INVESTIGATING LEAK RATES FOR “LEAK-BEFORE-BREAK” ASSESSMENTS

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Abstract

An investigation into the thermo-mechanical closure effect when a fluid leaks through a crack is presented here. The extended finite element method is the modelling scheme adopted for this, and the application of heat flux and pressure jump conditions along the crack is one of the novel contributions of this work. By modelling the fluid as one dimensional steady state and obtaining a heat transfer coefficient, it has been shown here that coupling the fluid with the structure is possible all within a single element. Convergence studies done with analytical models as a benchmark demonstrate the accuracy of the new method. Simulations are performed with the new element for conditions seen in both gas cooled and water cooled reactors. Significant crack closure is observed when the bulk fluid temperature is $20^\circ C$ hotter than the structure. It was also found that the amount of closure due to crack wall heating varies depending on the external boundary conditions, this is quantified in the thesis.
Declaration

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Nomenclature

\[ [[N]_I] \] Jump in shape functions \([N]_I\)

\([B]_I\) Matrix of shape function derivatives

\([D]\) Conductivity matrix

\([N]_I\) Matrix of shape functions \(N_i\)

\(\alpha_T\) Thermal expansion coefficient

\(\bar{\sigma}\) Flow stress

\(\dot{m}\) Mass flow rate

\(\epsilon_e\) Elastic strain

\(\epsilon_T\) Thermal strain

\(\eta\) Shape function parameter

\(\Gamma\) Boundary of finite element domain

\(\gamma\) Ratio of specific heats

\(\Gamma_c\) Crack contour

\(\gamma_k\) kth branch enrichment function

\(\kappa\) Kosolov coefficient

\(\lambda\) Shell parameter

\(\mu\) Lamé coefficient

\(\mu_f\) Fluid viscosity

\(\nu\) Poisson’s ratio

\(\nu_i\) Specific density of phase \(i\)

\(\Omega\) Finite element domain

\(\phi\) Level set function
Π  Pressure drop equation
ψ  Bimaterial enrichment function
ρ  Density
ρc  Crack outlet density
σ  Stress
σy  Yield stress
σref  Reference stress
τ  Shear stress
Θ  Relaxation time
θ  Crack tip angle
θc  Effective crack angle
τs  Surface traction
e  Unit vector
n  Normal vector
u  Displacement vector
Υ  Geometric correction factor for COA
Ξ  Critical mass flux equation
ξ  Shape function parameter
A  Crack opening area
a  Crack half length
CD  Discharge coefficient
cg  Specific heat of gas
cl  Specific heat of liquid
cp  Specific heat at constant pressure
cv  Specific heat at constant volume
Cd  Entrance discharge coefficient
Cijkl  Hooke tensor
Dh  Hydraulic parameter
$E$  Young’s modulus

$F$  Sum of pressure loss terms

$f$  Fanning friction factor

$F_{fric}$  Frictional pressure drop

$F_{inert}$  Inertial pressure drop

$F_{recirc}$  Recirculation pressure drop

$G$  Strain energy release rate

$g$  Plasticity correction factor for COA

$G_c$  Critical mass flux

$H$  Heaviside function

$h$  Enthalpy

$H^1$  Energy norm of a vector

$H_1$  Sobolev space

$h_c$  Heat transfer coefficient

$k$  Conductivity

$k_c$  Cohesive crack parameter

$K_e$  Elastic stress intensity factor

$k_f$  Fluid conductivity

$K_I$  Mode I stress intensity factor

$K_{ep}$  Elastic-plastic stress intensity factor

$K_{G+L,G}$  Channel length correction factor

$l$  Crack length

$L^2$  Norm of a vector

$l_e$  Outlet crack length

$l_i$  Inlet crack length

$L_r$  Ratio of applied load to limit load

$M$  Bulging Parameter

$m$  Ramsberg Osgood exponent
\( n \)  
Thermal equilibrium exponent

\( N_e \)  
Partial change of quality at throat

\( N_I \)  
Ith shape function

\( N_x \)  
Non-equilibrium parameter

\( n_{tL} \)  
Number of crack path turns

\( Nu \)  
Nusselt number

\( p \)  
Pressure

\( p_0 \)  
Stagnation pressure

\( p_a \)  
Phase change acceleration pressure drop

\( p_c \)  
Critical pressure

\( p_e \)  
Entrance pressure drop

\( P_f \)  
Wetted perimeter

\( p_f \)  
Frictional pressure drop

\( p_k \)  
Corners pressure drop

\( p_{aa} \)  
Area change pressure drop

\( p_{ex} \)  
Crack exit Pressure

\( Pr \)  
Prandtl number

\( Q \)  
Heat

\( q_i \)  
ith component of heat flux

\( R \)  
Radius of curvature

\( R_a \)  
Roughness

\( Re \)  
Reynolds number

\( s \)  
Ratio of applied stress to flow stress

\( S_0 \)  
Stagnation entropy

\( S_{gc} \)  
Gas entropy at critical plane

\( S_{Lc} \)  
Liquid entropy at critical plane

\( T \)  
Temperature

\( t \)  
thickness of structure
$T_\alpha$ $\alpha$th temperature degreee of freedom

$T_{bulk}$ Bulk fluid temperature

$t_{eff}$ Effective crack depth

$u_\alpha$ $\alpha$th displacement degreee of freedom

$v$ Fluid velocity

$W$ Strain Energy

$w$ Crack opening displacement

$w_e$ Outlet crack opening

$w_i$ Inlet crack opening

$w_{eff}$ Effective crack opening

$X$ Quality

$X_c$ Non-equilibrium quality

$X_e$ Equilibrium quality

$Y$ Ramsberg Osgood constant

$z$ Through thickness (channel) parameter
Acronyms

**AGR** Advanced Gas Cooled Reactor.
**BWR** Boiling Water Reactor.
**CCL** Critical Crack Length.
**CFD** Computational Fluid Dynamics.
**COA** Crack Opening Area.
**COD** Crack Opening Displacement.
**EVUT** Equal Velocity Unequal Temperature.
**FAD** Failure Assessment Diagram.
**FEM** Finite Element Method.
**HRM** Homogeneous Relaxation Model.
**HTC** Heat Transfer Coefficient.
**LbB** Leak-before-Break.
**NPP** Nuclear Power Plant.
**PDE** Partial Differential Equation.
**PIF** Possible-Impossible Flow.
**PUFEM** Partition of Unity Finite Element Method.
**PWR** Pressurised Water Reactor.
**RPV** Reactor Pressure Vessel.
**SIF** Stress Intensity Factor.
**XFEM** Extended Finite Element Method.
Chapter 1

Introduction

This thesis focusses on the calculation of leak rates for Leak-before-Break (LbB) assessments using a new finite element method. This new tool was developed to help investigate the effect of crack closure due to a leaking thermofluid heating the crack walls. The hypothesis is that as bulk fluid temperature increases, crack opening area will reduce and make leak rate calculations which ignore temperature effects non-conservative. The new element is built using the Extended Finite Element Method (XFEM), which is a new meshless method in finite elements based on the partition of unity method.

It is known that there can be substantial uncertainty when calculating leak rates and often safety factors are used to account for this. There is a motivation, therefore, to try and reduce this uncertainty. By bringing together state of the art leak rate models, and the latest finite element techniques in a new package, investigations into leak rates can be performed more effectively and potentially reduce uncertainty.

The new element will combine all the thermal hydraulics of the leak rate with the structural aspects of the crack in the component. This is achieved by implementing conditions along the crack which are dependent on the fluid, namely pressure and heat flux. These fluid parameters are derived from fluid mechanics which use the crack opening displacement as an input variable. Therefore there is a coupling between the fluid and the structure which must
be accounted for. Using the extended finite element method means that the coupling can be achieved on a sub element level. This is down to the ability of XFEM to augment the standard finite element approximation with enrichment functions which describe the physics. Therefore, special behaviour, like a jump in displacement across the crack, or the singularity in strain at the crack tip, can be added to the approximation to help the solution converge. The suitability of enrichment functions for the application of a leaking fluid through a crack are investigated in this thesis. The hypothesis implies that the investigations will require thermo-mechanical simulations. Therefore, the model presented here is thermo-mechanical, with thermal and mechanical boundary conditions imposed along the crack due to the presence of a leaking thermofluid.

By utilising the meshless properties of XFEM, and incorporating a fluid model within elements, the new finite element scheme will require no refined meshes, and output a leak rate straight from the simulation. The accuracy and effectiveness of this new scheme is compared to standard finite elements and analytical models.

The thesis will be structured in the following way; Firstly there will be a background to the LbB concept in Nuclear Power Plants (NPP). Then a literature review will give a summary of the state of the art in leak rate calculation, relevant fracture mechanics and XFEM. The next three chapters are the analysis and results. Chapter 4 focusses on the thermal hydraulics theory with some numerical results. Chapter 5 is the mathematical description of the new element, together with the results of a convergence study and example simulations. Chapter 6 presents the results of more simulations with a discussion of the thermal stresses and crack closure. The final chapter is a summary of the main findings.

The original contributions from this work are:

- A single phase fluid model was derived from the steady state transport equations for a 1-D channel and compared against an industry code. Good agreements are observed.
- Numerical experiments performed, show that heat transfer from fluid to crack walls
reduces leak rate due to crack closure, and also changes fluid properties.

- A jump condition was imposed along a crack in XFEM, to model heat flux and pressure jumps due to a leaking fluid. Convergence studies indicate that this was an accurate method of modelling this problem.

- A thermal finite element approximation, which can account for crack face conditions ranging from insulated to high heat flux is implemented.

- Numerical experiments done with the new finite element, show crack closure is sensitive to external boundary conditions, but in all cases leak rate is reduced when heat transfer is included.
Chapter 2

Background

The worldwide demand for energy is rising, and there is an ever increasing need for low carbon, reliable energy sources. Nuclear power provides an alternative to burning fossil fuels by harnessing the huge amount of energy released by nuclear fission. The potential dangers associated with this form of electricity generation dictate that the highest levels of safety are in place to allow their operation. The accident at Fukushima only served to re-inforce the need to have clear and stringent safety measures that give the public confidence in nuclear power.

There are many different designs of nuclear reactors around the world. However, all share a common design feature, which is that they all use a fluid to cool the fissile material in the core. This core can reach temperatures in excess of 2000 °K, therefore the fluid and flow must have the right characteristics to ensure adequate cooling. Various different fluids have been tried as coolants, however the most widely used is water, in either a Pressurised Water Reactor (PWR) or a Boiling Water Reactor (BWR). This is because it has both the correct coolant properties, and also acts as a moderater for the nuclear reaction. The water in a PWR is under high pressure in the primary circuit, so that it stays in the liquid phase when the temperatures exceed 300 °C. This hot water then enters the steam generators where the the heat is transfered to the secondary water, and steam is produced to drive the turbines.
A simplified illustration of the primary circuit of a PWR is shown in Fig. 2.1. The Reactor Pressure Vessel (RPV) contains the nuclear fuel and coolant, connecting pipes link the steam generators and pressuriser, and there is a primary pump to maintain the high coolant flow. Emergency coolant systems and other auxiliary systems are omitted here for simplicity.

![Diagram of a PWR primary circuit](image)

Figure 2.1: Main components in the primary circuit of a Pressurised Water Reactor (PWR)

The typical operating pressure for a PWR is 160 Bar. This, coupled with the fact that there is radioactive material in the reactor core, considerably increases the structural integrity requirements of components within these plants. The pressure vessels and piping must be designed to stay within code allowables. Also, due to the long periods of time that nuclear power stations are in operation for, there is material degradation and fracture issues that must be addressed. Nuclear components are manufactured to the highest specification, they are inspected for defects, and, if they pass these quality inspections, they can be commissioned for use. Despite the high resolution of modern day inspection techniques, there will still be some defects that are too small to be detected. Therefore structures have to be assessed using fracture mechanics principles to see how small flaws will develop over time. Structural Integrity Assessment procedures give guidance on how to assess these defects, then safety

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1The total reactor flow for Sizewell B is 18740 kg/s
cases can be built based on these analyses. In addition to, and supporting all this, there is another line of argument for the structural integrity of NPP and that is the LbB philosophy. This essentially says that if there is a crack that breaks through the wall of a component, then a leak will be detected well before that crack becomes so big that a sudden catastrophic failure would occur. So even if a crack developed larger than anticipated, LbB ensures that there will be sufficient time to carry out any corrective action before there is a full guillotine type fracture. This potentially alleviates the need for some of the costly pipe whip restraints and jet impingement shields in the primary circuit.
Chapter 3

Literature Review

3.1 Leak-before-Break

LbB is increasingly being used as part of safety justifications, particularly within the nuclear industry [1]. In order to make a LbB case for a pressurised component, it is necessary to determine leak rates through cracks under the operating load conditions. The R6 assessment procedure provides equations to calculate leak rates from a known Crack Opening Area (COA) [2]. However, leak rates evaluated from this calculational route, however, can be subject to significant safety factors being applied due to various uncertainties. As such there is a strong motivation to better understand the factors affecting leak rates through cracks in pipes, so that there is less conservatism in the leak rate estimation. To perform the investigations into these factors, a special finite element has been developed. This element uses the XFEM to model cracks with boundary conditions on the faces due to the leaking fluid. Previous work has shown that leak rates through a crack are affected by closure of the crack, which is due to convective heat transfer from the leaking fluid to the crack faces. Therefore, the new 2-D element is used to investigate the effect of heat transfer and pressure acting on the crack faces.
3.1.1 Leak-before-Break Concept

The formulation of a LbB argument can be explained with the aid of a diagram like the one shown in Fig. 3.1 [3]. This diagram shows crack depth (z) normalised to pipe wall thickness (t) as a function of crack length (2a). There is an initial part through crack which could grow by fatigue, tearing or any other process due to the operating load and environmental conditions. The crack will reach a point where the remaining ligament is sufficiently small to cause snapthrough. So long as this point is at a point well before the Critical Crack Length (CCL) but crack length is still large enough to allow a detectable leakage, Leak-before-Break can be applied.

![LbB Diagram](image)

*Figure 3.1: LbB diagram*

The case of multiple cracks in the context of LbB is considered in [4]. Distributions of cracks, crack growth laws and interaction laws are investigated, and it is concluded that catastrophic failure could occur without prior detectable leak, if the amount of initial cracks is high, and the degree of crack interaction is strong. Therefore, a multiple crack LbB case would require special treatment, and in most cases would probably not be possible. The LbB principle in the French Nuclear Industry was first documented in the work by Faidy [5]. This started a large research programme which resulted in a validated LbB methodology and computational tools to assist the calculation of leak rates. Stadmuller presents LbB applied to Nuclear Power Plant
(NPP) in Germany [6]. The paper discusses the results of a large research project dedicated to LbB, and the main observation was that with the use of an LbB curve, catastrophic failure before detectable leak could be taken as highly improbable. This load-bearing capacity diagram was a plot of external bending moment on a pipe against circumferential crack angle, and all failures occurred beneath the LbB curve, that is in the leakage region.

In terms of actually carrying out a LbB assessment, it may be sufficient to use the procedure and associated equations given in R6. This would typically be performed with an excel spreadsheet. However, if more accuracy is required it may be necessary to consider Finite Element Modelling. This motivates the development of a special LbB tool, namely, a special finite element which can model leak rates and is implemented in a FE code. This tool will be used to test the thermo-mechanical behaviour of a leaking fluid in a structure. It is thought that the leaking thermo-fluid will heat up the crack walls causing thermal expansion and reduction of the crack opening. Desirable properties of this finite element would be minimal meshing of the crack, no post processing to obtain COA and leak rate, and computational efficiency.

XFEM was chosen as the preferred modelling technique to solve the governing Partial Differential Equation (PDE). This uses information already known about the problem to augment the finite element approximation so that a solution is obtained with relative ease. The building of such an element requires the solution of fundamental problems, which are then used within individual elements so that complex behaviour can be captured without a refined mesh. So in summary, the new finite element will incorporate the discontinuities and singularities associated with mechanical and thermal fields in the solid, as well as a fluid mechanics model to account for the leak. The interaction between this fluid model and the solid model will be the convective heat transfer and pressure on the crack faces.
3.2 Crack Opening Area

3.2.1 Analytical Model

Crack opening shape in a pipe is generally assumed to be elliptical, so the crack opening area $A$ is calculated in terms of the crack opening displacement and crack length as follows [7]:

$$A = \pi a w$$  \hspace{1cm} (3.1)

where $a$ and $w$ are the crack half length and opening respectively. COA can also be obtained from the Stress Intensity Factor (SIF). Starting from the expression for strain energy release rate:

$$G = -\frac{1}{2t} \frac{\partial W}{\partial a}$$  \hspace{1cm} (3.2)

where $G$ is the strain energy release rate, $t$ is the thickness of the structure, $W$ is the potential energy and $a$ is crack half length. For thin plates and shells with membrane forces acting on them, the load on the crack can be treated as surface forces acting along the crack, see Fig. 3.2 [8]. The strain energy may be expressed in the form of the surface integral:

![Figure 3.2: Loading of a crack with superposition of membrane stress and pressure of leaking fluid](image)

Figure 3.2: Loading of a crack with superposition of membrane stress and pressure of leaking fluid
\[ W = -\frac{1}{2} \int_{\Gamma_c} \tau_s \cdot u d\Gamma \]  

(3.3)

where \( \tau_s \) and \( u \) are the surface traction and displacement vectors respectively. The integral extends over the surfaces \( \Gamma_c \) with non-zero forces, i.e. over the two crack surfaces. For the case of constant membrane stress, \( \sigma \), and internal pressure, \( p \), the integral becomes

\[ W = -\frac{1}{2}(\sigma + p) \int_{\Gamma_c} u \cdot n d\Gamma \]  

(3.4)

By introducing the average of the COA, \( A \), over the wall thickness

\[ A = \frac{1}{t} \int_{\Gamma_c} u \cdot n d\Gamma \]  

(3.5)

and the identity

\[ G = \frac{K_I^2}{E'} \]  

(3.6)

a relation between the COA and the SIF, \( K_I \), is obtained:

\[ K_I^2 = \frac{(\sigma + p)E'}{4} \frac{\partial A}{\partial a} \]  

(3.7)

where \( E' = E \) for plane stress and \( E' = E/(1-\nu^2) \) for plane strain with Young’s Modulus, \( E \), and Poisson’s ratio, \( \nu \). Thus if the SIF for the geometry under consideration is known, COA can be calculated from the determination of the integral

\[ A = \frac{4}{(\sigma + p)E'} \int_0^a K_I^2(x) dx. \]  

(3.8)

The derivation shown here does not take into account the fact that, for curved shells, the SIF depends on a variable perpendicular to the shell surface. This variable accounts for the bulging effect, which causes the COA to be different on each side of the shell. Using a mean value for the SIF can give an approximate value. In reality COA is affected by geometric and
loading conditions and material and thermal effects, so there is a large amount of literature
dedicated to quantifying these effects.

### 3.2.2 Cylindrical Shells

The SIF for cracks in shallow shells are expressed in the form

\[ K_I = M(\lambda)(\sigma + p)\sqrt{\pi a} \]  

(3.9)

where the bulging factor, \( M \), is a function of the shell parameter, \( \lambda \), where

\[ \lambda^4 = 12(1 - \nu^2) \frac{a^4}{R^2 t^2} \]  

(3.10)

where \( R \) describes the radius of curvature. Incorporating equation (3.9) into (3.8), the following expression for COA is obtained

\[ A = \frac{4\pi(\sigma + p)}{E'} \int_0^a M^2(\lambda)da. \]  

(3.11)

It is convenient to express COA as a multiple of the COA, \( A_0 \), for a crack in a plate, i.e.

\[ A = \Upsilon(\lambda)A_0 \]  

(3.12)

where

\[ A_0 = \frac{2\pi a^2(\sigma + p)}{E'} \]  

(3.13)

and where \( \Upsilon = \frac{2}{\lambda^2} \int_0^\lambda M^2(\lambda)\lambda d\lambda \) According to Kastner et. al. [9], for practical application it is convenient to use a simple analytical formula for axial cracks

\[ \Upsilon(\lambda) = 1 + 0.1\lambda + 0.16\lambda^2 \]  

(3.14)
and for circumferential cracks

\[ \Upsilon(\lambda) = (1 + 0.117\lambda^2)^{1/2} \]  

(3.15)

### 3.2.3 Elastic-Plastic

If the plastic effects are ignored for cracks in pressure vessels fabricated from ductile materials, the leak area may be underestimated considerably. This is because crack tip blunting leads to an increase in crack opening area. For the case of small scale yielding, Kastner [9] introduces a Irwin type correction, adding the plastic zone to the physical crack size. For cracks in plates, the factor \( g \) can be used as a plasticity correction, i.e.

\[ A = g(s)A_0 \]  

(3.16)

where

\[ g(s) = \left( 1 + \frac{s^2}{2} \right)^{3/2} - \left( \frac{s^2}{2} \right)^{3/2} \]  

(3.17)

and where \( s = \sigma/\bar{\sigma} \) and \( \bar{\sigma} \) is the flow stress. This is the solution given in R6 for COA, and it should be noted that this is limited to small plastic zones. To extend the range in which plasticity can be described, a Dugdale model can be used. The plasticity factor \( g(s) \) is a relatively complicated integral given in [8], and the area is calculated as follows:

\[ A = g(s)\Upsilon(\lambda)A_0 \]  

(3.18)

The analytical models considered thus far are the ones recommended in R6.

