SIMULATING THE EXPANSION PROCESS
OF INTUMESCENT COATING FIRE
PROTECTION

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<td>$A$</td>
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<tr>
<td>$A_s$</td>
<td>Shifting parameter</td>
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<tr>
<td>$C$</td>
<td>Specific heat</td>
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<td>Concentration</td>
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<td>Capillary number</td>
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<td>Colour function</td>
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<td>Speed of sound</td>
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<td>$C_{shift}$</td>
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<td>$d$</td>
<td>Coating thickness</td>
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<td>$D$</td>
<td>Diffusion coefficient</td>
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<tr>
<td>$dx$</td>
<td>Particle spacing in $x$-direction</td>
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<td>Convective heat transfer coefficient</td>
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<td>$h_{rad}$</td>
<td>Radiative heat transfer coefficient</td>
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<td>$i$</td>
<td>Interpolation particle</td>
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<tr>
<td>$j$</td>
<td>Neighbouring particles</td>
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<tr>
<td>$m$</td>
<td>Mass</td>
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<tr>
<td>$n$, $s$, $b$</td>
<td>Normal, tangent and binormal vectors to the surface</td>
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<tr>
<td>$N_{cells}$</td>
<td>Nucleation density</td>
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<tr>
<td>$P$</td>
<td>Pressure</td>
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\( Q \quad \text{Heat flux} \\
q \quad \frac{r_{ij}}{h} \\
R \quad \text{Radius} \\
\text{Distance magnitude between particles} \\
S \quad \text{Outer shell radius of a bubble} \\
T \quad \text{Temperature} \\
\text{Time} \\
V \quad \text{Volume} \\
v \quad \text{Particle velocity} \\
W \quad \text{Smoothing kernel function} \\
X \quad \text{Background pressure} \\

\textbf{Greek Symbols} \\
\alpha \quad \text{Artificial viscosity coefficient} \\
\alpha_d \quad \text{Kernel normalisation constant} \\
\alpha_{\text{shift}} \quad \text{Shifting free parameter} \\
\beta \quad \text{Second artificial viscosity coefficient} \\
\gamma \quad \text{Polytropic index} \\
\delta r \quad \text{Shifting distance} \\
\Delta T \quad \text{Temperature increase} \\
\Delta t \quad \text{Time step} \\
\varepsilon \quad \text{Porosity} \\
\lambda \quad \text{Thermal conductivity} \\
\mu \quad \text{Viscosity} \\
\Pi_{ij} \quad \text{Artificial viscosity} \\
\rho \quad \text{Density} \\
\sigma \quad \text{Stefan-Boltzmann constant} \\
\sigma_s \quad \text{Surface tension coefficient} \\
\tau \quad \text{Viscous stress tensor} \\
\Phi \quad \text{Continuum surface force tensor} \\
\Omega \quad \text{Interpolation region}
Subscripts

<table>
<thead>
<tr>
<th>Subscript</th>
<th>Definition</th>
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<tbody>
<tr>
<td>a</td>
<td>Ambient</td>
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<td>c</td>
<td>Coating</td>
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<td>f</td>
<td>Force</td>
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<td>fi</td>
<td>Fire</td>
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<td>g</td>
<td>Gas</td>
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<td>l</td>
<td>Liquid</td>
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<td>s</td>
<td>Steel</td>
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<td>st</td>
<td>Surface tension</td>
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Abbreviations | Definitions

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
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<tbody>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
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<tr>
<td>CPU</td>
<td>Central Processing Unit</td>
</tr>
<tr>
<td>DFT</td>
<td>Dry film thickness of intumescent coating</td>
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<tr>
<td>EOS</td>
<td>Equation of State</td>
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<td>FDM</td>
<td>Finite Differences Method</td>
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<td>FEM</td>
<td>Finite Element Method</td>
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<tr>
<td>FVM</td>
<td>Finite Volume Method</td>
</tr>
<tr>
<td>GPU</td>
<td>Graphic Processing Unit</td>
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<tr>
<td>SPH</td>
<td>Smoothed Particle Hydrodynamics</td>
</tr>
<tr>
<td>TGA</td>
<td>Thermogravimetric Analysis</td>
</tr>
<tr>
<td>VTU</td>
<td>Visual Toolkit Unstructured</td>
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ABSTRACT

Simulating the Expansion Process of Intumescent Coating Fire Protection
Burak Kaan Cirpici
Doctor of Philosophy
The University of Manchester
2015

The expansion ratio (defined as the ratio of the expanded thickness to the original thickness) of intumescent coatings is the most important quantity that determines their fire protection performance. This thesis explores two possible methods of predicting intumescent coating expansion: an analytical method, and a detailed numerical simulation method using Smoothed Particle Hydrodynamics (SPH).

The analytical method is based on a cell-model and predicts bubble growth due to pressure increase in viscous liquid with constant viscosity. It has been extended to non-uniform temperature field and temperature-dependent viscosity of intumescent melt. Accuracy of this extended analytical method is assessed by comparison against the cone calorimeter and furnace fire tests on intumescent coating protected steel plates with different intumescent coating thicknesses, steel plate thicknesses, and heating conditions.

The extended analytical method is then used to investigate how intumescent coating expansion and intumescent coating effective thermal conductivity are affected by changing the coating thickness, the steel thickness and the fire condition (including smouldering fire). The main conclusion is that the expansion ratio decreases as the rate of heating increases. Therefore, the intumescent coating properties obtained from the Standard fire exposure may be safely used for slower realistic fires, but would produce unsafe results for faster fires.

The second method explores the potential of a meshless numerical simulation: Smoothed Particle Hydrodynamics (SPH). SPH modelling of intumescent coating expansion has been implemented using the SPHysics FORTRAN open-source code as a platform. To check the validity of this modelling method, the modelling results are compared against theoretical solutions for surface tension (Young-Laplace theorem), and available numerical and analytical solutions for bubble expansion. A new algorithm for representing the mass transfer of gas into the bubble using SPH particle insertion and particle shifting scheme is presented to simulate the bubble expansion process. Close agreement with an analytical solution for the initial bubble expansion rate computed by SPH is obtained.

Whilst this research has demonstrated the potential of using SPH to numerically simulate intumescent coating expansion, it has also revealed significant challenges that should be overcome to make SPH a feasible method to simulate intumescent coating expansion. The main challenges include:

- Simulating gas-polymer flows when expansion is occurring where there are vastly different properties of these two fluids with a density ratio of about 1000. This high density ratio may easily cause numerical pressure noise, especially at the liquid-gas interface.
- Extremely high computational cost necessary to achieve sufficient accuracy by using a large number of particles (higher resolution), especially for the multi-phase SPH program, and very small time step for the lighter fluid (air).
- The behaviour of intumescent coatings involves expansion ratios on the order of 10-100 with thousands of bubbles which grow, merge and burst.

Based on the results of this exploratory research, future improvements are outlined to further develop the SPH simulation method.
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--- oOo ---

Burak Kaan Çırpıcı
July 2015

MACE Postgraduate Research Conference 2011, Manchester, UK (poster presentation)

MACE Postgraduate Research Conference 2014, Manchester, UK (oral presentation)
CHAPTER 1  INTRODUCTION

1.1 Research Background

Steel dominates the UK construction market and is used worldwide to construct modern, stylish and architecturally attractive structures. Due to the high thermal conductivity of steel and rapid loss of strength and stiffness of steel at elevated temperatures, fire attack can cause significant damage to steel structures. Therefore, fire protection is often necessary to protect steel structures against fire exposure. Among the many different types of passive fire protection materials (i.e. plaster boards, sprayed materials, and intumescent coatings); thin film intumescent coatings have become the preferable option owing to their many advantages such as flexibility, good appearance (aesthetics), light weight and fast application.

Intumescent coatings are inert at room temperature, but can swell up to 100 times the original thickness when being exposed to heat from the fire attack. It is the massively expanded thickness that protects the substrate steel structure from the fire attack.

Despite their widespread use, there is a lack of understanding of how intumescent coatings behave in fire. The majority of the previous research studies may be divided into two categories: studies by chemists to invent new ingredients and their mixture to pass the specified regulatory testing conditions, or studies by fire protection engineers based on phenomenological observations of the overall performance. There is very little link between studies of these two groups of researchers. As a result, there is still little understanding of how the physical and chemical changes (studied by chemists) would affect the fire protection performance (concerns of fire protection engineers) of intumescent coatings.

At high temperatures, intumescent coatings release gases. The released gases then expand due to high pressure. How intumescent coatings expand is the most important quantity that affects their fire protection performance. The expansion process clearly depends on the coating thickness, but also the speed of chemical reaction depends on the rate of heating. Therefore, it is expected that the fire protection performance of an intumescent coating will depend on the fire condition, the protected steel substrate (thickness) and the amount of coating used. However,
although intumescent coating expansion is the most important quantity, due to the complexity of intumescent coating behaviour, there has been very little research devoted to predicting expansion of intumescent coatings. Of the existing research studies that have attempted to incorporate expansion of intumescent coatings into the model of quantifying their fire protection performance, most have assumed the expansion as input data. Of the studies that have attempted to predict intumescent coating expansion, Butler (1997) and Butler et al. (1997) have tried to simulate the expansion process at the microscopic level. However, the detailed methodology of this model is not available and the simulation results have only demonstrated the feasibility of such an approach. Fresh efforts are required to develop this type of approach. Zhang et al. (2012a; 2012b) have developed a mathematical model to simulate the expansion process and global behaviour of intumescent coatings. In this approach, they assume that most of the gases produced in the intumescent coating are lost to the environment. The remaining amount is trapped in the intumescent coating and expands as ideal gas under the atmospheric pressure without any consideration of pressure equilibrium inside the coating. They relate the trapped gas (hence the local rate of expansion) to the local temperature and rate of temperature change. Although their comparison of model prediction results with their cone calorimeter and furnace fire test results suggests good accuracy, this model is based on many assumptions that do not reflect the physical and chemical behaviour of intumescent coatings. An alternative approach is necessary.

1.2 Objectives of This Project

Given the importance of understanding the expansion process of intumescent coatings, and the lack of methods to predict reliably the expansion process, the aim of this project is to explore the feasibility of two different modelling methods: detailed numerical simulation at the microscopic level that may be used to develop a detailed understanding of intumescent coating behaviour, and an analytical method quantifying the global expansion process that may be adopted for practical use by fire protection engineers and intumescent coating manufacturers. The detailed modelling will be developed using Smoothed Particle Hydrodynamics (SPH) and the global modelling will be based on the approach of Amon and Denson (1984).

The specific objectives of this research are:
For analytical modelling:

- To adapt the model of Amon and Denson (1984), originally developed for ambient temperature bubble expansion, due to pressure increase in a viscous liquid of constant viscosity, to intumescent coatings at high temperatures, including temperature change, conversion of intumescent coating mass into bubble pressure, temperature-dependent viscosity.
- To check the accuracy of the above analytical approach against the cone calorimeter and furnace fire tests of Zhang et al. (2012a), (2012b). Wherever possible, the expansion histories will be compared.
- To use the analytical model to investigate the effects of different fire protection design parameters (coating thickness, steel thickness, fire condition including smouldering fire) on the fire protection properties (expansion, thermal conductivity) of intumescent coatings and accuracy of predicting the steel substrate temperature.

For SPH modelling:

As explained in Chapter 2 and Chapter 5, SPH is a modelling technique ideal for non-linear deformation of different materials. The open source code SPHysics (Gomez-Gesteira et al., 2010b) will be used as the platform to model intumescent coating expansion. The aims include:

- To investigate the feasibility of simulating the evolution of the bubbles in 3-D using a multi-phase SPH model at the range of conditions typical for intumescent coatings.
- To validate the new SPH model with benchmark test cases including both analytical solutions and experimental data.
- To implement particle shifting techniques for multi-phase flows to maintain the particle spatial distribution in order to prevent non-physical numerical instability.
- To develop an approach to add additional mass into the bubble to represent the mass transfer, resulting in increase in pressure inside the gas bubble.
1.3 Structure of the Thesis

This thesis is divided into seven chapters as outlined below:

Chapter 1 gives a general introduction to the background and objectives of the project.

Chapter 2 provides a literature review of the physical and chemical processes of intumescent coatings, focusing particularly on previously developed quantification methods for modelling intumescent coatings, and SPH methods appropriate for modelling gas expansion and explosion.

Chapter 3 presents an analytical method of modelling the intumescent coating bubble growth and expansion, based on adaptation of the Amon and Denson (1984) model. The model prediction results will be compared against the furnace fire and cone calorimeter tests recently conducted at the University of Manchester to assess the accuracy of the analytical model.

Chapter 4 investigates in detail how intumescent coating properties (expansion, thermal conductivity) are affected by different fire protection design conditions (fire-temperature time curves (including smouldering fire), intumescent coating thickness and steel section factor) and how intumescent coating thermal conductivity may be assessed for accurate prediction of the protected steel temperature.

Chapter 5 describes the theoretical and mathematical background with detailed equations of the Smoothed Particle Hydrodynamics (SPH) method, which are required to simulate the bubbles in intumescent coatings.

Chapter 6 presents comparison of the SPH modelling results against a series of test cases, checking the accuracy of the SPH modelling method for different aspects related to intumescent coating expansion, including gas bubbles rising through a submerged orifice, surface tension for single and multi-phase liquid and air interaction and bubble growth. Significant challenges for future modelling of the entire intumescent coating expansion process are explained.

Chapter 7 summarises the main outcomes and findings of the research carried out in this project and suggests relevant future research studies to further develop the simulation and analytical methods for quantifying intumescent coating expansion.
CHAPTER 2 LITERATURE REVIEW

2.1 Introduction

Intumescent coatings are commonly used passive fire protection material that enables structures to survive under fire attack. This fire protection technique has several advantages compared to the other passive fire protection systems; it can be applied easily on to many types of materials such as metallic, polymer, textile, wood, steel, etc. The coating can be made in different colours to give an attractive appearance, and it is thin and lightweight. The required thickness of an intumescent coating depends on the type of fire exposure (cellulosic fire/hydrocarbon fire), the size and loading condition of the structural element. This coating thickness ranges typically from 0.2mm to a few mm. Depending on the type of intumescent coating, it can expand by a factor of between 5 to 100 times of the original thickness (Horacek and Pieh, 2000). The subject of this thesis is thin-filmed intumescent coating, used in building structures exposed to cellulosic fires. The coating thickness is typically around 1 mm and the expansion ratio is usually greater than 20.

Intumescent coatings consist of inorganic components and are designed to expand to form an insulative char. In a fire condition, the coating material melts first. After melting, several chemical reactions occur which release gases and cause the coating to expand (Bourbigot et al., 2004). In order to simulate accurately the intumescent coating expansion process, it is necessary to include the chemical reactions and the physical principles of conservation of mass, momentum and energy of the bubbles. The movement of the bubbles inside the intumescent coating is similar to the movement of any liquid or gas. Therefore, it is possible to model this process by the governing equations of fluid mechanics.

Based on the brief introduction above, the literature review will cover the following aspects:

- The physical and chemical processes of intumescent coatings which affect their fire protection performance, which is mainly thermal conductivity.
- Key models that have been developed by previous researchers to predict intumescent coating expansion.
- Relevant analytical models that may be adapted for predicting expansion of
intumescent coatings.
- Computational methodologies for simulating intumescent coating expansion and the novel meshless method Smoothed Particle Hydrodynamics (SPH) used in this work and previous research studies related to modelling bubble expansion.
- Methods of extracting thermal conductivity of intumescent coatings exposed to fire.

2.2 Effects of Physical and Chemical Processes of Intumescence on Fire Protection Performance of Intumescent Coatings

It is usually accepted that intumescent coatings have three generic agents in terms of the active components: acid source, blowing agent and charring agent (Jimenez et al., 2006). The physical and chemical mechanisms of the intumescent coatings under operation are still not well understood. It is therefore not possible to give a precise explanation of these processes. Here, a simple description of the processes, according to Anderson et al. (1985), is used to illustrate the different steps of intumescent coating behaviour:

1- The inorganic acid yields to acid at temperatures between 100°C and 250°C,

2- At around 300°C - 340°C, the phosphoric acid decomposes under heat evolution (Horacek, 2009).

3- After decomposing, a number of gases (e.g. CO₂, NH₃, etc.) evolve. This mixture is called the blowing agent. Bubbles are generated in this stage due to the production of these gases.

4- Formation of a char layer.

5- Oxidisation of the char.

Figure 2.1 illustrates a typical 1-D substrate (i.e. steel section-like plate) intumescent coating system. Depending on the substrate temperature, the unreacted zone may not exist (Di Blasi and Branca, 2001). The intumescent coating consists of three components (S₁, S₂ and S₃) which degrade according to three main reactions: melting, swelling and charring respectively. V₁, V₂ and V₃ are volatile species, C is the charred solid residue and v₁ and v₂ are stoichiometric coefficients. Subscripts “c” represents the coating and “s” represents the substrate.
The insulation efficiency of an intumescent coating depends on the cell (bubble) structure where the blowing process plays the key role during the intumescence process. If the blowing agent activates too early, the bubbles will burst without expansion because the viscosity of the molten material is too low. Furthermore, the bubbles that have not burst would form large bubbles that are relatively inefficient in terms of fire protection (i.e. insulation) due to high radiation within the large bubbles. Figure 2.2 shows typical fully grown bubble sizes, based on the tests of Yuan and Wang (2007) at the University of Manchester. The study of Yuan and Wang (2007) was continued by Zhang et al. (2012a; 2012b). Figure 2.3 and Figure 2.4 illustrate the cone calorimeter test setup of Zhang et al. (2012b) and the resulting expanded intumescent coatings.
Figure 2.2: Bubble size from a fire test (Yuan and Wang, 2007)

Figure 2.3: An example of the intumescent coating expansion process (a) the experimental setup for the cone calorimeter test, (b) top view of painted sample (plate) before the test, (c) side view during the test, (d) side view of expanded intumescent coating after the test (Zhang et al., 2012b)
Figure 2.4: Examples of bubble formation after the cone calorimeter tests with different heat fluxes (Zhang et al., 2012b)

The expanded thickness is clearly the most important quantity governing the fire protection performance of intumescent coatings. Furthermore, the bubble size has considerable influence on the fire protection performance since it affects the thermal conductivity of the expanded intumescent coating, as explained below.

2.2.1 Thermal Conductivity of Intumescent Coating

The expanded intumescent coating char is a highly porous material. Heat transfer through the expanded intumescent coating consists of conduction through the gas phase (movement of gas molecules) and the solid phase and radiation through the gas phase (i.e. bubbles or pores). The overall thermal conductivity of a porous material may be calculated according to the following equation (Yuan, 2009):

\[
\lambda^* = \lambda_s \frac{\lambda_g \varepsilon^2 + 1 - \varepsilon^2}{\lambda_s \left(\varepsilon^2 - \varepsilon\right) + 1 - \varepsilon^2 + \varepsilon} \tag{2.1}
\]

where \(\varepsilon\) is the porosity, \(\lambda_s\) is the thermal conductivity of the solid phase of the
expanded intumescent coating, $\lambda_g$ is the thermal conductivity of the gas that includes the combined effect of conduction (through the movement of gas molecules) and radiation.

Porosity ($\varepsilon$) is defined as the fraction of the volume occupied by the voids (empty spaces) over the total volume. Consider an intumescent coating which has an initial thickness of $d_{ini}$ and is expanded to the final thickness of $d$. The porosity can be calculated as follows:

$$\varepsilon = \frac{d - d_{ini}}{d} = 1 - \frac{d_{ini}}{d} = 1 - \frac{1}{E} = \frac{E - 1}{E}$$

(2.2)

where $E$ is the expansion ratio ($E = \frac{d}{d_{ini}}$).

Typically, thin-filmed intumescent coatings expand at least 20 times ($E = 20$). Therefore, the minimum value of porosity to achieve such an expansion of the intumescent coating, according to Equation (2.2), is 0.95.

The thermal conductivity of gas (through gas molecule movement) can be calculated as in Di Blasi and Branca (2001):

$$\lambda_{g_{cond}} = 4.815 \times 10^{-4}T^{0.717}$$

(2.3)

where the unit of the thermal conduction is W/mK and the temperature ($T$) is in Kelvin (K). The contribution of radiation through the intumescent coating bubbles may be calculated using the following equation (Yuan, 2009):

$$\lambda_{g_{rad}} = \frac{2}{3} \times 4de\sigma T^3$$

(2.4)

where the intumescent coating bubbles are assumed to be of the same spherical shape and size with a diameter of $d$, $e$ is the emissivity of the gas inside the bubbles and $\sigma$ is the Stefan-Boltzmann constant.

The total equivalent thermal conductivity of the gas is given by:

$$\lambda_g = \lambda_{g_{cond}} + \lambda_{g_{rad}} = 4.815 \times 10^{-4}T^{0.717} + \frac{2}{3} \times 4de\sigma T^3$$

(2.5)
Comparison of different contributions to total thermal conductivity of expanded intumescent coating

Figure 2.5 compares the expanded intumescent coating thermal conductivity (Equation (2.1)), the total gas equivalent thermal conductivity (Equation (2.5)), the gas thermal conductivity due to gas molecule movement (Equation (2.3)) and the contribution of radiation inside the bubbles to gas thermal conductivity (Equation (2.4)), based on an assumed bubble diameter of 3.5 mm (Figure 2.2) and a conservative estimate of the porosity (0.95, corresponding to an expansion ratio of 20). The thermal conductivity of the solid phase is taken as 0.5 W/mK. It can be seen that above approximately 327°C (600K), radiation within the bubbles dominates heat transfer within the bubbles. Furthermore, because the expanded intumescent coating is highly porous, the thermal conductivity of the solid phase has little effect on the overall thermal conductivity of the expanded intumescent coating (overall thermal conductivity of gas), including radiation, and is very close to the intumescent coating thermal conductivity.

