega \end{split}$$

$$F_{x}^{a}, i = \int_{\Omega} N_{i}X_{1}d\Omega + \int_{\Gamma_{t}} N_{i}\overline{t_{1}}d\Gamma + \int_{\Omega} \frac{\partial N_{i}}{\partial x}\gamma(\overline{\rho} - 1)d\Omega$$

$$F_{y}^{a}, i = \int_{\Omega} N_{i}X_{2}d\Omega + \int_{\Gamma_{t}} N_{i}\overline{t_{2}}d\Gamma + \int_{\Omega} \frac{\partial N_{i}}{\partial y}\gamma(\overline{\rho} - 1)d\Omega$$

$$F_{x}^{d}, i = \int_{\Omega} \Phi_{i}X_{1}d\Omega + \int_{\Gamma_{t}} \Phi_{i}\overline{t_{1}}d\Gamma + \int_{\Omega} \frac{\partial \Phi_{i}}{\partial x}\gamma(\overline{\rho} - 1)d\Omega$$

$$F_{y}^{d}, i = \int_{\Omega} \Phi_{i}X_{2}d\Omega + \int_{\Gamma_{t}} \Phi_{i}\overline{t_{2}}d\Gamma + \int_{\Omega} \frac{\partial \Phi_{i}}{\partial y}\gamma(\overline{\rho} - 1)d\Omega$$
(E.19)

The time integration can be treated using the Crank-Nicholson scheme for transient heat conduction or the Newmark method for the unsteady stress balance equation. Integration can be evaluated numerically using Gaussian quadrature and Lagrange basis functions. While the computational mesh is not refined futher when cracks develop, elements that are cut by crack or contain crack tips are divided for the integration purpose. The detailed description of the integration process can be found at [99]. The cracks can be described explicitly or implicitly using level set method with two unsigned level set functions and one signed level set function. In the latter approach, the local polar coordinate and the Heaviside function can be constructed from those three level set functions.

The direction for crack advancement is determined from the maximum circumferential stress criteria. Other studies use different crack advancement criterion, such as the maximum strain energy release rate, material force or minimal strain energy density. According to maximum circumferential stress criteria which is a local approach based on stress field near crack tip, crack extends in the direction θ_m that maximizes the tangential stress $\sigma_{\theta\theta}$ which is dependend on the stress intensity factors

$$\sigma_{\theta\theta} = \frac{1}{\sqrt{2\pi r}} \left(\frac{K_I}{4} \left(3\cos\frac{\theta}{3} + \cos\frac{3\theta}{2} \right) + \frac{K_{II}}{4} \left(-3\sin\frac{\theta}{2} - 3\sin\frac{3\theta}{2} \right) \right), \quad (E.20)$$

the condition $\frac{\partial \sigma_{\theta \theta}}{\partial \theta} = 0$ at $\theta = \theta_m$ leads to

$$K_I sin\theta_m + K_{II} (3cos\theta_m - 1) = 0.$$
(E.21)

The implementation of XFEM on Abaqus by User subroutines (UEL) is also done by other studies, such as [101] and [102] with success. XFEM, however, like Fracture Mechanics, is unable to predict crack initiation. This drawback is overcome by other fracture models such as phase field model, gradient damage model or continuum damage model.

APPENDIX F

A VARIATIONAL FORMULA FOR THE PHASE FIELD MODEL OF FRACTURE

Consider the elasticity problem described by Eq. (E.1). Since the constitutive relations between stress and strain is given by Eq. (E.4), the elastic strain energy density is

$$\psi^{e}(\varepsilon) = \frac{1}{2}\lambda\varepsilon_{ii}\varepsilon_{jj} + \mu\varepsilon_{ij}\varepsilon_{jj} + \frac{1}{2}\beta\chi\varepsilon_{ii}.$$
(F.1)