A summary of the state of the art models used for calculating COA is presented below. Ghosh provides estimations of crack opening area for curved shells such as pipes in the primary circuit of a nuclear reactor [10]. Elastic solutions are given for tension, bending and internal pressure
on a pipe. There are also solutions containing plastic corrections, as well as full elastic plastic fracture mechanics models. COA analyses for circumferential through-wall cracks in pipes are given by Rahman [11] [12] [13]. These papers provide the analytical models, followed by validations, and finally some realistic cases involving off centre cracks, weld residual stresses, thickness transitions and restraint of bending. It was found that weld residual stresses have a much bigger effect on COA when the pipe diameter and thickness is large. It was also shown that restraint of bending can in fact reduce the crack opening. This is particularly so if the crack is in areas close to a nozzle or restraint from the rest of the piping system. This means that the actual leak rate would be less than the leak rate calculated using analyses that assume that the pipe is free to rotate. Specific geometries require more careful analysis and often a full finite element simulation is required. However COA can often be conservatively estimated using simplified models, an example of this is given by Sharples et al. [14] where an COA is calculated for an attachment welded to a plate. It is shown that COA can be estimated conservatively by considering a crack in a plate, and that those solutions are within 20% of the actual values for the more complex geometry. Given that LbB is a defence in depth safety argument, this is acceptable, and can save considerable time and effort when carrying out an LbB assessment.

Takahashi [15] gives simplified evaluation methods for the COA and critical crack size for a circumferential through wall crack in a pipe subject to axial and bending loading. The paper shows that for the elastic case, COA is well estimated by formulae with corrections for geometric effects, and for plastic COA the reference stress method can be used. COA and leak rate calculations were performed in [16] using pipe elements. The procedure presented shows that a piping system with a cracked component can be studied with limited computer cost and manpower. This is a property that is desirable for a LbB finite element, one that is both easy to use and computationally efficient.
3.3 Fluid Mechanics

Flow through narrow channels can be likened to that of flow through channels with a geometry as shown in Fig. 3.3. Three distinct flow regions occur depending on the thermal hydraulic conditions. Compressible flow must be considered due to the large pressure difference. For cracks with large width and small depth, the pressure energy is mainly used to accelerate the flow and viscous force can be neglected, leading to critical flow. When the crack width is very small and the crack depth is very large, the flow in the crack will be compressible laminar flow. The next flow regime is compressible turbulent flow, which occurs when the crack depth is relatively large and the crack width is relatively small. The crack surfaces are very rough, so the flow is assumed to reach completely rough turbulent flow.

![Figure 3.3: Idealisation of flow channel](image)

3.3.1 Single phase

When considering leakage of a high pressure gas through a narrow orifice, it is assumed that the flow would attain critical conditions at the crack exit. However, if wall friction is sufficiently high, then choking may not occur. It is therefore important to obtain the correct correlation.
for friction. The surfaces of naturally occurring cracks are rough [17]. In the situation where there is a flow of single phase fluid through a narrow orifice, it is sufficient to use the steady state flow energy equation. Li. et al. [18] derive the following expressions for mass flow rate for lamina, turbulent and critical flow. Considering the pressure drop $dp$ over a length of channel $dz$:

$$-dp = 0.5 f \rho(z)v(z)^2 \frac{dz}{2w}$$

(3.19)

where at $z = -t/2$, $p = p_0$ and at $z = t/2$, $p = p_{ex}$ and where it is assumed that

$$\frac{p(z)}{\rho(z)} = \frac{p_0}{\rho_0}$$

(3.20)

and Reynolds number is defined to be $Re = \frac{\dot{m}}{\alpha \mu_f}$, where $\alpha$ is half the crack length, $f$ is the Fanning friction factor, $v$ is the fluid velocity and $\mu_f$ is the viscosity of the fluid. The leak rate is given by:

$$\dot{m} = 2\rho(z)awv(z)$$

(3.21)

which for turbulent flow becomes:

$$\dot{m} = 2awp(z)v(z) = 2aw \sqrt{\frac{(p_0^2 - p_{ex}^2)2w}{t(\rho_0/p_0)f}}$$

(3.22)

where $p_{ex}$ is the atmospheric pressure, $p_0$ and $\rho_0$ are the pressure and density in the pressure vessel.

Correlations for the friction factor are given by the following expressions.

$$f = [1.82 \log_{10}(w/R_a) - 0.77]^{-2}$$

(3.23)
from Spence et. al [19] and

\[ f = [2.035\log_{10}(w/R_a) - 0.657]^{-2} \tag{3.24} \]

from Gardiner and Tyrell [17]. In R6 the friction factor is given by the following [19]:

\[ f = [3.64\log_{10}(2w/R_a) - 2.636]^{-2} \tag{3.25} \]

which is eqn. (3.23) divided by four.

For critical flow the following formula is used in [18]:

\[ \dot{m} = A \sqrt{\frac{2}{\gamma + 1}} \left( \frac{2}{\gamma + 1} \right)^{\frac{2}{\gamma - 1}} p_0 p_0 \tag{3.26} \]

where \( \gamma \) is the ratio of the specific heats.

If the flow is lamina (\( Re < 2000 \)), the flow rate is given by [18]:

\[ \dot{m} = \frac{2(p_0^2 - p_{in}^2) A^2}{C \mu f p_0 / p_0 tk} \tag{3.27} \]

where \( C = 96 \).

Leak rate is calculated in R6 according to the formula:

\[ \dot{m} = C_D (p_0 p_0)^{1/2} w l \tag{3.28} \]

where \( C_D \) is a discharge coefficient, \( p_0, p_0 \) are the inlet density and pressure, and \( w, l = 2a \) are the crack width and length.

Figures 3.4, 3.5 and 3.6 show a comparison of the Li. [18] models with R6 for carbon dioxide at 800°C and various inlet pressures. Three different crack configurations were modelled in order to simulate lamina, turbulent and critical flow conditions. There is also a plot of the pressure drop for laminar flow shown in Fig. 3.7.
Figure 3.4: Comparison of leak rates between R6 and Li [18], crack length 80mm, width 0.015mm, depth 100mm

Figure 3.5: Comparison of leak rates between R6 and Li [18], crack length 120mm, width 0.07mm, depth 10mm
Figure 3.6: Comparison of leak rates between R6 and Li[18], crack length 5mm, width 0.5mm, depth 5mm

Figure 3.7: Pressure through thickness for Li[18] laminar flow model.
3.3.2 Crack Morphology

Cracks are known to have paths that change direction and as such there have been several investigations into the effect of crack path on leak rate. Typically there are pressure losses as a multiple of the pressure heads $\rho v^2/2$. Where the number of turns determines the losses. The discharge coefficient in Eq. (3.28) is related to the sum of the pressure loss terms through the crack by [20]:

$$C_D = \frac{1}{1 + \sqrt{F}}$$

(3.29)

In Eq. 3.29, $F$ is the sum of the pressure loss terms due to frictional, inertial, and recirculation effects, and is given by:

$$F = F_{fric} + F_{inert} + F_{recirc}$$

(3.30)

where

$$F_{fric} = \frac{f t_{eff}}{2 w_{eff}}$$

(3.31)

$$F_{inert} = \frac{w_{eff}}{w} n_t L 2 \theta_c$$

(3.32)

$$F_{recirc} = n_t L \left(1 - \left(\frac{w_{eff}}{w}\right)^2\right)$$

(3.33)

and where $w_{eff}$ and $t_{eff}$ are the effective width and depth of the crack after crack turns ($n_t L$) are considered, as shown in Fig. 3.8. The roughness is varied between a local and global value, depending on the crack opening displacement [21]. For smaller openings the fluid follows the contours of the crack and hence a longer crack is realised, with local roughness used. As the crack widens the fluid will follow a more direct path and so an interpolation between the local and global roughness values is required. The crack flow angle ($\theta_c$) and effective crack length are also interpolated in a similar way.
Figure 3.8: (a) Schematic of flow around two crack turns: crack width much less than roughness amplitude, $W_c < R_{glamp}$ (b) Schematic of flow around several crack turns: crack width much greater than roughness amplitude, $W_c > R_{glamp}$ [20]
This is consistent with the work in [22] and [23]. The different flow regimes are shown in [24] where different crack openings are modelled using Computational Fluid Dynamics (CFD) and compared with experiments. The experiments were performed with air as the fluid, and perspex as the medium containing the crack. Surface roughness is also looked at in some detail in the work by Manning [25] and Chivers [26]. Chivers [26] provides a bounding value for the maximum value of friction in practical cases. In Manning [25], crack face roughness was artificially created by grit blasting 32 idealized cracks and plotting friction against the Reynolds number for various roughnesses. It showed that for roughnesses greater than $4 \mu m$, the parameter $W/R_a$ could be used to characterise the friction factor. At lower roughnesses this was not the case, and a more detailed examination of the surface topography, indicated that this was due to the low slopes, and curvatures associated with low surface roughness.

The differences in leak rate observed in the figures 3.4, 3.5 and 3.6 is probably due to crack pathway losses which are included in the R6 models.

3.3.3 Two phase

As with the single phase case, the flow is assumed to be steady state. However, the problem is complicated due to water condensation and evaporation along the length of the flow path. The model presented here follows the Ecrevisse leak rate model in Code Aster, which is a development of the work by Feburie [27]. This gives a good summary of choked flow of subcooled water through slits. The usual mass, momentum, energy and entropy balance equations are considered, which reduce to a linear system of equations. This system of equations is complemented by an equation of state and solved, then a Runge-Kutta integration is done along the length of the channel to obtain the leak rate. The results of this model were compared against the measured leak rates of John et al. [28], see Fig. 3.9.

Depth of the slits was 46mm and length was 80mm. The crack opening displacement ranged from 250 to $440 \mu m$. Roughnesses ranged from 5.3 to $287 \mu m$. These cracks have a large crack opening, and it has been shown in the work of Rudland et. al. [21] that there is
Figure 3.9: Comparison of leak rates between Feburie model and measured results of John et al. [28]

larger uncertainty in leak rate estimation for narrower cracks. Inlet pressures of 40, 60, 80 and 100 bar were considered and outlet pressure ranged from 4 to 9 bar. For each pressure, temperatures between 2 – 60°C were tested. For these relatively large crack openings, there was reasonable agreement with the data, with an error of ±12%.

Other papers which provide a good background into critical two phase flow through slits are the papers by John [28], Morris [29] and Ghosh [30]. A wide range of test conditions were considered in experiments by John et al. [28]. These were varying inlet pressure, subcooling temperature of water, slit width and surface roughness. The results of these were used to modify the Pana model, and the measured data were predicted by this model with a relative standard deviation of less than 20%. Morris includes phase slip in his work, which is shown to have little effect on leak rate for high inlet pressures. However, differences emerge at lower pressures due to higher slip ratios. Nuclear power plants typically operate at high pressures, so it is acceptable to use homogeneous flow models for LbB in this environment. Ghosh modifies the Homogeneous Flow Model (HFM) taking into account the contribution of change in liquid phase kinetic energy. A computer code developed based on these models, gives results in good agreement with the published data. Leakage sizes are then estimated for different components in the primary circuit of Indian Pressurized Heavy Water Reactors.
Of prime importance when considering two phase flow through cracks, is the evolution of the mixture as it moves through the channel. Due to the small amount of time that the fluid is present in the crack, the fluid is in a state of mechanical and thermal non-equilibrium. The negligible interphase heat transfer during the expansion, translates into large heat transfer at the throat [31]. This leads to the assumption that the vapour at the throat behaves polytropically, with $n$ a thermal equilibrium polytropic exponent defined by Tangren at al. [32] and given by:

$$n = \frac{(1 - X)c_l / c_{pg} + 1}{(1 - X)c_l / c_{pg} + 1/\gamma}$$

where $X$ is the quality, $c_l$ is the specific heat of the liquid phase, $c_{pg}$ is the specific heat of the vapour phase at constant pressure and $\gamma = c_p / c_v$ is the isentropic exponent. Similarly, the mass transfer rate at the throat cannot be ignored. Taking the equilibrium quality, the mass transfer rate at the throat is correlated for steam-water critical flow through the parameter $N_e$, which is the partial change of quality at the throat [31].

$$N_e = \min(X_{exe}/0.14, 1)$$

The non-equilibrium interphase mass transfer is described in [33] by means of a relaxation equation. Acknowledging the complexity of the problem, the authors adopt a simple linear approximation to the vapour generation function:

$$\frac{DX}{Dt} = -\frac{X - \bar{X}}{\Theta}$$

where $\bar{X}$ is the equilibrium quality and $\Theta$ is the relaxation time. A correlation for the relaxation time is proposed in [33]. This gives the characteristic time for the non-equilibrium evaporation process as a function of void fraction, and non-dimensional pressure difference. This correlation was derived from runs of the Moby Dick experiments, for which flashing inception was situated in the test section. The Homogeneous Relaxation Model (HRM) is
implemented into a computer code using a Possible-Impossible Flow (PIF) procedure, similar to that used in Ecrevisse. The correlations presented are only a first approximation and there is a lot of scope to improve the relaxation models using more physically motivated relations. Recent work by Schmidt [34] utilises a multidimensional CFD implementation to study thermal non-equilibrium, two phase flows with flash-boiling and condensation. Results indicated that equal velocities and unequal temperatures was an acceptable assumption for most of the channel flows investigated.

3.3.4 Homogeneous non-equilibrium model

An early summary of the fundamentals of two phase flow was given by Fauske [35]. In this work, both theoretical and experimental analyses were used to derive critical flow expressions for nuclear reactor coolant systems. The idea that two phase flow could be approximated with a mixture was built on by Henry [31], who derived an expression for critical two phase flow from the solution of the momentum equation. Subsequent work has built on this concept, and a summary of models and their validity is given by Elias et al. Elias [36] and Wallis [37]. More recent work focusses on the thermal disequilibrium and slip between phases. Valero [38] considers an Equal Velocity Unequal Temperature (EVUT) model to analyse the significance of thermal disequilibrium in dispersed bubbly flow under critical conditions. The Lattice-Boltzmann method has been employed in [39] based on the work of Shan et al. [40] to simulate the movement of Taylor bubbles and to investigate the two-phase flow in a narrow channel. Investigations into non-homogeneous non-equilibrium flow are presented in [41] through constitutive relations for interfacial transfer rates. Modeling of mechanical non-equilibrium for choking flow is particularly important, as the pressure drop is mainly caused by the accelerations of each phase which, near the choking point, are different.

A comparison of the SQUIRT code is given against experimental data in Figure 3.10. The data is obtained from reports on two phase flow through long tubes by Sozzi and Sutherland [42], two phase flow through slits by Collier et. al [43], Amos and Schrock [44], and Yano
and two phase flow through actual cracked pipe reported by Collier [43]. There are lines showing errors up to a factor of ten. It is the narrow stress corrosion cracks (denoted by E and F in the figure) which give the largest error. This is put down to the crack pathway losses. The latest version of SQUIRT accounts for these losses based on the work of Rudland et. al. [21]. More detailed models that investigate the movement of bubbles through channels can be found in the literature. For example [39], [46] and [38]. When the void fraction is small, slip between phases can be neglected. In this case, the fluid can be thought of as a bubbly mixture, where the vapour bubbles are carried along by the liquid.

Many other models are available in the literature and a brief summary of some of those models is given here. Friedel [47] uses experiments on more than 80 model cracks over wide parameter ranges to assess the validity of a theoretical mechanistic model. One of the key conclusions from this work, is that slip between vapour and liquid phases in water leakage models can generally be ignored, because its omission from the model only causes minor errors in the prediction of pressure drop. Therefore, homogenous models are sufficiently accurate for predicting leakage rates through cracks. Leakage through concrete walls has
been investigated in [48] and [49]. These models would not be directly applicable to LbB, as none of the components suitable for an LbB assessment are made out of concrete. Instead they are used for simulating accident conditions in PWR plants. However, the fundamental principles of the model are the same and simply require modification of the friction relations. An experimental program that validates the theoretical work in [24] was done by Clark et. al. [50]. This gives relationships between leak rate and crack opening for narrow cracks where there are pressure drops due to bends and changes in area, and wider cracks which are modelled by flow between parallel plates. For irregular shaped paths such as those seen by a fluid flowing through a crack, it is possible to perform a mesh partitioning strategy along a path [51]. This technique uses a shortest path algorithm to obtain the shortest path along a tortuous path, and at each stage calculates a circumferential seam path around the centroid. The method has been applied to cooling channels in pressure die casting [52]. This could be applied to cracks. However, the actual condition of the crack path is subject to some uncertainty, and it is more suitable to use coefficients on friction to account for crack path effects. When there is confidence in the number and angle of turns through the crack depth, this method would be become very useful in obtaining the minor losses terms.

3.3.5 Probabilistic leak rate analysis

There is a considerable level of uncertainty in the leak rate due to the lack of precise knowledge of the exact crack shape. This is accounted for in the computer code PSQUIRT which gives probabilistic evaluations of leak rates in nuclear piping [53]. By taking a statistical distribution of input parameters, a sensitivity analysis can be performed to give a distribution of leak rates. Multiple cracks and their interaction are considered in [54], where Monte Carlo simulations are performed to simulate multiple crack growth/coalescence, along with the corresponding leak rate. It was concluded that the magnitude and statistical property of the leak rate in the multiple crack situations, are considerably different from those in a single crack situation. This highlights the need for special treatment of LbB analysis when multiple cracks are present.
3.4 Crack Tip Singularity

The gradient of displacement and temperature are both singular at the crack tip. Analytical solutions exist for the thermal and stress fields in plates with central cracks. The singular behaviour of the temperature gradient in the vicinity of a macrocrack tip is analysed in [55] and [56], and a term analogous to the stress intensity factor is presented. This is called the intensity factor of thermal gradient, and gives an indication of the power of the singularity in heat flux at the crack tip. This intensity of heat flux at the crack tip causes high thermal stresses and can cause crack propagation. In [57] the thermal stresses are derived by the complex variable method. Thermal stress fields near the tip of a mode I crack in a functionally graded material are derived based on the method of displacement potentials in [58]. It is observed that the temperature field disturbed by the crack influences the maximum shear stress. In [59], a method of Fourier Integral Transform is used, in conjunction with the coordinate transformations of field variables in the basic thermoelasticity equations. Heat flux and stress singularities are analysed for different orientations of crack and combinations of material, and geometric parameters. The paper addresses the fact, that when crack closure occurs due to heating, the frictional contact of the crack faces would invalidate the traction free boundary condition. Also, a partially insulated crack face condition is considered, to see what effect this has on stress. The thermal stress is shown to be less severe when the crack is partially insulated compared to a fully insulated crack. Results obtained for a fully insulated crack were verified with a closed form solution [60], and gave exact agreement.

Elastic crack tip stress fields can be derived from the complex stress potentials of [61], leading to the well known solution of Williams [62]. The solution is an expansion in powers of \( r^{m/2} \) for integers \( m \), so taking the derivative gives a singularity of \( r^{-1/2} \) at \( r = 0 \). The mathematical crack tip, \( r = 0 \), is non physical because in reality plasticity would blunt the sharp crack tip. However, with the small scale yielding assumption, the asymptotic form of the crack tip field is suitable beyond a small radius surrounding the crack tip.