To summarise, in order to quantify accurately the fire protection performance of intumescent coatings, the most important factors are the expansion thickness and the internal structure of the expanded char. Section 2.4 will review past research studies related to these aspects.
2.3 Current Method of Assessment for Intumescent Coatings

In the current Eurocode (EN 13381-4:2013) for assessment of intumescent coatings (CEN, 2013a), the equivalent thermal conductivity of an intumescent coating (related to the original coating thickness), is obtained by using the following equation:

\[ \lambda_{p,t} = \left[ d_p \times \frac{V_s}{A_p} \times C_s \times \rho_s \times \left(1 + \frac{\phi}{3}\right) \times \frac{1}{(T_{fi} - T_s) \times \Delta t} \right] \times \left[ \Delta T_s + \left( e^{\frac{\phi}{10}} - 1 \right) \Delta T_{fi} \right] \]  

(2.6)

where \( \phi = \frac{C_p \rho_p A_p t_p}{C_s \rho_s V_s} \).

In the above equation, \( T_{fi} \) and \( T_s \) are the fire and steel temperatures respectively, \( \Delta T_{fi} \) and \( \Delta T_s \) are the temperature increments of the fire and the steel respectively, \( \Delta t \) is the time increment, \( A_p \) is the exposed surface area of the fire protection material, \( t_p \) is the thickness of the fire protection material, \( C_p \) is the specific heat of the fire protection material, \( \rho_p \) is the density of fire protection material, \( C_s \) is the specific heat of the steel member, \( V_s \) and \( \rho_s \) are the volume and density of the steel member respectively.

The above assessment method is the inverse solution of the equation for calculating the temperature of a protected steel section in Eurocode 3 Part 1.2 (CEN, 2005), as follows:

\[ \Delta T_s = \left( \frac{T_{fi} - T_s}{A_p} \right) \frac{V_s}{C_s \rho_s \left(1 + \frac{1}{3} \phi\right)} \Delta t - \left( e^{\frac{\phi}{10}} - 1 \right) \Delta T_{fi} \]  

(2.7)

The current assessment method in Eurocode gives temperature-dependent thermal conductivity of the fire protection material. Two fundamental assumptions are made in this equation: (1) the temperature of the fire protection material is uniform, being the average of the fire and the protected steel temperatures; (2) the thermal conductivity of the fire protection material is temperature-dependent only. Assumption (1) is strictly not true because the fire protection material temperature varies from that of the fire to that of the steel section. Assumption (2) is acceptable.
for non-reactive materials whose thermal conductivities are only temperature-dependent. However, it is not suitable for intumescent coatings. Intumescent coatings are chemically active and the speed of reaction will not only depend on temperature, but also on the rate of heating. It is important to examine the applicability of these assumptions to intumescent coatings.

2.4 Intumescent Coating Models

The expansion process of intumescent coating is highly complicated, involving a complicated mixture of gases, liquid and solid phases and many components which are difficult to measure. Very few studies have been conducted to investigate the performance of intumescent coatings, and these have had very limited success in modelling. The developed intumescent models can be classified depending on their complexity.

The earliest model was developed by Cagliostro et al. (1975), who investigated the sensitivity of protected steel plate temperatures to the swelling behaviour of intumescent coatings. An empirical form for the expansion factor ($E$) was proposed. This first modelling approach became quite popular, and was adopted by many researchers (Di Blasi and Branca, 2001) and (Di Blasi, 2004). However, this approach relies on providing the expansion ratio as input. Also this expansion ratio was assumed to be constant regardless of the heating condition. In reality, the expansion ratio varies from a value of less than 10 to a value close to 100, depending on the heating rate and temperature of the coating.

In the model of Di Blasi and Branca (2001) and Di Blasi (2004), the different stages of chemical reactions are included through modelling of mass transfer. The reaction rates are governed by the Arrhenius equation. However, the chemical reactions are decoupled from the expansion process because the expansion ratio is treated as input. The framework of this approach became the basis of the model developed by Yuan and Wang (2009).

The work of Yuan and Wang (2009) still had the same shortcomings as the above in terms of modelling the expansion ratio. However, this study has demonstrated that accurate prediction of intumescent coating behaviour is possible if the expansion ratio can be accurately calculated. Furthermore, this study clarified the role of the internal bubble size in affecting the thermal conductivity of intumescent coatings.
coatings (see section 2.2.1) and has provided some experimental data for the bubble size.

Continuing from the work of Yuan and Wang (2009), Zhang et al. (2012a) and (2012b) focused on the need to predict accurately the expansion ratio under different heating conditions. In their research, they assumed that the intumescent coating pressure is maintained at the atmospheric pressure. If all the released gases are used to expand the intumescent coating, the expansion ratio would be hundreds or thousands of times (the ratio of density of solid intumescent coating to gas is about 1100). Therefore, in order to overcome this problem, they stipulate that only a certain amount of the released gas would be trapped inside the bubble to expand the intumescent coating and the remainder of the gases is lost to the environment. They have compared their model predictions against their own cone calorimeter tests (Zhang et al., 2012b) and furnace fire tests (Zhang et al., 2012a) and have demonstrated good accuracy of the model. Nevertheless, their assumption is open to question since the escaped gases would need to travel from the intumescent coating melt through the coating, including the char, to the outside air simultaneously.

At the most complicated level, the intumescent coating behaviour may be studied from the fundamental microscopic level of chemical reaction, individual bubble generation, growth, movement and interaction with other bubbles and collapse. The most well-known study is that described by Butler (1997) and Butler et al. (1997). Their model is divided into three sub-models; namely hydrodynamic, growth rate and heat transfer. Whilst these studies have demonstrated the possibility of microscopic level modelling, the modelling procedure is not clearly explained and the modelling results are only available for the initial phase of the expansion process.

As a summary, there is clearly a need to calculate accurately the expansion ratio of intumescent coatings under different heating conditions. Although the existing approaches have identified the important controlling factors that affect intumescent coating behaviour and hinted at the possible modelling approaches, they all have major shortcomings. This thesis will explore the potential of two alternative approaches: using a novel meshless numerical method, Smoothed Particle Hydrodynamics (SPH) for detailed modelling, and an analytical approach. The basis of analytical modelling methods will be reviewed in the next section.
2.5 Relevant Expansion Modelling Methods

2.5.1 Analytical Modelling

The problem of bubble nucleation and growth inside foams plays an important role in the chemical industry.

The two well-known bubble growth models are those of Patel (1980) and Amon and Denson (1984). The Amon and Denson (1984) model itself is based on the Patel (1980) model. As the Amon and Denson (1984) model will form the basis of the analytical study of this thesis, this section presents a summary of the main assumptions and conclusions of this study.

2.5.2 Governing Bubble Growth Equations

Figure 2.6 shows a sketch of the main quantities involved in bubble growth where the radius of the bubble is $R$. The main driving force for bubble growth is the increased gas pressure inside the bubbles ($P_g$). The resistance forces, which control the bubble growth process, are due to the viscosity ($\eta$) and surface tension force ($F_s$) due to surface tension at the interface. These forces act on the interface, which has infinitesimally small thickness, shown in Figure 2.6 by zooming in to the interface.

![Figure 2.6 A sketch of the forces acting on a bubble](image)

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2.5.3 The Single Bubble Growth Model (Patel’s Model)

Patel (1980) made the following assumptions;

- The gas inside the bubble behaves according to the ideal gas law and there is always thermodynamic equilibrium at the gas-liquid interface according to the gas concentration (Henry’s law).
- None of the physical properties of the polymer liquid and gas change with time.
- The bubble is assumed to have a spherical shape.

Based on the conservation of mass and momentum, Patel (1980) has obtained the following equation to predict the rate of bubble growth;

\[
\frac{dR}{dt} = R \left( \frac{P_g - P_a - 2\sigma_s/R}{4\eta_o} \right)
\]

In the above equation, \(P_g\) and \(P_a\) are the gas pressure inside the bubble and the ambient pressure respectively. \(R\) is the radius of the bubble, \(\sigma_s\) is the surface tension coefficient and \(\eta_o\) is the viscosity of the polymer liquid.

As this bubble growth model describes a very large single bubble growth due to the assumption of unlimited supply of blowing agent, it does not consider the influence of surrounding bubbles. Therefore, this model overpredicts the actual bubble growth in polymer foaming. Another shortcoming of this model is that the polymer liquid is assumed to be a Newtonian fluid while the bubble forming in intumescent coatings behaves as a non-Newtonian fluid and the physical properties such as viscosity and surface tension change with time. However, this model is still applicable to this kind of modelling of bubbles in intumescent coatings by making necessary changes to the assumptions.

2.5.4 Multi-Cell Model


Referring to Figure 2.7, which shows the uniformly distributed bubbles having the same radii and masses, the initial polymer shell with an outer shell radius \(S(t)\) decreases with increase of the bubble radius \(R(t)\) over time, controlled by mass
transfer. By assuming that the number of nucleation sites remains the same, the outer shell radius is calculated at each time step based on the conservation of volume, giving:

\[ S(t) = \left( S_o^3 + R(t) - R_o^3 \right)^{1/3} \]  

(2.9)

where \( S_o \) is the initial outer shell radius containing the polymer liquid. It is calculated depending on the number of nucleation sites per volume (nucleation density):

\[ S_o = \left[ \frac{3}{4\pi N_{\text{cells}}} \right]^{1/3} \]  

(2.10)

where \( N_{\text{cells}} \) is the nucleation density. Each cell has a volume of \( \left[ (4/3)\pi S_o^3 \right] \) of the volume at time \( t = 0 \).

Figure 2.7 Schematic representation of the multi-cell model, Amon and Denson (1984)

Amon and Denson (1984) obtained the following equation to calculate the expansion rate of the bubbles:

\[ \frac{dR}{dt} = R \left( \frac{P_g - P_a - 2\sigma_s/R}{4\eta_o} \right) \left( \frac{S^3 - R^3}{S^3} \right) \]  

(2.11)
This multi-cell model predicts actual bubble growth much more realistically compared to Patel’s (1980) model, because it considers the neighbouring bubble effect in the bubble growth model. As the distance between growing bubbles decreases, the growth of the bubbles will be limited with time.

In this thesis (Chapter 3), the Amon and Denson (1984) multi-cell model will be adapted to model the expansion process of intumescent coatings. For this purpose, a number of modifications will be necessary to take account of the different driving force (release of gas) and temperature-dependent material properties (viscosity, surface tension). Details will be presented in Chapter 3.

As explained in Section 2.5.3, this approach is based on certain assumptions, most notably that the bubble shape is spherical. This thesis also aims to investigate the possibility of using modelling techniques that capture the nonlinearity of the flow. Herein, the smoothed particle hydrodynamics (SPH) is investigated.

2.6 Bubble Formation and Growth in Polymer Foam Processing

The foaming of a polymer melt is an important issue for applications such as insulation, personal care and fire retardation. The main feature, which has an effect on the quality of the thermoplastic foam product, is the cell size distribution (CSD). Many factors influence the final CSD of a foam, including bubble nucleation, growth, deformation, possible coalescence and bursting, while each of these depends on many sub-factors such as temperature, pressure, blowing agent and the use of nucleating agents (Feng and Bertelo, 2004).

The foaming process, dominated by the dynamics of the gas-liquid interface and using physical blowing agents, is a complex process which consists of three main stages. The first is “nucleation”, where the gas in the gas-liquid mixture diffuses into gas clumps and begins to form bubbles. The second is essentially “bubble growth”, where bubbles grow due to a gas source from the liquid or smaller neighbouring bubbles. The third step is “coarsening”, where the bubbles come together and combine into larger bubbles (Naber et al., 2008). This foaming process represents exactly the intumescent coating expansion process described in Section 2.2.

Although numerous works have been conducted on the theoretical study of bubble growth including experiments, only a limited number of studies have reported the issue of the dynamic behaviour of bubble growth in the molten polymer. It is
mentioned in the work of Tuladhar and Mackley (2004) that the classical and well-known theory of nucleation is based on Gibbs free energy, which is appropriate for creating a void in a liquid and assumes that the critical bubble is in equilibrium in terms of mechanical and thermodynamic properties. In their model, bubbles larger than the critical bubble size keep growing while smaller ones dissolve. As the bubble growth is mainly related to the pressure, the growth does not continue infinitely because the concentration of the dissolved gas $c_r(t)$ in the surrounding polymer melt also reduces with respect to time. Hence, the rate of bubble growth is a function of the polymer viscosity, diffusivity of the gas (mass conversion from liquid to gas) and pressure inside the bubble. In reality and for any numerical model for multi-bubble growth, expanded bubbles that are in close proximity to another bubble or bubbles cannot grow infinitely, since only a finite supply of gas is available for the growth (Amon and Denson, 1984). The prediction of the nucleation process is therefore difficult, but if it occurs, bubble growth is controlled by the fundamental laws where the pressure of the gas within the bubble provides a driving force to expand the bubble whereas the viscosity of the polymer and surface tension of the bubble wall provide opposing forces (resistance) to bubble growth. The schematic of a single bubble can be shown in Figure 2.8.

Figure 2.8: Schematic diagram of a single bubble growth model (Tuladhar and Mackley, 2004)
With many variables influencing the bubble modelling simultaneously, sensitivity studies for the parametric values should be conducted (Tuladhar and Mackley, 2004). For instance, some of those parameters are initial bubble radius, influence cell radius, melt viscosity, diffusion coefficient, initial gas concentration, etc. Initial bubble size is directly related to the surface tension, so as the bubble size increases, the importance of the surface tension decreases. According to Tuladhar and Mackley (2004), the low viscosity values of the melt (< 10 Pa s) have less influence on the bubble growth while the gas diffusion rate is important in that condition. However, if it is a highly viscous melt (> 10 Pa s), the viscosity of the material controls the growth. The important parameters for the bubble growth in the polymer melt are the viscosity, surface tension and the pressure increase inside the bubble, and they can be modelled using other computational approaches.

2.7 General Computational Fluid Dynamics (CFD) Approaches for Modelling Bubbles

Multi-fluid flows which have an interface have been considered in various industrial processes such as chemistry, polymer foaming, etc. However, simulating these kinds of flows is particularly challenging since the interface separating the fluids needs to be treated such that the models are computationally efficient, while surface tension for the cases of highly curved interfaces needs to be treated accurately and efficiently. A number of techniques have been developed and applied to simulate complex multi-phase flows (van Sint Annaland et al., 2005). For moving grid methods such as the finite element method (FEM), mesh generation is also necessary to simulate the flow, because mass, momentum and energy are transported with the movement of mesh cells. However, it can be time consuming when the objects have large deformations and distortions. It may even introduce inaccurate results (Liu and Liu, 2003). In terms of high velocity impact (HVI), shock waves can be given as an example where the behaviour involves large deformations, moving material interfaces and deformable boundaries. This situation is also difficult to model using grid-based numerical methods. Some of these mesh-based or meshless techniques are briefly reviewed with their advantages and disadvantages herein. The approaches can be broadly classified as Eulerian, involving variation of flow quantities at fixed points in space, and Lagrangian where the flow properties can move in space and time. Here we give an overview of some common approaches for
modelling the interface computationally:

- **Front Tracking Method**
  
The interface between fluids is tracked by using a set of points connected to each other (i.e. triangles). A fixed or Eulerian grid is used to solve the governing Navier-Stokes equations. Although this method is accepted as accurate, its implementation is rather complex due to meshing of the interface and because all the data is required to be transferred from a mesh on to another mesh, especially when the multiple interfaces interact with each other, such as in bubble growth in polymer foaming (intumescent coating). This method has recently been used by Pivello et al. (2014) to simulate the motion of a single bubble rising in a liquid with low and high flow rates.

- **Level Set Method**
  
  This method has been accepted as being relatively easy to implement as the interface is defined by a set of distance functions considering steady flow, but it can suffer in a case where the interface is destroyed or significantly deformed. Modelling of the sharp interface can also be problematic. Therefore, the main drawback is the loss of accuracy due to loss of mass (Osher and Fedkiw, 2001). A single droplet’s drop on to a liquid interface with the effect of gravity has been modelled by Balcázar et al. (2015) using a multiple marker level-set method. In this study, the droplet and fluid bed have been described separately by separate level-set functions which help to avoid unphysical coalescence of fluid particles. However, due to the nature of mesh generation, mass especially at the interface may not be conserved when two interfaces are in the same computational mesh.

- **Marker Particle Method**
  
  The idea to identify the multiple fluids is similar to the use of a colour function explained in detail in Chapter 5. In this method, marker particles are assigned to a specific fluid to track the motion of the flow, and hence the interface of the fluids. This method is Eulerian, and is used to solve the Navier-Stokes equations. Although the marker particle method is accurate and robust in 2-D, it is computationally very expensive in 3-D. Besides, problems arise when the interface stretches or shrinks, since the addition of fresh marker particles is required during the simulation. Using this method, the numerical predictions for 2-D bubble collapse within a viscous fluid surrounded by a rigid boundary have recently been presented by Lind and Phillips (2013) with a small density ratio of 4 between phases. As this marker particle method
is based on the mesh nature, the mesh is refined around the area of interest, mainly at the interface of the bubble and inside the bubble in this study.

- **Volume-of-Fluid Method**

  In this method, a colour function is employed to indicate the fluids at certain positions \((x, y, z)\) at a certain time. The interface is determined by the gradient of the colour function. However, there is limited accuracy in gas bubbles’ modelling, especially at the interface and coalescence of bubbles when the distance of the fluids and multiple bubbles is less than the size of the computational cell (Bussmann \textit{et al.}, 1999). A coupled level set and volume-of-fluid method has been used to simulate single condensing bubble behaviour in a cooled flow (Zeng \textit{et al.}, 2015). This phase change model has been developed to analyse certain parameters such as the condensing bubble deformation, bubble lifetime and the history of bubble size.

- **The Lattice Boltzmann Method**

  This method is one of the attractive methods as an alternative to the classical finite difference methods (FDM) or finite element methods (FEM) for multiple moving simulations such as bubbles or droplets. Ladd (1994) has used this method to simulate a gas particle drug in special suspension fluids and more recently Cheng \textit{et al.} (2010) has developed 3-D multiple bubble rising under buoyancy force considering bubble-bubble interaction while rising in a viscous incompressible fluid using the Lattice Boltzmann method. However, serious problems such as interface deformations similar to the volume-of-fluid method can be seen in this method (van Sint Annaland \textit{et al.}, 2005), where the interface is not sharply defined.

  The numerical methods explained above are the alternative methods to the meshless methods for multi or single bubble formations, modelling of multi-phase surface interactions and are defined at points connected to each other by a computational grid or mesh. This is precisely based on the Eulerian scheme or concept of the flow (i.e. the observer is stationary). The governing equations are computationally solved by the interaction between different points of the grid defining efficient mathematical operators such as the derivative.

  However, points in the mesh or grid need to be destroyed in a case where significant deformation appears or sharp changes of geometry occur, such as in a violent fluid flow. Therefore, these grids need to be remeshed or refined for these
kinds of problem, which leads to a computationally expensive process.

- **Meshless Methods**

Recently, meshless methods have been developed in order to tackle exactly these kinds of problem (Belytschko *et al.*, 1996). They are based on the Lagrangian concept of flow (i.e. the observer and the flow move with the same velocity). The computational domain is defined with particles which are used to solve the fluid properties such as conservation of mass or momentum (Monaghan, 2005). The basic idea of the meshless methods is that the computational points are free to move, making them ideal for problems with nonlinear distortion. In addition, the discontinuities of the flow in possible locations of the computation domain such as sharp interfaces can be numerically well-computed due to the Lagrangian nature.

With the general advantages and disadvantages of the meshless method making them good candidates for modelling the expansion process of intumescent coatings, the Smoothed Particle Hydrodynamics (SPH) method is particularly attractive and is considered in this research study for simulating the bubble growth model with its sub-models (viscosity, surface tension, etc.). The brief background and range of applications of SPH is given in the following section.

### 2.8 Smoothed Particle Hydrodynamics (SPH) modelling

#### 2.8.1 General Background of SPH and the Range of Applications

Smoothed particle hydrodynamics (SPH) is a meshless method which was initially developed for solving astrophysical problems (Gingold and Monaghan, 1977; Lucy, 1977). It is still in use for simulations of star formation (Katz, 1992) and coalescence of black holes (Springel, 2010).

In the past two decades, the method has been used extensively to tackle fluid dynamics problems, especially free-surface flows (Monaghan and Kos, 1999), (Monaghan, 1994) as well as solid dynamics problems (Benz and Asphaug, 1994), and brittle solids (Benz and Asphaug, 1995). The range of applications of SPH is very broad and varied, encompassing areas such as solid and fluid mechanics, heat conduction (Jeong *et al.*, 2003), fracture mechanics (Benz and Asphaug, 1994), fluid-solid modelling (Antoci *et al.*, 2007), modelling of water waves, sloshing, etc. (Dalrymple and Rogers, 2006).
Multi-phase models such as those encountered here, and will be discussed in Section 2.8.3, have also been developed with the aid of the meshless nature of the SPH method (Colagrossi and Landrini, 2003).

As a meshless method, the Smoothed particle hydrodynamics (SPH) method obtains approximate numerical solutions to the set of equations representing the dynamics by replacing the medium with a set of particles. The particles are free to move according to the governing dynamics and interact with each other by means of overlapping influence areas known as smoothing kernels or weighting functions. These kernels have a characteristic spatial distance, generally known as the “smoothing length”, which is represented by “h”. The physical property of any particle can be estimated by summing weighted contributions of all the surrounding particles that are located within the radius of influence (support) of the kernel. Detailed information for the smoothing function is given in Chapter 5. The method has many attractive features, which are summarised below.

1- The conservation of mass without extra computational process is exact since the mass of each particle remains constant.

2- SPH evaluates the pressure from the contributions of neighbouring particles rather than by solving linear systems of equations.

3- With the governing equations expressed in Lagrangian form, nonlinear advection terms are implicitly included such that SPH provides pure advection. For example, if the particles are given a colour and the velocity is specified, the transport of the colour by particles is exact (Monaghan, 2005).

4- An important advantage directly relevant to this thesis is that it is possible to deal with interface problems, since each material is described by its own set of particles. As explained in Section 2.7, this is difficult to achieve with mesh-based methods.

5- SPH computation takes place only where the particles are located.

6- There is no limit to the complex physical geometries.

7- Unlike grid-based methods which must have fluid boundaries, simulation of interfacial flows, such as intumescent paints, is straightforward. Hence, this method is applicable and preferable for simulating the intumescent coating in terms of fluid motion.