The total potential energy of the body equal to the summation of elastic energy and fracture energy

$$\psi^{p}(u) = \int_{\Omega} \psi^{e}(\varepsilon) d\Omega + \int_{\Gamma} G_{c} ds$$
(F.2)

where G_c is the fracture energy per unit crack area. If steady-state assumption is taken, the Lagragian of the system will include a kinetic term which is

$$\psi^{k}(u) = \frac{1}{2} \int_{\Omega} \rho \frac{\partial u_{i}}{\partial t} \frac{\partial u_{i}}{\partial t} d\Omega$$
(F.3)

For quasi-steady state condition, the kinetic potential is negligible in the Lagragian. The potential by external force is

$$\psi^{f}(X,t) = \int_{\Omega} X_{i} u_{i} d\Omega + \int_{\Gamma_{t}} \overline{t_{i}} u_{i} ds$$
(F.4)

Now turning to the variational formula of fracture using the phase field. In phase field model, the crack is described as smeared over a length l_c by a scalar variable c that can get any value between unity and zero. In 1D, c can be assumed of taking the exponential form as

$$c(x) = exp\left(-\frac{x - x_0}{l_c}\right) \tag{F.5}$$

in which x_0 specifies the location of the crack where reas c gets the value of unity. Far away from x_0 , c drops to zero value. Obviously, c(x) is the solution of the following differential equation

$$\frac{c}{l_c^2} - \frac{d^2c}{dx^2} = 0 \tag{F.6}$$

subjected to boundary conditions $c(\pm \infty) = 0$. Following the variational principle, the weak form of (F.6) is

$$\int_{-\infty}^{\infty} \frac{dv}{dx} \frac{dc}{dx} + \frac{vc}{l_c^2} dx = 0$$
 (F.7)

and the functional associated with the weak form is

$$I(c) = \frac{1}{2} \int_{-\infty}^{\infty} \left(\frac{dc}{dx}\right)^2 + \frac{c^2}{l_c^2} dx.$$
 (F.8)

Thus the expression of I(c) in 2D is given by

$$I(c) = \frac{1}{2} \iint_{\Omega} \nabla c \cdot \nabla c + \frac{c^2}{l_c^2} dx dy.$$
(F.9)

The fracture surface energy density is defined in term of the phase field function c(x, y) as

$$\gamma(c) = \frac{1}{2} \left[l_c \nabla c. \nabla c + \frac{c^2}{l_c} \right]$$
(F.10)

From (F.10) and (F.2), the modified total potential energy of the system include the strain energy and the crack surface energy which is

$$\psi(u,c) = \iint_{\Omega} g(c)\psi^{e}(\varepsilon)d\Omega + \frac{G_{c}}{2}\iint_{\Omega} \left[l_{c}\nabla c.\nabla c + \frac{c^{2}}{l_{c}} \right] d\Omega$$
(F.11)

in which ψ^e is given by Eq. (F.1), g(c) is some degradation function, taken by [103] as

$$g(c) = [(1-c)^2 + d]$$
 (F.12)

d is a small positive number for numerical stability. From (F.11), (F.4) and principal of virtual displacement, the governing equations are derived, which are

$$[(1-c)^{2}+d]\frac{\partial\sigma_{ij}}{\partial x_{j}} + X_{j} = 0 \quad in \quad \Omega$$

$$[(1-c)^{2}+d]n_{j}\sigma_{ij} = \overline{t_{i}} \quad on \quad \Gamma_{t}$$

$$u_{i} = \overline{u_{i}} \quad on \quad \Gamma_{u} \qquad (F.13)$$

$$-G_{c}l_{c}\frac{\partial c}{\partial x_{i}}\frac{\partial c}{\partial x_{i}} + \left[\frac{G_{c}}{l_{c}} + 2\psi^{e}(\varepsilon)\right] = 2\psi^{e}(\varepsilon) \quad \in \Omega$$

$$\frac{\partial c}{\partial x_{i}}n_{i} = 0 \quad on \quad \Gamma$$

The stiffness and residual matrices of the FEM formulation are derived for the phase field variable c and the displacement fields u in [104].

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