Thermomechanical stress fields and strain energy associated with a mixed-mode propagating
crack, again using the displacement potentials and asymptotic approach, are presented in [63]. Anisotropic thermoelastic crack problems are analysed in [64] and [65], where solutions for temperature are presented, with boundary conditions imposed on the crack front. A Green’s function method for concentrated thermal/mechanical loading of the faces of a crack in a coupled thermo-elastic solid is considered in [66]. Crack surface convection is considered in [67], where Green’s function method is used. It is shown that convection can give rise to temperature changes in the crack plane that are both more prominent and extensive than those that occur for an insulated crack surface. For thermal problems of plates containing cracks with heat transfer, [68] and [69] provide explicit solutions based on integrals of Bessels Functions. The temperature field is also derived based on a similar method for plates containing a disc with non-ideal thermal contact between them [70]. Stress intensity factor solutions are given in [71] for plates containing cracks with various boundary conditions on the crack. The plate is modeled with the Poisson equation and is solved using potential theory. This leads to integral equations containing modified Bessel functions of the second kind.

3.5 XFEM

XFEM is a development of the finite element method which utilises the partition of unity concept [72]. The Partition of Unity Finite Element Method (PUFEM) has many useful features, the most salient of these being the ability to include information about local behaviour in the finite element solution. This puts the PUFEM into the category of 'meshless' methods, due to the fact that there does not need to be a complicated mesh around the area of significant interest. One physical problem, which is difficult to obtain accurate results from using finite element methods, is cracks in elastic solids. This is down to the fact that there is a discontinuity in displacement across the crack, as well as a singularity in strain at the crack tip.

Conventional finite elements requires the mesh to conform to the geometry of the crack, with
smaller elements surrounding the crack tip to ensure accuracy. Belytschko [73] was the first to apply the PUFEM to crack problems, and showed that optimum convergence rates could be achieved. This is when XFEM became more widely accepted as a practical tool. Since then, many researchers have investigated XFEM for a wide variety of problems. For example, Bayesteh et. al. [74] presented enriched shell elements and showed that a far more accurate estimation of the singular stress field near the crack tip was achievable over standard finite elements.

Solidification has also been modeled using XFEM in [75]. Here the discontinuity in the derivative of temperature was captured within elements by the level set method. Two phase flow contains a discontinuity between the liquid and vapour phase, and as such there have been attempts to model this using XFEM [76]. The condition number for the system matrices were investigated in this work, which are known to be very high in XFEM system matrices. The so called stable XFEM or sXFEM, introduced by Babuska and Banerjee [77], is investigated. This is claimed to offer the same convergence properites as the standard method, while the conditioning remains in the range of the standard Finite Element Method (FEM). This is made possible by modifying the step enrichment. It was shown in [76] that improved iterative solver performance was achieved with sXFEM with similar accuracy to conventional XFEM.

Elastic-plastic fracture mechanics in XFEM was considered by Elguedj et. al. [78] using the Hutchinson-Rice-Rosengren fields to represent the singularities. A Newton like iterative algorithm, and the radial return mapping scheme was used to compute plastic flow. Very good accuracy is obtained for numerical evaluation of J integral, indicating the plastic solution is well captured by the tip enrichment.

XFEM has also been exploited for applications in electrostatics [79] due to the moving discontinuities that occur in these problems. Both the bi-material [80] and void material enrichments [81] have been studied for this application.

For a comprehensive overview of the XFEM methodology and applications, the paper by Fries and Belytschko [82] is recommended.
3.5.1 Integration

Integration is more complicated in XFEM due to the fact that there are non-linear, singular and discontinuous functions included in the approximation space. For the crack tip elements, the strain singularity requires there to be extra integration points focussed around the crack tip. Domain integration is used, and this involves subdividing the element into triangles, each having a vertex at the crack tip so that almost polar integration is performed \[83\] \[84\]. Singular mapping \[85\] has also been used. This maps a real triangular interpolation cell onto a reference quadrangular cell. In this way the singular functions are transformed into regular ones. However, both these techniques come at an extra computational cost, and the accuracy is dependent on the number of integration points. Strain smoothing has been proposed as one method to alleviate some of these problems \[86\] \[87\]. It uses boundary integration instead of a domain integral, so the singular strain fields no longer need to be integrated. This has been shown to be robust, stable and of low computational cost. Convergence is improved, but there is a greater error than using element decomposition \[88\].

Schwarz-Christoffel mapping have also been used for integrating crack tip elements \[89\] \[90\] \[91\]. A Schwarz-Christoffel map takes an n sided polygon to a unit disc, and a midpoint quadrature rule is used on this disc. This method eliminates the need for a two-level isoparametric mapping which is usually required. For problems in linear elasticity, this was shown to give good convergence and accuracy, compared to the usual bi-mapping technique based on triangulation. However, it was slightly less accurate for the crack problem tested.

Displacement regularisation in the context of XFEM was introduced by Benvenuti et. al. \[92\] \[93\]. This essentially regularises the Heaviside function with a smooth function which varies from -1 to 1 over a characteristic length. This length is sufficiently small and in the limit as it tends to zero, the regularized functions becomes the Heaviside function.
The analytical expression of the regularised function $H_\rho(x)$ is:

$$H_\rho(\phi(x)) = \begin{cases} 
-1 + e^{\phi(x)/\rho} & \text{if } \phi(x) < 0 \\
1 - e^{-\phi(x)/\rho} & \text{if } \phi(x) > 0 
\end{cases}$$

(3.37)

The limit as $\rho \to 0$ gives the Heaviside function.

$$H(\phi(x)) = \begin{cases} 
-1 & \text{if } \phi(x) < 0 \\
1 & \text{if } \phi(x) > 0 
\end{cases}$$

(3.38)

Where $\phi(x)$ is the level set function. Using a function like the one in [3.37] means that all the fields are continuous and differentiable. Hence, standard quadrature can be used. The regularisation function is replaced with continuous polynomials that exactly integrate to give the stiffness coefficients. This is an extension of the method proposed by Ventura [94], to avoid quadrature subcells in XFEM for strong discontinuities. This is shown to be accurate, and can be used as an alternative to subdividing enriched elements into integration subdomains.

### 3.5.2 Blending elements

There have been reports of poor convergence rates due to the elements on the edge of the enriched group of elements. These elements contain nodes that are enriched and non-enriched, and these so-called blending elements are the reason for poor rates of convergence in XFEM. A corrected XFEM formulation [95] was proposed which circumvents the problem of these blending elements with the use of an additional function. The main problem in these elements, is that the interpolation is not a partition of unity, therefore the approximation is no longer able to represent the enrichment function exactly. Also, there are unwanted terms for elements with only some nodes in the enrichment zone. The modified enrichment [95]
uses a ramp function in these blending elements, which varies continuously between zero and one. Therefore, in these elements, all the nodes are enriched, and still serve the purpose of blending the approximation in the enriched part with that in the standard FE part.

3.5.3 Cohesive cracks

Cohesive cracks have been successfully modelled in [96] and [97]. A traction separation law, which depends on the crack opening displacement, characterises the softening due to the presence of a crack. Essentially, the cohesive stress depends on the crack opening displacement in the fracture process zone, and decreases as the crack opening displacement increases. In [98], all cracked elements are enriched by the step function, with a cohesive zone accounting for the crack tip. This avoids some of the difficulties associated with branch functions in the tip element. In [99], the growth of the cohesive zone is governed by SIFS at the tip of the cohesive zone to vanish. Using this approach, avoids the evaluation of stresses at the mathematical tip of the crack. Wells and Sluys [100] also applied the XFEM concept to cohesive cracks, but this formulation limited the enrichment to the case where cracks end at element edges.

3.5.4 Some novel applications of XFEM

The physical problem considered here is similar to that of hydraulic fractures. The cracks are subject to a pressure, and there is a thermal field disturbed by insulated discontinuities at the cracks. Lecampion [101] couples the fluid in the crack with the solid, and defines two regimes. One is the toughness dominated zone, which has the standard XFEM asymptotic functions, and the other is the viscosity dominated regime with an $r^{-2/3}$ approximation. Thermal fields are included in the analysis of Khoei et al. [102], however only insulated or fixed temperature boundary conditions are considered. The flow here is modeled using the Reynolds equation for viscous flow, as such there is a stronger link between the fluid pressure and the crack
opening. In the problem of a high pressure leak through a narrow crack, it is more appropriate to consider critical flow. Therefore, in this work, more focus is given to critical flow, and the heat transfer to the crack walls. The fluid pressure is taken to be constant.

XFEM has also been applied to problems in leakage from multilayer aquifers [103]. The multiple material discontinuities and fractures arising in this problem, mean that XFEM is a good method to accurately model this. Couple this with the fact that there are multiscale effects, where the local scale phenomena (resolved at a resolution smaller than that of the mesh) have a well understood functional form. This second property is taken advantage of in [103]. Promising convergence rates were quoted for these multi scale systems, and the meshless property of XFEM was shown to increase the flexibility of models.

3.5.5 Application to a leaking thermofluid through a crack

The problem of a leaking fluid through a crack, requires thermo-mechanical modelling due to the presence of a hot fluid at high pressure escaping through the crack. Therefore, the LbB element must be thermo-elastic and include the contribution of heat flux and pressure on the crack walls. Duflot [104] was the first to explore thermo-elastic fracture mechanics with XFEM. Isothermal cracks and insulated cracks are considered, where the isothermal crack requires Lagrange multipliers to apply the Dirichlet conditions along the crack front. This is different to what is required here, where a non-Dirichlet condition is applied, so effectively it is more straightforward. The crack temperature can still be specified with this method by setting the heat transfer coefficient to be very large, so that the crack face temperature assumes the bulk fluid temperature. In this work, the heat flux and pressure will be specified along the crack, by integrating the necessary terms along the level set. This is in addition to the element integral, and will require special treatment. Essentially the level set will be populated with Gauss points and a line integral will be performed. A jump in temperature based on thermal resistance model was considered by Yvonet et. al. [105]. This assumed a constant heat flux across the crack. The thermal model that will be presented here assumes a heat flux along
the crack imposed by a Robin type boundary condition. The change in heat flux is accounted for by the relevant enrichment function. Recent work of Gong et. al. [106] demonstrates the use of XFEM for temperature fields in heterogenous materials. Material discontinuities within elements are modeled with the level set enrichment, and excellent agreement was observed with analytical and standard FEM solutions.
Chapter 4

Thermal Hydraulics

4.1 Introduction

The calculation of leak rates through narrow cracks is of prime importance when carrying out a LbB assessment. The prediction of leak rate is required to ensure that a crack would produce a detectable leak, well before it was large enough to cause a large break. There is currently some uncertainty in the prediction of leak rates due to the complexity in the flow path, and the effect of phase change in the two phase case.

Current thermal hydraulic codes for leak rate prediction such as DAFTCAT [107] and SQUIRT [108], assume the channel to be straight walled with an empirical relation for roughness. However, cracks can meander through the wall of the vessel meaning that the straight walled assumption is inaccurate. The latest models try and account for this uncertainty, with crack morphology parameters that modify the pressure losses. These are discussed in the thesis.

For the case of two phase flow, which may occur when there is a through wall crack in a vessel containing subcooled water, there are vaporisation effects which change the mass flow rate. A summary of two phase flow models is presented, as well as a detailed analysis of the Henry-Fauske model [31] for a leaking crack situation. Finally, a model which treats single and two phase flow in the same model is derived. This is then used to perform leak rate
calculations with the finite element software Code Aster.

In the next section, fluid models to calculate leak rates will be presented. The steady-state transport equations describe the physics for fluid flow through a pipe. These are used to derive an ordinary differential equation for single phase critical flow that can be solved numerically. Two two-phase models are presented. One is based on the Henry-Fauske thermal non-equilibrium model, the other comes from the transport equations and uses the mixture properties of the water-steam flow. This second model requires a special solution procedure which is implemented in Ecrevisse, a thermal hydraulics code in Code Aster.

4.2 Single phase

The three steady-state transport equations applicable in this case are:

\[ \int_{\Gamma} \rho v \cdot n d\Gamma = 0 \]  
\[ \int_{\Gamma} \rho v \cdot v d\Gamma = - \int_{\Gamma} \sigma \cdot n d\Gamma + \int_{\Gamma} \tau \cdot n d\Gamma \]  
\[ \int_{\Gamma} \rho (h + \frac{1}{2}v \cdot v) u \cdot n d\Gamma = - \int_{\Gamma} q \cdot n d\Gamma \]

where \( dh = c_p dT \) is the enthalpy of the fluid, \( \tau \) is the shear stress, \( v \) is the fluid velocity, \( \rho \) is the density and \( p \) is the pressure. The heat transfer to the fluid is given by \( q \). The equations in (5.36) can be applied to an elemental volume of measure \( dV = Adz \), whose axis is in the unit direction \( e \) with swept surface area \( dS = P_f ds = P_f (e^\perp \cdot n)^{-1} dz \), where \( e^\perp \) is perpendicular to \( e \). The continuity equation immediately reveals

\[ d(\rho v A) = 0 \Rightarrow \frac{dp}{\rho} + \frac{dv}{v} + \frac{dA}{A} = 0 \]  

\[ d(\rho v A) = 0 \Rightarrow \frac{dp}{\rho} + \frac{dv}{v} + \frac{dA}{A} = 0 \]  

50
Resolving the momentum equation along the axis gives

\[ \int_{\Gamma} \rho e \cdot v \cdot n d\Gamma = -\int_{\Gamma} p e \cdot I \cdot n d\Gamma + \int_{\Gamma} \epsilon \cdot T \cdot n d\Gamma \]  \hspace{1cm} (4.3)

which reduces to

\[ d(pAv^2) + Adp = e \cdot \tau \cdot ndS = \tau_w P_f dz \Rightarrow \frac{dv}{v} + \frac{dp}{\rho v} = \frac{\tau_w P_f}{\rho Av} dz \]  \hspace{1cm} (4.4)

where \( \tau_w = \frac{1}{2} \rho v^2 f \). Likewise the energy equation gives

\[ d(pAv(h + \frac{1}{2} v^2)) = qdS = qP_f ds \Rightarrow dh + vdv = \frac{qP_f}{\rho Av} ds = q_w P_f dz \]  \hspace{1cm} (4.5)

where \( q_w = q/(\rho A v^2 \cdot n) \)

Assuming a polytropic process gives

\[ d(p\rho^{-k}) = 0 \Rightarrow \frac{dp}{p} - k \frac{d\rho}{\rho} = 0 \]  \hspace{1cm} (4.6)

whilst the gas law gives

\[ d(p\rho^{-1}T^{-1}) = 0 \Rightarrow \frac{dp}{p} - \frac{d\rho}{\rho} - \frac{dT}{T} = 0 \]  \hspace{1cm} (4.7)

Taking the Mach number to be \( M_a = \frac{u}{e} \) where \( e = (\frac{kp}{\rho})^{1/2} \) and where \( k \) is the polytropic index. Taking \( k = 1 \) and contrasting equations (4.6) and (4.7) one can deduce that \( dT = 0 \), i.e. temperature is constant. This immediately infers that \( dh = C_p dT = 0 \). So for isothermal conditions, equations (4.2) and (4.4) and (4.6) give the following expression

\[ \frac{1}{2} M_a^2 f P_f dz = \frac{dA}{A} + \frac{dM_a}{M_a} (1 - M_a^2) \]  \hspace{1cm} (4.8)

Expression (4.8) can be solved using Runge Kutta step integration with boundary conditions of \( M_a = 1 \) at the crack exit (choked at exit). This is a valid assumption given the high
pressure difference between inlet and outlet. The area $A$ is assumed to vary linearly through the thickness according to the inner and outer crack openings, $A(x) = W(x)L(x)$ for a rectangular opening where $W$ is the crack opening displacement and $L$ is the crack length.

$$W = w_i + \left( \frac{w_e - w_i}{2t} \right)z$$ \hspace{1cm} (4.9)

and

$$L = l_i + \left( \frac{l_e - l_i}{2t} \right)z$$ \hspace{1cm} (4.10)

where $t$ is plate thickness. Inserting equations (4.9) and (4.10) into equation (4.8), an ordinary differential equation is obtained which can be solved numerically, i.e.

$$\frac{dM_a}{dz} = \frac{M_a^2 f(A + (B + C)z) - L_i B + w_i C + 2BCz}{[(1 - M_a^2)/M_a](w_i + Bx)(l_i + Cz)}$$ \hspace{1cm} (4.11)

where $A = w_i + l_i$, $B = (w_e - w_i)/2t$ and $C = (l_e - l_i)/2t$. This is solved for $M_a$ using ODE45 in MATLAB, where $M_a = M_e = 1$ at $x = x_e = t$. $M_i$ is then obtained at $x = x_i = 0$ and substituted into the following expression to obtain mass flow rate:

$$\dot{m} = M_i (\rho_i p_i)^{\frac{1}{2}} A_i$$ \hspace{1cm} (4.12)

Plots of the Mach number against distance through the channel are given in Fig. 4.1 for friction and no friction.

Various conditions were simulated and compared against the current R6 equations and good agreement is observed when the initial conditions are chosen to give critical flow. The leak rate is given by the following formula in R6, where $C_D$ is a discharge coefficient which can account for lamina turbulent and critical flow.

$$\dot{m} = C_D (\rho_i p_i)^{\frac{1}{2}} A$$ \hspace{1cm} (4.13)
Figure 4.1: Mach number against through thickness parameter. Thickness $t = 10\,\text{mm}$, $W = 100\,\mu\text{m}$, $L = 100\,\text{mm}$. Plots are for smooth and rough channels, i.e. no friction and friction.
where $A$ is the COA. The discharge coefficient also contains information about the pressure losses due to crack path directional changes through the channel. This is discussed in the next section. A plot of equations (4.12) and (4.13) is given in Fig. 4.2.

![Figure 4.2: Comparison of R6 and ODE model from equations 4.13 and 4.12.](image)

### 4.3 Two Phase

In this section a presentation of the Henry Fauske model [31][35] is given. This accounts for the thermal disequilibrium in critical two phase flow [36][38].
4.3.1 Homogeneous non-equilibrium model

The mass flux and pressure constraints form a simultaneous non-linear system which can be solved by Newton-Raphson iteration, i.e.

\[
\Xi(G_c, p_c) = G_c^2 - \frac{1}{X_c \nu_{gc} - (\nu_{gc} - \nu_{Lc}) N_x \frac{dX_E}{d\rho}} = 0 \quad (4.14a)
\]

\[
\Pi(G_c, p_c) = p_c + p_e + p_a + p_f + p_k + p_{aa} - p_0 = 0 \quad (4.14b)
\]

where the non-equilibrium and equilibrium mixture qualities, \(X_c\) and \(X_E\), are given by:

\[
X_c = N_x X_E (1 - e^{(-B((L/D_i - 12))}) \quad (4.15a)
\]

\[
X_E = \frac{[S_0 - S_{Lc}]}{[S_{gc} - S_{Lc}]} \quad (4.15b)
\]

where \(N_x = 20\) for \(X_E < 0.05\) and \(N_x = 1\) for \(X_E \geq 0.05\). The constant \(B\) is an empirical fit and is taken as 0.0523. The entropies \(S_0, S_{Lc}\) and \(S_{gc}\) and specific densities \(\nu_0, \nu_{gc}, \nu_{Lc}\) are taken at the stagnation point (0) and critical planes for the liquid (L) and gas (g).

The pressure losses are due to entrance effects, friction, head loss, area change and phase change. These are described in more detail below. The entrance pressure drop is

\[
p_e = \frac{G_0^2 \nu_{L0}}{2 C_{De}^2} \quad (4.16)
\]

where \(C_{De}\) is the entrance discharge coefficient, taken to be 0.95 for tight cracks. The frictional pressure drop is given by:

\[
p_f = \left( f \frac{L}{W} \right) \frac{G^2}{2} \left[ (1 - \bar{X}) \bar{\nu}_L + \bar{X} \bar{\nu}_g \right] \quad (4.17)
\]

where \(W\) is the average crack width and \(R_s\) is the crack surface roughness. Symbols with a
bar indicate average values over the channel.