8- Potentially expensive grid generation is avoided.
In this work, the main interest lies in the modelling of a gas bubble in the surrounding fluid. Therefore, the model is considered as multi-phase modelling. A model of this kind of multi-phase flow is quite complex and includes an interface between the air and fluid phase with numerous discontinuities and stability problems. Moreover, different models (i.e. surface tension, no-penetration force), correction methods (e.g. shifting method) and the new particle generation method have been added to develop a robust modelling scheme and to improve the accuracy of the modelling. A more detailed literature review of multi-phase fluid-air interaction is given in Section 2.8.3.

2.8.2 The Need for SPH

Although mesh-based methods such as FDM or FEM have been used to solve the wide range of problems numerically, they can struggle to model the different shape, complex geometries and highly nonlinear behaviour of sharp interfaces, which may require extensive meshing and interface treatments, as explained in Section 2.7. In all grid-based methods, the first step is the mesh generation for the numerical simulations. If the Eulerian grid method is considered as an FDM, preparing the grid for the irregular case problems which have undefined geometries can be a difficult issue. Therefore, Eulerian grid-based methods possess disadvantages with regard to overcoming the problems, such as bubble modelling and growth in the polymer foaming, which have complex geometries in a regular fixed space. As a meshless method, SPH is applicable for many problems from free surfaces to a moving interface, and a deformable boundary to complex mesh generation. Furthermore, the change of properties on the particles is easily tracked since the particles carry the material properties and can also move due to the internal interactions and external forces.

Hence, using the SPH method is a very promising alternative for bubble modelling in the polymer melt of intumescent coating.

2.8.3 Multi-Phase SPH Modelling

As mentioned in the previous section, SPH is a Lagrangian method which enables the simulation of multi-phase flows such as explosive multi-phase pipe flow, wave breaking, and air bubble formation (gas expansion) in a liquid. It can be a difficult and complex task to apply the Eulerian grid-based methods to these kinds of
multi-phase flow simulation, as the creation of mesh requires a significant amount of
time, complex algorithms and high quality computational resources (Sussman et al.,
1994).

Extensive research methods with the SPH scheme have already been proposed
for multi-phase modelling, including both liquid-gas and liquid-liquid flows. One of
the most attractive features of SPH is to include more than one fluid with a separate
set of particles in each phase by assigning different equations of state (Monaghan,
2005). This is explained in this thesis in detail (see Section 5.3.4.1). However, the
accuracy of the multi-phase modelling results is greatly dependent on the ratio of
their hydrodynamic properties such as density and viscosity (Hu and Adams, 2006),
(Hu and Adams, 2007).

One of the first multi-phase SPH schemes examined the motion of dust and gas
by movement of the dust into a static gas phase (Monaghan and Kocharyan, 1995).
Shortly after, Monaghan and Kos (1999) proposed a multi-phase SPH for the
interaction of multiple fluids to simulate the gravity current free-surface problems
with a ramp. The results were satisfactory, with a correction to the velocity keeping
the particles more orderly and preventing the particle penetration. As the density
ratio between the fluids was small, using the classical SPH formulation without
applying any corrections at the interface could be acceptable. However, when
simulating large density ratios (e.g. 1:1000), several instability problems in the
region between the two substances can occur due to the high density gradient at the
interface and the presence of density in the denominator of SPH summations.
Colagrossi and Landrini (2003) proposed one of the first treatments for this problem
by modifying the expressions for SPH gradients.

A different approach was conducted by Hu and Adams (2006), in which the
density is only affected by the particle’s own volume rather than the volumes of
neighbouring particles. They also expressed the shear stress contribution in terms of
the colour function (see Section 5.3.4.4) such that the surface tension term could be
evaluated using that colour function.

The previous work was followed by the incompressible model developed by the
same authors (Hu and Adams, 2009). A constant density approach has been
introduced by correcting the density errors at a half-time step to simulate the flows
with high density ratios (i.e. a density ratio of 100 or more). As this more recent incompressible model requires greater computational resources, the method of Hu and Adams (2006) has been applied directly to surface tension modelling test cases, and the bubble growth test case (see Chapter 6).

Grenier et al. (2009) proposed a multi-fluid model combining the viscosity and surface tension of Hu and Adams (2006) based on the specific volume of particle approach with Colagrossi and Landrini (2003) scheme. The formulation was used for both phases separately, including an additional repulsive force similar to the non-penetration force expressed by Das and Das (2009) and used in the modelling of bubble generation through a submerged orifice in this thesis (see Section 6.3). The method of Grenier et al. (2009) was used to simulate an air bubble rising in water (multi-phase flow) and also gravity currents (free-surface flows).

Similar to that used by Grenier et al. (2009), a repulsion term is proposed for the lighter phase where the speed of sound is larger than that of the denser fluid (i.e. the ratio of speed of sounds is around 3) to simulate the multi-phase simulations (Monaghan, 2011). This was later improved by involving the free-surface problem with no rigid boundaries being applied to non-linear oscillation of the fluids, the simulation of waves at the interface between two fluids, the Rayleigh-Taylor instability test case and simulating the gravity currents with density ratios of 2-30 (Monaghan and Rafiee, 2013).

In recent years, SPH has been applied to simulate the phenomena of bubbles rising and multiple bubbles coalescing in viscous fluids in 3-D (Sun et al., 2015). Although SPH is becoming an increasingly popular method for free-surface flows (i.e. single phase flows), it can suffer from non-physical particles mixing at the interface of immiscible phases due to the current SPH formulations for multi-phase flows. Szewc et al. (2013) and Szewc et al. (2014) has also studied the single bubbles rising through viscous fluids by choosing the speed of sound carefully to set the incompressibility of the fluid in order to minimise the density fluctuations due to the high density ratio between fluids. Similar care has also been taken in the simulation of bubble growth in intumescent coatings, explained in detail in Section 6.4.
2.8.4 Modelling of Bubble Formation and Rise through a Submerged Orifice by SPH

Formation of bubbles with the aid of a submerged orifice, shown in Figure 2.9, is another attractive way for a large number of researchers to represent the physical process of bubble formation. An example of SPH being used to simulate the bubble evolution in a liquid pool through a submerged orifice has been shown by Das and Das (2009). In their work, the model is considered as a multi-phase problem including a gas compartment and a liquid compartment separated by a rigid partition with a central circular hole. The multi-phase SPH algorithm was applied to the setup shown in Figure 2.9. The Das and Das (2009) SPH scheme used artificial viscosity (Monaghan, 1992) to ensure that stress due to viscosity was continuous across the material interfaces. In this thesis, the SPHysics code is modified to simulate the bubble growth via an orifice similar to Das and Das (2009) but using the 3-D multi-phase SPHysics code. The modifications made in the SPHysics FORTRAN code are explained in detail in Chapter 5.

![Figure 2.9: Schematic view of problem domain (Das and Das, 2009)](image)

The parameters that have an influence on the bubbling process from a submerged orifice are the gas pressure, the density and the viscosity of the fluids, their
interfacial tension, the orifice diameter and the magnitude of the body force.

This model gives an opportunity to examine the details of the movement of two different liquids (liquid and gas) with a density ratio of 1:800, their interface and interfacial mass transfer from the lower chamber into the liquid pool using the SPH modelling technique. As shown in Figure 2.6 and explained in Section 2.6, growth of the bubbles in the intumescent coating and therefore expansion of the polymer foam significantly depend on the pressure coming from conversion of mass from solid to liquid and eventually gas. Hence, the process of the bubble forming with a submerged orifice is quite similar in terms of the pressure difference being the main driving force for the expansion.

However, the pressure of the air phase (air chamber) was kept constant throughout the simulation. This phenomenon is quite different from calculating the pressure according to the Equation of State in terms of being complex and challenging, as explained in detail in Section 5.3.4.1 based on the nature of SPH. Therefore, rather than assigning a higher constant pressure, other ways to obtain a higher pressure using that Equation of State need to be investigated. This is one of the motivations for conducting this thesis, as explained in Section 6.3 in Chapter 6.

2.9 Gas Expansion/Explosion Simulations using SPH Method

SPH is evidently an attractive method for treating the simulation of large deformation problems, and it can be used to investigate the complicated expansion process of bubbles. In the general expansion process of gaseous products towards the surrounding liquid (e.g. melted paint in intumescent process), there are free surfaces and moving interfaces involved. Research in a similar area of underwater explosion and expansion was conducted by Liu et al. (2003) and Wataru and Akiko (2006). The basic physics can be divided into two processes. One is the detonation process through the high explosive (HE) and the second step is the interaction process between the produced gas and surrounding water after explosion. Therefore, this expansion process behaviour is similar to the expansion process in the intumescent paint in terms of gasification due to intense heat and pressure.

In the interaction process, two pressure processes are involved in water: a shock wave proceeding through the water and a bubble pulse related to the expansion depending on the gas. The main differences between the work conducted by Liu et
al. (2003) and the intumescence process of the intumescent coating are that they assumed the water and gas phases to be inviscid and compressible while the expansion process occurs, and that the timescales over which the expansion of the intumescent coating occurs are far greater than in an underwater explosion. The Jones-Wilkins-Lee (JWL) equation of state, which is used in that work, is quite different since it corresponds to a detonation velocity and a Chapman-Jouget (C-J) pressure whereas Tait’s equation of state for nearly incompressible water is the most common approach for presenting fluids. The other major numerical aspects applied in the modelling of underwater explosion/expansion in terms of using artificial viscosity (Monaghan (1992), the boundary treatment as well as the material interface treatment are identical to the research methodology of this thesis.

The violent reaction between the gas and liquid phase leads to unphysical penetration or mixing near the interface in SPH. In order to solve this stability problem, some SPH models such as that of Das and Das (2009) add a repulsive force to the particles from different phases in the vicinity of the interface (i.e. boundary-fluid, gas-fluid or boundary-gas particles). This penetration force is also considered in the work explained in detail in Section 2.8.4.

2.10 Originality, Objectives and Assumptions of This Research

The literature review has revealed that the currently available methods for assessing the fire protection performance of intumescent coatings all have major shortcomings. Alternative predictive methods should be developed. This thesis aims to explore two possible developments, one using an analytical approach and one making use of numerical simulation using SPH. The main objectives of this research are:

- To extend the analytical method for multiple bubble growth of Amon and Denson (1984) to predict expansion of intumescent coatings with temperature-dependent properties and non-uniform temperature field, and to check the accuracy of this method against fire and heating test results for one type of intumescent coating where most of the necessary input information is available.

- To use the extended analytical method to assess the applicability of the current Eurocode method for calculating thermal conductivity of intumescent coatings, and to provide an insight into how different fire protection design
parameters (fire conditions including smouldering fire and parametric fires, intumescent coating thickness, steel section factor) affect intumescent coating thermal conductivity.

- To investigate the feasibility of using the meshless method, Smoothed Particle Hydrodynamics (SPH) to model the growth of a single intumescent coating bubble.

- To identify the challenges and possible methods to overcoming these challenges in order to develop a reliable detailed numerical simulation method for modelling the entire expansion process of intumescent coatings using SPH.

Although the development of the two modelling methods will be based on the other research studies reviewed in this chapter, modifications of their assumptions are necessary to tackle the specific problem of modelling intumescent coating expansion. Table 2.1 lists the main assumptions that will be employed in this research.

**Table 2.1 Main assumptions and shortcomings of both theoretical and SPH modelling methods for bubble growth**

<table>
<thead>
<tr>
<th>Theoretical Approach</th>
<th>SPH Approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>The expansion is in one-dimensional, perpendicular to the direction of heating with different heating conditions.</td>
<td>Isothermal condition.</td>
</tr>
<tr>
<td>The pressure increase comes from mass conversion of solid-liquid polymer melt to gas. All the releases gas is trapped inside the coating.</td>
<td>The pressure increase due to the mass conversion is represented by additional new gas particles.</td>
</tr>
<tr>
<td>Thermodynamic equilibrium is instantly achieved with changing temperatures.</td>
<td>Thermodynamic equilibrium exists continuously between the gas pressure inside the bubble and polymer-gas solution.</td>
</tr>
<tr>
<td>The material properties of intumescent coating such as viscosity, surface tension changes with temperature and time.</td>
<td>The viscosity changes according to the Laminar Viscosity equation in the SPH formulation and the surface tension is constant throughout the simulation.</td>
</tr>
</tbody>
</table>
2.11 Concluding Remarks

This chapter has provided a review of the physical processes of intumescent coatings and methods of predicting their performance in providing insulation to steelwork. This review has identified that the most important quantity controlling the fire protection performance of intumescent coatings is the expansion ratio. However, there is a lack of detailed studies that develop reliable methods for predicting this value. Most of the current research studies on intumescent coatings assume the expansion ratio is provided as input. The research studies of Butler (1997), Butler et al. (1997) and Zhang et al. (2012a; 2012b) are the only studies attempting to predict the expansion ratio. However, they have some major shortcomings and alternative research studies are required. This will be examined in this thesis.

The alternative modelling methods to be developed in this thesis will use the Smoothed Particle Hydrodynamics (SPH) method to model the intumescent coating expansion process at the microscopic level, and an analytical method based on the multi-cell model of Amon and Denson (1984). The SPH method is far from being mature enough to be used as a viable tool to investigate intumescent coating behaviour, and the objective of this research is to explore its capabilities and to identify future improvements. The analytical method will be further applied to conduct a detailed parametric study to investigate the applicability of the current Eurocode assessment to obtain thermal conductivity of intumescent coatings, and to provide an insight into how different fire protection parameters (fire condition, coating thickness, steel section factor) affect intumescent coating thermal conductivity and hence the accuracy of predicting steel temperature.
CHAPTER 3  A THEORETICAL MODEL FOR QUANTIFYING THE EXPANSION OF INTUMESCENT COATINGS

3.1  Introduction

When an intumescent coating is exposed to heat, it melts into a viscous fluid. Gases are then released from the blowing agent to expand the viscous fluid. Afterwards, the intumescent coating solidifies to form a stable char layer. The expanding process and the final expansion are the most critical factors in determining the fire protection performance of the intumescent coating.

This chapter presents an analytical method for bubble growth based on Amon and Denson (1984), which gives a solution to the expansion of spherical bubbles in viscous fluid when subject to an increase in pressure within the bubbles. This analytical method has been extended to non-uniform temperature field and temperature-dependent viscosity of intumescent melt. The pressure increase inside the bubbles is a result of conversion of the intumescent coating from melt to gases at high temperatures. The extended analytical method has been used to predict the expansion process of an intumescent coating tested by Zhang et al. (2012a; 2012b) under the cone calorimeter heating condition and also under furnace fire condition with different fire temperature-time curves. In these tests, an intumescent coating was applied to steel plates and the tests examined the effects of different coating thicknesses and steel plate thicknesses, therefore allowing the fire and cone calorimeter tests to encompass a wide range of temperatures and rates of heating.

3.2  Assumptions

The Amon and Denson (1984) bubble growth model has been described in Section 2.5.4. Its derivation was based on a number of idealised assumptions (see Section 2.5.3). In order to apply this model to calculate the expansion of intumescent coatings, the following adaptations are made:

- The expansion of intumescent coating is assumed to be one-dimensional, perpendicular to the direction of heating. In the coating thickness direction, the coating is divided into a large number of layers, each of which has the same temperature.
The driving force (pressure) inside the bubbles is due to the release of additional gas from the intumescent coating melt. All the released gas is trapped inside the coating and there is no diffusion from the released gas.

- Thermodynamic equilibrium is instantly achieved with changing temperatures.
- The material properties of the intumescent coating (viscosity, gas release, surface tension) change with temperature and time. This is explained in detail in Section 3.3.

### 3.3 Input properties of intumescent coating

#### 3.3.1 Mass Conversion (loss)

In the literature on intumescent coatings, the conversion of intumescent melt into gases is often referred to as mass loss. This is a misconception because the intumescent melt mass that has been converted into gases has not been lost. However, this is understandable because such tests are carried out using very small volumes and small quantities of intumescent coating mass in thermogravimetric analysis (TGA) tests. With the small sample size in the TGA test, the released gases can easily escape, hence giving rise to the appearance of mass loss. However, in large test samples such as in the cone calorimeter or furnace fire tests that are modelled in this study, the gases are assumed to be retained. Thus, the mass loss from the TGA test is alternatively referred to as mass conversion in this study.

Figure 3.1 shows the mass conversion – temperature relationship for the intumescent coating studied by Zhang et al. (2012b).
3.3.2 Pressure increase

The mass conversion value can be used to calculate the pressure increase inside intumescent coating bubbles that drives the expansion process. Consider an initial bubble of volume $V$. When the intumescent coating is converted from melt to gas, it is assumed that the mass of total converted gas is $\Delta m$, which is associated with the bubble volume $V$. If the pressure inside the bubble is maintained, the bubble would have to increase in volume by:

$$\Delta V = \frac{\Delta m}{\rho_g}$$  \hspace{1cm} (3.1)

where $\rho_g$ is the density of the gas inside the bubble.

However, before expansion occurs, the volume of the bubble is maintained. Therefore, the pressure inside the bubble has to increase. According to the ideal gas law, the initial state of the bubble is:

$$P_a V = nRT$$  \hspace{1cm} (3.2)
where \( R \) is the ideal gas constant, \( n \) is the amount of gas in moles, \( V \) is the volume of the gas and \( T \) is the temperature, \( n = \frac{m}{MW} \) in which \( m \) is the mass of gas and \( MW \) is the molar mass.

With the volume unchanged and the temperature maintained, when the additional \( \Delta m \) is included, the state of the bubble is:

\[
(P + \Delta P)V = (n + \Delta n)RT
\]  

(3.3)

where \( n = \frac{m}{MW} \).

Therefore, the new pressure in the bubble can be calculated using:

\[
\frac{P_g}{P_a} = \frac{(m + \Delta m)}{m} = \frac{(V + \Delta V)}{V}
\]  

(3.4)

\[
P_g = \left(\frac{\Delta V + V}{V}\right)P_a
\]  

(3.5)

where \( P_a \) is the initial gas pressure inside the bubble before mass conversion and expansion.

### 3.3.3 Surface Tension

In order to use Equation (2.11), the surface tension coefficient \((\sigma_s)\) of the intumescent coating melt is required. Since there has been no measurement of this property for intumescent coating melt, the values of Kwok et al. (1998) for polyethylene are adopted. This is shown in Figure 3.2.
Fortunately, prediction of intumescent coating expansion is not sensitive to the value of surface tension coefficient. Figure 3.3 indicates that when using the variable surface tension in Figure 3.2 and a constant value of 20 N/m² for predicting one (C12L1) of the tests of Zhang et al. (2012b), the results are very similar.
3.3.4 Viscosity

For the intumescent coating studied by Zhang et al. (2012a; 2012b), there was no measurement of viscosity. Therefore, for the purpose of this research, the viscosity value has to be estimated. This estimate is based on the results of Bugajny et al. (1999) which provided viscosity data for a number of intumescent melts given by Bourbigot et al. (2004). Comparing the mass conversion (loss) data shown in Figure 3.1 for the intumescent coating studied by Zhang et al. (2012b) with the TGA data of Figure 3.4, it can be seen that the intumescent coating of Zhang et al. (2012b) is similar to the curve for PP-APP/PEN. Therefore, in this study, it is assumed that the viscosity of the intumescent coating studied by Zhang et al. (2012b) is that of the curve for PP-APP/PEN. Figure 3.5 shows the recorded viscosity-temperature relationship for PP-APP/PEN and the fitted 5th-order polynomial curve for use in this study.
**Figure 3.4** TGA curves of different mixtures of intumescent paints (Bourbigot et al., 2004)

**Figure 3.5** Assumed viscosity – temperature relationship, based on heat-treated PP/PER/APP system of Bugajny et al. (1999)
3.4 Mathematical Model Results and Comparison

Zhang et al. (2012a; 2012b) carried out two series of tests, one under furnace fire exposure and one with a cone calorimeter. Comparison will be made for both series of tests.

3.4.1 Comparison for furnace fire tests

The furnace fire tests of Zhang et al. (2012a) were conducted by exposing intumescent coated steel plates, measuring 100 mm by 100 mm in planar dimensions and varying heights, coated with the same thickness on both sides, to fire from both sides. Three fire temperature-time curves were used for the furnace fire test condition. They are shown in Figure 3.6 and are referred to as fast fire, International Organization for Standardization (ISO) fire and slow fire.

When the intumescent coating protected steel plate was exposed to fire, the temperature distribution in the intumescent coating was non-uniform. When using the Amon and Denson model, the intumescent coating was divided into a large number of slices, each having its own temperature. The temperatures of these slices are based on the assumed temperature distributions shown in Figure 3.7. In this figure, the temperature of the intumescent coating in contact with the fire has the same temperature as the fire and the coating in contact with the steel plate has the same temperature as the steel plate.

Due to the very small mass of intumescent coating used, the effect of heat capacitance in heat transfer may be neglected. Therefore, heat transfer within the intumescent coating may be considered steady state. Under this condition, the temperature gradient within the intumescent coating is inversely proportional to the thermal conductivity of the intumescent coating. The effective thermal conductivity (based on the original thickness) of intumescent coating decreases as the temperature increases. Therefore, it is expected that the temperature gradient within the intumescent coating will increase from the steel plate to the fire side. The two temperature distribution bounds in Figure 3.7 represent the possible lower and upper bounds with the middle distribution in Figure 3.7, representing possible realistic temperature distribution inside the intumescent coating. The three temperature distributions in Figure 3.7 are used to demonstrate sensitivity of the results calculated using the Amon and Denson model to the assumed temperature distribution.
Figure 3.6 Furnace fire – temperature curves (Zhang et al., 2012b)

Figure 3.7 Different possible temperature assumptions throughout the intumescent coating thickness (D: Coating thickness, T: Temperature)
The steel plate thicknesses were 6, 10 and 20 mm and the nominal dry film thicknesses (DFTs) were 0.4, 0.8 and 1.2 mm respectively. However, in this modelling, the actual measured DFTs were used.

In the following sections, A, B and C refer to 6, 10 and 20 mm steel plate thicknesses respectively, while 04, 08, 12 refer to 0.4, 0.8 and 1.2 mm DFTs respectively. For example, A04SLOW refers to a steel plate of thickness 6 mm with 0.4 mm DFT subjected to slow fire conditions.