There is the pressure drop due to changes in crack direction of the form

$$p_k = n_t L \bar{G}_c^2 \left[ (1 - \bar{X})\bar{\nu}_L + \bar{X}\bar{\nu}_g \right] \quad (4.18)$$

where $n_t L = e L_c$ is the total loss coefficient over the crack flow path length and $e$ is the number of turns per mm. Pressure drop due to phase change acceleration is given by

$$p_a = \bar{G}_c^2 \left[ (1 - X_c){\nu}_L + X_c{\nu}_g - \nu_L \right] \quad (4.19)$$

Pressure drop due to area changes:

$$p_{aa} = \frac{G_c^2}{2} \nu_{L0} \left[ \left( \frac{A_c}{A_i} \right)^2 - \left( \frac{A_c}{A_e} \right)^2 \right] + \frac{G_c^2}{2} \left[ (1 - \bar{X})\nu_L + \bar{X}\nu_g \right] \left[ 1 - \left( \frac{A_c}{A_i} \right)^2 \right] \quad (4.20)$$

where the subscripts $i$, $c$ and $e$ represent the area at the inlet, critical and outlet plane. The Newton Raphson technique for a linear system can be summarised by the following formula:

$$\bar{x}_{new} = \bar{x}_{std} + \delta \bar{x} \quad (4.21)$$

where $\delta \bar{x}$ is defined by

$$J \cdot \delta \bar{x} = -F \quad (4.22)$$

so

$$\delta \bar{x} = -J^{-1} F \quad (4.23)$$
and \( F = (\Psi, \Omega)^T \), \( J \) is the Jacobian.

\[
J = \begin{pmatrix}
\frac{\partial \Xi}{\partial G^2_c} & \frac{\partial \Xi}{\partial p_c} \\
\frac{\partial \Omega}{\partial G^2_c} & \frac{\partial \Omega}{\partial p_c}
\end{pmatrix}
\]

where

\[
detJ = \frac{\partial \Xi}{\partial G^2_c} \frac{\partial \Omega}{\partial p_c} - \frac{\partial \Xi}{\partial p_c} \frac{\partial \Omega}{\partial G^2_c}
\]  

(4.24)

so

\[
J^{-1} = \frac{1}{detJ} \begin{pmatrix}
\frac{\partial \Omega}{\partial p_c} & -\frac{\partial \Xi}{\partial p_c} \\
-\frac{\partial \Omega}{\partial G^2_c} & \frac{\partial \Xi}{\partial G^2_c}
\end{pmatrix}
\]

This is solved in a computer code. Values for the density, enthalpy and entropy are taken from IAPWS 97 steam tables, and a MATLAB script which interpolates.

### 4.3.2 Crack Morphology

For the two phase case, modifications to the surface roughness, channel length and number of turns are made with the following approximate interpolations

\[
\mu = \begin{cases}
R_{aL}, & 0.0 < \frac{R_a}{W} < 0.1 \\
R_{aL} + \frac{\mu_{G} - R_{aL}}{9.9} \left( \frac{W}{R_{aG}} - 0.1 \right), & 0.1 < \frac{R_a}{W} < 10 \\
R_{aG}, & \frac{R_{aG}}{W} > 10
\end{cases}
\]  

(4.25)

\[
n = \begin{cases}
n_{tL}, & 0.0 < \frac{R_a}{W} < 0.1 \\
n_{tL} - \frac{n_{tL}}{10} \left( \frac{W}{R_{aG}} - 0.1 \right), & 0.1 < \frac{R_a}{W} < 10 \\
0.1n_{tL}, & \frac{R_{aG}}{W} > 10
\end{cases}
\]  

(4.26)
\[
\frac{L_c}{l} = \begin{cases} 
K_{G+L}, & 0.0 < \frac{R_a}{W} < 0.1 \\
K_{G+L} - K_{G+L} \left( \frac{W}{R_{ag}} - 0.1 \right), & 0.1 < \frac{R_a}{W} < 10 \\
K_G, & \frac{R_{ag}}{W} > 10
\end{cases}
\]  

These are based on the ratio of crack opening displacement to global roughness, \(W/R_{ag}\) \[21\]. An illustration of this is given in Figs 4.3 and 4.4. Values for \(K_G\) are typically around one for intergranular stress corrosion (IGSCC) and fatigue cracks, and \(K_{G+L} = 1.33\) for IGSCC and again about one for fatigue cracks. For more details on the values used in the above equations, see [21]. The plot in Fig. 4.5 shows simulations done with SQUIRT, with and without the crack morphology model. There is a factor of two difference between the models at \(COD = 140 \mu m\)

### 4.3.3 Ecrevisse model characteristics

A more general model is presented here which makes no assumption about the temperature effects on the flow. The same formulation is used for single and two phase flow, and lamina, turbulent and critical flow can all be modelled. Again the model is 1D where \(z = 0\) at the crack entrance, \(z = L\) at the outlet. The friction of the fluid with the crack walls is taken into account, as is the convective heat transfer. The change of phase of the water is also included in the model and it is assumed that critical flow can be reached. In terms of the flow cross section, the crack opening is simplified as an ellipse or a rectangle and the flow path dimensions can change linearly along the flow path. It is assumed that the flow is homogeneous for the air, steam, water mixture, and that all phases are at the same temperature. If water is present then the following conditions hold:

\[ T = T_{sat}(P_{vap}) \]
Figure 4.3: Effect of COD on flow path length
Figure 4.4: COD and roughness
Figure 4.5: Leak rate of subcooled water with and without crack morphology models. $P_0 = 155\text{Bar}$, $T_0 = 300^\circ\text{C}$, $\mu_G = 40.513\ \mu\text{m}$, $\mu_L = 8.81\ \mu\text{m}$, pipe wall thickness = 10 mm, Crack length = 100 mm. In the crack morphology model, the number of velocity heads per mm, $e = 6.73\text{turns/mm}$. 
where $P_{vap}$ is the steam partial pressure in the gas phase.

**Main equations for air/water flow**

<table>
<thead>
<tr>
<th>Variables characterising the fluid state inside the crack</th>
<th>air</th>
<th>steam</th>
<th>water</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity (m/s)</td>
<td>$v$</td>
<td>$v$</td>
<td>$v$</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>$T$</td>
<td>$T$</td>
<td>$T$</td>
</tr>
<tr>
<td>Pressure (Pa)</td>
<td>$P_{air}$</td>
<td>$P_{vap}$</td>
<td>$P = P_{air} + P_{vap}$</td>
</tr>
<tr>
<td>Mass Fraction (-)</td>
<td>$x_a$</td>
<td>$(1 - x_a) \cdot x$</td>
<td>$(1 - x_a) \cdot (1 - x)$</td>
</tr>
</tbody>
</table>

with $x_a = \frac{m_{air}}{m_{tot}}$, $x = \frac{m_{vap}}{m_{vap} + m_{liq}}$

The initial mass flow rate ($z=0$) is denoted by $G_0 = A \rho_m v_0$, and the air fraction at $z = 0$, $x_a = x_{a0}$, due to air mass conservation. It can be shown that for all cases, given $x_{a0}$ and $G_0$, the seven parameters characterising the fluid state can be deduced from only two of them, say $P$ and $T$. Therefore, $\frac{d\nu_m}{dz}$ and $\frac{dh_m}{dz}$ in the balance equations can be written in terms of $\frac{dP}{dz}$ and $\frac{dT}{dz}$. Ignoring the effects of gravity, the following linear system of equations in matrix form is obtained from equations (4.2), (4.4) and (4.5):

$$
\begin{bmatrix}
\frac{\partial \nu_m}{\partial T} & \frac{\partial \nu_m}{\partial P} & -\frac{\nu_m}{v} \\
0 & 1 & \frac{w}{\nu_m} \\
\frac{\partial h_m}{\partial T} & \frac{\partial h_m}{\partial P} & \frac{\nu_m}{v}
\end{bmatrix}
\begin{bmatrix}
\frac{d\nu_m}{dz} \\
\frac{dP}{dz} \\
\frac{dh_m}{dz}
\end{bmatrix}
= 
\begin{bmatrix}
\frac{\nu_m}{A} \frac{dA}{dz} \\
\frac{P_f}{A} \tau_v \\
\frac{P_f q_{sw}}{A_m}
\end{bmatrix}
$$

The convection from the fluid to the structure is defined from Newton’s law of cooling, $q_w = h(T_{bulk} - T_w)$. The subscript $m$ indicates that properties are taken for the mixture.
Solution procedure

The calculational philosophy adopted here is the same as that used in many two-phase pipe flow computer programs. Choose a length of pipe increment, and solve the momentum and energy equations simultaneously to obtain the pressure drop for which this length of pipe is realised. This process is repeated until the whole length of pipe is traversed.

This philosophy is followed in the Ecrevisse solution procedure, where a possible/impossible flow criteria is used. The full procedure is described below:

1. Calculation of a maximum flow rate \( G_{\text{max max}} \) (assuming adiabatic, frictionless and isentropic flow between the crack upflow and the first point inside the crack: \( z = 0 \));
   \( G_{\text{min}} = 0; G_{\text{max}} = G_{\text{max max}} \)

2. Test of \( G \), with \( G_{\text{min}} < G < G_{\text{max}} \)
   (a) Calculation of fluid state at \( z = 0 \) (head loss at crack entrance)
   (b) From \( z = 0 \) to \( z = L \) (or \( z < L \) if critical conditions are reached, i.e. the matrix in 4.29 has a determinant of zero): calculation of \( dP/dz, dT/dz, du/dz \) by solving the linear system, integration from \( z \) to \( z + \Delta z \) (Runge Kutta method with integration step fitting), calculation of new fluid state
   (c) If \( P(L) > P_{\text{downflow}} \), \( G \) too low \( \Rightarrow G_{\text{min}} = G \)
   If \( P(L) < P_{\text{downflow}} \), \( G \) too high \( \Rightarrow G_{\text{max}} = G \)
   If critical conditions reached, \( G \) too high \( \Rightarrow G_{\text{max}} = G \)
   (d) If \( (G_{\text{max}} - G_{\text{min}}) > \epsilon \), return to 2) to test a new \( G \) value

3. End of calculation, printing of results (final \( G \), and fluid state along the crack)

The correlations used in Ecrevisse for wall friction and wall heat transfer are now described:
Pressure drop due to friction

Friction is summarised in the following formula:

$$\frac{P_f \tau_w}{2A} = \frac{f \rho_m v^2}{D_h}$$

(4.30)

The friction coefficient $f$ is calculated in two different ways depending on lamina ($Re \leq 5000$) or turbulent ($Re > 5000$) conditions. For $Re \leq 2000$:

$$f = K \frac{64}{Re}$$

(4.31)

The coefficient $K$ depends on the geometry of the crack opening. It takes the value 1 for the case of a circular opening, 1.5 for elliptic and varies between 0.89 and 1.5 for a rectangular opening.

For $Re > 2000$ the correlation of Colebrook and White [109] is used:

$$\frac{1}{\sqrt{f}} = -2 \log[10]\left(\frac{e}{3.715 D_h} + \frac{2.514}{Re \sqrt{f}}\right).$$

(4.32)

For two phase flow the mass fractions of the gas and liquid part determine the friction.

$x_l < 0.02$, $f = f_g$

$x_l > 0.05$, $f = f_l$

$0.02 \leq x_l \leq 0.05$, $f = f_g + \frac{f_l - f_g}{0.03} [x_l - 0.02]$

Fluid/wall heat exchange

The wall heat flux is given by:

$$q_w = h_w (T_{bulk} - T_w)$$

(4.33)
The wall heat transfer coefficient \( h \) is calculated using various correlations based on whether the flow is laminar or turbulent, single-phase or two-phase. For single-phase flow with \( Re \leq 2100 \) the correlation of Sieder and Tate is used [110]:

\[
h_c = 1.86 \frac{k_f}{D_h} \left( Re Pr \frac{D_h}{L} \right)^{\frac{1}{3}}
\]

(4.34)

where \( k_f \) is the fluid conductivity and \( D_h \) is the hydraulic diameter.

For larger Reynolds numbers \( (Re > 2100) \), McAdam’s correlation can be used [111]:

\[
h_c = 0.023 \frac{G}{A} C_p Re^{-0.2} Pr^{-\frac{2}{3}}
\]

(4.35)

For two phase flow, the calculation depends on the liquid mass fraction and \( v_g/v_{tot} \):

\( \alpha = v_g/v_{tot} < 0.3 \): \( h_c = h_l \)

For all other cases \( (\alpha > 0.3) \), a combination of \( h_l \) or \( h_g \) with \( h_{wtp} \) given by Chen correlation [112]: Liquid mass fraction \( x_l < 0.02 \): \( h_c = h_g \)

\( x_l > 0.05 \) and \( \alpha \geq 0.5 \):

\[
h_c = h_{tp1} = F_J 0.023 Re^{0.8} Pr^{0.4} \frac{k_f}{D_h}
\]

(4.36)

\( F_J \) is a correction coefficient which is dependent on the Martinelli parameter \( x_{tt} \)

\[
x_{tt} = \sqrt{\left( \frac{x_l}{1-x_l} \right)^{2-Blasius} \frac{v_l}{v_g} \left( \frac{\mu_l}{\mu_g} \right)^{Blasius}}
\]

(4.37)

where \( Blasius = 0.25 \) for a smooth pipe

\( F_J = 1 \) for \( x_{tt} > 10 \) or \( x_l \geq 0.999 \) and for all other situations:

\[
F_J = 2.35 \left( \frac{1}{x_{tt} + 0.213} \right)^{0.736}
\]

(4.38)
for $0.02 < x_l \leq 0.05$ and $\alpha \geq 0.5$:

$$h_c = h_{tp} = h_g + \frac{h_{tp1} - h_g}{0.03}(x_l - 0.02)$$ (4.39)

$x_l > 0.05$ and $\alpha < 0.5$:

$$h_c = \frac{(\alpha - 0.3)h_{tp1} + (0.5 - \alpha)h_l}{0.2}$$ (4.40)

$0.02 < x_l \leq 0.05$ and $\alpha < 0.5$:

$$h_c = \frac{(\alpha - 0.3)h_{tp} + (0.5 - \alpha)h_l}{0.2}$$ (4.41)

This fluid model is coupled to a thermo-mechanical finite element model in the open source software Code Aster. The structural model is transient and uses an iterative solver to converge on a leak rate. Boundary conditions are imposed on the faces of the crack, based on the fluid conditions within the crack. This changes the crack opening displacement through the channel. Two simulations were performed, one using air as the coolant and the other one water. The geometry and mesh of the structure is shown in Fig. 6.10, where there is a focused region at the crack inlet.

The plate was fixed at the left and right ends with Encastre boundary conditions, so that any expansion due to heat transfer from the fluid could cause crack closure. Two different situations were considered, to investigate both the structural response when a leaking single phase fluid is present, and the thermal hydraulic behaviour of a water-steam mixture. For the air model, inlet conditions of the fluid were a pressure of 1MPa, and temperature of 140°C. For the water model, inlet conditions were a pressure of 16MPa, and a temperature of 300°C. The crack was considered to have parallel walls with no change in crack length in the out of plane direction. The Crack Opening Displacement (COD) for the air model ranged from 90 to 140 µm, and the length was 100mm, where a rectangular opening was considered. For the water model, the crack was 60mm in length, and the COD was 50 µm. Material prop-
erties are approximate, and correspond to those of Austenitic Steel with a Young’s modulus of $E=200\text{GPa}$, Poisson’s Ratio $\nu = 0.3$, Thermal Conductivity $k=20\text{W/mK}$, and Thermal Expansion Coefficient $\alpha = 1.282 \times 10^{-5}$. Heat transfer occurs at the inner and outer surfaces and along the crack walls. The Heat Transfer Coefficient (HTC) is fixed at $8\text{W/m}^2\text{K}$ on the inner surface, and $4\text{W/m}^2\text{K}$ on the outer surface. Along the crack walls, correlations are used to calculate the HTC. Ambient temperatures on the inside are inlet fluid temperatures, and for the outside they are $20^\circ\text{C}$ for the air model, and $100^\circ\text{C}$ for the water model.

Pressure and temperature plots in Figs. 4.7 and 4.8 show the difference between when there is heat transfer at the walls, and when they are insulated. Leak rates for air with and without heat transfer are given in Fig. 4.9, a factor of ten difference is seen at $COD = 110\mu\text{m}$.
Figure 4.7: Pressure of water through thickness with and without heat transfer to crack walls
Figure 4.8: Temperature of water through thickness with and without heat transfer to crack walls

Figure 4.9: Leak rate of air with and without heat transfer, \( P_0 = 10 \) Bar, \( T_0 = 140^\circ C \), Crack length=100mm
Chapter 5

New finite element

5.1 Introduction

It is apparent that LbB has both structural and fluid mechanics considerations. It is present practice to analyse these two aspects independently [3]. However, modern computational techniques are making a coupled approach more feasible. The motivation for a coupled approach stems from the fact that thermal heat transfer from the fluid to the crack walls is known to affect leak rate [113]. Two phase flow is particularly sensitive to wall heat transfer [114]. This is due to the steam evolution as pressure and temperature changes through the thickness. Also, the additional heating of the crack walls, due to a leaking fluid, causes thermal expansion, which changes the crack opening displacement. So it is clear that there should be a link between fluid and structure through a thermal coupling. In addition to this, there should be a consideration for the end user, so a model which can be efficiently used in an industrial context is essential. To facilitate this requirement, a new finite element has been developed which accounts for all the physics that affects leak rate. The approach outlined is founded on the XFEM as this provides a framework to build an element that can capture the essential behaviour, as well as being simple to use once implemented into a finite element code. This chapter provides a description of the mathematical formulation of the new element, as well
as a test of its accuracy with a convergence study. Finally, there is an example simulation for the case of a plate with conditions similar to those experienced in a PWR.

## 5.2 Mathematical formulation

Steady state conditions are assumed in this analysis, as well as small deformation theory for the strains. The crack is considered to be a one dimensional line discontinuity in a two dimensional domain, see Fig. 5.1. The crack reduces to a single contour when the two faces are assumed to collapse to the same line, with a jump condition imposed due to the change in the sign of the normal. The governing equations are the equilibrium equation and heat equation on a domain $\Omega$ bounded by $\partial \Omega$. Respectively, these are given by:

\begin{align}
\sigma_{ij,j} &= f_i \\
q_{i,i} &= Q
\end{align}

where $f_i$ is the body force, $Q$ is the heat source (which in this case will be zero, so the heat equation reduces to the Laplacian $T_{jj} = 0$). The $j$ denotes differentiation with respect to the jth coordinate. The constitutive equations in thermoelasticity are given by

\begin{align}
\underline{\sigma} &= \sigma_{ij} = C_{ijkl}\epsilon^e_{kl} \\
\epsilon^e &= \epsilon^t_{ij} = \epsilon_{ij} - \epsilon^t_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) - \alpha T \Delta T \delta_{ij} \\
q_i + kT, i &= 0
\end{align}

where $C_{ijkl}$ is the isotropic fourth order tensor, $\epsilon_{ij}$ is the strain tensor, $\alpha_T$ is the thermal expansion coefficient, $k$ is the thermal conductivity, $\Delta T$ is the change in temperature with respect to some reference temperature, and $\delta_{ij}$ is the Kronecker delta. The superscripts $e$ and $t$ represent the elastic and thermal components of the total strain and $u$ is the displacement vector.
Neumann and Dirichlet boundary conditions in the form of the traction/heat flux and displacement/temperature are imposed on the body, with additional conditions on the crack.
\[ u = \bar{u} \text{ on } \Gamma_u \tag{5.3a} \]
\[ t = \sigma \cdot n = \bar{t} \text{ on } \Gamma_t, \Gamma_c \tag{5.3b} \]
\[ T = T_0 \text{ on } \Gamma_T \tag{5.3c} \]
\[ q \cdot n = \bar{q} \text{ on } \Gamma_q \setminus \Gamma_c \tag{5.3d} \]
\[ [[q \cdot n]] = [[q_c \cdot n]] \text{ on } \Gamma_c \tag{5.3e} \]
\[ [[\sigma \cdot n]] = [[-pn]] \text{ on } \Gamma_c \tag{5.3f} \]

where \( p \) and \( q_c \) are obtained from the pressure and heat flux of the leaking fluid respectively. \( \bar{I} \) is the second-order identity matrix. The boundary conditions in 5.3 satisfy \( \Gamma_T \cup \Gamma_q = \Gamma \) and \( \Gamma_T \cap \Gamma_q = \emptyset, \Gamma_u \cup \Gamma_t = \Gamma \) and \( \Gamma_u \cap \Gamma_t = \emptyset, \Gamma_c \subset \Gamma_t, \bar{t} = -pn_c \) for the crack surface.

In the case of a thermo-elastic crack with convection on the faces \( \Gamma_c \subset \Gamma_q, q = q_c \).