3.5 Results and discussions

3.5.1 Sensitivity of modelling results to the number of nucleation sites

When intumescent coating starts to expand, many bubbles will be created at different nucleation sites. The Amon and Denson model calculates expansion of the bubbles, from which the total expansion of the intumescent coating is calculated, as explained in Section 2.5.4. In theory, it is necessary to know the number of bubbles (nucleation sites) from which expansion occurs. However, since the nucleation sites share the same amount of gas conversion, it is expected that the expansion result will not be sensitive to the number of nucleation sites provided there is a sufficient number to smooth out the expansion. To check this, different numbers of nucleation sites have been considered in the theoretical model to investigate their influence on the final expansion thickness. Figure 3.8 shows the results for the final thickness when we vary the number of nucleation sites (number of bubbles in this case). It can be seen that the final thickness of the intumescent coating after full expansion is the same regardless of the number of bubbles once the number of nucleation sites reaches about 3,600. For further investigation of this research, a total number of bubbles of 36,000 will be used, which for a 100mm×100mm plate represents 60 nucleation sites in the planar direction and 10 nucleation sites in the thickness direction.
Using Equation (2.11) and (3.5), we can compute three representative expansion-time relationships for respectively 18,000, 36,000 and 144,000 bubbles are shown in Figure 3.9. It can be seen that the time history of expansion is also independent of the total number of nucleation (initial bubble) sites.

**Figure 3.8** Effect of number of bubbles on the final expanded thickness of intumescent coating

**Figure 3.9** Expansion-time relationship for various numbers of bubbles (nucleation sites)
3.5.2 Slow Fire Results

Figures 3.10 to 3.12 compare modelling results for different coating thicknesses and different assumed temperature distributions, for 6 mm, 10 mm and 20 mm steel plate thicknesses respectively. Figure 3.10 shows that using different temperature distributions has some effect on intumescent coating expansion, but the results are quite close to each other. Therefore, for further comparisons, only the realistic temperature distribution shown in Figure 3.7 will be used.

Figures 3.11 and 3.12 indicate moderate differences in the final expansion ratio under different conditions (coating thickness/steel plate thickness) for the 6 mm and 10 mm thick steel plates. However, for the 20mm thick plate tests, as shown in Figure 3.12, the theoretical model predicts quite a large difference in the final expansion ratios. This may be used as convincing data to support validation of the prediction results because the large reductions in expansion for C08 and C12 specimens are in excellent agreement with the test results. In fact, Table 3.1 compares the theoretically calculated and measured fire expansion ratios for all the slow fire tests. Despite the various assumptions of the Amon and Denson theoretical model and the further assumptions made by the authors to adapt the Amon and Denson model, the agreement is surprisingly good. In fact, the agreement is better than that between the test results and the predictions by Zhang et al. (2012a).
Figure 3.10  Sensitivity of predicted expansion process to assumed temperature distributions, for slow fire, 6 mm steel plate thickness

Figure 3.11  Predicted expansion ratios for slow fire, 10 mm steel thickness
Figure 3.12 Predicted expansion ratios for slow fire, 20 mm steel thickness

Table 3.1 Comparison between measured and predicted final expansion ratios for the slow fire tests

<table>
<thead>
<tr>
<th>SAMPLE ID</th>
<th>E.R(^a) Measured Zhang et al. (2012a)</th>
<th>E.R(^a) Predicted Zhang et al. (2012a)</th>
<th>E.R(^a) Current prediction</th>
</tr>
</thead>
<tbody>
<tr>
<td>A04SLOW</td>
<td>39.2</td>
<td>40.8</td>
<td>39.1</td>
</tr>
<tr>
<td>A08SLOW</td>
<td>40.5</td>
<td>30.1</td>
<td>37.3</td>
</tr>
<tr>
<td>A12SLOW</td>
<td>48.6</td>
<td>31.4</td>
<td>32.2</td>
</tr>
<tr>
<td>B04SLOW</td>
<td>42.9</td>
<td>37.7</td>
<td>39.5</td>
</tr>
<tr>
<td>B08SLOW</td>
<td>39.3</td>
<td>30.5</td>
<td>37.9</td>
</tr>
<tr>
<td>B12SLOW</td>
<td>37.5</td>
<td>32.6</td>
<td>36.0</td>
</tr>
<tr>
<td>C04SLOW</td>
<td>42.3</td>
<td>28.3</td>
<td>41.2</td>
</tr>
<tr>
<td>C08SLOW</td>
<td>20.2</td>
<td>24.2</td>
<td>21.5</td>
</tr>
<tr>
<td>C12SLOW</td>
<td>16.4</td>
<td>26.4</td>
<td>19.8</td>
</tr>
</tbody>
</table>

E.R\(^a\): Expansion Ratio
3.5.3 ISO Fire Results

Figures 3.13 to 3.15 present expansion-time relationships for the ISO fire tests. Table 3.2 compares the theoretical expansion ratios with those measured and calculated by Zhang et al. (2012a). Again, the agreement between the theoretical and measured results is quite good. It is particularly interesting to note the trend of expansion for the C-series tests whose steel plate thickness was the highest, being 20 mm. The theoretical model predicted the highest expansion ratio for the 0.8 mm DFT of A-B series tests and the smallest expansion ratio for the C-series test compared to those of the 0.4 mm and 1.2 mm DFT tests. This is in agreement with the test observation. In contrast, the predictions of Zhang et al. (2012a) indicate a monotonic change in the expansion ratio as the DFT changes.

![Figure 3.13 Predicted expansion ratios for ISO fire tests, 6 mm steel thickness](image)

Figure 3.13 Predicted expansion ratios for ISO fire tests, 6 mm steel thickness
Figure 3.14 Predicted expansion ratios for ISO fire tests, 10 mm steel thickness

Figure 3.15 Predicted expansion ratios for ISO fire tests, 20 mm steel thickness
Table 3.2 Comparison between measured and predicted final expansion ratios for the ISO fire tests

<table>
<thead>
<tr>
<th>SAMPLE ID</th>
<th>E.R\textsuperscript{a} Measured</th>
<th>E.R\textsuperscript{a} Predicted</th>
<th>E.R\textsuperscript{a} Current prediction</th>
</tr>
</thead>
<tbody>
<tr>
<td>A04ISO</td>
<td>34.2</td>
<td>37.1</td>
<td>24.71</td>
</tr>
<tr>
<td>A08ISO</td>
<td>36.6</td>
<td>35.3</td>
<td>34.80</td>
</tr>
<tr>
<td>A12ISO</td>
<td>28.2</td>
<td>30.3</td>
<td>27.82</td>
</tr>
<tr>
<td>B04ISO</td>
<td>29.9</td>
<td>33.1</td>
<td>24.68</td>
</tr>
<tr>
<td>B08ISO</td>
<td>23.0</td>
<td>25.7</td>
<td>28.47</td>
</tr>
<tr>
<td>B12ISO</td>
<td>21.0</td>
<td>25.7</td>
<td>27.50</td>
</tr>
<tr>
<td>C04ISO</td>
<td>26.2</td>
<td>29.6</td>
<td>26.94</td>
</tr>
<tr>
<td>C08ISO</td>
<td>18.5</td>
<td>23.3</td>
<td>21.53</td>
</tr>
<tr>
<td>C12ISO1</td>
<td>21.3</td>
<td>20.9</td>
<td>26.49</td>
</tr>
</tbody>
</table>

E.R\textsuperscript{a}: Expansion Ratio

3.5.4 Fast Fire Results

Figures 3.16 to 3.18 compare the modelling expansion ratio results for the fast fire tests and Table 3.3 summarises the final expansion results. Similar to the slow and ISO fire results from Sections 3.5.2 and 3.5.3, the current theoretical results are generally in good agreement with the experimental results of Zhang et al. (2012a). As can be seen from Table 3.3, there is a monotonic change in expansion-time relationships for each series of the fast fire test specimens. The theoretical results follow this trend except for the sample with 6 mm steel thickness (A12).
Figure 3.16 Predicted expansion ratios for fast fire tests, 6 mm steel thickness sample

Figure 3.17 Predicted expansion ratios for fast fire tests, 10 mm steel thickness
Figure 3.18 Predicted expansion ratios for fast fire tests, 20 mm steel thickness

Table 3.3 Comparison between measured and predicted final expansion ratios for the fast fire tests

<table>
<thead>
<tr>
<th>SAMPLE ID</th>
<th>E.R&lt;sup&gt;a&lt;/sup&gt; Measured Zhang et al. (2012a)</th>
<th>E.R&lt;sup&gt;a&lt;/sup&gt; Predicted Zhang et al. (2012a)</th>
<th>E.R&lt;sup&gt;a&lt;/sup&gt; Current prediction</th>
</tr>
</thead>
<tbody>
<tr>
<td>A04FAST</td>
<td>24.8</td>
<td>30.8</td>
<td>24.82</td>
</tr>
<tr>
<td>A08FAST</td>
<td>21.8</td>
<td>25.5</td>
<td>21.45</td>
</tr>
<tr>
<td>A12FAST</td>
<td>28.8</td>
<td>25.2</td>
<td>16.81</td>
</tr>
<tr>
<td>B04FAST</td>
<td>31.5</td>
<td>31.5</td>
<td>35.24</td>
</tr>
<tr>
<td>B08FAST</td>
<td>23.7</td>
<td>25.8</td>
<td>21.49</td>
</tr>
<tr>
<td>B12FAST</td>
<td>20.7</td>
<td>26.1</td>
<td>16.02</td>
</tr>
<tr>
<td>C04FAST</td>
<td>32.2</td>
<td>27.6</td>
<td>34.09</td>
</tr>
<tr>
<td>C08FAST</td>
<td>19.7</td>
<td>23.4</td>
<td>22.39</td>
</tr>
<tr>
<td>C12FAST</td>
<td>20.5</td>
<td>22.6</td>
<td>18.00</td>
</tr>
</tbody>
</table>

E.R<sup>a</sup>: Expansion Ratio
3.6 Modelling the Cone Calorimeter Tests

The same intumescent coating as in the furnace fire tests was used in the cone calorimeter tests (see Figure 2.3). In addition, the same steel plate thicknesses and nominal DFTs were used. The cone calorimeter tests were performed for two radiating heat flux: 50 kW/m² and 65 kW/m². The steel temperature was measured in the experiments. However, there was no measurement of the intumescent coating surface temperature. In order to obtain the intumescent coating surface temperature to approximate the temperature profiles within the intumescent coating, the intumescent coating surface temperature \( T_{surface} \) calculation method developed by Omrane et al. (2007) was used. A summary of this method is provided below:

Considering the test sample as one-dimensional, the surface temperature of the intumescent coating is calculated using the following heat balance equation:

\[
e_{c} \sigma T^4 + h_c (T - T_\infty) = e_c Q_e - Q_{loss} - \frac{(\Delta T + \Delta T_s)}{2\Delta t} \rho_p C_p d_p - \frac{\Delta T_s}{\Delta t} \rho_s C_s d_s
\]  

(3.6)

where \( Q_e \) is the incident irradiance (heat flux) from the cone calorimeter on the surface of the specimen, \( e_c \) is the surface emissivity of the intumescent coating, \( h_c \) is the convective heat transfer coefficient, \( T_\infty \) is the environment temperature and \( \rho_p, C_p, d_p, \rho_s, C_s, d_s \) are the density, specific heat and the original thickness of the coating and steel plate respectively.

The first and second terms on the left-hand side of Equation (3.6) are radiation and convection heat losses from the surface of the intumescent coating to the space respectively. The first term on the right-hand side of the equation is the heat flux irradiance; the second term is the conductive heat loss from the steel plate to the mineral wool, while the third and fourth terms are the heat stored in the intumescent coating and in the steel plate respectively. In the calculation of the intumescent coating surface temperature in this study, the conductive heat loss from the steel plate to the insulation and heat stored in the coating are neglected due to good insulation and negligible coating mass respectively. The predicted surface temperature using Equation (3.6) rapidly increases to the final steady value within 8-10 minutes.

After obtaining the intumescent coating surface temperature, the same
temperature distribution profile, as shown by the middle (realistic) curve of Figure 3.7, was used in the theoretical calculations using the Amon and Denson model.

During the cone calorimeter tests, continuous measurement of the expanded thickness of the intumescent coating was made. This makes it possible to compare the theoretical prediction of the expansion process with the test results. In Sections 3.6.2 and 3.6.3, H and L refer to the heat fluxes of 65 kW/m$^2$ and 50 kW/m$^2$ respectively, while 1 and 2 refer to the sample number. For example, A04L1 refers to a steel plate of thickness 6 mm with 0.4 mm DFT subjected to radiant heat flux of 50 kW/m$^2$ having a sample number of 1.

3.6.1 Modification to Surface Temperature Prediction

Since some of the heat loss terms (heat conduction to insulation, heat stored in intumescent coating) in Equation (3.6) were neglected and a high surface emissivity was assumed from the beginning, using Equation (3.6) of Omrane et al. (2007) produced a very high initial increase in the intumescent coating surface temperature, causing the predicted intumescent coating expansion to increase rapidly when the experimental results indicated near zero expansion. To avoid this problem, the predicted surface temperature – time curve using Equation (3.6) was shifted by a small amount of time so that the prediction and measurement of intumescent coating thickness would start at the same time. This is shown in Figure 3.19 as an example.
Figure 3.19 Comparison of predicted and measured expansion ratios using two predicted surface temperature-time relationships (one using Equation (3.6), one using Equation (3.6) with a shift in time), test sample B08L1

3.6.2 Results for low heat tests (50 kW/m²)

The measured results of Zhang et al. (2012b) show that specimens A04L1, B08L1 and C12L1 achieved maximum expansion, medium (average) expansion and minimum expansion. These three tests are used here to show a detailed comparison between the theoretical prediction and test results.

Figure 3.20 compares the expansion ratio–time relationships for these three tests, where “Test” refers to the measured expansion ratio by Zhang et al. (2012b) and “Prediction” refers to the current predicted expansion ratio. Figures 3.21 and 3.22 also compare the expansion ratio-time relationships for other samples with different DFTs and steel thicknesses.
Figure 3.20 Comparison of predicted and measured expansion histories for three representative tests (maximum expansion (A04), minimum expansion (C12), average expansion (B08))

Close agreement is clearly shown between the prediction and test results for the intumescent coating expansion process and the maximum expansion ratio. The small difference may be due to the assumed coating temperature profile, and this difference is considered acceptable. Some of the test results indicate reduction in expansion after reaching the maximum. Zhang et al. (2012b) attributed this to oxidation of the surface layers at high temperatures after reaching the maximum value and proposed a simplified equation to deal with this. Since the main interest of this study is the intumescent coating expansion process until attainment of maximum expansion, this has not been implemented in the current theoretical prediction, although the same procedure may easily be used.
Figure 3.21 Comparison of predicted and measured expansion histories for three low heat tests (nominal DFT=0.4 mm)

Figure 3.22 Comparison of predicted and measured expansion histories for three low heat tests (nominal DFT=1.2 mm)
Table 3.4 compares the predicted and measured expansion thicknesses and ratios for all the cone calorimeter tests at 50kW/m$^2$. The predicted results from this study are the final thickness of the coating at the end of the one hour prediction. Overall, the agreement with the measured results is very good, considering that the complex physical and chemical behaviour of the intumescence process and many of the necessary assumptions may not be exact. There is much closer agreement for the new expansion model results with the experimental results of Zhang et al. (2012b) than predicted results of Zhang et al. (2012b).

Table 3.4 Summary of comparison between predicted and measured final thicknesses/expansion ratios of samples exposed to 50 kW/m$^2$

<table>
<thead>
<tr>
<th>SAMPLE ID</th>
<th>Measured Final Thickness (mm) / Expansion Ratio Zhang et al. (2012b)</th>
<th>Predicted Final Thickness (mm) / Expansion Ratio Zhang et al. (2012b)</th>
<th>Current prediction Final Thickness (mm) / Expansion Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>A04L1</td>
<td>22/63</td>
<td>17.3/48.6</td>
<td>23.8/68.0</td>
</tr>
<tr>
<td>A08L2</td>
<td>36/36</td>
<td>34/34.1</td>
<td>39.3/38.3</td>
</tr>
<tr>
<td>A12L1</td>
<td>48/38</td>
<td>32.9/26.4</td>
<td>42.8/37.5</td>
</tr>
<tr>
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<td>21.6/42.0</td>
<td>28.4/55.8</td>
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<td>41.4/48.7</td>
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<td>41/37</td>
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<td>49.8/38.2</td>
</tr>
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<td>21.8/40.7</td>
<td>20.9/37.8</td>
</tr>
<tr>
<td>C08L2</td>
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<td>33.5/33.0</td>
<td>34.0/33.0</td>
</tr>
<tr>
<td>C12L1</td>
<td>40/27</td>
<td>35.0/23.3</td>
<td>40.0/26.7</td>
</tr>
</tbody>
</table>

3.6.3 Results for high heat tests (65 kW/m$^2$)

The same exercise as described above was repeated for the tests under heat flux of 65 kW/m$^2$. Figure 3.23 compares the expansion ratio–time relationships for these three tests, where “Test” refers to the expansion ratio measured by Zhang et al. (2012b) and “Prediction” refers to the current predicted expansion ratio. Figures 3.24
to 3.26 show the comparison of the expansion ratios between predicted and measured results for all samples. Again the predicted results are in good agreement with the measured results.

Table 3.5 compares the predicted and measured expansion ratios. There are some relatively large differences for some of the tests (A08H1, B04H1). This is because the measured values were the final values and the predicted values were the maximum values, and for these tests, there was a substantial amount of shrinkage after the intumescent coating had reached maximum expansion, as shown in Figure 3.23.

![Graph comparing predicted and measured expansion ratios](image)

**Figure 3.23** Comparison between predicted and measured expansion histories for three representatives (maximum expansion B04H1, minimum expansion A12H1, average expansion C08H1) of the high heat tests
Figure 3.24 Comparison of predicted and measured expansion histories for three high heat tests (nominal DFT=0.4 mm)

Figure 3.25 Comparison of predicted and measured expansion histories for three high heat tests (nominal DFT=0.8 mm)
Figure 3.26 Comparison of predicted and measured expansion histories for three high heat tests (nominal DFT=1.2 mm)

Table 3.5 Summary of comparison between predicted and measured final thicknesses/expansion ratios of samples exposed to 65 kW/m²

<table>
<thead>
<tr>
<th>SAMPLE ID</th>
<th>Measured Final Thickness (mm) / Expansion Ratio Zhang et al. (2012a)</th>
<th>Predicted Final Thickness (mm) / Expansion Ratio Zhang et al. (2012a)</th>
<th>Current prediction Final Thickness (mm) / Expansion Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>A04H1</td>
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<td>21.3/68.8</td>
</tr>
<tr>
<td>A08H1</td>
<td>26/39</td>
<td>25.6/38</td>
<td>38.2/53.6</td>
</tr>
<tr>
<td>A12H1</td>
<td>31/19</td>
<td>37.4/23</td>
<td>37.5/23.4</td>
</tr>
<tr>
<td>B04H1</td>
<td>13/46</td>
<td>13.5/48</td>
<td>21.2/75.7</td>
</tr>
<tr>
<td>B08H1</td>
<td>26/39</td>
<td>25.6/38</td>
<td>31.7/44.2</td>
</tr>
<tr>
<td>B12H1</td>
<td>38/25</td>
<td>37.6/25</td>
<td>45.4/29.2</td>
</tr>
<tr>
<td>C04H1</td>
<td>21/37</td>
<td>19.8/35</td>
<td>24.8/44.1</td>
</tr>
<tr>
<td>C08H1</td>
<td>24/30</td>
<td>29.7/37</td>
<td>31.7/38.2</td>
</tr>
<tr>
<td>C12H1</td>
<td>35/28</td>
<td>32.3/26</td>
<td>37.8/29.5</td>
</tr>
</tbody>
</table>
3.7 Concluding Remarks

This chapter has assessed the feasibility of extending the theoretical model of Amon and Denson (1984) to predict expansion of intumescent coating in fire. The Amon and Denson theoretical model calculates the increase in diameter of spherical bubbles in viscous liquid when the pressure inside the bubbles increases. For application to calculation of intumescent coating expansion, the driving pressure comes from conversion of intumescent melt to gases. The main extensions to the Amon and Denson model include non-uniform temperature field and temperature-dependent viscosity. Calculation results from the extended Amon and Denson (1984) model have been compared to the cone calorimeter test results of Zhang et al. (2012b) and the furnace fire test results of Zhang et al. (2012a). These tests included different steel plate thicknesses, intumescent coating thicknesses and fire/cone calorimeter heating conditions. The following conclusions may be drawn:

1. The extended model prediction results are insensitive to the number of initial nucleation sites (where the expanding bubbles start) provided a sufficiently large number is used.
2. The surface temperature of the intumescent coating melt has only a minor effect on expansion.
3. Expansion of the same intumescent coating varies depending on the heating condition. This variation is not monotonic with heating rate.
4. The extended Amon and Denson model has been demonstrated to give prediction results of the maximum intumescent coating expansion in good agreement with the measured results of Zhang et al. (2012a) and Zhang et al. (2012b).

The following chapter will examine the effects of different steel thicknesses/coating thicknesses on intumescent coating fire protection performance.
CHAPTER 4  FIRE BEHAVIOUR OF INTUMESCENT COATING

4.1  Introduction

In Chapter 3, the Amon and Denson (1984) model has been extended to quantify the expansion process of intumescent coatings. It has been found that with suitable modifications and input reaction data (mass loss, viscosity), the Amon and Denson (1984) model is applicable. The validation of the model is based on comparison of the intumescent expansion process and the maximum expansion ratio between the calculation results and the test results of Zhang et al. (2012a; 2012b) under different heating and fire testing conditions. In this comparison, the measured steel temperatures were used as input data. However, due to the limited number of tests, it is not possible to examine in detail the influences of changing the various design conditions on the behaviour and thermal conductivity of intumescent coatings. These design conditions include the fire temperature-time curve, the intumescent coating thickness and the steel section factor. The purpose of this chapter is an attempt to address this deficiency, by using the analytical method based on the Amon and Denson (1984) model as presented in detail in Chapter 3.

4.2  Procedure

To achieve the aim of this chapter, which is to examine the effects of changing different design parameters on the behaviour and thermal conductivity of intumescent coatings, the following procedure is applied:

(1) Obtaining the thermal conductivity of the intumescent coating as a function of its temperature and rate of temperature increase. This will be done by assuming a uniform temperature field in the coating. The thermal conductivity of the coating will be expressed as the effective thermal conductivity (for the original coating thickness). The apparent thermal conductivity of the coating (for the expanded coating thickness) is almost independent of the rate of temperature rise. Temperature rates of 2°C/minute (based on the protected steel reaching 600°C at 300 minutes in a standard fire) to 100°C/minute (near the fire exposure surface) will be used.

(2) The effective thermal conductivity of the coating will then be used to
calculate the protected steel temperatures using the equation in EN 1993-1-2 (CEN, 2005) for protected steel sections. The calculation results will be compared with the fire test results of Zhang et al. (2012a) to check validity of the model.

(3) Using the analytical method, the intumescent coating effective thermal conductivity at different uniform temperatures and different rates of temperature increase, a parametric study will be carried out to calculate the protected steel temperatures under different fire temperature-time curves, using different steel section factors and different coating thicknesses.

(4) Using the protected steel temperatures calculated from (3), the effective thermal conductivity of the intumescent coating with non-uniform coating temperature distribution will be calculated, through inverse solution of the protected steel temperature equation according to EN 13381-4:2013 (CEN, 2013a).

The same intumescent coating as in Chapter 3, which was used in the studies of Yuan (2009) and Zhang et al. (2012a; 2012b), will be used.

4.3 Effective Thermal Conductivity of Intumescent Coating

After expansion, the intumescent coating becomes a porous material. According to Yuan (2009), the apparent thermal conductivity of the coating is:

$$\lambda^* = \lambda_s \left( \frac{\lambda_g}{\lambda_s} \frac{2}{\varepsilon^2} + \frac{1}{\varepsilon^2} + \varepsilon^2 \right)$$

where $\varepsilon$ is the volume fraction (or porosity), $\lambda_g$ is the thermal conductivity of the gas within the pore (or bubble) and $\lambda_s$ is the thermal conductivity of the solid part of the porous structure. After full expansion, there is very little solid left in the coating char and the thermal conductivity of the solid has little influence on the thermal conductivity of the coating. For simplicity, a value of 0.5 W/mK may be used (Yuan, 2009).

Porosity ($\varepsilon$) is defined as the fraction of the total volume occupied by the bubbles to the total volume. If the expansion ratio of the intumescent coating is $E$, then the porosity is simply:
\[ \varepsilon = \frac{E - 1}{E} \]  

(4.2)

The thermal conductivity of the gas \( (\lambda_g) \) comprises pure conduction \( (\lambda_{g\text{cond}}) \) and radiation \( (\lambda_{g\text{rad}}) \) inside the bubbles (pore). The contribution of gas conduction is given by Di Blasi and Branca (2001) as:

\[ \lambda_{g\text{cond}} = 4.815 \times 10^{-4}T^{0.717} \]  

(4.3)

The contribution to overall thermal conductivity of the coating due to thermal radiation inside the bubbles is calculated using the following equation (Yuan, 2009):

\[ \lambda_{g\text{rad}} = \frac{2}{3} \times 4\varepsilon\sigma T^3 \]  

(4.4)

where \( d \) is the pore (bubble) diameter. For this study, the bubbles of the fully expanded intumescent coating are assumed to be identical, all spherical in shape with a diameter of 3.5 mm (Yuan, 2009). "\( \varepsilon \)" is the emissivity of the gas inside the bubbles and "\( \sigma \)" is the Stefan-Boltzmann constant. \( 2/3 \) is the shape factor of spherical pores for radiation. If the intumescent coating is not fully expanded, it is assumed that the diameter of the bubbles is proportional to the maximum expansion ratio (Yuan, 2009), i.e.

\[ d = d_b \frac{E}{E_{\text{max}}} \]  

(4.5)

The total thermal conductivity of the gas through the bubbles is given by:

\[ \lambda_g = \lambda_{g\text{cond}} + \lambda_{g\text{rad}} = 4.815 \times 10^{-4}T^{0.717} + \frac{2}{3} \times 4\varepsilon\sigma T^3 \]  

(4.6)

Figure 4.1 presents the expansion ratio-temperature relationships of the intumescent coating under different rates of temperature increase. For the heating rate of 100\(^{\circ}\)C/min, the intumescent coating has only expanded to a few times its original thickness, and has not reached full expansion, because this heating rate is too high. In general, when the heating rate increases, the expansion ratio decreases.
Figure 4.1 Effects of heating rates on intumescent coating expansion

Figure 4.2 compares the apparent thermal conductivities of expanded intumescent coating under different rates of temperature increase in the coating. The apparent thermal conductivity values for different heating rates are almost the same, except for the heating rate of 100°C/min. The apparent thermal conductivity at high temperatures for 100°C/min is lower than others because at this high heating rate, the intumescent coating has not fully expanded. When the heating rate is too high, the amount of gases released is low during the optimal expansion window (between 250°C - 400°C, see Figure 3.5) when the viscosity of the coating is low. Therefore, the bubble size is smaller (Equation (4.5)), leading to a lower apparent thermal conductivity (Equation (4.1)).
The “Effective Thermal Conductivity” of the intumescent coating is related to the apparent thermal conductivity of the coating consideration of equal thermal resistance of the same coating, whether using the initial coating thickness (effective thermal conductivity) or the expanded coating thickness (apparent thermal conductivity). Therefore, the effective thermal conductivity is:

$$\lambda_{\text{effective}} = \frac{\lambda_{\text{apparent}}}{E}$$ (4.7)

Figure 4.3 compares the effective thermal conductivities of the intumescent coating with different heating rates. Since the intumescent coating has not fully expanded when the rate of heating is 100˚C/min, the effective thermal conductivity of the coating is much higher than for other heating rates. At other heating rates, there are also large differences in effective thermal conductivity of the coating after full expansion (temperature from about 300˚C). The same trend of thermal conductivity – temperature relationships shown in Figure 4.2 has been reported by another of other researchers, based on experimental results. Muller et al. (2013) measured the effective thermal conductivities of intumescent coatings using X-ray computed tomography and Gardelle et al. (2013) using heat radiator test. They gave thermal
conductivity values at ambient temperature and at 300°C of 0.30±0.01 W/mK and 0.10±0.01 W/mK respectively. These values are similar to the values of this study. At higher temperatures, their measured effective thermal conductivity values increase. Wang et al. (2015) obtained the effective thermal conductivities of an intumescent coating based on back calculation (using the same equation as 4.19) of measured steel and fire temperatures for intumescent coating protected steel plates exposed to three non-standard fire conditions. They reported the same trend as shown in Figure 4.2. In contrast, Staggs (2010) showed a monotonic trend of increasing thermal conductivity value from 0.1 W/mK at ambient temperature to 0.4 W/mK at 600°C. However, his prediction model was based on the fully expanded intumescent coating char and did not consider the initial stage of intumescent coating behaviour during the expansion phase. It is this varying thermal conductivity-temperature relationship under different heating rates that makes it important to understand how different fire conditions, different coating thicknesses and different steel section factors will affect intumescent coating behaviour, because these design parameters influence the intumescent coating heating rate.

![Figure 4.3 Effective thermal conductivity of the expanded intumescent coating under different heating rates](image)

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4.4 Temperatures of Steel Sections Protected by Intumescent Coating in Fire

According to Eurocode EN 1993-1-2 (CEN, 2005), the temperature of protected steel can be calculated using the following equation:

\[
\Delta T_s = \left( \frac{T_{fi} - T_s}{\frac{A_p}{V_s}} \right) \frac{\lambda_p}{\rho_s C_s} \left( 1 + \frac{1}{3} \phi \right) \Delta t - \left( e^{\frac{\phi}{10}} - 1 \right) \Delta T_{fi}
\]

where \( \phi = \frac{c_p \rho_p v_p}{c_s \rho_s v_s} \).

In this equation, the thermal boundary condition of the fire is ignored. It is also assumed that the temperature of the fire protection material is the average of the steel section temperature and the fire temperature. Although this is sufficiently accurate for calculating the protected steel temperature, because of the critical influence of intumescent coating temperature on its thermal conductivity, it is necessary to calculate the intumescent coating temperature more accurately. For this purpose, it is necessary to include the thermal resistance of the fire in the denominator of the above equation, so that:

\[
\Delta T_s = \left( \frac{T_{fi} - T_s}{\frac{A_p}{V_s}} \right) \frac{\lambda_p}{\rho_s C_s} \left( 1 + \frac{1}{3} \phi \right) \Delta t - \left( e^{\frac{\phi}{10}} - 1 \right) \Delta T_{fi}
\]

where \( h \) is the total heat transfer coefficient of the fire layer, calculated as:

\[
h = h_{rad} + h_{conv}
\]

where \( h_{rad} \) is calculated as:

\[
h_{rad} = e \sigma (T_{fi}^2 + T_s^2) (T_{fi} + T_s)
\]

in which \( h_{conv} = 25 \text{ W/m}^2\text{K} \) is the convective heat transfer coefficient.

Since the intumescent coating is very thin, the heat stored in the intumescent coating is negligible. Therefore, given the fire temperature and the steel section temperature, heat transfer through the intumescent coating may be assumed to be steady state.
Consequently, the surface temperature of the intumescent coating may be calculated using the following equation (Wang, 2002):

\[
T_{\text{surface}} = T_{fi} - \frac{\left(\frac{1}{t_f} + \frac{t_p}{\lambda_p}\right) \left(T_{fi} - T_s\right)}{h}
\]  

(4.12)

As a first approximation, the intumescent coating is assumed to be at uniform temperature and the coating temperature is the average of the coating surface temperature and the steel section temperature, given below:

\[
T_{\text{coating}} = \frac{T_{\text{surface}} + T_s}{2}
\]  

(4.13)

The rate of heating of the coating is thus:

\[
\Delta T_{\text{coating}} = \frac{T_{\text{coating}_{(t+\Delta t)}} - T_{\text{coating}_{(t)}}}{\Delta t}
\]  

(4.14)

Based on the coating temperature (Equation (4.13)) and the heating rate (Equation (4.14)), the effective thermal conductivity of the intumescent coating can be calculated by interpolation based on the results in Figure 4.3. In this research, this is referred to as the “one-layer” model.

However, because temperature distribution in the intumescent coating is non-uniform, and hence the rate of heating is non-uniform, and because the heating rate of the intumescent coating influences the coating thermal conductivity – temperature relationship (see Figure 4.3), it is necessary to calculate the intumescent coating temperature more accurately. To do so, the intumescent coating is divided into a number of layers and each layer is assumed to have the same temperature. To obtain the temperatures of the layers, the steady state heat conduction within the intumescent coating, given the coating surface temperature and the substrate steel temperature, can be calculated as follows (Wang et al., 2012):

\[
\dot{Q} = \frac{T_{fi} - T_s}{R_{\text{total}}}
\]  

(4.15)

where the total thermal resistance, for the five layers of intumescent coating and the
thermal boundary layer of the fire, is:

\[ R_{total} = R_{fi} + R_{12} + R_{23} + R_{34} + R_{45} + R_{56} \]  \( (4.16) \)

in which \( R_{ij} \) is the thermal resistance of layer \( ij \), given by:

\[ R_{ij} = \frac{\Delta x_{ij}}{\lambda_{ij}} \]  \( (4.17) \)

where \( \lambda_{ij} \) is the thermal conductivity, \( \Delta x_{ij} \) is the layer thickness.

\[ R_{fi} = \frac{1}{h_{fi}} \]  \( (4.18) \)

where \( h_{fi} \) is the heat exchange coefficient on the fire side.

In this procedure, the steel temperature is calculated using Equation (4.9), by replacing the thermal resistance term \( \left( \frac{1}{h} + \frac{t_p}{\lambda_p} \right) \) with \( R_{total} \). To obtain the intumescent coating layer temperatures, the steady state heat conduction is calculated using Equation (4.15). The layer temperatures, and the associated heating rates, are then used to obtain the layer thermal conductivity values according to Figure 4.3. This procedure is implemented incrementally with a time interval of 10s.

In this chapter, this model is referred to as the “multi-layer” model. This chapter will assess the accuracy of these two different models.

### 4.5 Validation of Calculations of Temperature of Intumescent Coating Protected Steel under Different Fire Conditions

The method described so far is predictive: using the thermal conductivity-temperature relationships at different heating rates in Figure 4.3, the protected steel temperature can be calculated. To check the accuracy of this predictive method, the fire test results of Zhang et al. (2012a) are compared in this section. Table 4.1 lists the fire tests conducted by Zhang et al. (2012a). Figure 4.4 shows the three furnace temperature-time curves.
Table 4.1 Steel thicknesses and dry film thicknesses (DFT) for all tests

<table>
<thead>
<tr>
<th>Sample ID*</th>
<th>Steel Thickness (mm)</th>
<th>Target DFT (mm)</th>
<th>Measured DFT_A side (mm)</th>
<th>Measured DFT_B side (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A04ISO</td>
<td>6</td>
<td>0.4</td>
<td>0.301</td>
<td>0.447</td>
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<td>0.8</td>
<td>0.706</td>
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<td>0.8</td>
<td>0.737</td>
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<tr>
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<td>1.067</td>
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<td>1.049</td>
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<td>1.014</td>
<td>1.063</td>
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</tbody>
</table>


Sample ID*: Steel thickness (A – 6 mm, B – 10 mm, C – 20 mm) + target DFT (04, 08, 12 mm) + fire type (ISO – ISO, SLOW – slow, FAST – fast)
4.5.1 Standard Fire (ISO) Results

Figure 4.5 and Figure 4.6 compare the measured steel temperatures and the predicted steel temperatures with single and multi-layer coating models, with respect to time. In the multi-layer model, the coating is divided into 5 layers. Thicknesses of the steel plate samples are 6, 10 and 20 mm. For clarity, only results for the minimum and maximum coating thicknesses (nominal coating thickness of 0.4 mm and 1.2 mm, indicated by 04 and 12 in the designations in Table 4.1) and the minimum and maximum steel thicknesses (6 mm and 20 mm, indicated by the letters A and C in the designations in Table 4.1) are presented. Comparison of results for other tests is presented in Appendix A. Close agreement can be seen between the prediction and test results. In most cases, the predicted results tend to be lower than the experimental results, especially at the end of the test. This behaviour has also been seen in the studies of Zhang et al. (2012a) and Yuan (2009). The reason for this is that cracks were present in the intumescent char in tests at very high temperatures but they cannot be included in the current model. In general, the predicted and measured steel temperatures are within 10% of each other. Also, Figures 4.5 and 4.6 show that the multi-layer model gives better prediction than the single layer model.
**Figure 4.5** Comparison between measured and predicted steel temperatures based on single and multi-layer models for ISO fire: steel plate thickness 6 mm

**Figure 4.6** Comparison between measured and predicted steel temperatures based on single and multi-layer models for ISO fire: steel plate thickness 20 mm
4.5.2 Slow and Fast Fire Results

Figure 4.7 to Figure 4.10 present the same sets of results for the Slow and Fast fire tests. Similar to the results for the standard fire tests, agreement between the simulation and test results is very good.

The effective thermal conductivity results in Figure 4.3 show the drastic effects of a high rate of heating on intumescent coating behaviour. This is reflected in the difference in results between using the single and multi-layer models. For the Slow fire tests, because the heating rate is predominately moderate, the difference in thermal conductivity between different layers is relatively small. Therefore, using the single layer model produced similar results to using the multi-layer model. However, for the Fast fire tests, because of large temperature differences between different layers and the critical influence of a high heating rate on the effective thermal conductivity of the intumescent coating, using the single layer model introduces quite noticeable inaccuracy in the prediction results.

![Comparison between measured and predicted steel temperatures based on single and multi-layer models for slow fire: steel plate thickness 6 mm](image)

**Figure 4.7** Comparison between measured and predicted steel temperatures based on single and multi-layer models for slow fire: steel plate thickness 6 mm
**Figure 4.8** Comparison between measured and predicted steel temperatures based on single and multi-layer models for slow fire: steel plate thickness 20 mm

**Figure 4.9** Comparison between measured and predicted steel temperatures based on single and multi-layer models for fast fire: steel plate thickness 6 mm
Figure 4.10 Comparison between measured and predicted steel temperatures based on single and multi-layer models for fast fire: steel plate thickness 20 mm

4.6 Influences of Different Parameters on Effective Thermal Conductivity of Intumescent Coatings

At present, in Eurocode EN 13381 Part 4 (CEN, 2013a), assessment of intumescent coating is essentially considered in the same way as for other non-reactive fire protection materials. In this approach, the standard fire resistance test results are used to output thermal conductivity of intumescent coatings, as a function of temperature. This section will assess whether or not this approach is suitable under different design conditions, considering influences of different design fire temperature – time curves, different steel section factors and different intumescent coating thicknesses. In EN 13381-4, the effective thermal conductivity of the intumescent coating is calculated by the inverse solution of the equation for calculating protected steel temperature, given as:

\[
\lambda_{p,t} = \left[ t_p \times \frac{V_s}{A_p} \times C_s \times \rho_s \times (1 + \phi / 3) \times \frac{1}{(T_{fi} - T_s) \times \Delta t} \right] \\
\times \left[ \Delta T_s + (e^{\phi / 10} - 1) \Delta T_{fl} \right]
\]  

(4.19)
where $\Delta t \leq 0.5$ minutes.

Note that in the above equation, the effect of the thermal boundary condition is neglected.

In this approach, the intumescent coating is considered to be only one layer. However, when calculating the steel temperature to be used in the above equation, the multi-layer model is used to obtain more accurate steel temperature results.

The following results will be used to examine how the effective thermal conductivity of the intumescent coating is influenced by changing the design conditions as follows:

Steel section factor: (A) 333 m$^{-1}$, (B) 200 m$^{-1}$, (C) 100 m$^{-1}$ and (D) 50 m$^{-1}$

Intumescent coating thickness: 0.4, 0.8, 1.2, 1.6 and 2.0 mm

Fire exposure condition: Fast, ISO, Slow fires as in Figure 4.4 and Smouldering fire as defined in EN 13381-8:2013 (CEN, 2013b):

During the period between $t = 0$ min and 20 min, the temperature – time relationship is:

$$T = 154\sqrt{t} + 20$$

(4.20)

After $t = 20$ min, the fire temperature-time relationship follows the standard fire curve, i.e:

$$T = 345\log_{10}[8(t - 20) + 1] + 20$$

(4.21)

**4.6.1 Effects of Fire Exposure**

Figures 4.11 to 4.13 show representative results of comparison for effective thermal conductivity–temperature relationships under the four fire conditions, for the maximum steel temperature (0.4 mm coating thickness with section factor 333 m$^{-1}$), intermediate steel temperature (1.2 mm coating thickness with section factor 100 m$^{-1}$) and minimum steel temperature (2 mm coating thickness with section factor 50 m$^{-1}$). Figure 4.14 - Figure 4.16 compare the calculated steel temperatures, using Equation (4.9) and the effective thermal conductivity – temperature relationship extracted under the standard fire condition for the three corresponding combinations of coating thickness and steel section factor.
The results in Figures 4.11 – 4.13 indicate that the results for Smouldering fire and for Standard fire are similar at high temperatures. This is reasonable because at high temperatures, the two fire curves are the same. The Fast fire thermal conductivity values are the highest because the expansion ratio decreases at a faster heating rate, as shown in Figure 4.1. For the same reason, the slow fire thermal conductivity results are lower than the Standard fire results.

Figure 4.1 also shows that except for very fast heating rates, the intumescent coating behaviour is similar for other heating rates. Since the results in Figures 4.11-4.13 differ only in the steel section factor and this difference only causes the heating rate to be different near the steel plate where the heating rate is low, these different figures show very similar patterns.

The calculated steel temperatures, shown in Figures 4.14 to 4.16, reflect the trends in thermal conductivity. Therefore, using the thermal conductivity extracted from the Standard fire underestimates the actual steel temperature for the fast fire case; while it slightly over-predicts steel temperatures for the Slow and Smouldering fire cases. The latter is acceptable because it is on the safe side. However, the former is unsafe and should not be used.

![Figure 4.11](image.png)

**Figure 4.11** Comparison of thermal conductivity-temperature relationships for maximum steel temperature case under different fire conditions (steel section factor: $333 \, \text{m}^{-1}$, coating thickness: 0.4 mm)
Figure 4.12 Comparison of thermal conductivity-temperature relationships for intermediate steel temperature case under different fire conditions (steel section factor: 100 m$^{-1}$, coating thickness: 1.2 mm)

Figure 4.13 Comparison of thermal conductivity-temperature relationships for minimum steel temperature case under different fire conditions (steel section factor: 50 m$^{-1}$, coating thickness: 2 mm)
Figure 4.14 Comparison of the steel temperatures calculated using extracted thermal conductivity under ISO fire and Equation (4.9) and the steel temperatures using multi-layer for the maximum steel temperature case (steel section factor: 333 m$^{-1}$, coating thickness: 0.4 mm)

Figure 4.15 Comparison of the steel temperatures calculated using extracted thermal conductivity under ISO fire and Equation (4.9) and the steel temperatures using multi-layer for the intermediate steel temperature case (steel section factor: 100 m$^{-1}$, coating thickness: 1.2 mm)
Figure 4.16 Comparison of the steel temperatures calculated using extracted thermal conductivity under ISO fire and Equation (4.9) and the steel temperatures using multi-layer for minimum steel temperature case (steel section factor: 50 m$^{-1}$, coating thickness: 2 mm)

4.6.2 Effects of Coating Thickness

To demonstrate the effects of intumescent coating thickness on the effective thermal conductivity–temperature relationship, representative comparisons are again used: for the minimum steel temperature (Slow fire, section factor = 50 m$^{-1}$), the intermediate steel temperature (ISO fire, section factor = 100 m$^{-1}$) and the maximum steel temperature (Fast fire, section factor = 333 m$^{-1}$). The comparisons are shown in Figure 4.17 - Figure 4.19. Also, Figure 4.20 - Figure 4.21 show corresponding comparisons of steel temperatures when calculated using Equation (4.9) and the thermal conductivity–temperature relationship extracted from the Standard fire condition.