Integration of the variational terms \( f \cdot \delta u \) and \( \delta TQ \) over the domain, and on application of the divergence theorem, provides the weak form of equation \( (5.1) \), with the prescribed boundary conditions, i.e.

\[
\int_\Omega \sigma : \delta \epsilon d\Omega = \int_\Omega f \cdot \delta u d\Omega + \int_{\Gamma_t \setminus \Gamma_c} \delta u \cdot \bar{t} d\Gamma + \int_{\Gamma_c} [[-pn \cdot \delta u]] d\Gamma \tag{5.4}
\]
\[
\int_\Omega \delta q \cdot D^{-1} q d\Omega = \int_{\Gamma_q \setminus \Gamma_c} \delta T \bar{q} \cdot n d\Gamma + \int_{\Gamma_c} [[q_c \cdot n \delta T]] d\Gamma \tag{5.5}
\]

where \( D \) is the conductivity matrix and the following solution spaces \( u_0 \) and \( T_0 \) of the test functions \( \delta T \) and \( \delta u \) are given by:

\[
u_0 = \{u \in H_1(\Omega) : u = \bar{u} \text{ on } \Gamma_u, u \text{ possibly discontinuous on } \Gamma_c\}
\]
\[
T_0 = \{T \in H_1(\Omega) ; T = \bar{T} \text{ on } \Gamma_T, q \text{ possibly discontinuous on } \Gamma_c\}
\]

Where \( H_1 \) is the Sobolev space.

The formulation is similar to a traditional FE formulation, but in this case the stiffness
matrix has an additional contribution arising from an integral along the crack. The heat vector also has a contribution due to the bulk fluid temperature along the crack.

The discretized form is:

\[
\mathbf{u}(x) = \sum_{I \in S} N_I(x) u_I + \sum_{I \in S_c} N_I(x) \left[ H(\phi(x)) - H(\phi(x_I)) \right] a_I + \sum_{I \in S_t} N_I(x) \sum_{k=1}^4 \left[ \gamma_k(x) - \gamma_k(x_I) \right] b_{kI}
\]

(5.6)

and

\[
T(x) = \sum_{I \in S} N_I(x) T_I^a + \sum_{I \in S_c} N_I(x) \left[ H(\phi(x)) - H(\phi(x_I)) \right] T_I^a + \sum_{I \in S_t} N_I(x) \left[ \gamma_1(x) - \gamma_1(x_I) \right] T_I^b
\]

(5.7)

or

\[
T(x) = \sum_{I \in S} N_I(x) T_I^a + \sum_{I \in S_c} N_I(x) \psi(x) T_I^c + \sum_{I \in S_t} N_I(x) \left[ \gamma_2(x) - \gamma_2(x_I) \right] T_I^b
\]

(5.8)

where \(a_i, b_i, T_i^a, T_i^b\) and \(T_i^c\) are additional unknowns that need to be solved for. \(S_c\) are nodes whose parent element is completely cut by the crack, \(S_t\) are nodes whose parent element is partially cut by the crack. Equation 5.7 is the approximation for a discontinuous temperature across the crack, and equation 5.8 is for a discontinuous heat flux across the crack.

For a more general formulation, the temperature can be approximated using both the weak and strong discontinuity enrichments, i.e.

\[
T(x) = \sum_{I \in S} N_I(x) T_I^a + \sum_{I \in S_c} N_I(x) \left[ H(\phi(x)) - H(\phi(x_I)) \right] T_I^a
\]

\[
+ \sum_{I \in S_c} N_I(x) \psi(x) T_I^c + \sum_{I \in S_t} \sum_{k=1}^2 N_I(x) \left[ \gamma_k(x) - \gamma_k(x_I) \right] T_{kI}^b
\]

(5.9)

Here, \(H\) is the step function which is +1 on one side of the crack and -1 on the other. \(\gamma_i\) is the
crack tip enrichment, \( \phi \) is the level set function employed to locate the crack. An important property of a traditional finite element approximation, is the kronecker delta property of the shape functions, i.e. \( N_i(x_j) = \delta_{ij} \). This ensures that the computed unknowns \( u_I \) are the actual values required of \( u(x) \) at nodes \( I \), i.e. \( u(x_I) = u_I \). It also makes imposing Dirichlet boundary conditions \( u(x) \) simple: \( u_I = \bar{u}(x_I) \) for \( x \in \Gamma_u \). The shifting of the enrichment functions \( (\gamma_j(x) - \gamma_j(x_I)) \) is done to ensure that the finite element scheme has this property. The weak discontinuity enrichment is defined in such a way that is has this feature (see equation 5.10). For the temperature field, it is possible to model a jump in heat flux on either side of the crack. This requires an enrichment function that can account for a change in the derivative of temperature across the crack. Moës Bimaterial formulation [80] is used to account for this. Moës Bimaterial formulation is:

\[
\psi(x) = \sum_I |\phi_I| N_I(x) - |\sum_I \phi_I N_I(x)| \tag{5.10}
\]

where \( \phi(x) \) is the level set and

\[
\phi(x) = \sum_I \phi_I N_I(x) \tag{5.11}
\]

\( \phi_I \) is the normal distance from the interface to the node. If the crack is assumed insulated, i.e. when there is no fluid in the gap, it is more appropriate to use the Heaviside function to give a jump in temperature. However, this does not account for different fluxes on each side of the crack. The enrichment function in 5.10 is used in 5.8 to account for the jump in heat flux at the crack. A plot of the enrichment function in 5.10 is given in Fig. 5.2 along with the derivative in Fig. 5.3. The resulting second order function has a discontinuity in the first derivative. This gives the jump in heat flux that is required. The enrichment functions describe the singular behaviour at the crack tip, and are based on the Westergaard solution.

\[
\gamma \in \left\{ \sqrt{r} \cos\left(\frac{\theta}{2}\right), \sqrt{r} \sin\left(\frac{\theta}{2}\right), \sqrt{r} \sin\left(\frac{\theta}{2}\right) \sin(\theta), \sqrt{r} \cos\left(\frac{\theta}{2}\right) \sin(\theta) \right\} \tag{5.12}
\]
where \( r \) and \( \theta \) are polar coordinates, with origin at the crack tips. For the thermal field, it is appropriate to use the following enrichment function, when a constant temperature is imposed on the crack faces:

\[
\gamma_1(r, \theta) = \sqrt{r} \cos \left( \frac{\theta}{2} \right)
\]  

(5.13)

This is suitable, because it is constant along \( \pi \) and \( -\pi \), which are the respective crack faces. Hence the temperature is continuous across the crack, when this enrichment function is used (see Fig. 6.1). Taking the derivative with respect to \( \theta \), gives sinusoidal behaviour, which is discontinuous across the crack, giving a discontinuity in heat flux, as shown in Fig. 6.4 When
the crack faces are subject to a constant heat flux, this enrichment function should be used:

$$\gamma_2(r, \theta) = \sqrt{r} \sin \left( \frac{\theta}{2} \right)$$  \hspace{1cm} (5.14)

This is discontinuous from $\pi$ to $-\pi$, hence the temperature can be discontinuous across the crack. See Figs. 6.2 and 6.3 for a plot of equation 5.14 and its derivative respectively.

The pressure term given in the weak form (5.5) is now analysed. There is a non-zero traction on each face of the crack, which is equal in magnitude but in opposite directions. The normals $\mathbf{n}_1$ and $\mathbf{n}_2$ are defined on each face of the crack $\Gamma_1$ and $\Gamma_2$, and $\mathbf{n}$ is the global normal, as shown in Fig 5.1. The relationship between the crack face normals is defined to be $\mathbf{n}_1 = -\mathbf{n}_2$.

The crack is taken to be a single contour $\Gamma_c = \Gamma_1 \cup \Gamma_2$ as shown in Fig. 5.4. This is physically justified for small crack openings, where the crack is taken to be the limit as the two faces converge, with a jump term along the contour to account for the pressure of heat flux acting on the walls. The pressure term becomes:

$$\int_{\Gamma_c} [-p \mathbf{n} \cdot \delta \mathbf{u}] d\Gamma = \int_{\Gamma_c} -p((\mathbf{n}_1 \cdot \delta u_1) + (\mathbf{n}_2 \cdot \delta u_2)) d\Gamma$$

$$= \int_{\Gamma} -p\mathbf{n}_2 \cdot (\delta u_2 - \delta u_1) = \int_{\Gamma_c} -2p\delta u_n d\Gamma$$  \hspace{1cm} (5.15)

where $\delta u_n$ is variation along the crack, symmetry is assumed on either side of the crack.

Similarly, for the thermal case, there is a heat flux on each face of the crack, equal in magnitude but in opposite directions. This flux is defined by a convection law ($q_i = h(T - T_{bulk})\mathbf{n}_i$),
therefore:

\[
\int_{\Gamma_c} [q \cdot n] \delta T d\Gamma = \int_{\Gamma_c} (q_1 \cdot n_1 \delta T_1 + q_2 \cdot n_2 \delta T_2) d\Gamma = \int_{\Gamma_c} (h(T_{bulk} - T_1) \delta T_1 + h(T_{bulk} - T_2) \delta T_2) d\Gamma \\
= \int_{\Gamma_c} (hT_{bulk}(\delta T_1 + \delta T_2) - h(T_1 \delta T_1 + T_2 \delta T_2)) d\Gamma \\
= \int_{\Gamma_c} (hT_{bulk}[[\delta T]] - h[[T \delta T]]) d\Gamma
\]

(5.16)

Considering equation 5.5, \(T_{bulk}\) and \(h\) are known \textit{a priori}, but \(T\) must be obtained from the solution, therefore it is incorporated into the left hand side.

\[
\int_{\Omega} \delta q \cdot D^{-1} q d\Omega + \int_{\Gamma_c} h[[T \delta T]] d\Gamma = \int_{\Gamma_q \setminus \Gamma_c} \delta T q \cdot n d\Gamma + \int_{\Gamma_c} h[[\delta T]] T_{bulk} d\Gamma
\]

(5.17)

With the current formulation it is possible to model either a discontinuity in heat flux or temperature. This is because the temperature approximation can contain the Heaviside, or the level set enrichment which account for the strong or weak discontinuity respectively.

Using the convection law above, means that prescribing a temperature along the crack is simply a case of fixing the heat transfer coefficient to be very large. This would give a constant temperature along the crack, without the need to use Lagrange multipliers. Currently this is what is done for imposing Dirichlet conditions in XFEM [104].

5.3 Finite Element Equations

Inserting the test functions and trial functions into the weak form leads to the fully coupled mechanical system of equations which can be solved simultaneously with respect to the mechanical and thermal degrees of freedom:

\[
[K][\xi] = [F]
\]

(5.18)
with the vectors \([\xi] = [U, A, B, T_u, T_a, T_b, T_c]^T\) and \([F] = [F^u, F^a, F^b, Q^u, Q^a, Q^b, Q^c]^T\).

Here, the subscripts \(u, a, b\) and \(c\) denote the standard, step enriched, tip enriched and weak discontinuity enriched degrees of freedom. The upper case letters, \(U, A, B\) are DoF for mechanical, \(T_u, T_a, T_b, T_c\) are DoF for thermal. The same standard linear shape functions \(N\) are used for both the mechanical and thermal fields.

**Submatrices**

The thermo-mechanical and thermal element matrices are structured as follows:

\[
[K_{\text{mech}}] = \begin{bmatrix}
K^{uu}_M & K^{ua}_M & K^{ub}_M & K^{uu}_TM & K^{ua}_TM & K^{ub}_TM & K^{uc}_TM \\
K^{au}_M & K^{aa}_M & K^{ab}_M & K^{au}_TM & K^{aa}_TM & K^{ab}_TM & K^{ac}_TM \\
K^{bu}_M & K^{ba}_M & K^{bb}_M & K^{bu}_TM & K^{ba}_TM & K^{bb}_TM & K^{bc}_TM \\
\end{bmatrix}
\]

\[\text{(5.19)}\]

\[
[K_{\text{ther}}] = \begin{bmatrix}
K^{uu}_T & K^{ua}_T & K^{ub}_T & K^{uc}_T \\
K^{au}_T & K^{aa}_T & K^{ab}_T & K^{ac}_T \\
K^{ba}_T & K^{bb}_T & K^{bc}_T \\
K^{cu}_T & K^{ca}_T & K^{cb}_T & K^{cc}_T \\
\end{bmatrix}
\]

\[\text{(5.20)}\]

where the subscripts \(M, T\) and \(TM\) correspond to the mechanical, thermal and thermo-mechanical components respectively.
Mechanical

\[
[K_{M}]_{IJ} = \int_{\Omega} [B]_{I} [C] [B]_{J} d\Omega \quad (5.21a)
\]

\[
[K_{M}]_{IJ} = \int_{\Omega} [B]_{I} [C] [B]_{J} d\Omega \quad (5.21b)
\]

\[
[K_{M}]_{IJ} = \int_{\Omega} [B]_{I}^{\alpha} [C]^{\beta} [B]_{J}^{\beta} d\Omega \quad (5.21c)
\]

and

\[
[F_{I}] = \int_{\Gamma_1 \setminus \Gamma_c} [N]_{I} \bar{t} d\Gamma - \int_{\Gamma_c} [N]_{I} 2pd\Gamma \quad (5.22a)
\]

\[
[F_{I}] = \int_{\Gamma_1 \setminus \Gamma_c} [N]_{I} \bar{t} d\Gamma - \int_{\Gamma_c} [N]_{I} 2pd\Gamma \quad (5.22b)
\]

where \( \alpha, \beta \in \{0, 1, 2, 3, 4\} \) denote the extra degrees of freedom, 0 corresponds to Heaviside enriched, 1 – 4 are the branch term enriched.

The first order elasticity tensor \([C]\), for plane stress, is given by:

\[
[C] = \frac{E}{1- \nu^2} \begin{bmatrix}
1 & \nu & 0 \\
\nu & 1 & 0 \\
0 & 0 & \frac{1- \nu}{2}
\end{bmatrix} \quad (5.23)
\]

where \( E \) is the elastic modulus and \( \nu \) is Poisson’s ratio.
Thermomechanical

\[
[K_{TM}^{uu}]_{IJ} = \int_{\Omega} [B]_I [C] \alpha_T [N]_J d\Omega 
\]
(5.24a)

\[
[K_{TM}^{u\alpha}]_{IJ} = \int_{\Omega} [B]_I^{\alpha} [C] \alpha_T [N]_J d\Omega 
\]
(5.24b)

\[
[K_{TM}^{\alpha u}]_{IJ} = \int_{\Omega} [B]_I [C]^{\alpha} \alpha_T [N]_J d\Omega 
\]
(5.24c)

\[
[K_{TM}^{\alpha\beta}]_{IJ} = \int_{\Omega} [B]_I^{\alpha} [C]^{\beta} \alpha_T [N]_J d\Omega 
\]
(5.24d)

where \( \alpha \in \{0, 1, 2, 3, 4\} \) and \( \beta \in \{0, 1\} \), where the 0 corresponds to the weak or strong discontinuity enrichment and the 1 is either a cosine or sine enrichment. If the enrichment in Eqn. 5.9 is used, \( \beta \in \{0, 1, 2, 3\} \).

Thermal

The Conductivity matrix is made up of the standard matrix plus the contribution from the crack face condition.

\[
[K_{T}^{uu}]_{IJ} = \int_{\Omega} [B]_I [D] [B]_J d\Omega + \int_{\Gamma_e} h_e [[[N]_I][N]_J] d\Gamma 
\]
(5.25a)

\[
[K_{T}^{u\alpha}]_{IJ} = \int_{\Omega} [B]_I^{\alpha} [D] [B]_J d\Omega + \int_{\Gamma_e} h_e [[[N]_I][N]_J^{\alpha}] d\Gamma 
\]
(5.25b)

\[
[K_{T}^{\alpha u}]_{IJ} = \int_{\Omega} [B]_I [D]^{\alpha} [B]_J d\Omega + \int_{\Gamma_e} h_e [[[N]_I^{\alpha}][N]_J] d\Gamma 
\]
(5.25c)

\[
[K_{T}^{\alpha\beta}]_{IJ} = \int_{\Omega} [B]_I^{\alpha} [D]^{\beta} [B]_J d\Omega + \int_{\Gamma_e} h_e [[[N]_I^{\alpha}][N]_J^{\beta}] d\Gamma 
\]
(5.25d)

and

\[
[Q^u]_I = \int_{\Gamma_q \setminus \Gamma_e} [N]_I \bar{q} d\Gamma + \int_{\Gamma_e} [[[N]_I]] h_e T_{bulk} d\Gamma 
\]
(5.26a)

\[
[Q^\alpha]_I = \int_{\Gamma_q \setminus \Gamma_e} [N]_I^{\alpha} \bar{q} d\Gamma + \int_{\Gamma_e} [[[N]_I^{\alpha}]] h T_{bulk} d\Gamma 
\]
(5.26b)

where \( \alpha, \beta \in \{0, 1\} \) or \( \{0, 1, 2, 3\} \) depending on the approximation used. \([D]\) contains the
conductivity, \( k \), i.e.

\[
[D] = k \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
\] (5.27)

For the two-dimensional case, the \([B]\) matrices for the mechanical part are:

\[
[B]_I = 
\begin{bmatrix}
[N]_{I,x} & 0 \\
0 & [N]_{I,y}
\end{bmatrix}
\] (5.28)

For the heaviside enriched nodes

\[
[B^0]_I = 
\begin{bmatrix}
([N]_I(H(\phi(x)) - H(\phi(x_I))))_{x,x} & 0 \\
0 & ([N]_I(H(\phi(x)) - H(\phi(x_I))))_{y,y}
\end{bmatrix}
\] (5.29)

For the branch enriched nodes

\[
[B^\alpha]_I = 
\begin{bmatrix}
([N]_I(\gamma_\alpha(x)) - \gamma_\alpha(x_I)))_{x,x} & 0 \\
0 & ([N]_I(\gamma_\alpha(x)) - \gamma_\alpha(x_I)))_{y,y}
\end{bmatrix}
\] (5.30)

For \( \alpha \in \{1, 2, 3, 4\} \).

For the thermal part, the \( B \) matrix for the standard shape functions is:

\[
[B]_I = 
\begin{bmatrix}
[N]_{I,x} \\
[N]_{I,y}
\end{bmatrix}
\] (5.31)

For the thermo-mechanical part of the structure matrix, the \((N)\) matrix for the standard shape
functions is:

\[
[N]_I = \begin{bmatrix} [N]_I & [N]_I \end{bmatrix}
\]  

(5.32)

Enriched shape functions are treated in exactly the same way as the standard functions.

The structure matrix for two dimensions reduces to:

\[
[K]_{struc} = \begin{bmatrix} [K^M]_{11} & [K^M]_{12} & [K^{TM}]_1 \\
[K^M]_{21} & [K^M]_{22} & [K_{TM}]_2 \\
0 & 0 & [K^T] \end{bmatrix}
\]  

(5.33)

Where \( K^T \) is a 12x12 matrix, \( K^M_{ij} \) are 24x24 matrices and \( K^{TM}_{ij} \) are 24x12 matrices.

If we consider a 4 noded quadrilateral linear element, the standard shape functions in a reference domain are:

\[
[N]_I(\xi, \eta) = \frac{1}{4} \begin{bmatrix} (1 + \xi)(1 + \eta) \\
(1 - \xi)(1 + \eta) \\
(1 - \xi)(1 - \eta) \\
(1 + \xi)(1 - \eta) \end{bmatrix}
\]  

(5.34)

where \( \xi, \eta \in [-1, 1] \). The reference domain is mapped to the real element under a smooth map.

## 5.4 Fluid models

The crack is modelled using the single and two phase formulations in section 4.2 and 4.3 respectively. For the case of two phase flow, the mass flux and pressure constraints form a
A simultaneous non-linear system which can be solved by Newton-Raphson iteration, i.e.

\[ C^2_c = \frac{1}{\frac{X_{\nu gc}}{\gamma_0 p_c} - (\nu_{gc} - \nu_{Lc}) N \frac{dX_E}{dp}} = 0 \]  

\[ p_c + p_e + p_a + p_f + p_k + p_{aa} - p_0 = 0 \]

where \( G_c \) is the critical mass flux, \( \nu_{gc} \) and \( \nu_{Lc} \) are the specific enthalpy of the vapour and liquid respectively, \( \gamma \) is the isentropic exponent and \( X_c \) and \( X_E \) are the non-equilibrium and equilibrium mixture quality, given by:

\[ X_c = N X_E (1 - e^{[-B(L/D_i-12)]}) \]  

\[ X_E = \left[ \frac{S_0 - S_{Lc}}{S_{gc} - S_{Lc}} \right] \]

where \( N = 20 \) for \( X_E < 0.05 \) and \( N = 1 \) for \( X_E \geq 0.05 \). The constant \( B = 0.0523 \). The subscripts 0, c, e, a, f, k and aa denote the vessel pressure, critical, entrance, phase change acceleration, frictional, corners, and area change acceleration pressure losses respectively.

Properties of steam are obtained from IAPWS IF-97 steam tables [115]. The thermal non-equilibrium is accounted for by a relaxation condition which is an expression derived from experimental data [33]. This is the most practical way of accounting for heat transfer between the liquid and vapour. To model this process in detail using CFD would be prohibitively expensive.

For the single phase case, the situation is much more simple:

\[ \dot{m} = C_D (\rho_0 p_0)^{1/2} A \]

where \( C_D \) is the discharge coefficient, \( p_0 \) and \( \rho_0 \) are the inlet pressure and density and \( A \) is the average COA. The heat transfer coefficient is calculated from on the flow rate, channel dimensions and fluid properties. The Dittus Boelter correlation can be used as a good
approximation:

\[ Nu = 0.023Re^{0.8}Pr^{0.4} \]  \hspace{1cm} (5.38)

where \( Re = \dot{m}D_h/A\mu \), \( Pr = cp\mu f/k_f \) and

\[ h_c = \frac{k_f}{D_h}Nu \]  \hspace{1cm} (5.39)

where \( D_h \) is the hydraulic diameter of the channel, \( c_p, k_f, \mu_f \) is the specific heat, conductivity and viscosity of the fluid respectively.

### 5.5 Integration

Numerical integration is complicated somewhat by the fact that there are discontinuous and singular functions in the approximation. These non-polynomial functions cannot be accurately integrated using standard Gaussian quadrature. Therefore, there have been various methods proposed that are designed to overcome these problems, one such method is to subdivide elements into smaller integration regions [95] [116] [73]. Crack tip elements are broken down into triangles, which have a vertex at the crack tip. Crack front elements are dissected into sub quadrilaterals which are aligned with the level set. For integration along the level set itself, there is a 1-d integral performed and the integration points are distributed along the level set.

The method of subdivision is chosen here due to its robustness and accuracy, as well as it being relatively simple to implement. Figure 5.5 shows the integration points in a cracked element. The quadrangles have a side which align with the discontinuity. The level set integration points are also shown and the contribution from both of these sets of integration points gives the total integral for the element. Figure 5.6 shows the integration points in the crack tip.
Six triangles decompose the element, all of which have a vertex at the crack tip. Within each of these triangles are twenty five integration points. Along the crack, an algorithm populates the segment of the level set that is cracked.

Figure 5.5: Integration points in the reference element containing part of the crack front, (a) in the element and (b) along the crack

Figure 5.6: Integration points in the reference element containing the crack tip, (a) in the element and (b) along the crack
5.6 Implementation

The 2-D code developed here has the ability to model plates with cracks placed anywhere, and with any configuration without any need to change the mesh. The user supplies the dimensions of the plate with a mesh size, along with the crack tips and enrichment radius. The code then generates the mesh and level set it then finds the enriched elements. After all the initial conditions have been input, the code runs and outputs a leak rate as well as any other quantities of interest. The coupling between the fluid and the structure can be summarised with the help of Fig. 5.7. The initial temperature field is input to the thermomechanical model, and a crack opening displacement is obtained from the solution. This COD is used in the leak rate calculation to give the leak rate and heat transfer coefficient. A new temperature is then calculated and fed into the thermomechanical model to obtain a new COD. This process is repeated until a steady COD or leak rate is obtained.

5.6.1 One dimensional case

For the 1-d case, a single element is considered which contains a cohesive crack. This is necessary to maintain the integrity of the element, so a traction separation law which related the stress to the displacements on each side of the crack [96] is used, i.e.

\[ t_c = k_c (u^+ - u^-) \]  

(5.40)

Hooke’s law is assumed applicable everywhere else.

Expressions below are obtained by considering the stresses and strains in the element and following some manipulation give:

\[ u_c^+ = \frac{-E u_1 - k_c L u_1 + p x_c + k_c u_1 x_c - k_c u_2 x_c}{E + k_c L} \]  

(5.41)

\[ u_c^- = \frac{-L p_c - k_c L u_1 - E u_2 + p x_c + k_c u_1 x_c - k_c u_2 x_c}{E + k_c L} \]  

(5.42)
Figure 5.7: Schematic of the code used to find leak rate based on thermo-mechanical simulation.
where $L$ is the original length of the element, $k_c$ is the crack stiffness parameter, $p$ is the internal pressure, $x_c$ is the location of the crack, $u_1$ and $u_2$ are the displacements at nodes 1 and 2 respectively. The magnitude of the difference between $u_c^-$ and $u_c^+$ provides an expression for the crack opening displacement, i.e.

$$
COD = |u_c^- - u_c^+| = \frac{-Eu_1 + Eu_2 + Lp}{E + k_cL} \tag{5.43}
$$

For the thermal case, there can be different temperatures on either side of the crack. The heat transfer is defined by the convection law:

$$
q_{1,2} = h_c(T_{bulk} - T_{1,2})n_{1,2} \tag{5.44}
$$

where $n_{1,2}$ are the normals on face 1 and 2 respectively. Balancing heat flux gives:

$$
T_c^- = h_cT_{bulk} - kT_1/(h_c x_c - k) \tag{5.45}
$$

$$
T_c^+ = kT_2/(L - x_c) - h_c T_{bulk} / \{k/(L - x_c) - h_c\} \tag{5.46}
$$

Given the linear nature of this problem, the single elements agree exactly with the analytical models. This is shown in Figs. 5.8 and 5.9.

As another example, the Heaviside and Bimaterial formulation are used in conjunction by multiplying them together, so the new approximation becomes:

$$
T(x) = \sum_{I \in S} N_I(x)T_{I}^u + \sum_{I \in S_c} N_I(x)[H(\phi(x)) - H(\phi(x_I))]\psi(x)T_{I}^a \tag{5.47}
$$

where there is a term in the conductivity matrix like the following:

$$
\int_{\Gamma_c} [N][N]^T d\Gamma \tag{5.48}
$$

which for the 1d case is simply $[N][N]^T$ evaluated at the crack location. Evaluating the
Figure 5.8: Comparison between mechanical 1-D finite element and theoretical.

Figure 5.9: Comparison between thermal 1-D finite element and theoretical.
Heaviside enriched shape functions in the one dimensional element considered here, gives the following:

\[ N_1H_1 = N_1(H(x) - H(x_1)) = \begin{cases} 0 & \text{if } x \leq x_c; \\ 2N_1 & \text{if } x > x_c. \end{cases} \] (5.49)

\[ N_2H_2 = N_2(H(x) - H(x_2)) = \begin{cases} -2N_2 & \text{if } x \leq x_c; \\ 0 & \text{if } x > x_c. \end{cases} \] (5.50)

The distances of each node from the level set are \( \phi_1 = x_1 - x_c = -x_c \) and \( \phi_2 = x_2 - x_c = x_l \), so the enrichment function in equation 5.10 for the one dimensional element becomes:

\[ \psi(x) = N_1(x)x_c + N_2(x)x_l - | - N_1(x)x_c + N_2(x)x_l | \] (5.51)

A plot of \( H(x)N_1(x) \) and \( H(x)N_1(x)\psi(x) \) for a 1D element with a crack at its midpoint is given in Figs. 5.10 and 5.11 respectively.

The components of the stiffness matrix for a Moës bi-material enrichment (temperature) from analytical integration are given in Appendix D. The results of the simulation for various conditions are given in Fig. 5.12. When the heat transfer coefficient is zero, and there is a linear temperature profile through the element, there is a jump in temperature at the crack. For non-zero heat transfer coefficient, and a bulk temperature higher than the ends of the element, there is a temperature spike within the element.

The one dimensional study indicates that, in principle, an XFEM element can model the thermal and mechanical effects of a leaking fluid within an element. The traction separation law, which was introduced to keep the element held together, is not necessary for a full two dimensional model. This is because the surrounding material holds the structure together.
Figure 5.10: Shape functions multiplied by shifted Heaviside function

Figure 5.11: Shape functions multiplied by shifted Heaviside function and bimaterial enrichment
could occur at the crack. However, if the heat transfer coefficient was sufficiently large, then the temperature on each side of the crack would be the same. For the case of a leaking fluid through a crack, the heat transfer coefficient in most practical situations will be large enough for the crack temperatures to attain the same temperature. Therefore, it would be more appropriate to use an enrichment which can account for a discontinuity in the derivative of temperature. Both the Heaviside and Moës enrichments are investigated in the following section for the temperature model.

The 1-D example was further extended to a three element system, this was to check continuity between enriched and non-enriched elements. It was found that the transition between elements was continuous, so in principle this should be the same for a 2-D implementation. The details of the structure matrices for this model are in Appendix C.
5.6.2 Two dimensional case

The mesh used for the 2D model is shown in Fig. 5.13. Enriched elements are those that are cut by the crack, and are within a certain radius of the crack tip. These elements are enriched with the Heaviside and branch functions respectively. A visualisation of the opening of an angled crack is given in Fig. 5.14. Analytical models (see Appendix A) show that in reality the heat flux singularity is logarithmic, whereas the selected enrichment function gives singular behaviour like $1/\sqrt{r}$. As will be seen in this chapter, the $\sqrt{r}$ is a pragmatic choice for the approximation of thermal fields around crack tips. This is because differentiation is more straightforward and high accuracy is achieved.
Figure 5.14: Close up of crack opening displacement
5.7 Results

5.7.1 Convergence

In order to assess the accuracy and convergence performance of the element in a full finite element model, analytical models were derived and energy and temperature error norms calculated. The analytical expression for a prescribed temperature on the crack embedded in an infinite 2-D domain is:

\[ T(x, y) = -\frac{T}{\pi \ln(a/2)} \oint_{\Gamma} \frac{\ln[(x-s)^2 + y^2]^{1/2}}{\sqrt{a^2 - s^2}} d\Gamma \]  \hspace{1cm} (5.52)

where \( \Gamma \) is the contour of the crack, \( s \) is a parameter which traverses the length of the crack, \( a \) is the crack length and \( (x, y) \) is a point on the plate. The \( H^1 \) and \( L^2 \) norm are used to show the relative error in the energy and temperature respectively, where \( T^h \) is the numerical approximation and \( T \) is the exact solution, i.e.

\[ ||T - T^h||_{H^1(\Omega)} = \frac{\sqrt{\int_{\Omega} (\nabla T - \nabla T^h)^T D (\nabla T - \nabla T^h) d\Omega}}{\sqrt{\int_{\Omega} (\nabla T)^T D (\nabla T) d\Omega}} \]  \hspace{1cm} (5.53)

\[ ||T - T^h||_{L^2(\Omega)} = \frac{\sqrt{\int_{\Omega} (T - T^h)^T (T - T^h) d\Omega}}{\sqrt{\int_{\Omega} T^2 d\Omega}} \]  \hspace{1cm} (5.54)

where the denominator terms are included for normalisation purposes.

The singularity in heat flux is obtained in the approximation by choosing a \( r^{1/2} \) enrichment function for the temperature field. On differentiation this gives a \( r^{-1/2} \), which is singular. In order to get a \( \ln r \) singularity, an enrichment function like \( r \ln r - r \) would be required. The \( r^{1/2} \) was chosen as this is straightforward to work with when differentiating and integrating.
For the displacement, an analytical expression is derived based on a method of complex potentials. The pressure term is included via the principle of superposition. The displacements are:

\[ 2\mu u_1 = \frac{\kappa - 1}{2} Re\phi - x_2 Im\phi' \]
\[ 2\mu u_2 = \frac{\kappa + 1}{2} Im\phi - x_2 Re\phi' \]  

(5.55)

where \( \phi \) is the complex potential according to Muskhelishvili [61], \( \mu \) is a Lamé coefficient and \( \kappa \) is the Kosolov constant. The variables \( x_1, x_2, u_1, u_2 \) represent the coordinates and displacements in the 1 and 2 directions. So the COD at the midpoint of the crack is:

\[ COD = (\sigma_0 + p)\left(\frac{\kappa + 1}{2\mu}\right)a \]  

(5.56)

where \( p \) and \( \sigma_0 \) are the pressure and far field stress respectively. This is then compared with COD obtained from the finite element solution, which is given by the expression:

\[ COD = 2 \sum_i N_i(x_0)a_i \]  

(5.57)

where \( x_0 \) is the mid-point of the crack. This is due to the fact that standard shape functions are equal along the crack, and the enriched shape functions are \( \pm 1 \), so taking the difference gives a factor of two.

There is an option to modify this crack opening displacement due to plasticity effects, which are known to increase the crack opening area considerably [8]. Currently, the code uses a relationship between elastic and elastic plastic stress intensity factor \( (K) \) from the R6 Failure Assessment Diagram (FAD), and the fact that COD is proportional to \( K^2 \). The results of the convergence study are shown in Figs 5.15, 5.16 and 5.17.

Figure 5.15 shows that the error in temperature is less than 0.001% for a mesh size smaller than 0.01, and the slope of the line is 1.7 when the weak enrichment is used. The mesh
Figure 5.15: Thermal $L_2$ error norm against relative mesh size, $h$ for weak and strong discontinuity enrichments.

Figure 5.16: Thermal Energy error norm against mesh size, $h$ for weak and strong discontinuity enrichments
size is defined to be the width of an individual element divided by the width of the plate. When a strong enrichment is used the slope of the line is 1. The optimal convergence rate for a smooth function in standard finite elements is $O(h^2)$ if the $L^2$ norm is being used. Therefore when the correct enrichment is used, the convergence is getting close to optimal. This comes about because a fixed area, or geometric enrichment is used. By utilising such an enrichment, optimal convergence can be achieved, however this is at the expense of a huge increase in condition number. Ways to avoid such increases in condition number are discussed in [83]. Implementing this method on a larger scale would required more consideration of the condition number to improve solver performance, however only the accuracy was of interest for this study. For the energy error the error is less than 5% for a mesh size smaller than 0.01 and the slope of the line is 0.9 for when weak enrichment is used. This is close to 1, which is the optimal convergence rate of the energy error norm. For a cracked domain, the optimal convergence of standard finite elements is $O(\sqrt{h})$. When the strong enrichment is used for this problem, the slope of the convergence curve is 0.5, so the convergence is no better than
standard finite elements. The integration was 3rd order for standard and crack face elements, and 5th order for the crack tip elements.

5.7.2 Stress and Heat Flux

The stress component $\sigma_{yy}$ after application of 155 bar of pressure on the crack faces is given in Fig. 5.18 where the upper and lower surfaces are fixed in the $y$ direction. The stress pattern is very similar to the situation of a far field stress being applied, and the crack faces are traction free. Heat flux and temperature are shown for an angled crack in figures 5.19, 5.20 and 5.21. A fluid temperature of 295 °C was taken, and the upper and lower surfaces were fixed at 290 °C. The singular behaviour in Fig. 5.20 can be clearly seen at the crack tips. Figure 5.22 is a plot of heat flux vectors. This demonstrates how the heat flows in a plate containing an angled crack with heat transfer on the faces.
5.7.3 Temperature using all enrichment functions

Using the approximation given in equation 5.9, it is possible to exploit the properties of all the enrichment functions so that no assumption is made about the continuity of temperature or heat flux at the crack. A temperature gradient was imposed across a 1mx1m plate by fixing temperatures of 292°C and 290°C on the upper and lower surfaces. A horizontal crack of length 0.2m was centred about the origin and the bulk fluid temperature was 295°C. The heat transfer coefficient was varied between 0 and 1000 W/m²K. The results for temperature along the y axis are shown in Fig 5.23.

5.7.4 Leak Rates

Leakage rates are calculated for water, which is slightly subcooled at high pressure. Thermo-mechanical simulations are performed using approximate values for standard operating conditions of a Pressurised Water Reactor (PWR), i.e. $p_0 = 155$ Bar, $T = 300$°C. Various crack
Figure 5.20: Heat flux in the x-direction
Figure 5.21: Heat flux in the y-direction
lengths are simulated at three different fluid temperatures of 290°C, 295°C and 300°C. Approximate material properties of stainless steel are taken with $E = 200$ GPa, $\nu = 0.3$, $\alpha = 1.282 \times 10^{-5}$ and $k = 20$ W/mK. The dimensions of the plate are 1mx1m with a thickness of 25mm, see Fig 6.10. Displacements of 0.1mm and -0.1mm are imposed on the upper and lower sides of the plate, and the temperatures were fixed at 290°C, which is also taken as the reference temperature in the thermal strain calculation. The effect of bulk fluid temperature on leak rate for a horizontal crack is shown in Figure 5.24.
Figure 5.23: Temperature along the y axis for a plate with temperature gradient and crack with different heat transfer coefficients
Figure 5.24: Leak rate against crack length for PWR conditions with three different fluid temperatures
Chapter 6

Thermal stresses and crack closure

6.1 Introduction

When carrying out a LbB, it is important to obtain an accurate prediction of leak rate. This can be done using fracture mechanics to calculate the COA. Then from this, a mass flow rate can be deduced based on the channel depth and inlet conditions. The fracture mechanics and fluid mechanics are generally considered separately. In this chapter, more analysis on the new finite element method is presented, with a focus on thermal stresses and crack closure.

When a fluid which is at high temperature and pressure leaks through a crack, there is an influence on the structure. This is due to the additional heating from the fluid to the structure along the crack walls, as well as the pressure acting to open the crack. These two effects necessitate the use of thermo-mechanical models, which can account for the local behaviour at the crack. Analytical models which use complex stress potentials to solve the case of an insulated crack in a uniform stress field are well established [60]. However, these are limited to the case of a crack in a plate, and more complex cases require numerical analysis.

The finite element method presented here is designed to capture all the relevant physics when a fluid leaks through a crack within a single element. This is achieved using the XFEM, which
can embed discontinuities and singular behaviour within elements. In addition to this, special
jump terms are added to the approximation space to account for the pressure and heat flux
of the leaking fluid acting along the crack. The new element will be referred to as xLbB.

The enrichment of the temperature field is sufficiently general to model discontinuities in
temperature along the crack, as well as a discontinuity in the heat flux. The justification of
these enrichment terms is based on a convergence study performed using analytical solutions
derived via a Green’s function method.

This chapter is structured as follows. First a description of all the enrichment functions is
given, then a comparison of crack opening displacement for a hot crack under pressure is
presented in Section 6.3, where the model used for comparison is a focussed mesh in Abaqus
using standard elements. The heat flux and stress plots are then discussed, as well as the leak
rates for Pressurised Water Reactor (PWR) conditions.

6.2 Enrichment functions

Figures 6.1, 6.2, 6.3 and 6.4 show plots of the thermal enrichment functions and their deriva-
tives with respect to $y$. The crack is located along the x-axis with tip at $(0, 0)$. If the crack is
insulated, there is a discontinuity in temperature across the crack and the enrichment function
$\gamma_2 = \sqrt{r} \sin(\theta/2)$ captures this behaviour. This is because the crack is defined to have faces
at $\pm \pi$, therefore $\gamma_2(\pm \pi) = \pm 1$. When the crack is hotter than the surrounding structure,
for example, when a hot fluid is escaping, the temperature is continuous. Therefore, under
these circumstances, the enrichment function $\gamma_1 = \sqrt{r} \cos(\theta/2)$ is more appropriate, as this
is continuous across the crack, $\gamma_1(\pm \pi) = 0$. The derivative of temperature would be discon-
tinuous across the crack in this case, and the enrichment function has this property, as seen
in Fig. 6.4. The derivative of $\sqrt{r} \sin(\theta/2)$ is continuous across the crack as seen in Fig. 6.3.
Both Figs. 6.3 and 6.4 show a singularity at the crack tip, which is what is predicted by linear
elastic fracture mechanics. The final two enrichment functions are given in Figs. 6.5 and 6.6.
both of which are continuous across the crack.

Figure 6.1: Enrichment function $\gamma_1 = \sqrt{r} \cos(\theta/2)$

Figure 6.2: Enrichment function $\gamma_2 = \sqrt{r} \sin(\theta/2)$
Figure 6.3: Derivative of enrichment function $\frac{\partial \gamma_2}{\partial y}$

Figure 6.4: Derivative of enrichment function $\frac{\partial \gamma_1}{\partial y}$
Figure 6.5: Enrichment function $\gamma_3 = \sqrt{r} \cos(\theta/2) \sin(\theta)$

Figure 6.6: Enrichment function $\gamma_4 = \sqrt{r} \sin(\theta/2) \sin(\theta)$
The code simply requires the user to input the coordinates of two crack tips, then a straight line is automatically drawn between these points, which would define the level set. This is a thermo-elastic formulation. However, it is well known that plasticity can significantly increase the COA due to blunting at the crack tip [8]. Therefore, in order for this model to be adequate for nuclear applications, where extensive plasticity is accepted in the design, a correction must be included for these effects.