The results in Figures 4.17 - 4.19 show that as the coating thickness increases, the effective thermal conductivity also increases. This may be explained as follows. The average coating temperature is used when plotting the results. At the same average coating temperature, the coating surface temperature for higher coating thickness would be higher than for lower coating thickness. In contrast, the steel temperature for the higher coating thickness would be lower than that for the thinner
coating. This is illustrated in Figure 4.22, which shows the temperature distributions in the coating thickness direction for different coating thicknesses which all have an average temperature of 500°C under the Standard fire condition. However, because the coating behaves similarly when the heating rate is low (Figure 4.1) while the high heating rate has more influence on the coating behaviour, the effective thermal conductivity for the higher coating thickness is higher than for the thinner coating. As in the previous section, using the thermal conductivity values extracted under the Standard fire underestimates the steel temperatures for Fast fire (see Figure 4.20) and over-predicts the steel temperatures for Slow fire (see Figure 4.21). Under-predicting the temperature leads to unsafe results. Whilst over-predication of the steel temperature is on the safe side, the results in Figure 4.21 shows that the over-predication can be quite high, which could lead to unduly conservative specification of fire protection.

![Comparison of effective thermal conductivity – temperature relationships for different coating thicknesses, minimum steel temperature rise (Slow fire, steel section factor: 50 m⁻¹)](image)

Figure 4.17 Comparison of effective thermal conductivity – temperature relationships for different coating thicknesses, minimum steel temperature rise (Slow fire, steel section factor: 50 m⁻¹)
Figure 4.18 Comparison of effective thermal conductivity – temperature relationships for different coating thicknesses, intermediate steel temperature rise (ISO fire, steel section factor: 100 m$^{-1}$)

Figure 4.19 Comparison of effective thermal conductivity – temperature relationships for different coating thicknesses, maximum steel temperature rise (Fast fire, steel section factor: 333 m$^{-1}$)
**Figure 4.20** Comparison of the steel temperatures calculated using extracted thermal conductivity under ISO fire and Equation (4.9) and the steel temperatures using multi-layer for the maximum steel temperature case (A04-12-20FAST)

**Figure 4.21** Comparison of the steel temperatures calculated using extracted thermal conductivity under ISO fire and Equation (4.9) and the steel temperatures using multi-layer for minimum steel temperature case (D04-12-20SLOW)
4.6.3 Effects of Steel Section Factor

To examine the effects of the steel section factor on the effective thermal conductivity–temperature relationship, the following representative comparisons are used: for the minimum steel temperature (Slow fire, intumescent coating thickness = 2.0 mm), the intermediate steel temperature (ISO fire, intumescent coating thickness = 1.2 mm) and the maximum steel temperature (Fast fire, intumescent coating thickness = 0.4 mm). The comparisons are shown in Figure 4.23 to Figure 4.25. Also, Figure 4.26 - Figure 4.27 show corresponding comparisons of steel temperatures when calculated using Equation (4.9) and the thermal conductivity–temperature relationship extracted from the standard fire condition.

Figures 4.22 to 4.24 show that increasing the steel section factor (in descending order from A to D) results in increasing effective thermal conductivity. Again, as for changing the coating thickness, this may be explained by considering the coating temperatures on the steel plate and on the surface. For thicker steel plates (low section factors), the steel temperatures are low, requiring the coating surface temperatures to be higher so that the average coating temperature is the same for
different steel section factors. For confirmation, Figure 4.28 shows the temperature distributions in the coating thickness direction for different steel section factors which all have an average coating temperature of 500°C under the Standard fire condition. Since the higher coating temperature rates (near the surface) are more influential on the coating expansion (see Figure 4.1) and coating effective thermal conductivity (see Figure 4.3), the effective thermal conductivity of the coating for a higher steel section factor is lower than for a lower steel section factor. Nevertheless, when only changing the steel thickness without changing other parameters (fire type, coating thickness), the coating on the fire side, where the heating rate is high, exhibits similar behaviour. The coating behaviour on the steel side, where the heating rate is lower, is different. However, because the coating behaviour does not vary so much when the heating rate is low, changing the steel thickness does not tend to have as much effect as changing the coating thickness. The exception is when the steel section factor is very low (case D, section factor = 50 m⁻¹).

![Figure 4.23](image)

**Figure 4.23** Comparison of thermal conductivity – temperature relationships for different steel section factors, minimum steel temperature case (intumescent coating thickness: 2 mm)
Figure 4.24 Comparison of thermal conductivity – temperature relationships for different steel section factors, intermediate steel temperature case (intumescent coating thickness: 1.2 mm)

Figure 4.25 Comparison of thermal conductivity – temperature relationships for different steel section factors, maximum steel temperature case (intumescent coating thickness: 0.4 mm)
Figure 4.26 Comparison of the steel temperatures calculated using extracted thermal conductivity under ISO fire and Equation (4.9) and the steel temperatures using multi-layer for maximum steel temperature case (A04-B04-C04FAST)

Figure 4.27 Comparison of the steel temperatures calculated using extracted thermal conductivity under ISO fire and Equation (4.9) and the steel temperatures using multi-layer for minimum steel temperature case (A20-B20-C20-D20SLOW)
4.7 Concluding Remarks

This chapter has presented a detailed assessment of intumescent coating behaviour (expansion ratio, apparent thermal conductivity, effective thermal conductivity) under different heating conditions (temperature, rate of temperature) and how the intumescent coating behaviour affects prediction of effective thermal conductivity and steel temperatures under different design conditions (changing fire condition, changing coating thickness and changing steel section factor). The main findings of this chapter are:

- The analytical model for the bubble growth described in Chapter 3 is able to predict accurately the expansion ratio of intumescent coatings and steel temperatures under different heating rates and fire conditions, when compared to the test results of Zhang et al. (2012a; 2012b).
- Increasing the heating rate of the intumescent coating decreases the effectiveness of intumescent fire protection: decreasing the expansion ratio and increasing the effective thermal conductivity.
- As the temperatures and rate of heating within the intumescent coating are

![Temperature distributions throughout the coating thickness for an average coating temperature of 500°C (A12-B12-C12-D12ISO)]
different, different layers of the intumescent coating have different thermal conductivities. When predicting the temperature of intumescent coating protected steel, using the multi-layer model gives more accurate results than using the single layer model. The single layer model is currently used in design codes such as EN 1993-1-2.

- The effective thermal conductivity of the coating extracted from the Standard fire tests may be used to predict steel temperatures for other heating conditions if the fire condition is less severe than the Standard fire condition because the prediction results are on the safe side.

- The effective thermal conductivity of the coating extracted from the Standard fire tests should not be used to predict steel temperatures for other heating conditions if the fire condition is more severe than the Standard fire condition.

The next chapter will present the Smoothed Particle Hydrodynamics (SPH) method with its theoretical and numerical features in detail.
CHAPTER 5 SPH METHOD FOR MODELLING BUBBLE FORMATION

5.1 Introduction

As introduced earlier in Chapter 1, one of the main aims of this project is to develop a detailed methodology to model the expansion process of intumescent coating incorporating the physical and chemical behaviour of the coating at the microscopic level. At a continuum level, the modelling of bubbles and their movement in the melted liquid intumescent coating obey the principles of conservation of mass, momentum and energy.

Many computational methods can be used to solve the conservation equations for problems in computational fluid dynamics (CFD), such as the finite difference method (FDM), finite volume method (FVM) and finite element method (FEM) (Anderson, 1995). However, these methods use a grid to solve the governing equations. Moreover, when simulating problems with large distortions, moving materials, free surfaces, etc., these grid-based methods can face difficulties. These problems often require large mesh distortion, particularly for problems with large nonlinear deformation. Even though Coupled Eulerian-Lagrangian (CEL) and Arbitrary Lagrange-Eulerian (ALE) methods have been developed by combining the Lagrangian and Eulerian methods and work well, they are complicated and may also cause inaccurate results in numerical treatments (Liu and Liu, 2003).

Meshless methods have recently seen significant development to simulate computational fluid dynamic problems. As mentioned in the literature review in Chapter 2, one of the most popular is the smoothed particle hydrodynamics (SPH) method, a Lagrangian method which is efficient for large deformation, moving interfaces and free surfaces. The SPH method can be applied to various systems from the micro-scale to the macro-scale.

This chapter starts with an introduction to the conservation equations needed to describe bubble growth, followed by a detailed overview of SPH methodology. Finally, this chapter is concluded by describing the SPHysics FORTRAN open-source code and its modifications used to model the bubble growth and the other test cases described in Chapter 6.
5.2 Model Description

5.2.1 Physical Processes to be modelled by SPH

Smoothed particle hydrodynamics (SPH) is a truly meshless method. It was first invented to solve astrophysical problems by Lucy (1977) and Gingold and Monaghan (1977), but has since found widespread applications in many areas of engineering. In this method, the system (i.e. problem) is represented by a set of particles which carry physical properties such as an individual mass, volume, density, position, velocity, temperature and other physical quantities. With the advantages of the Lagrangian nature of SPH, this method can be applied to a wide range of applications, for example, incompressible, free-surface and compressible flows with applications in fluid mechanics and moving interfaces, large deformations and distortions in both fluid and solid mechanics (Gomez-Gesteira et al., 2010a), (Monaghan, 2005), (Liu and Liu, 2010).

For the general expansion process of the gaseous products towards the surrounding liquid such as foam formation and therefore bubble production, SPH is an attractive method to simulate those physical processes, as free surfaces and moving interfaces are involved in those systems. Foam formation and bubble growth processes are of great importance in the chemical and process applications. For those applications, the physical foaming process is the result of the mixing of the gas-generating substance (e.g. blowing agent) with molten polymer at elevated pressure and temperature to generate the gas-polymer melt solution. These are exactly the same processes that intumescent coatings go through when expanding on heating. There are a number of physical parameters (mainly cell size, nucleation density, cell structure, etc.) which control and optimise the mechanical properties of the actual thermoplastic foam (Elshereef et al., 2010).

In this thesis, SPH will be employed to investigate the feasibility of modelling the bubble growth process of the well-known model of Patel (1980) which is described by coupled conservation of mass and momentum equations. The bubble growth rate is mainly a function of the polymer melt viscosity, the diffusivity of the gas from melted liquid to bubble, and therefore the pressure inside and outside of the bubble. Das and Das (2009)’s SPH bubble evolution model through a submerged orifice has a close resemblance with Patel (1980)’s model in terms of the pressure
difference being the main driving force for the bubble growth. This model will be further explored herein. In the next chapter, the SPH model will be applied to simulating the expansion process of intumescent coatings where the pressure difference that drives bubble growth, and hence intumescent coating expansion, comes from conversion of the intumescent coating melt to gas.

5.2.2 A Brief Description of the Physical Processes to be Modelled

In order to describe the bubble growth model, a single bubble surrounded by a liquid molten polymer is shown in Figure 5.1.

![Figure 5.1 Schematic representation of a single spherical bubble surrounded by molten polymer (Elshereef et al., 2010)](image)

For the single bubble shown, $R$ is the bubble radius and $r$ is the radial distance from the centre of the bubble to the point of interest. The pressure at a distance in the molten polymer is considered to be ambient pressure ($P_a$) and is lower than the gas pressure inside the bubble ($P_g$). Therefore, bubble growth begins at $t = 0$ where the gas pressure reduces to the ambient pressure. However, the bubble keeps growing by consuming gas from the surrounding liquid. Thus, the concentration of the dissolved gas in the polymer melts changes (increases) with respect to time as shown in Figure 5.1. This physical phenomenon of bubble growth in Newtonian fluids is based on the simultaneous mass and momentum transfer.

Modelling the bubble growth model in a pool of polymer melt obeys the governing equations which include the continuity equation (conservation of mass)
and conservation of momentum equation. For intumescent coatings, the dissolved gas in the surrounded liquid melt comes from the chemical reactions when the intumescent coating experiences heating. This dissolved gas supply is limited and changes with respect to time and radial position as shown in Figure 5.2. The concentration of the gas results in pressure increase inside the bubble.

In this thesis, we will make some assumptions to enable the feasibility of using SPH to be investigated.

![Diagram](image)

**Figure 5.2** The dissolved gas concentration gradient with respect to time and radius of the bubble

### 5.2.3 Model Assumptions

Patel (1980) developed a bubble growth model in a viscous fluid by considering the diffusion from the polymer liquid to the gas phase. The assumptions in that model were:

- The system is isothermal and a thermodynamic equilibrium exists continuously between the gas pressure inside the bubble and polymer-gas solution at the interface.

- All physical properties of the liquid and gas are constant. This assumption is also applicable for SPH bubble growth modelling except that the density changes according to the conservation of mass.
• The normal stresses at the interface are the surface tension and viscosity, neglecting the inertial terms.

• As mentioned earlier in Section 5.2.2, the rate of the bubble’s growth is related to the pressure increase inside the bubble, whereas ambient pressure $P_a$ is assumed to be constant,

$$\frac{dR}{dt} = R \left( \frac{P_g - P_a - 2\sigma_s/R}{\eta_o} \right) - 3P_g \left( \frac{\dot{R}}{R} \right)$$  \hspace{1cm} (5.1)

It is assumed that the initial bubble radius should be greater than the critical bubble radius, which comes from the Young-Laplace equation,

$$R_{cr} = \frac{2\sigma_s}{P_g - P_a}$$  \hspace{1cm} (5.2)

• The density of the gas inside the bubble $\rho_g$ is calculated according to the Ideal Gas law.

$$\rho_g = \frac{P_g M}{R_g T}$$  \hspace{1cm} (5.3)

The assumptions above are applied to the SPH bubble growth modelling. Instead of calculating the pressure increase inside the bubble, a higher pressure is assigned to the gas phase. The details of the test cases will be given in the next chapter.

### 5.3 SPH Methodology

#### 5.3.1 SPH Integral Interpolant

The formulation of the SPH method is composed of two main steps. The first is the integral representation (kernel approximation) of field functions and the second is the particle approximation.

The discrete or particle representation of an arbitrary function is approximated by summing up the function values of the nearest neighbour particles in the interpolation region. However, first the interpolation procedure for SPH starts from the integral interpolation for the value of a function $f(\mathbf{x})$, given by:
\[ f(x) = \int_{\Omega} \delta(x - x') f(x') \, dx' \]  

(5.4)

where \( f(x) \) is the function of a three-dimensional position vector \( x \), \( \Omega \) is the volume of the integral that depends on \( x \) and \( \delta(x - x') \) is the Dirac delta function given by:

\[
\delta(x - x') = \begin{cases} 
1 & x = x' \\
0 & x \neq x' 
\end{cases}
\]  

(5.5)

Any function can be represented in an integral form as shown in Equation (5.4). From the point of computational procedure, the delta function cannot be used since it is infinitesimally narrow and small. For the later discretisation process, the interpolation region, \( \Omega \), of \( \delta(x - x') \) will not overlap other particles. Therefore, the delta function is replaced by a weighting function, called the smoothing kernel function \( W(x - x', h) \), where \( h \) is a characteristic length called the smoothing length and \( W \) has a radius of influence around \( x \) defining a compact support (described below).

By replacing the \( \delta \) function with a smooth weighting function \( W \) (referred to herein as the smoothing kernel), Equation (5.4) becomes an integral approximation written as:

\[
\langle f(x) \rangle = \int_{\Omega} W(x - x', h) f(x') \, dx'
\]  

(5.6)

where \( \langle \ldots \rangle \) denotes the approximation and \( dx' \) is the infinitesimal volume of the particle \( j \). The integral representation of Equation (5.6) is an approximation when \( W \) is not a Dirac delta function.

The smoothing kernel, \( W(x - x', h) \), is a function of the interpolation distance, \( x - x' \), and the smoothing length, \( h \). The smoothing length defines the extent of the kernel with the radius of each kernel \( r \) often set to be twice the smoothing length as shown in Figure 5.3. The particles outside the radius of influence have no effect on the influence domain. The region inside the radius of
influence is called the compact support of the kernel.

![Figure 5.3 Kernel and its support domain](image)

As mentioned in the definition of the smoothing length, the influence area is a domain where a particle at $\mathbf{x}$ interacts with another particle at point $\mathbf{x}'$, whereas the support domain is a domain where the information for all the points inside this domain is used to estimate all properties at the point $\mathbf{x}$ (Liu and Liu, 2003). Hence, the influence domain is related to a node in the mesh-free methods (as opposed to the meshless methods such as SPH), and the support domain is about any field point $\mathbf{x}$ that can be, but is not necessarily a node.

Different weighting or smoothing functions, $W$, have been proposed for the SPH method (Monaghan, 2005). Smoothing kernels must obey key requirements with specific properties. The main properties are summarised below (Monaghan, 1992).

1. Since the integral of the delta function on its own is 1, $W$ should be normalised over its support domain such that

   $$\int_{\Omega} W(\mathbf{x} - \mathbf{x}', h) \, d\mathbf{x}' = 1 \quad (5.7)$$

2. $W$ should have compact support (Monaghan, 1992), i.e.,

   $$W(\mathbf{x} - \mathbf{x}') = 0 \quad \text{for} \quad |\mathbf{x} - \mathbf{x}'| > \kappa h \quad (5.8)$$

   where $\kappa$ is a free parameter to define the extent of the kernel, (e.g. in Figure 5.3, $\kappa = 2$).

3. $W(\mathbf{x} - \mathbf{x}') \geq 0$ for any neighbour particle at point $\mathbf{x}'$ within the support domain of the particle at point $\mathbf{x}$.

4. The value of the smoothing kernel function should decrease with an increase
in distance away from the particle. This means that the closest particle has a greater effect on the particle under consideration.

5. The smoothing function should satisfy the Dirac delta function condition when the smoothing length approaches zero.

\[ \lim_{h \to 0} W(x - x', h) \to \delta(x - x') \quad (5.9) \]

6. The smoothing kernel should be symmetric (i.e. an even function), such that two particles have an identical kernel value to the other particle.

7. \( W \) should be sufficiently smooth to obtain accurate results and it should also be sufficiently continuous (Quinlan et al., 2006).

Any function having the above properties can be considered as SPH smoothing function.

The following are some of the most commonly used smoothing kernels: Cubic Spline Kernel, Quadratic Kernel and Wendland Kernel. These are considered as the smoothing functions in the developed models and are also available in the SPHysics code.

**Cubic Spline Kernel:**

This is a third-order approximation to a Gaussian kernel:

\[
W(r, h) = \alpha_d \begin{cases} 
1 - \frac{3}{2}q^2 + \frac{3}{4}q^3 & 0 \leq q \leq 1 \\
\frac{1}{4}(2 - q)^3 & 1 \leq q \leq 2 \\
0 & q \geq 2 
\end{cases} \quad (5.10)
\]

where \( q = \frac{r_{ij}}{h} = \frac{r_i - r_j}{h} \geq 0 \) and \( r_{ij} \) is the distance between the particles. \( \alpha_d \) is the normalisation factor for the kernel to ensure the integral of the kernel itself reproduces the unity obeying Equation (5.7), which is defined as \( 1/h, 10/(7\pi h^2) \) and \( 1/(\pi h^3) \) for the Cubic Spline kernel in one-, two- and three-dimensional space respectively.
Quadratic Kernel:

This is a second-order computationally less expensive kernel:

\[
W(r, h) = \alpha_d \begin{cases} 
\frac{3}{16} q^2 - \frac{3}{4} q + \frac{3}{4} & 0 \leq q \leq 2 \\
0 & q \geq 2
\end{cases}
\]  

(5.11)

where \(\alpha_d\) is equal to \(2/(\pi h^2)\) for 2D and \(5/(4\pi h^3)\) for 3D.

Wendland Kernel:

This is a fifth-order kernel that is relatively cheap to compute:

\[
W(r, h) = \alpha_d \begin{cases} 
\left(1 - \frac{q}{2}\right)^4 (2q + 1) & 0 \leq q \leq 2 \\
0 & q \geq 2
\end{cases}
\]  

(5.12)

where \(\alpha_d\) is equal to \(7/(4\pi h^2)\) for 2D and \(7/(8\pi h^3)\) for 3D.

Their functions and their derivatives have been plotted in Figure 5.4, Figure 5.5 and Figure 5.6 based on their functions, taken from Liu and Liu (2003).

Figure 5.4 The Cubic Spline Kernel and its first derivative
The choice of kernel tends to have a limited effect on most problems, but there is still uncertainty as to the best kernel to choose (Robinson, 2009). Herein, we choose the cubic spline, as this has been shown to be robust for a variety of applications (Liu and Liu, 2003).

Figure 5.5 The Quadratic Kernel and its first derivative
5.3.2 SPH Summation Approximation

In the SPH method, the system is presented by a finite number of particles which carry individual mass and have individual space. The particle approximation procedure is defined in this section.

If the infinitesimal volume $d\mathbf{x}'$ which has been defined in the integral representation (in Section 5.3.1) is replaced by the finite volume of the particle $\Delta V_j$, the mass of the $j^{th}$ particle is,

$$m_j = \Delta V_j \rho_j$$  \hspace{1cm} (5.13)

where $\rho_j$ is the density of particle $j$ ($j = 1, 2, 3, \ldots, N$) and $N$ is the number of particles within the support domain. The continuous SPH integral representation for $f(x)$ is written in the form of particle approximation, i.e.:

$$\langle f(\mathbf{x}) \rangle = \int_{\Omega} f(\mathbf{x}') W(\mathbf{x} - \mathbf{x}', h) d\mathbf{x}'$$  \hspace{1cm} (5.14)
becomes in discrete form,

\[
\langle f(\mathbf{x}) \rangle = \sum_{j=1}^{N} f(\mathbf{x}_j) W(\mathbf{x} - \mathbf{x}_j, h) \Delta V_j
\]  

(5.15)

Using Equation (5.13), this can be rewritten as:

\[
\langle f(\mathbf{x}_i) \rangle = \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(\mathbf{x}_j) W(\mathbf{x} - \mathbf{x}_j, h)
\]  

(5.16)

By writing \( W_{ij} = W(\mathbf{x}_i - \mathbf{x}_j, h) \) and \( f_j = f(\mathbf{x}_j) \), the particle approximation for a function at the location of particle \( i \) is written as:

\[
\langle f(\mathbf{x}_i) \rangle = \sum_{j=1}^{N} \frac{m_j}{\rho_j} f_j W_{ij}
\]  

(5.17)

Equation (5.17) shows that the interpolation of the function \( f \) at particle \( i \) is approximated using all particles in the support domain of particle \( i \), which is weighted by the smoothing kernel \( W \) given by the equations in Section 5.3.1.