6.3 Effects of plasticity

Blunting of the crack tip occurs due to void growth and coalescence in the material ahead of crack tip [117]. This plasticity is accounted for in the model with a correction factor based on the R6 Failure Assessment Diagram (FAD) [2]. The COA is proportional to the square of the SIF, and the FAD gives a relationship between elastic and elastic plastic SIF’s. Therefore, as a good first approximation, the elastic plastic COD can be obtained from the elastic COD and FAD via the equation

\[ COA_{ep} = COA_e \times \left(1/f_1^2\right) \]  (6.1)

where \( f_1 = K_e/K_{ep} \) and is a function of \( L_r \), an R6 parameter defined by

\[ L_r = \frac{\sigma_{ref}}{\sigma_y} \]  (6.2)

where \( \sigma_{ref} \) is a reference stress, which accounts for an increase in stress in the remaining ligament of material when a crack is present and where \( \sigma_y \) is the yield stress of the material. For a plate of width \( 2W \) containing a central crack of length \( 2a \), loaded with a constant membrane stress of \( \sigma \), the reference stress is

\[ \sigma_{ref} = \sigma (1 - a/W)^{-1} \]  (6.3)
A plot of $f_1$ against $L_r$ is given in Fig. 6.7. A plot of elastic and elastic-plastic crack opening displacements is given in Fig. 6.8. The material used in the elastic-plastic Abaqus simulation obeyed a Ramberg Osgood law for isotropic hardening given by:

$$\epsilon = \frac{\sigma}{E} + Y\left(\frac{\sigma}{\sigma_y}\right)^m$$  \hspace{1cm} (6.4)

where $E = 200$ GPa, $\sigma_y = 344.8$ MPa, $m = 5$, $Y = 0.002$.

![Figure 6.7: R6 failure assessment diagram (FAD)](image)

### 6.4 Abaqus model

The Abaqus model uses linear plane stress elements CPS4 and the thermal model uses linear heat transfer elements DC2D4. A quarter model is considered and the crack is defined as a traction free surface by imposing a fixed displacement boundary condition on the remaining ligament. Meshing around the crack tip is focussed and the singularity at the tip uses a
Figure 6.8: Crack opening displacement from Abaqus simulation and with R6 correction factor collapsed element side with single node at the crack tip. The thermal model is solved separately on the same mesh, then the solution is input into the thermo-mechanical model as a predefined field in a load step.

6.5 Results

6.5.1 Verification with Abaqus

To test the thermomechanical behaviour of the new element, a comparison between the new method and a model using standard elements in Abaqus was undertaken. Standard crack meshing techniques were used, with a focussed region surrounding the crack as shown in Fig. 6.9. The mesh used for the xLbB model, used the same linear elements. However, there was no focussed region, the crack is defined by a level set within elements, see Fig. 6.10. Boundary conditions were imposed on the upper and lower surfaces in the form of zero displacement. Crack face temperatures ranging from 290°C to 300°C were imposed, and the crack opening
displacement at the midpoint of the crack was calculated. The initial plate temperature was 290°C. A comparison of the two is given in Fig. 6.11. A visualisation of the crack opening area is given for both models in Figs. 6.12 and 6.13. The corresponding leak rate is given in Fig. 6.14.

6.5.2 Temperature, heat flux and stress

It is clear from Fig. 6.14 that the leak rate is reduced to near zero as bulk fluid temperature is increased. This is due to the fixed zero displacement boundary condition on the upper and lower surfaces forcing the crack to close as the fluid heats the plate. For a fixed displacement of ±0.1 mm on the upper and lower surfaces respectively, the closure is not as large, although it is still significant. Leak rates were simulated based on realistic conditions from an Advanced Gas
Figure 6.10: Close up of mesh used for xLbB simulations, crack front enriched nodes shown with circles, crack tip enriched nodes shown with squares.

Figure 6.11: Comparison of COD from Abaqus and xLbB after thermomechanical simulation for different crack face temperatures.
Figure 6.12: Crack opening for crack with (a) no additional heating and (b) 5°C of heating. Scale factor=1000
Figure 6.13: Crack opening from xLbB model with (a) no additional heating and (b) $5^\circ C$ of heating. Scale factor=$1000$
Cooled Reactor (AGR). The fluid was taken to be CO$_2$ at standard AGR operating conditions, giving bulk temperature of 800-820K and a pressure of 4MPa. The initial temperature of the plate was 800°C. The COD and leak rate results are shown in Figs. 6.15 and 6.16. So from Figures 6.14 and 6.16 it is clear that far field boundary conditions can have a large influence on the amount a crack closes due to wall heating.

The temperature along the x-axis is given in Fig. 6.17, where a peak of 300°C is observed when the heat transfer coefficient is sufficiently large. Heat flux in x and y-direction along the x-axis is given in Fig. 6.18, where the peaks are clearly visible at the crack tips. The heat flux in the y direction along the y axis is given in Fig. 6.19. $\sigma_{yy}$ along the x-axis is given in Fig. 6.20. There are the characteristic peaks at the crack tips. After the temperature field is imposed, there is a reduction in the stresses. $\sigma_{xx}$ along the x-axis has similar behaviour to $\sigma_{yy}$ as can be seen in Fig. 6.21. $\sigma_{yy}$ along the y-axis, shown in Fig. 6.22, shows the jump at the crack and the slowly decaying field towards the edges of the plate. $\sigma_{xy}$ along the x-axis is plotted in Fig. 6.23, and there is an oscillating stress pattern with peaks at the crack tips.
Figure 6.15: COD against fluid temperature for AGR conditions and displacements of ±0.1 mm on the upper and lower surfaces of the plate.

Figure 6.16: Leak rate against fluid temperature for AGR conditions and displacements of ±0.1 mm on the upper and lower surfaces of the plate.
Figure 6.17: Temperature along the x axis for different heat transfer coefficients and a bulk fluid temperature of 300°C

Figure 6.18: Heat flux in x and y direction along x axis
Figure 6.19: Heat flux in y direction along y axis

Figure 6.20: $\sigma_{yy}$ along the x axis

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Figure 6.21: $\sigma_{xx}$ along the x axis

Figure 6.22: $\sigma_{yy}$ along the y axis
Figure 6.23: $\sigma_{xy}$ along the x axis
Chapter 7

Summary and Conclusions

7.1 Conclusions

The results in chapter 4 show that thermal effects in LbB assessments are important for both the fluid and structural elements. The heating of crack faces from the leaking fluid causes an expansion of the surrounding material, which reduces the crack opening displacement. The fluid also loses heat during this process, which changes the fluid properties through the channel. It is suggested that further refinements should be made to the Ecrevisse model, by incorporating more detailed pressure loss terms, as well as accounting for thermal non-equilibrium effects. The benefit of using this model is that there is consistency between the single and two phase models, as well as a thermal coupling to the structure.

Presented in chapter 5 is an implementation of XFEM using boundary conditions that are dependent on a fluid model. The heat flux is obtained from Newton's law of cooling, where the heat transfer coefficient is obtained from empirical formulae. This provides a coupling of the fluid to the structure, which is modelled thermo-mechanically, thereby providing a means of studying changes in crack opening area due to crack wall heating. In order to test the accuracy and hence suitability of the model, convergence studies were undertaken for a 2D test case. Provided the correct enrichment function is chosen, the convergence rates proved
to be optimum for the thermal case. For the mechanical model, the crack opening area was
chosen as the parameter on which to base convergence. When the relative mesh size was
about 0.01, the relative error in crack opening displacement was less than 1%.

A more general temperature model was then presented, which made no restrictions on the
continuity of temperature or heat flux at the crack. This indicated that when using an approx-
imation containing both the weak and strong discontinuity enrichment functions, situations
ranging from low to high heat transfer could be modelled with the same model.

A test case to demonstrate the features of the new finite element method was undertaken.
This test was based on conditions experienced in nuclear reactor primary circuits, specifically
those seen in PWR’s. As shown in Fig 5.24, there is a 30% reduction in leak rate when the
fluid is 10°C hotter than the structure. These results proved the hypothesis that heat flux due
to a leaking thermofluid has a noticeable closure effect on the crack opening, and ultimately
reduces leak rate.

Performing a leak rate calculation can be done more efficiently using the new finite element
tool than using conventional finite elements and post-processing. This is because a) the
meshing of the crack and calculation of COD from nodal displacements is not required, b) the
leak rate is calculated within the procedure and c) the thermal and mechanical simulations
are all done within the main program.

Chapter 6 shows crack opening area is reduced when a hot fluid is present, especially when the
ends of the plates are fixed. Leak rate reduces to almost zero in this case, indicating the crack
is completely closed. The reduction in leak rate has consequences for an LbB assessment. This
is because if the reduction is ignored, then the leak rate would be overpredicted for a given
crack size, hence a LbB argument would be made incorrectly. Stresses are reduced with this
additional heating, this would have an effect on the critical crack size, an important parameter
when performing an LbB assessment. It is important to note here that this simulation was
performed for a specific set of boundary conditions. More cases would need to be examined
before there was sufficient confidence in the precise effects of thermal interaction between
fluid and structure for a leaking fluid. Essentially the finite element tool presented here gives a convenient way to analyse this effect quickly and with good accuracy.

7.2 Further Work

As stated in the conclusions, more test cases need to be performed with different boundary conditions to fully assess the thermal effects in Leak-before-Break. An extension of this work would be to implement this new method in a finite element code to enable 3D simulations. Once the thermo-mechanical XFEM framework is in place, it will be possible to carry out tests to assess the viability for using this in LbB assessments. Further to this, there is still much scope to improve thermal hydraulic codes used in this method. Two-phase flow is an area of active research \[34\] [41], particularly for nuclear applications, and the current state of the art could be phased into the scheme presented in this thesis. By having a heat component in the fluid models, there can be two way heat transfer between the fluid and structure. This would enable investigations into how the fluid properties change, and hence how this affects leak rate, when there is heat transfer to and from the crack walls.
Bibliography


Appendix A

Analytical models

A.1 Temperature

The problem involves an infinite 2-D plate which contains a jump in heat flux or a specified temperature along a line. The temperature field is governed by the Laplacian ($\nabla^2 T = 0$), or the screened Poisson equation ($\nabla^2 T - \chi^2 T = 0$) if there is heat transfer from the faces of the plate. The jump in heat flux condition is defined to be

$$\left. \frac{\partial T}{\partial n} \right|_{g(s) \in \Gamma^+} - \left. \frac{\partial T}{\partial n} \right|_{g(s) \in \Gamma^-} = f(s) \quad (A.1)$$

For the specified temperature

$$\left. T \right|_{g(s) \in \Gamma^+} = \left. T \right|_{g(s) \in \Gamma^-} = g(s) \quad (A.2)$$

and for a jump in temperature

$$\left. T \right|_{g(s) \in \Gamma^+} - \left. T \right|_{g(s) \in \Gamma^-} = h(s) \quad (A.3)$$
where \( s \) parametrises the crack contour. The solution is obtained by applying Green’s third identity to obtain the fundamental solution for the Laplacian, then using single layer potential theory. The fundamental solution for the Laplacian in 2-D is

\[
w(x, x') = -\frac{1}{2\pi} \ln |x - x'|
\]

(A.4)

where \( x' \) is a point along the crack contour and \( x \) is any point. Green’s identity is

\[
\int_{\Omega} \phi(x') \nabla^2 w(x, x') \, d\Omega - \int_{\Omega} w(x, x') \nabla^2 \phi(x') \, d\Omega = \oint_{\Gamma} \phi(x') \frac{\partial w(x, x')}{\partial n} \, d\Gamma - \oint_{\Gamma} w(x, x') \frac{\partial \phi(x')}{\partial n} \, d\Gamma
\]

(A.5)

where \( n \) is the outward pointing normal to the boundary \( \Gamma \). Application of \( \nabla^2 \phi = 0 \) and \( \nabla^2 w = \delta(|x - x'|) \) the temperature can be expressed as

\[
\phi(x) = \oint_{\Gamma} \phi(x') \frac{\partial w(x, x')}{\partial n} \, d\Gamma - \oint_{\Gamma} w(x, x') \frac{\partial \phi(x')}{\partial n} \, d\Gamma
\]

(A.6)

considering the condition \( \phi = \bar{T} = \text{constant} \) on \( \Gamma \). The density of dipoles is zero, \( \frac{\partial w}{\partial n} = 0 \), so the problem is reduced to finding a function for the density of sources \( p(x') = \frac{\partial \phi}{\partial n}(x') \) such that the following integral equation is satisfied

\[
\bar{T} = -\frac{1}{2\pi} \oint_{\Gamma} p(x') \ln(|x - x'|) \, dx'
\]

(A.7)

The crack contour \( \Gamma \) is a line from \( -a \) to \( a \), on the x-axis. Equation A.7 is an inhomogeneous Fredholm equation and there exists a solution for \( p(x, 0) \):

\[
p(x, 0) = \frac{1}{\pi \sqrt{(x + a)(a - x)}} \left[ \frac{1}{\ln(a/2)} \oint_{\Gamma} \frac{-2\bar{T}\pi}{\sqrt{(t + a)(a - t)}} \, dt \right]
\]

(A.8)
performing the integration gives:

\[
p(x) = \frac{2\bar{T}}{a^2 - x^2 \ln(a/2)} \tag{A.9}\]

So the temperature at any point in \(\Omega\) can be expressed as:

\[
T(x, y) = -\frac{\bar{T}}{\pi \ln(a/2)} \int_{\Gamma} \frac{\ln[(x-s)^2 + y^2]^{1/2}}{\sqrt{a^2 - s^2}} ds \tag{A.10}
\]

The integral in equation (A.10) has no closed form solutions so is solved numerically.

This expression can be differentiated with respect to \(x\) and \(y\) and multiplied by \(-k\) to give the \(x\) and \(y\) components of the heat flux:

\[
q_x = -k \frac{\partial T}{\partial x} = \frac{kT}{\pi \ln(a/2)} \int_{-a}^{a} \frac{(-s + x)}{((-s + x)^2 + y^2)^{1/2} \sqrt{a^2 - s^2}} ds \tag{A.11}
\]

\[
q_y = -k \frac{\partial T}{\partial y} = \frac{kT}{\pi \ln(a/2)} \int_{-a}^{a} \frac{y}{((-s + x)^2 + y^2)^{1/2} \sqrt{a^2 - s^2}} ds \tag{A.12}
\]

In the case for a specified heat flux on each side of the line, the source density \(p(x') = -2q/k\), so the integral in equation (A.7) reduces to

\[
T(x, y) = -\frac{q}{\pi k} \int_{\Gamma} \ln[(x-s)^2 + y^2]^{1/2} ds \tag{A.13}
\]

which integrates to give

\[
T(x, y) = \frac{-q}{2\pi k} \left[-4a + 2y(\tan^{-1} \left(\frac{a-x}{y}\right) + \tan^{-1} \left(\frac{a+x}{y}\right)) + (a-x) \ln((a-x)^2 + y^2) + (a+x) \ln((a+x)^2 + y^2)\right] \tag{A.14}
\]

Finally, there is the situation where there is a jump in crack face temperature: Take \(h(s) = [\bar{T}]\), so the density of sources \(\frac{\partial \phi}{\partial n} = 0\), and density of dipoles is \(\frac{\partial w}{\partial n} = \gamma(x') = -2[\bar{T}]\).
Therefore the temperature is the solution of the equation:

\[
T(x, y) = -\frac{1}{2\pi} \int_{\Gamma_c} \gamma(x') \frac{\partial}{\partial y} \ln[(x - s)^2 + y^2]^{1/2} ds
\]  

(A.15)

\[\Rightarrow T(x, y) = \frac{[|T|]}{\pi} \int_{-a}^{a} \frac{\partial}{\partial y} \ln[(x - s)^2 + y^2]^{1/2} ds \]  

(A.16)

so

\[
T(x, y) = \frac{[|T|]}{\pi} \int_{-a}^{a} \frac{y}{(x - s)^2 + y^2} ds = -\tan^{-1}\left(\frac{x - s}{y}\right) \bigg|_{-a}^{a}
\]  

(A.17)

therefore

\[
T(x, y) = \frac{[|T|]}{\pi} \left(\tan^{-1}\left(\frac{x + a}{y}\right) - \tan^{-1}\left(\frac{x - a}{y}\right)\right)
\]  

(A.18)

### A.2 Displacement

The problem involves an infinite plate under membrane loading with a central crack which has a pressure acting perpendicular to the crack faces.

One can think of a crack in a plate as the superposition of a plate without a crack under membrane loading, plus the contribution of a compressive stress \((\sigma_0)\) along the crack, enforcing the traction free condition. In addition to this there is the pressure \((p)\) within the crack that acts in the same direction of the compression stress. The stresses and displacements in the
plate can be expressed in terms of the complex potentials \( \phi \) and \( \psi \):

\[
2\mu(u + iv) = \kappa \phi(z) - z\psi'(z) - \overline{\psi(z)} \quad (A.19)
\]

\[
\sigma_{xx} + i\tau_{xy} = \phi'(z) + \overline{\phi'(z)} - z\phi''(z) - \psi'(z) \quad (A.20)
\]

\[
\sigma_{yy} - i\tau_{xy} = \phi'(z) + \overline{\phi'(z)} + z\phi''(z) + \psi'(z) \quad (A.21)
\]

Restraining attention to the Mode-I case, where \( \sigma_{12} = 0 \), which can be enforced by setting \( \psi'' = -z\phi'' \). In this case \( \phi' = -z\phi' + \phi + \text{const} \). If there exists equal and opposite tractions on the top and bottom surfaces of the crack then there exist general solutions for \( \phi' \) of the form

\[
\phi' = \frac{1}{\pi \sqrt{z^2 - a^2}} \int_{-a}^{a} p \frac{\sqrt{a^2 - t^2}}{z - t} dt \quad (A.22)
\]

where \( p \) is the pressure acting on the crack faces. The stresses can be expressed as:

\[
\sigma_{11} = \text{Re}\phi' + x_2 \text{Im}\phi''
\]

\[
\sigma_{22} = \text{Re}\phi' + x_2 \text{Im}\phi'' + \sigma_0 \quad (A.23)
\]

\[
\sigma_{12} = -x_2 \text{Re}\phi''
\]

where

\[
\phi' = (\sigma_0 + p) \left[ \frac{z}{\sqrt{z^2 - a^2}} - 1 \right]
\]

\[
\phi = (\sigma_0 + p) \left[ \sqrt{z^2 - a^2} - z \right] + \text{const}
\]

\[
\phi'' = x_2 \text{Im} \left[ \frac{1}{\sqrt{z^2 - a^2} - \left(\frac{z}{(z^2 - a^2)^{3/2}}\right) (\sigma_0 + p)} \right]
\]

and \( z = x_1 + ix_2 \). The displacements are:

\[
2\mu u_1 = \frac{\kappa - 1}{2} \text{Re}\phi - x_2 \text{Im}\phi'
\]

\[
2\mu u_2 = \frac{\kappa + 1}{2} \text{Im}\phi - x_2 \text{Re}\phi' \quad (A.25)
\]
From these expressions the crack opening displacement can be found at the origin:

\[ COD = (\sigma_0 + p) \frac{\kappa + 1}{4\mu} a \]  

(A.26)
Appendix B

Enrichment functions

B.1 Mechanical enrichment functions

The stresses in two dimensions can be expressed with the complex potentials $\phi(z)$ and $\psi(z)$, i.e.

$$\begin{align*}
\sigma_x + \sigma_y &= 2[\phi'(z) + \bar{\phi}'(z)] \\
\sigma_y - \sigma_x + 2i\tau_{xy} &= 2[\bar{z}\phi''(z) + \psi''(z)] \\
2\mu(u + iv) &= \kappa\phi(z) - \bar{z}\phi'(z) - \psi'(z)
\end{align*}$$

(B.1)

where $\mu = E / (1 + \nu)$, $\kappa = 3 - 4\nu$ for plane strain and $\kappa = (3 - \nu)/(1 + \nu)$ for plane stress.