Similarly, the derivative of the function can be expressed as,

\[
\langle \nabla f(\mathbf{x}_i) \rangle = \sum_{j=1}^{N} \frac{m_j}{\rho_j} f_j \nabla_i W_{ij}
\]  

(5.18)

where \( \nabla_i W_{ij} \) is

\[
\nabla_i W_{ij} = \frac{\mathbf{x}_i - \mathbf{x}_j}{r_{ij}} \frac{\partial W_{ij}}{\partial r_{ij}}
\]  

(5.19)

It is clear from Equations (5.17) and (5.18) that the continuous integral representations of a function can be converted to the discretised summations based on the particles with a random spatial distribution. For a constant field, for example \( f = \text{constant} \), the gradient should be zero, but Equation (5.18) rarely gives zero. Hence, Equation (5.18) is replaced by:
\[
\langle \nabla f(x_i) \rangle = \sum_{j=1}^{N} \frac{m_j}{\rho_j} (f_j - f_i) \nabla_i W_{ij}
\] (5.20)

This will be revisited in Section 5.3.3.4.

5.3.3 Governing Equations in Lagrangian form

Two fundamental physical principles, namely conservation of mass and momentum, are employed to describe the fluid flows in this thesis. There are two approaches to describe the physical governing equations: Eulerian description and Lagrangian description. The Lagrangian description represents the total rate of change as a point moves through space, and therefore uses the total time derivative as the combination of local and convective derivatives. The Eulerian description represents the rate of flow quantities at a fixed point in space. In this section, the derivation of the basic governing equations of a fluid in motion will be briefly described in Lagrangian form by considering an infinitesimal fluid control volume, \( \delta V \).

The control volume can move with the fluid flow in the Lagrangian description, provided that the material type remains the same inside the control volume. Therefore, the Lagrangian control volume may have expansion, compression and even deformation and the mass of the fluid contained in the infinitesimal fluid element will be conserved.

5.3.3.1 Conservation of Mass (The Continuity Equation)

The conservation of mass relates the change of mass inside a control volume to the net flow of mass out of the control volume. Its volume and shape will change from one point to another point as it moves. For a Lagrangian specification of a flow field, the mass contained in the control volume is:

\[
\delta m = \rho \delta V
\] (5.21)

where \( \rho \) is the fluid density.

Mass is conserved, therefore the total time rate of change of the mass (substantial derivative of the mass) will be zero,
\[ \frac{D(\delta m)}{Dt} = 0 \quad (5.22) \]

where the operator \( \frac{D}{Dt} \) represents the total rate of change and is the sum of the Eulerian rate of change \( \frac{\partial}{\partial t} \) and the nonlinear advective acceleration \( \mathbf{v} \cdot \nabla \).

By substituting Equation (5.21) into (5.22), the mass conservation equation becomes:

\[ \frac{D(\rho \cdot \delta V)}{Dt} = \delta V \frac{D\rho}{Dt} + \rho \frac{D(\delta V)}{Dt} = 0 \quad (5.23) \]

\[ \frac{D\rho}{Dt} + \rho \left[ \frac{1}{\delta V} \frac{D(\delta V)}{Dt} \right] = 0 \quad (5.24) \]

The term in the brackets is related to the divergence theorem. In other words, the net flow of out of region for a vector is equal to the volumetric integral of the divergence. Equation (5.24) can be written:

\[ \frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0 \quad (5.25) \]

Due to consideration of the infinitesimally small fluid element, the equation is obtained in partial differential equation form. The final version of the continuity equation is often written with the divergence term on the right hand side as:

\[ \frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v} \quad (5.26) \]

### 5.3.3.2 Conservation of Momentum

Newton’s second law states that the net force on an object is proportional to the rate of change of momentum. Two types of forces considered are body forces and surface forces.

Body forces can be the gravitational forces which have an effect on the volumetric mass of the fluid element (e.g. gravitational, electric, etc.). On the other hand, surface forces can originate either from pressure distribution or from the shear and normal stress distribution. The pressure on the surface is due to the outside fluid surrounding the fluid element. The shear and normal stress result in deformation of
the fluid elements.

The time rate of change of deformation is mainly due to the shear and normal stresses. In addition, the deformation results in the time rate of change of volume of the fluid element.

Writing the total accelerations of a fluid cell in three Cartesian coordinate directions as \( \frac{Dv_x}{Dt} \), \( \frac{Dv_y}{Dt} \) and \( \frac{Dv_z}{Dt} \), the derivation of the momentum equation in the \( x \)-direction will be presented below.

Applying Newton’s second law in the \( x \)-direction to an elemental volume of mass \( \delta m \) gives:

\[
\delta m \frac{Dv_x}{Dt} = \rho dx dy dz \frac{Dv_x}{Dt} = -\frac{\partial p}{\partial x} dx dy dz + \left( \frac{\partial \tau_{xx}}{\partial x} dx dy dz + \frac{\partial \tau_{yx}}{\partial y} dx dy dz + \frac{\partial \tau_{zx}}{\partial z} dx dy dz \right) + \delta m g_x
\]

(5.27)

where \( p \) is pressure, \( m \) is mass, \( \tau_{xx}, \tau_{yx} \) and \( \tau_{zx} \) are shear stresses acting on the surface, \( dx dy dz \) is equal to the volume of the fluid and \( g_x \) is the gravitational force.

Dividing through by the mass \( \delta m = \rho dx dy dz \), the momentum equation in the \( x \)-direction is:

\[
\frac{Dv_x}{Dt} = -\frac{1}{\rho} \left[ \frac{\partial p}{\partial x} - \left( \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \right) \right] + g_x
\]

(5.28)

Similarly for the \( y \)- and \( z \)-directions, the full momentum equation can be written as:

\[
\frac{Dv}{Dt} = -\frac{1}{\rho} \left[ \nabla p - \nabla \cdot \mathbf{\tau} \right] + \mathbf{g}
\]

(5.29)

where \( \mathbf{\tau} \) is the shear stress tensor and \( \mathbf{g} \) is gravitational force vector.

### 5.3.3.3 SPH Continuity Equation (Density summation approach)

The use of particle summation for the approximation of the integral enables the creation of a simple interpolation method without using any mesh. One approach to estimate the density is to use the SPH interpolation process itself. Using \( f(x) = \rho \) in
Equation (5.17) gives:

$$\rho_i = \sum_{j=1}^{N} m_j W_{ij}$$  \hspace{1cm} (5.30)

However, this approach is rarely used since an incomplete support leads to a low estimate for $\rho(x)$ without kernel correction, which is often unstable and therefore not used.

### 5.3.3.4 SPH Continuity Equation (Continuity density approach)

An alternative approach to estimating the change in density is to use the SPH technique applied to the equation for conservation of mass.

Equation (5.26) is the continuity equation in Lagrangian form. SPH formulations for partial differential equations (PDEs) can be derived from the equations that are in conservation form where the formulation uses a differentiable interpolation function with its values at the particles (Monaghan, 1992).

To ensure zero divergence of a constant velocity field, the interpolant is found by using a prior manipulation of the gradient.

$$\rho \nabla f(x_i) = \nabla (\rho f(x_i)) - f(x_i) \nabla \rho$$  \hspace{1cm} (5.31)

By using Equation (5.31) for velocities in Equation (5.26), the discretised form of the continuity equation is:

$$\frac{D \rho_i}{Dt} = \mathbf{v}_i \cdot \sum_{j=1}^{N} m_j \nabla_i W_{ij} - \sum_{j=1}^{N} m_j \mathbf{v}_j \cdot \nabla_i W_{ij}$$  \hspace{1cm} (5.32)

or simply:

$$\frac{D \rho_i}{Dt} = \sum_{j=1}^{N} m_j (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij}$$  \hspace{1cm} (5.33)

Another form of density approximation equation is obtained by using Equation (5.20) (Colagrossi and Landrini, 2003):
\[
\frac{D\rho_i}{Dt} = \rho_i \sum_{j=1}^{N} \frac{m_j}{\rho_j} (v_i - v_j) \cdot \nabla_i W_{ij}
\]  
(5.34)

Both formulations are used to evaluate the density change of a particle. However, Equations (5.33) and (5.34) use the velocity difference for the derivative and this is usually preferred in the SPH formulations, because it gives zero error for constant velocity fields. Equation (5.34) is used throughout the SPH modelling in the next chapter because it has been shown by Colagrossi and Landrini (2003) to give better behaviour for multi-phase flows.

5.3.3.5 SPH Momentum Equation (Particle approximation of momentum)

The SPH formulation method for the momentum approximation is similar to the continuity density approach. It also involves some different transformations which lead to different forms of momentum approximation equations. If we write the conservation of momentum equation as \( \frac{Dv_i}{Dt} = \frac{1}{\rho} \nabla \cdot \sigma \), then apply the SPH particle approximation to the stress divergence part of the momentum equation, we get:

\[
\frac{Dv_i}{Dt} = \frac{1}{\rho_i} \sum_{j=1}^{N} m_j \frac{\sigma_i}{\rho_j} \nabla_i W_{ij}
\]  
(5.35)

However, this form does not conserve momentum (Monaghan, 2005).

Given that \( \sum_{j=1}^{N} \frac{m_j}{\rho_j} \nabla_i W_{ij} \approx 0 \), if we add the following equation

\[
\sum_{j=1}^{N} m_j \frac{\sigma_i}{\rho_i \rho_j} \nabla_i W_{ij} = \frac{\sigma_i}{\rho_i} \left( \sum_{j=1}^{N} \frac{m_j}{\rho_j} \nabla_i W_{ij} \right)
\]  
(5.36)

into Equation (5.35), we arrive at:

\[
\frac{Dv_i}{Dt} = \sum_{j=1}^{N} m_j \frac{\sigma_i + \sigma_j}{\rho_i \rho_j} \nabla_i W_{ij}
\]  
(5.37)

This form guarantees momentum conservation (Monaghan, 1992).

If the stress term (\( \sigma \)) is now rewritten in terms of the pressure, \( P \), and shear stress, \( \tau \),
\[ \sigma = -P\delta + \tau \]  \hspace{1cm} (5.38)

Equation (5.37) becomes:

\[
\frac{D\mathbf{v}_i}{Dt} = - \sum_{j=1}^{N} m_j \left( \frac{P_i + P_j}{\rho_i \rho_j} - \frac{\tau_i + \tau_j}{\rho_i \rho_j} \right) \nabla_i W_{ij} \]  \hspace{1cm} (5.39)

In many SPH formulations such as those used here, the shear stress terms are represented by an alternative form \( \Pi_{ij} \) described below and in Section 5.3.4.3.

A different approximation can be derived to form a slightly different momentum equation:

\[
\frac{D\mathbf{v}_i}{Dt} = \sum_{j=1}^{N} m_j \left( \frac{\sigma_i}{\rho_i} + \frac{\sigma_j}{\rho_j} \right) \nabla_i W_{ij} \]  \hspace{1cm} (5.40)

which using Equation (5.38) can be written in pressure form as:

\[
\frac{D\mathbf{v}_i}{Dt} = - \sum_{j=1}^{N} m_j \left( \frac{P_i}{\rho_i} + \frac{P_j}{\rho_j} + \Pi_{ij} \right) \nabla_i W_{ij} \]  \hspace{1cm} (5.41)

However, Colagrossi and Landrini (2003) showed that this produces inferior behaviour for multi-phase flows compared to Equation (5.39).

In summary, the equations for conservation of mass and momentum being solved are:

\[
\frac{D\rho_i}{Dt} = \sum_{j=1}^{N} m_j \mathbf{v}_{ij} \cdot \nabla_i W_{ij} \]  \hspace{1cm} (5.42)

\[
\frac{D\mathbf{v}_i}{Dt} = - \sum_{j=1}^{N} m_j \left( \frac{P_i + P_j}{\rho_i \rho_j} + \Pi_{ij} \right) \nabla_i W_{ij} + \mathbf{g} \]  \hspace{1cm} (5.43)

\( \mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j \), which is the relative velocity of particles \( i \) and \( j \).

In the following section, surface tension effects will be included in the momentum equation.
5.3.4 Closure Submodels

5.3.4.1 Equations of State

The SPH formulation represented by Equations (5.42) and (5.43) is known as the weakly compressible SPH (WCSPH) formulation. In WCSPH, very small compressibility effects ($< 1\%$) are permitted such that the fluid pressure for each particle is calculated using an equation of state as in (Monaghan, 1994). This equation of state, often referred to as Tait’s, used in the present work has the form:

$$P = B \left[ \left( \frac{\rho}{\rho_o} \right)^\gamma - 1 \right] + X$$

where

$$B = \frac{\rho_o c_s^2}{\gamma}$$

$\rho_o$ and $c_s$ are the reference density and speed of sound respectively, $X$ is background pressure and $\gamma$ is a polytropic index of value $\gamma = 7$ to approximate incompressible fluids. However, this results in pressure being significantly sensitive to density variation. The pressure will go to zero for free surface flows if the reference density is equal to the density. By choosing the speed of sound, compressibility effects which are in the order of the Mach number squared, can be kept to less than 1%, which is acceptable for engineering applications. The equation of state takes the form given in Equation (5.44), with $\gamma = 1.4$ for the gas (air) phase of multi-phase simulations (Colagrossi and Landrini, 2003). Therefore, Equation (5.44) has been applied to the air and water phases separately, with different $\gamma$ values explained above.

Another equation of state has been developed by Morris et al. (1997) for quasi-incompressible SPH flows. The use of $\gamma = 1$ may remove the boundary effects at a free surface, so it can cause numerical instabilities. The Morris equation of state is:

$$P = c_s^2 (\rho - \rho_o)$$

Tait’s equation of state for multi-phase flows is used in SPHysics simulations (test cases) shown in detail in Chapter 6.
5.3.4.2 Density (Shepard) Filter

In weakly compressible SPH used in this thesis, it is common to use a Shepard or density filter to maintain a noise-free pressure field especially when using Tait’s equation of state (Equation (5.44)) due to the polytropic index (Gomez-Gesteira et al., 2012b). The Shepard density filter is a zeroth-order kernel correction as:

\[
\tilde{W}_{ij} = \frac{W_{ij}}{\sum_j m_j \rho_j W_{ij}} \tag{5.47}
\]

The corrected density \(\rho_i^{\text{new}}\) is recomputed using the corrected kernel by:

\[
\rho_i^{\text{new}} = \sum_{j=1}^{N} \rho_j \tilde{W}_{ij} \tag{5.48}
\]

The Shepard density filter is usually applied every 10-20 time steps.

5.3.4.3 Viscous Effects

The most commonly used representation of viscous effects in SPH is to use artificial viscosity by Monaghan (1992) which is applied to allow viscosity to be variable and makes sure that stress due to viscosity is continuous across the material interfaces. The artificial viscosity formulation, \(\Pi_{ij}\), is added to the momentum equation as:

\[
\frac{D\mathbf{v}_i}{Dt} = -\sum_{j=1}^{N} m_j \left( \frac{p_i + p_j}{\rho_i \rho_j} + \Pi_{ij} \right) \nabla_i W_{ij} + g \tag{5.49}
\]

The artificial viscosity formulation considered in this study is:

\[
\Pi_{ij} = \begin{cases} 
-\alpha \tilde{c}_{ij} \mu_{ij} + \beta \mu_{ij}^2 & \mathbf{v}_{ij} \cdot \mathbf{r}_{ij} \leq 0 \\
0 & \mathbf{v}_{ij} \cdot \mathbf{r}_{ij} > 0 
\end{cases} \tag{5.50}
\]

where \(\alpha\) and \(\beta\) are constants depending on the test case and \(\beta\) is usually set to 0, \(\tilde{c}_{ij}\) and \(\tilde{\rho}_{ij}\) are the average value of speed of sound and density respectively, with \(\mu_{ij}\) is given by:
\[
\begin{align*}
\mu_{ij} &= \frac{h v_{ij} \cdot r_{ij}}{r_{ij}^2 + \eta^2} \\
\bar{c}_{ij} &= \frac{c_i + c_j}{2} \\
\bar{\rho}_{ij} &= \frac{\rho_i + \rho_j}{2}
\end{align*}
\]

where \( \eta \) is the constant and is equal to 0.01 \( h \).

In order to keep the multi-phase problem (e.g. bubble growth model) stable and reduce the effects of pressure fluctuations and the artificial viscosity, Equation (5.50) is applied separately to different phases with a viscosity ratio. The use of very different viscosities in Equation (5.51) allows the viscosity \( (\Pi_{ij}) \) to be variable and also ensures that shear stress due to the viscosity effect is continuous across the phase interface. For two particles of different phases (i.e. \( i \) and \( j \) particles), \( \alpha \) has been considered as the average value of \( \alpha_i \) and \( \alpha_j \) as:

\[
\bar{\alpha}_{ij} = \frac{1}{2} (\alpha_i + \alpha_j) \tag{5.54}
\]

**Laminar viscosity:**

For low Reynolds number flows, formulations for Laminar viscosity have proven robust and accurate. The simplified laminar viscosity formulation introduced by Morris et al. (1997) is given as:

\[
(v \nabla^2 v)_i = \sum_j m_j \left( \frac{2 v_{ij} r_{ij} \cdot v_{ij}}{\bar{\rho}_{ij} \left( |r_{ij}|^2 + \eta^2 \right)} \right) \nabla_i W_{ij} \tag{5.55}
\]

where \( v_o \) is the kinematic viscosity of laminar flow. Equation (5.55) is added to momentum equation (Equation (5.43)) such that

\[
\Pi_{ij} = -\frac{2 v_{ij} r_{ij}}{\bar{\rho}_{ij} \left( |r_{ij}|^2 + \eta^2 \right)} \tag{5.56}
\]

where \( v_{ij} \) is given as:
\[ v_{ij} = \frac{v_i \times v_j}{v_i + v_j} \]  

(5.57)

The choice of using artificial or laminar viscosity is explained in Chapter 6.

### 5.3.4.4 Surface Tension

Surface tension can be explained as the resistance force of the fluid against extension of a free surface. In order to model the surface tension force, the continuum surface force (CSF) is applied in the momentum equation of the particles based on the flow geometry (Brackbill et al., 1992). In the CSF model, surface tension is transformed into a force per unit volume, \( F_s \) with the following equation:

\[ F_s = f_s \delta_s \]  

(5.58)

where \( \delta_s = |n| \), a normalised function (the surface delta function) and \( f_s \) is the force per unit area given by:

\[ f_s = \sigma_s \kappa \hat{n} + \nabla_s \sigma_s \]  

(5.59)

where \( \sigma_s \) is the surface tension coefficient, \( \hat{n} \) is the unit normal to the interface, \( \kappa \) is the curvature of the interface (\( \kappa = -\nabla \cdot \hat{n} \)), \( \nabla_s \) is the surface gradient (it will be neglected as surface tension is assumed to be constant throughout the fluid).

Figure 5.7 shows the sketch of continuum surface force acting at the interface of an air bubble. Contour colourings separate the different fluids with colour function values of \( C_i^1 \) and \( C_i^2 \) given in Equation (5.61). The transition region represents the interface between fluid and air particles. Fluid 1 in this model is air and fluid 2 is the water or polymer’s melt for bubble modelling of intumescent coating. \( \hat{n} \) represents normals given below in Equation (5.60). \( P_1 \) and \( P_2 \) are pressures of the different phases.
To determine the surface normal $\mathbf{n}$, we use a scalar colour function ($C$) such that its gradient determines the $\mathbf{n}$ in Equation (5.59) as follows:

$$\mathbf{n} = \frac{\nabla C}{|\nabla C|}$$  \hspace{1cm} (5.60)

where $C$ is defined as colour function.

In order to evaluate the derivatives, each different phase is assigned to a colour function defined as,

$$C_i^s = \begin{cases} 1 & \text{if particle belongs to phase } s \\ 0 & \text{otherwise} \end{cases} \hspace{1cm} (5.61)$$

Hu and Adams (2006) developed an approach to avoid the problem of particles far from the interface influencing the surface tension calculation by adopting the suggestion of Wu et al. (1998), who expressed the shear stress contributions directly in terms of the colour function gradients to calculate the surface tension.
\[
\frac{Dv_i}{Dt} = -\sigma_s (\nabla \cdot \hat{n}) \hat{n} = \frac{1}{\rho} \nabla \Phi^{st} = \sum_j m_j \left( \frac{\Phi_i}{\rho_i^2} + \frac{\Phi_j}{\rho_j^2} \right) \nabla_i W_{ij} \tag{5.62}
\]

where the CSF force is given in a tensor form, which is \( \Phi = \sigma_s (I - \hat{n}\hat{n}) |\nabla C| \). This tensor is given as (Wu et al., 1998):

\[
\Phi = \frac{\sigma_s}{|\nabla C|} \left( \frac{1}{d} |I| |\nabla C|^2 - \nabla C \nabla C \right) \tag{5.63}
\]

where \( \nabla C \nabla C = \frac{\partial c}{\partial x_\alpha} \frac{\partial c}{\partial x_\beta} \), \( d \) is the spatial dimension, \( I \) is the unit vector and \( \alpha \) and \( \beta \) are the Einstein notations.

To be consistent with the pressure gradient term in the momentum equation (5.43), another form of the Equation (5.62) will be used in the developed models shown in the following chapter. This equation is:

\[
\frac{Dv_i}{Dt} = \sum_j m_j \left( \frac{\Phi_i}{\rho_i} + \frac{\Phi_j}{\rho_j} \right) \frac{\partial W_{ij}}{\partial x_i} \tag{5.64}
\]

Including viscous effects and surface tension, the full momentum equation can therefore be written as:

\[
\frac{Dv_i}{Dt} = -\sum_{j=1}^{N} m_j \left( \frac{P_i + P_j}{\rho_i \rho_j} + \Pi_{ij} \right) \nabla_i W_{ij} + \sum_{j=1}^{N} m_j \left( \frac{\Phi_i + \Phi_j}{\rho_i \rho_j} \right) \nabla_i W_{ij} + g \tag{5.65}
\]

5.3.4.5 Particle Shifting

In SPH simulations, the particle spatial arrangement can sometimes create situations where the particles are too close or too far from each other, leading to numerical instability. A variation of the particle shifting algorithm originally proposed by Xu et al. (2009) for ISPH will be used to solve the stability and accuracy problems such as clumping due to irregular particle distributions.
Shifting based on particle concentration gradients

The initial shifting algorithm of Xu et al. (2009) has some significant problems such as noise in the pressure field inside the air bubble and also at the interface of the multi-phase, leading to stability problems in the simulation. Therefore, a treatment is necessary, especially for the air-water interface. A modified algorithm was proposed by Lind et al. (2012) to change the shifting magnitude and direction according to Fick’s law in order to obtain stable and accurate solutions for both internal and free-surface flows. This will help the particles to be shifted by preventing highly anisotropic distributions. This behaviour is expected for the air particles. Hence, shifting distance can be calculated as:

\[ \delta \mathbf{r}_i = -D \nabla C_i \]  
(5.66)

where \( \delta \mathbf{r}_i \) denotes the shifting distance, \( D \) is a diffusion coefficient which controls the shifting magnitude and \( C \) is the particle concentration. The approach proposed by Skillen et al. (2013) to calculate the diffusion coefficient has been used as:

\[ D = -A_s h \| \mathbf{u} \|_i \Delta t \]  
(5.67)

where \( A_s \) is a parameter taking a value from 1 to 6 and \( \| \mathbf{u} \|_i \) is the velocity magnitude of the particle \( i \). The value of \( A_s \) is the minimum possible value to present effective shifting. The recommended value of 2 has been used.