Taking the complex potentials to be $\phi(z) = \sum_{n=0}^{\infty} B_n z^{\lambda_n}$ and $\psi(z) = \sum_{n=0}^{\infty} C_n z^{\lambda_n+1}$ where $B_n = b_{1n} + ib_{2n}$ and $C_n = c_{1n} + ic_{2n}$ then these be substituted the expansions into equations (B.1) and the following identities are obtained (62):

$$2\mu u = \sum_{n=0}^{\infty} r^{-\lambda_n} \left\{ \kappa (b_{1n} \cos \lambda \theta - b_{2n} \sin \lambda \theta) \\
+ \lambda_n [-b_{1n} \cos(\lambda_n - 2)\theta + b_{2n} \sin(\lambda_n - 2)\theta] \\
+ (\lambda_n + 1) [-c_{1n} \cos \lambda_n \theta + c_{2n} \sin \lambda_n \theta] \right\}$$

(B.2)
\[ 2\mu v = \sum_{n=0}^{\infty} r^{-\lambda_n} \{ \kappa (b_{1n} \sin \lambda \theta - b_{2n} \cos \lambda \theta) \]
\[ + \lambda_n [b_{1n} \sin (\lambda_n - 2) \theta + b_{2n} \cos (\lambda_n - 2) \theta] \]
\[ + (\lambda_n + 1) [c_{1n} \sin \lambda_n \theta + c_{2n} \cos \lambda_n \theta] \} \]

(B.3)

\[ \sigma_x = \sum_{n=0}^{\infty} r^{-\lambda_n-1} \{ 2\lambda_n (b_{1n} \cos (\lambda - 1) \theta - b_{2n} \sin (\lambda_n - 1) \theta) \]
\[ - \lambda_n (\lambda_n - 1) [b_{1n} \cos (\lambda_n - 3) \theta - b_{2n} \sin (\lambda_n - 3) \theta] \]
\[ - (\lambda_n + 1) [c_{1n} \cos (\lambda_n - 1) \theta - c_{2n} \sin (\lambda_n - 1) \theta] \} \]

(B.4)

\[ \sigma_y = \sum_{n=0}^{\infty} r^{-\lambda_n-1} \{ 2\lambda_n (b_{1n} \cos (\lambda - 1) \theta - b_{2n} \sin (\lambda_n - 1) \theta) \]
\[ + \lambda_n (\lambda_n - 1) [b_{1n} \cos (\lambda_n - 3) \theta - b_{2n} \sin (\lambda_n - 3) \theta] \]
\[ + (\lambda_n + 1) [c_{1n} \cos (\lambda_n - 1) \theta - c_{2n} \sin (\lambda_n - 1) \theta] \} \]

(B.5)

\[ \tau_{xy} = \sum_{n=0}^{\infty} r^{-\lambda_n-1} \{ \lambda_n (\lambda_n - 1) [b_{1n} \sin (\lambda_n - 3) \theta + b_{2n} \cos (\lambda_n - 3) \theta] \]
\[ + (\lambda_n + 1) \lambda_n [c_{1n} \sin (\lambda_n - 1) \theta + c_{2n} \cos (\lambda_n - 1) \theta] \} \]

(B.6)

This is subject to the traction free boundary condition: \( \sigma_{yy} = 0 \) and \( \tau_{xy} = 0 \) at \( \pm \pi \); after substitution this gives the eigenvalues and coefficient relations:

\[ \lambda_n = \frac{n}{2} \]
\[ c_{in} = \frac{1 - n/2}{1 + n/2} b_{in}, \; n \text{ odd} \]
\[ c_{in} = -b_{in}, \; n \text{ even} \]

(B.7)
The near tip closed form solution contains only the asymptotic terms and is shown here:

\[
\begin{align*}
    u_x(r, \theta) &= \frac{K_I}{\mu} \sqrt{\frac{r}{2\pi}} \cos \frac{\theta}{2} \left[ \frac{1}{2} (\kappa - 1) + \sin^2 \frac{\theta}{2} \right] \\
    u_y(r, \theta) &= \frac{K_I}{\mu} \sqrt{\frac{r}{2\pi}} \sin \frac{\theta}{2} \left[ \frac{1}{2} (\kappa + 1) + \cos^2 \frac{\theta}{2} \right]
\end{align*}
\] (B.8)

\[
\begin{align*}
    \sigma_x(r, \theta) &= \frac{K_I}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \left[ 1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right] \\
    \sigma_y(r, \theta) &= \frac{K_I}{\sqrt{2\pi r}} \sin \frac{\theta}{2} \left[ 1 + \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right] \\
    \tau_{xy}(r, \theta) &= \frac{K_I}{\sqrt{2\pi r}} \sin \frac{\theta}{2} \cos \frac{\theta}{2} \cos \frac{3\theta}{2}
\end{align*}
\] (B.9)

where \( K_I \) is the mode I stress intensity factor. For the branch enrichment in XFEM, the four angular terms are extracted from the displacement approximation (B.8):

\[
\gamma = \{ \sqrt{r} \cos \frac{\theta}{2}, \sqrt{r} \sin \frac{\theta}{2}, \sqrt{r} \cos \frac{\theta}{2} \sin \theta, \sqrt{r} \sin \frac{\theta}{2} \sin \theta \} \] (B.10)

### B.2 Thermal enrichment functions

Assuming an isotropic and homogenous material

\[
g = -k \nabla T
\] (B.11)

In polar coordinates centred at the crack tip, the gradient is:

\[
\nabla T = T_r \varepsilon_r + \frac{1}{r} T_\theta \varepsilon_\theta
\] (B.12)
where $\mathbf{e}_r$ and $\mathbf{e}_\theta$ represent unit vectors in the $r$ and $\theta$ direction respectively. The steady state energy equation is the Laplacian, which in polar coordinates centred at the crack tip is:

$$\nabla^2 T = T_{rr} + \frac{1}{r}T_r + \frac{1}{r^2}T_{\theta\theta} = 0 \quad (B.13)$$

This is subject to a constant heat flux on the crack face, which, without loss of generality can be set to zero:

$$\mathbf{n} \cdot \nabla T = \frac{1}{r}T_{\theta\theta} = 0 \quad \text{at } \theta = \pm \pi \quad (B.14)$$

where $\mathbf{n}$ is the normal to the crack contour. Only the crack line itself is being considered here so the dot product of the radial component of the gradient and the normal is zero. Expressing the temperature in terms of a complex function $F(z)$, with $z = x_1 + ix_2$, in the form

$$T(x_1, x_2) = \frac{1}{2} \{ F(z) + \overline{F(z)} \} \quad (B.15)$$

where $F(z) = \sum_{n=0}^{\infty} A_n z^{\lambda_n + 1}$, $A_n = a_{1n} + ia_{2n}$, and $a_{in} \in \mathbb{R}$

Differentiation of (B.15) with respect to $\theta$ and on application of condition (B.14) gives

$$\sum_{n=0}^{\infty} (\lambda_n + 1)(a_{1n} + ia_{2n})(-\sin[\pi(\lambda_n + 1)] + i \cos[\pi(\lambda_n + 1)]r^{\lambda_n + 1} = 0 \quad (B.16)$$

which on setting the real parts to zero provides

$$a_{1n} \sin(\lambda_n + 1)\pi - a_{2n} \cos(\lambda_n + 1)\pi = 0$$

$$a_{1n} \sin(\lambda_n + 1)\pi + a_{2n} \cos(\lambda_n + 1)\pi = 0 \quad (B.17)$$
which by inspection reduces to

\[
\sin[2(\lambda_n + 1)\pi] = 0
\]

\[\Rightarrow \lambda_n + 1 = n/2, \; n = 0, 1, 2, \ldots\]  \hspace{1cm} (B.18)

Clearly, the \(a_{1n} = 0\) for \(n\) odd, and \(a_{2n} = 0\) for \(n\) even.

Using equation (B.15), the temperature is obtained in terms of \(r\) and \(\theta\), i.e.

\[
T(r, \theta) = \sum_{n=0}^{\infty} r^{\lambda_n + 1}[a_{1n} \cos(n\theta/2) - a_{2n} \sin(n\theta/2)]
\]

(B.19)

Differentiating with respect to \(r\) and expanding this for the first few terms of \(n\) gives,

\[
T_r(r, \theta) = \frac{a_{11}}{2\sqrt{r}} \sin(\theta/2) + a_{22} \cos \theta + r[(3/2)a_{13} \sin(\frac{3\theta}{2})] + O(r^{n/2}) \text{ for } n > 2
\]

as \(r \to 0\). Near the crack the first term dominates so the asymptotic form is

\[
T_r(r, \theta) \approx \frac{a_{11}}{2\sqrt{r}} \sin(\theta/2)
\]

(B.20)

A similar analysis can be performed to derive the temperature expansion for a constant temperature boundary condition along the crack. Again, without loss of generality, take the temperature to be zero along the crack:

\[
T = 0 \text{ at } \theta = \pm\pi
\]

(B.22)

Application of B.22 to B.15 provides the following expressions

\[
\sum_{n=0}^{\infty} (\lambda_n + 1)(a_{1n} + ia_{2n})(\cos[\pi(\lambda_n + 1)] + i \sin[\pi(\lambda_n + 1)])r^{\lambda_n + 1} = 0
\]

\[
\sum_{n=0}^{\infty} (\lambda_n + 1)(a_{1n} + ia_{2n})(\cos[-\pi(\lambda_n + 1)] + i \sin[-\pi(\lambda_n + 1)])r^{\lambda_n + 1} = 0
\]

(B.23)
and on setting the real parts to zero gives

\[ a_{1n} \cos(\lambda_n + 1)\pi - a_{2n} \sin(\lambda_n + 1)\pi = 0 \]

\[ a_{1n} \cos(\lambda_n + 1)\pi + a_{2n} \sin(\lambda_n + 1)\pi = 0 \]

which on inspection reveals

\[ \sin[2(\lambda_n + 1)\pi] = 0 \]

\[ \Rightarrow \lambda_n + 1 = n/2, \ n = 0, 1, 2, \ldots \] (B.25)

Only this occasion, the \( a_{1n} = 0 \) for \( n \) even and \( a_{2n} = 0 \) for \( n \) odd. Therefore, by expanding and finding the asymptotic terms

\[ T_{\varphi}(r, \theta) \sim \frac{a_{11}}{2\sqrt{r}} \cos(\theta/2) \] (B.26)
Appendix C

1-d Three element system

The derivation of the finite element equations are derived separately in the work by Asferg [96] and Unger [97], who present a model for cohesive cracks in the extended finite element method. Both methods are based on a similar principle only with slightly different step functions, the method by Asferg [96] uses the conventional Heaviside step function, which is also used in this three element system. The jump in the displacement field (which can be considered to be the strain distribution in the crack) is expressed as:

\[
[u_j](x) = (N_j H(x \in \Omega_+) - N_j H(x \in \Omega_-)) a_j = \bar{B}_j^a a_j
\]

As \( H(x) = 0 \) in \( \Omega_- \) and \( 1 \) in \( \Omega_+ \), the value of \( \bar{B}_j^a \) simply becomes \( N_j \). So the extra term in the stiffness matrix due to the crack is:

\[
\int_{\Gamma_{coh}} (\bar{B}_i^a)^T k_c (\bar{B}_j^a)
\]

In the 1-d example presented in this thesis, the curve \( \Gamma_{coh} \) is just a single point so the integral becomes the value of integrand evaluated at the point of the crack, which is \( L/2 \) in this case.

The structure stiffness matrix for the arrangement shown in Fig. C.1 is as follows:
Figure C.1: Three element structure with crack in second element. The displacement $u_i$ are the standard finite element displacements, the $a_i$ are the extra degrees of freedom associated with the cut element.

Figure C.2: Illustration of first order finite element shape functions $N_1$ and $N_2$ on single element.

**Element 1:**

Here, $H(x) = 0$, so

$$
N_i = [1 - \eta, \eta] \quad E_i = H(x)[1/L] 
$$

$$
B_i^u = [-1/L, 1/L] \quad B_i^a = 0
$$

Calculating the stiffness matrix gives:

$$
K_{uu}^{ij} = \frac{EA}{L^2} \begin{pmatrix} -L & -L \\ L & L \end{pmatrix} \begin{pmatrix} -L & L \\ -L & L \end{pmatrix} = \frac{EA}{L} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}
$$

and $K_{ua}^{ij} = k_{ua}^{ij} = K_{aa}^{ij} = 0$, so we have, for the element

$$
K_{e1} = \frac{EA}{L} \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}
$$
Element 2:

There is a step function giving a discontinuity at $D$. This means integration over the element must be performed in two separate domains, denoted by $\Omega_+$ and $\Omega_-$, for the postive and negative sides of the crack respectively. The Heaviside function is 0 in $\Omega_-$ and 1 in $\Omega_+$.

$$\int_{\Omega} = \int_{\Omega_-} + \int_{\Omega_+}$$

where $\Omega_- = [0, D]$ and $\Omega_+ = [D, L]$ in the 1-d example. Where $D$ is the distance to the crack. The standard shape functions are integrated along the whole element as they are not discontinuous.

$$K_{ij}^{uu} = \frac{EA}{L^2} \int_0^L \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} dx = \frac{EA}{L} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \quad (C.7)$$

The term $K_{ij}^{ua}$ is calculated in the two domains:

$$K_{ij}^{ua} = \frac{EA}{L^2} \int_0^D 0 dx + \frac{EA}{L^2} \int_D^L \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} dx = \frac{EA}{L} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

The final part of this element matrix contains the extra crack terms and is calculated as follows:

$$K_{ij}^{aa} = \frac{EA}{L^2} \int_0^D 0 dx + \frac{EA}{L^2} \int_D^L \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} dx + \left( \begin{pmatrix} 1 - \eta \\ \eta \end{pmatrix} k_c \left( \begin{pmatrix} 1 - \eta & \eta \end{pmatrix} = \frac{EA(L - D)}{L} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \right) +$$
\[
    k_c \begin{pmatrix}
        (1 - \eta)^2 & (1 - \eta)(\eta) \\
        (\eta)(1 - \eta) & \eta^2
    \end{pmatrix}_D
\]

The reason for taking just the value of the integrand at \( L/2 \) is because it is a single point so the integral just picks out the value at that point.

\[
    K^\text{ea}_{ij} = \frac{EA(L - D)}{L} \begin{pmatrix}
        1 & -1 \\
        -1 & 1
    \end{pmatrix} + \frac{k_c}{4} \begin{pmatrix}
        1 & 1 \\
        1 & 1
    \end{pmatrix}
\]

Giving a total stiffness matrix for element 2 as:

\[
    K_{el2} = \begin{pmatrix}
        \frac{EA}{L} & -\frac{EA}{L} & \frac{EA(L-D)}{L^2} & -\frac{EA}{L^2} \\
        -\frac{EA}{L} & \frac{EA}{L} & -\frac{EA(L-D)}{L^2} & \frac{EA(L-D)}{L^2} \\
        \frac{EA(L-D)}{L^2} & -\frac{EA(L-D)}{L^2} & \frac{EA}{L} + \frac{k_c}{4} & -\frac{EA}{L} + \frac{k_c}{4} \\
        -\frac{EA(L-D)}{L^2} & \frac{EA(L-D)}{L^2} & -\frac{EA}{L} + \frac{k_c}{4} & \frac{EA}{L} + \frac{k_c}{4}
    \end{pmatrix}
\]

**Element 3:**

Element 3 is calculated in a similar way to element 1 only this time \( H(x) = 1 \), so we have:

\[
    N_i = [1 - \eta, \eta] \quad E_i = H(x)[-1/L] \quad (C.8)
\]

\[
    B^a_i = [-1/L, 1/L] \quad B^a_i = -1/L \quad (C.9)
\]

The stiffness matrix becomes:

\[
    K^\text{wu}_{ij} = \frac{EA}{L^2} \begin{pmatrix}
        -L \\
        L
    \end{pmatrix} \begin{pmatrix}
        -L & L
    \end{pmatrix} = \frac{EA}{L} \begin{pmatrix}
        1 & -1 \\
        -1 & 1
    \end{pmatrix} \quad (C.10)
\]
and

\[
K_{ij}^{aa} = \frac{EA}{L} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}
\]

so we have, for the element

\[
K_{e3} = \frac{EA}{L} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}
\]

Therefore the overall structure stiffness matrix is:

\[
K_{str} = \begin{pmatrix}
\frac{EA}{L} & -\frac{EA}{L} & 0 & 0 & 0 & 0 \\
-\frac{EA}{L} & \frac{2EA}{L^2} & -\frac{EA}{L} & 0 & \frac{EA(L-D)}{L^2} & -\frac{EA(L-D)}{L^2} \\
0 & -\frac{EA}{L} & \frac{2EA}{L^2} & -\frac{EA}{L} & -\frac{EA(L-D)}{L^2} & \frac{EA(2L-D)}{L^2} \\
0 & 0 & -\frac{EA}{L} & \frac{EA}{L} & 0 & -\frac{EA}{L} \\
0 & \frac{EA(L-D)}{L^2} & -\frac{EA(L-D)}{L^2} & 0 & \frac{EA}{L} & -\frac{EA}{2L} + \frac{k_c}{4} \\
0 & \frac{EA(L-D)}{L^2} & \frac{EA(2L-D)}{L^2} & -\frac{EA}{L} & -\frac{EA}{2L} + \frac{k_c}{4} & -\frac{3EA}{2L} + \frac{k_c}{4}
\end{pmatrix}
\]

The conductivity matrix is calculated in a similar fashion by simply replacing \( E \) with \( k_c \), the conductivity, and \( k_c \) with \( h \), the heat transfer coefficient across the crack.

The additional terms \( D \) and \( k_c \) provide information about the location and traction law of the crack respectively. The results of a simulation are given in Fig. C.3 where the jump at the crack is clearly visible. An illustration of the shape functions is given in Fig. C.2.
Figure C.3: Results of XFEM model of cracked bar, the x-axis shows the distance along the element in the coordinate space, and the y-axis is the calculated displacement along the element.
Appendix D

Moës and Heaviside enrichment combined

\[
K_1 = kA \begin{pmatrix}
1/L^2 & -1/L^2 & 0 & -(4x_c^2(x_c - 1))/L^2 \\
-1/L^2 x_c & 1/L^2 x_c & 0 & (4x_c^2(x_c - 1))/L^2 \\
0 & 0 & 0 & 0 \\
-(4x_c^3(x_c - 1))/L^2 & (4x_c^3(x_c - 1))/L^2 & 0 & (64x_c^3(x_c - 1)^2)/3L^2
\end{pmatrix}
\]

\[
K_2 = kA \begin{pmatrix}
1/L^2(L - x_c) & -1/L^2(L - x_c) & -(4x_c(L - x_c)(x_c - 1))/L^2 & 0 \\
-1/L^2(L - x_c) & 1/L^2(L - x_c) & (4x_0(L - x_c)(x_c - 1))/L^2 & 0 \\
-(4x_c(L - x_c)(x_c - 1))/L^2 & (4x_c(L - x_c)(x_c - 1))/L^2 & K_2^{33} & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\]

\[
K_2^{33} = 16Lx_c^2/3 - ((16x_c^2(4x_c^3 - 6x_c^2 + 3x_c))/3 - (16Lx_c^2(6x_c^2 - 6x_c + 3))/3 - 16x_c^3)/3
\]

\[
K_{c_1} = h_cA \begin{pmatrix}
(1 - x_c)^2 & x_c/L(1 - x_c/L) & 0 & -2\psi(x_c)x_c(1 - x_c/L) \\
x_c/L(1 - x_c/L) & x_c^2/L^2 & 0 & -2\psi(x_c)x_c^2/L^2 \\
0 & 0 & 0 & 0 \\
-2\psi(x_c)x_c/L(1 - x_c/L) & -2\psi x_c^2/L^2 & 0 & 4\psi^2 x_c^2/L^2
\end{pmatrix}
\]
$Kc_2 = h_c A \begin{pmatrix}
(1 - x_c/L)^2 & x_c/L(1 - x_c/L) & 2\psi(x_c)(1 - x_c/L)^2 & 0 \\
 x_c/L(1 - x_c/L) & x_e^2/L^2 & 2\psi(x_c/L)x_c/L(1 - x_c/L) & 0 \\
 2\psi(x_c)(1 - x_c/L)^2 & 2\psi(x_c)x_c/L(1 - x_c/L) & 4\psi(x_c)^2(1 - x_c/L)^2 & 0 \\
 0 & 0 & 0 & 0
\end{pmatrix}$

where $K_{cond} = K1 + K2 + Kc_1 + Kc_2$ and $k$ is the conductivity and $h_c$ is the heat transfer coefficient at the crack wall.