The particle concentration value can be calculated from the sum of the smoothing kernel function as:

\[ C_i = \sum_{j=1}^{N} \frac{m_j}{\rho_j} W_{ij} \]  
(5.68)

The concentration gradient can be found as in (Mokos, 2013):

\[ \nabla C_i = \sum_{j=1}^{N} (C_j - C_i) \frac{m_j}{\rho_j} \nabla W_{ij} \]  
(5.69)

As shown by Lind et al. (2012) and Mokos et al. (2013), a better particle distribution has been obtained when this shifting method is introduced.
Since the present study (air bubble modelling) uses dynamic boundary particles (Crespo et al., 2007) in the nature of SPHysics FORTRAN code (Gomez-Gesteira et al., 2010b), the boundary particles should be used to calculate the concentration and concentration gradient of the particles ensuring that the fluid particles near the edge of the domain have complete kernel support. Otherwise, the fluid particles near the edge tend to leave the system due to high forces (i.e. pressure) and acceleration from the other particles. Therefore, the concentration for the boundary particles has been assigned as approximately 1.0 to prevent this unphysical behaviour.

**Modifications of the free-surface correction**

Besides the treatments based on the concentration to determine the shifting distance and its direction explained above, Lind et al. (2012) presented a correction method for the free-surface flows. Equation (5.66) shifts all the particles with a constant movement. Thus, the fluid particles at the interface are moved towards the interface to the air particles. This will result in mixing fluid and air particles together and creating instabilities. This has been seen in air bubble growth test cases with Xu et al. (2009)’s shifting algorithm. In order to prevent unphysical mixing or movement at the interface, the concentration gradient near the surface should not be controlled by using global coordinates. Following from that, the binormal, tangent and normal vectors are considered for the 3-D model, allowing the shifting only in the tangent and binormal directions. Therefore, Equation (5.66) becomes (Mokos et al., 2013):

\[
\delta \mathbf{r}_s = -D \left( \frac{\partial C_i}{\partial s} \mathbf{s} + \frac{\partial C_i}{\partial b} \mathbf{b} + \alpha_n \left( \frac{\partial C_i}{\partial n} - \beta_n \right) \mathbf{n} \right)
\]

where \( \mathbf{s}, \mathbf{n} \) and \( \mathbf{b} \) are the tangent, normal and binormal vector respectively to the surface. \( \beta_n \) is a reference concentration gradient for the water phase in the free surface. The parameter \( \alpha_n \) limits the diffusion in the normal direction, so the water particles are prevented from moving through the air particles. It is set to 0.1 in this study as air bubble modelling can be assumed as slow flows (Lind et al., 2012).

To identify free-surface particles, the divergence of particle position is used (Lee et al., 2008).
\[ \nabla \cdot \mathbf{r} = \sum_{j=1}^{N} \frac{m_j}{\rho_j} \mathbf{r}_{ij} \cdot \nabla_i W_{ij} \] (5.71)

This divergence of the particle position equals 2 for 2-D and 3 for 3-D simulations. Hence, for the 3-D simulations a threshold value of 2.5 is used to determine the particles belonging to the surface and particle shifting is applied to the phases due to this value, i.e. if \( \nabla \cdot \mathbf{r} < 2.5 \), the particles are considered to belong to the surface.

The shifting algorithm should be applied carefully, as it has the potential to disrupt the interface. The initial algorithm proposed by Xu et al. (2009) had significant issues at the interface, creating unphysical particle movements.

In order to be effective and to obtain accurate results, Equation (5.66) has been performed for air particles so as to allow them to expand without mixing with the fluid phase. The same equation is also applied to the fluid particles, except it is applied at the interface. The treatment or surface correction term shown in Equation (5.70) has only been applied to the interface particles. This method was also conducted by Mokos et al. (2013) to prevent the air phase dispersing in the water phase and creating voids.

5.3.5 Time Stepping (Time Integration)

5.3.5.1 Time Integration Schemes

The equations for conservation of mass and momentum need to be integrated forward in time. Common methods are Leap-Frog (LF), predictor-corrector and Runge-Kutta (Gomez-Gesteira et al., 2012b). There are some advantages and disadvantages of these methods themselves. For instance, Leap-Frog is good at using low memory storage in the computation as the acceleration is evaluated per time step, whereas the Runge-Kutta method requires four evaluations of the acceleration for an RK4 (i.e. Runge-Kutta 4th order) scheme and six for an RK45 (i.e. Runge-Kutta 4th and 5th order). Choosing a time integration scheme is generally based on the problem type and computational simulations of physical processes. For example, if it is intended to solve pure heat conduction problems, an optimum integration scheme such as predictor-corrector should be preferred as it allows longer time steps. Ideally, a good time integration algorithm should conserve the mass, momentum and energy
and keep errors bounded (Monaghan, 2005). It should also be efficient in terms of computational time and be capable of allowing as large a time step as possible.

The set of ordinary differential equations for the fundamental governing equations can be solved via time integration. In terms of SPH time integration, the scheme must be at least 2nd-order accurate in time since the particles (computation points) move. Herein, we use the 2nd-order predictor-corrector method of Monaghan (1992), as it is robust and well used. The predictor-corrector method is explained in detail below as it will be applied to the SPHysics simulations herein.

Following Gomez-Gesteira et al. (2012a), the governing equations are rewritten as:

\[
F_i = \frac{Dv_i}{Dt} \quad \text{(Momentum)} \tag{5.72}
\]

\[
D_i = \frac{D\rho_i}{Dt} \quad \text{(Continuity)} \tag{5.73}
\]

\[
v_i = \frac{Dr_i}{Dt} \quad \text{(Position)} \tag{5.74}
\]

2nd-order accurate Predictor-Corrector

There are three steps for this time integration scheme, namely predictor step, corrector step and final step.

**Predictor step:** The existing assigned properties such as density, velocities, thermal energy, and temperature etc., are used to predict the new values at the midpoint of the time step:

\[
v_i^{n+1/2} = v_i^n + \frac{\Delta t}{2} F_i^n \quad \rho_i^{n+1/2} = \rho_i^n + \frac{\Delta t}{2} D_i^n \tag{5.75}
\]

\[
r_i^{n+1/2} = r_i^n + \frac{\Delta t}{2} v_i^n \tag{5.76}
\]
Corrector step: The predicted values in the predictor step are then corrected using forces at half step:

\[
\begin{align*}
\mathbf{v}_i^{n+1/2} &= \mathbf{v}_i^n + \frac{\Delta t}{2} \mathbf{F}_i^{n+1/2} \\
\rho_i^{n+1/2} &= \rho_i^n + \frac{\Delta t}{2} D_i^{n+1/2}
\end{align*}
\] (5.77)

\[
\begin{align*}
\mathbf{r}_i^{n+1/2} &= \mathbf{r}_i^n + \frac{\Delta t}{2} \mathbf{v}_i^{n+1/2}
\end{align*}
\] (5.78)

Final step: The corrected values are calculated at the end of the time step.

\[
\begin{align*}
\mathbf{v}_i^{n+1} &= 2\mathbf{v}_i^{n+1/2} - \mathbf{v}_i^n \\
\rho_i^{n+1} &= 2\rho_i^{n+1/2} - \rho_i^n \\
\mathbf{r}_i^{n+1} &= 2\mathbf{r}_i^{n+1/2} - \mathbf{r}_i^n
\end{align*}
\] (5.79)

5.3.5.2 Variable Time Step

For the simulations presented herein, a variable time step is used for efficient computation. The time step depends on conditions such as internal and external forces, viscous forces, surface tension, etc. In other words, the time step for an SPH application is related to the physical nature of the simulation.

Time step based on forces

The particles should be prevented from being too close to each other. If particles clump together, this produces unphysical densities and pressures during their motion when they are exposed to external and internal forces (e.g. gravity, acceleration, and etc.). Therefore, the time step based on this condition is given by Monaghan (1989), Monaghan (1992), Monaghan and Kos (1999):

\[
\Delta t_f = \min \sqrt{\left( \frac{h}{|f_i|} \right)}
\] (5.81)

where \( f_i \) denotes all forces associated with particle \( i \) per unit mass.
**Time step based on viscous forces**

\[
\Delta t_{CV} = \min_i \frac{h}{c_s + \mu_i}
\]  

(5.82)

where

\[
\mu_i = \max_j \left| \frac{v_{ij} \cdot r_{ij}}{r_{ij}^2 + 0.01h^2} \right|
\]  

(5.83)

where \(c_s\) is the speed of sound and the term on the denominator is related to the viscous term.

**Time step based on surface tension**

For problems involving surface tension, the time step criteria must satisfy the surface tension condition as in (Brackbill et al., 1992):

\[
\Delta t_{st} = \sqrt{\frac{\rho h^3}{2\pi \sigma_s}}
\]  

(5.84)

where \(\rho\) is the reference density and \(\sigma_s\) is the surface tension coefficient.

The final time step should be the minimum value of the conditions above. It can be expressed as:

\[
\Delta t \leq C_r \min(\Delta t_f, \Delta t_{CV}, \Delta t_{st})
\]  

(5.85)

where \(C_r\) is the Courant number which typically has a value between 0.1 and 0.5.

**5.4 SPHysics Code and Modifications**

SPHysics is a platform of free open-source codes (Gomez-Gesteira et al., 2010b) for SPH and it is written in different programming languages (e.g. FORTRAN) for the simulation of free-surface hydrodynamics. The SPHysics code is capable of simulating many different test cases such as wave breaking, dam breaks, sloshing, floating objects, laser cutting processes etc.. The code can be run on Windows and
Linux with the relevant compilers (e.g. Silverfrost FTN95, Intel, GNU GFortran compiler). The results can be visualised either with Matlab or ParaView. In order to visualise with ParaView, the data files require post-processing to generate visual toolkit unstructured (VTU) files. There are two main sources in the code. One is used to generate the geometry and create the initial conditions of the run and is called SPHysicsGen, while the other is SPHysics, which mainly involves the main source codes (i.e. viscosity, kernel calculations, time step calculations). This open-source code has recently been modified to model the dry and wet laser cutting process by Muhammad et al. (2013) and it is used for this research with the required modifications to simulate the bubble generation and growth for intumescent paints.

As the current code was for a laser cutting process, there were two phases (i.e. solid and water) in the model. Many generic changes have been made to the code.

- First of all, the applied laser power was removed. The phases in the current code have been changed to the required phases (i.e. air and water). In terms of arranging the locations of particles, boundary particles in the domain are considered as stationary fluid particles, where they are arranged as two layers and their movements restricted such that their velocities are zero.

- The artificial viscosity formulation explained in Monaghan (1992) and also laminar viscosity formulation given in Section 5.3.4.3 is considered in the model, therefore the multi-phase modifications have been implemented in the viscosity subroutine.

- The general problem of unphysical penetration or mixing of two different particles especially near the boundaries (fluid boundary particles and gas particles) and also newly-introduced air particles in the liquid chamber which have different physical properties (i.e. density, pressure, etc.), can occur in the simulation. In order to prevent penetration, a no penetration force formulation has been taken into consideration and implemented to the related subroutines. The formulation is given by Das and Das (2009):

\[
 f_{pi} = \begin{cases} 
 \frac{\xi(p_d^6 - p_i^6)(x_i - x_j)}{r^2 m_i} & \text{if } P_d \geq 1 \\
 0 & \text{if } P_d < 1 
\end{cases} 
\]  

(5.86)

where \( P_d = (h_i + h_j)/2r \) and \( r \) is the scalar distance between the interfacial
particles. \( \xi \) is an empirical constant which depends on the type of fluids and flow situations.

- Implementation of the surface tension, which is based on Hu and Adams (2006) shown in Section 0, into the particle interaction subroutines of SPHysics code (i.e. ac_3D.f, celij_3D.f and self_3D.f) has been performed for the simulation of the single bubble growth and the surface tension model has been validated with Rogers et al. (2009). The detailed explanation and results are shown in the next chapter.

- Implementation of the shifting algorithm based on Xu et al. (2009) and Lee et al. (2008) (see Section 5.3.4.5) has been performed on the SPHysics code by creating the necessary subroutines (i.e. particle_shifting_3D.f, ac_Shifting_3D.f, pre_celij_Shifting_3D.f, pre_self_Shifting_3D.f). The shifting of the particles is restricted at the surface of the bubble modelling by implementing the surface particle tracking method.

- For the bubble growth modelling with SPH, the pressure should be increased inside the bubble to force growth of the bubble. Two methods have been conducted to increase the pressure. One is to assign a higher pressure than one atmospheric pressure inside the bubble by keeping the pressure as atmospheric pressure outside of the bubble (i.e. the pressure for the surrounding liquid is kept at 1 atm). This has been done by choosing a higher density than the reference density of gas to predict a higher pressure according to Tait’s equation of state. This is described in detail in Chapter 6.

The other method is to add additional mass into the bubble to represent mass transfer (see Section 6.4 in the next chapter), which will result in an increase in pressure inside the gas bubble. This has been done by implementing the particle insertion (i.e. increasing the number of gas particles inside the bubble). The algorithm has been implemented to SPHysics (i.e. step_predictor_corrector_3D.f subroutine) to create new gas particles at the surface of the bubble at certain time steps depending on the growth of the bubble. A detailed explanation with a test case will be given in the next chapter.

### 5.5 Concluding Remarks

In this chapter, the SPH methodology with its theoretical and numerical features was explained in detail. The formulations presented throughout this chapter are used
in the following chapter to solve the numerical problems and test cases in this research. The open-source code SPHysics is used to model the surface tension, actual bubble growth and bubble growth with orifice test case. The next chapter will present the 3-D bubble modelling and rise through submerged orifice, validation of the surface tension modelling and single bubble growth model.
CHAPTER 6 SPH MODELLING OF BUBBLE GROWTH

6.1 Introduction

This chapter presents the results of an investigation into the feasibility of using smoothed particle hydrodynamics (SPH) to model bubble growth in intumescent coatings. As introduced earlier in Chapter 2, the intumescent coating is a polymer material used for fire protection which can swell up to 100 times the original thickness when exposed to fire attack. The fire protection performance of the intumescent coating is related to its expansion ratio. It expands at high temperatures such as under fire condition by melting and releasing gases due to various chemical reactions occurring with the temperature increase. Those gases generate bubbles of different sizes during the expansion process. The growth of a bubble in the polymer melt depends on forces such as gas pressure inside the bubble, the pressure and viscosity of the surrounding liquid and surface tension between the bubble and polymer melt (liquid). The main driving force for bubble generation and growth is the increased gas pressure inside the bubble due to conversion of mass from solid to liquid and eventually gas. This increase in pressure is directly related to the amount of mass loss (or mass conversion), which is not infinite. Apart from the pressure increase inside the bubble, the viscosity and the pressure of the surrounding liquid (or polymer melt) and also the other bubbles’ growth act as resistance forces to control the bubble’s growth. Therefore, bubble growth is limited based on these factors.

As mentioned in Chapter 1, one of the objectives of this research project is to model the expansion process of intumescent coating in detail by modelling bubble growth. As a Lagrangian method, the smoothed particle hydrodynamics (SPH) method is foreseen to be able to demonstrate numerical simulation of bubble expansion. The meshless nature of SPH, represented by a set of particles where each particle moves according to the fundamental governing equations (conservation of mass, momentum), has been explained in Chapter 5. The open-source code SPHysics (Gomez-Gesteira et al., 2010b) is used to model three different cases presented herein; a 3-D static surface tension case, bubble formation through submerged orifice (Das and Das, 2009) and air bubble growth in liquid respectively.
This chapter presents the results for the three test cases. Finally, the main conclusions of those test cases will be presented, along with an outline of the significant challenges and recommendations of possible methods that could be applied to overcome them.

6.2 Test Case 1: Surface Tension Modelling

6.2.1 Introduction

Surface tension exists at the interface of two materials (e.g. two liquids in fluid dynamics) and it is a macro (continuum scale) force representing the combined effects of molecular attraction and repulsion. Surface tension plays an important role in many application areas, for instance food processing, cosmetics, fuel injection, enamelling, metal casting, etc. (Morris, 2000). Many different techniques have been developed and used to simulate multi-phase flows with surface tension for many engineering applications such as a dam break problem, an oscillating bubble, two-liquid interface problem, coalescence of two initially stationary drops, equilibrium and oscillating rod, etc. (Wu et al., 1998), (Morris, 2000). Nugent and Posch (2000) used SPH to model the formation of a liquid drop surrounded by its vapour in 2-D. The cohesive pressure due to the equation of state results in pressure increase, and therefore the forces between the particles exceed the interaction range of all the other smoothed forces in the equation of motion. With the effect of surface tension, stable drops are formed. Colagrossi and Landrini (2003) used the idea of Nugent and Posch (2000) to model two-dimensional interfacial flows with different fluids separated by sharp interfaces using different equations of state for each different fluid and some changes to the kernel summations. The results showed that their surface tension formulation gives stable solutions for low density ratios. The approach of Hu and Adams (2006) for the surface tension calculation given in detail in Section 5.3.4.4 eliminates the problem of particles far from the interface influencing the surface tension calculation. Each phase is assigned a colour function which results in surface tension stress acting on particles of the same phase. Therefore, the Hu and Adams (2006) surface tension approach has been used herein. Two validation test cases for the surface tension modelling have been developed. One of them is single phase (liquid-liquid interaction without density ratio) and the other one is multi-phase (liquid-air interaction with a density ratio of 800). Surface tension has also been used
to model the bubble growth explained in Section 6.4.

### 6.2.2 Model Description

The surface tension test case consists of a circular region (bubble) of one fluid surrounded completely by another fluid. The sketch of the surface tension test case is shown in Figure 6.1.

![Surface tension definition sketch](image)

**Figure 6.1** Surface tension definition sketch

By assigning different densities to each phase and a surface tension coefficient $\sigma_s$ (given in Equation (5.59)) for the interface, the pressure inside the bubble will be different. The properties of both fluids are given in Table 6.1.
Table 6.1 The properties of the 3-D surface tension test cases

<table>
<thead>
<tr>
<th>Properties of the cases</th>
<th>Water-water</th>
<th>Water - air</th>
</tr>
</thead>
<tbody>
<tr>
<td>Box dimension – L (m)</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>Radius of Fluid 1 – R (m)</td>
<td>0.02</td>
<td>0.02</td>
</tr>
<tr>
<td>Density of Fluid 1 (kg/m$^3$)</td>
<td>1000</td>
<td>1.25</td>
</tr>
<tr>
<td>Density of Fluid 2 (kg/m$^3$)</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>Speed of Sound of Fluid 1 (m/s)</td>
<td>50</td>
<td>200</td>
</tr>
<tr>
<td>Speed of Sound of Fluid 2 (m/s)</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>Surface tension coefficient - $\sigma_s$ (N/m)</td>
<td>0.5</td>
<td>0.07</td>
</tr>
<tr>
<td>Gravity – g (m/s$^2$)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Theoretical pressure drop (Pa)</td>
<td>25</td>
<td>3.5</td>
</tr>
<tr>
<td>Artificial viscosity</td>
<td>0.1</td>
<td>0.1 (water)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.0 (air)</td>
</tr>
</tbody>
</table>

The artificial viscosity formulation of Monaghan (1992) explained in detail in Section 5.3.4.3 has been used with a value of 0.1 for water – water and 0.01 for water-air surface tension simulations. The 3-D simulation for the first test case (water-water) and second test case (water-air) has been run up to 0.02 and 0.2 seconds respectively to obtain steady-state condition. To assess numerical convergence, three different resolutions have been used in the simulations: $\Delta x/R = 0.25$, 0.2 and 0.1 corresponding to particle sizes of $\Delta x = 5$ mm, 4 mm and 2 mm respectively.

6.2.3 Results

6.2.3.1 Water – water bubble

For the first case in Table 6.1, the water, which has a density of 1000 kg/m$^3$, is separated from water by an interface with the surface tension coefficient $\sigma_s$ of 0.5 N/m. According to the Young-Laplace equation, the pressure drop from fluid 1 to fluid 2 is given by:
\[ \Delta P = \frac{\sigma_s}{R} \]  
(6.1)

which gives a theoretical pressure drop (\(\Delta P = 25 \text{ Pa}\)) for the properties in Table 6.1.

The pressure inside fluid 1 is higher than in fluid 2 due to the effect of surface tension between fluids. Figures 6.2 to 6.4 show the comparison of pressure with respect to the distance \(x/R\) (the particle position over radius). The formulation of Hu and Adams (2006) predicts almost zero pressure in the surrounding fluid when the simulation has been performed with resolution of \(\Delta x/R = 0.1\) where the distance between particles is 2 mm. However, the pressure is not well predicted in the surrounding fluid, at the interface and inside fluid 1 (i.e. the water bubble) (see Figure 6.2) for low resolution simulation where the distance between particles is 5 mm. The reason for this is the formulation nature of Hu and Adams (2006) and coarse resolution. The \(d\) (dimension) parameter in Equation (5.63) also has a significant effect on the pressure prediction (unphysical pressure drop). This can be solved by setting \(d = 1\) in the simulation (Rogers et al., 2009).

To assess numerical convergence, the \(L_2\) error norm has been computed according to:

\[
L_2(P) = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left( \frac{P_i - P_{i,\text{theoretical}}}{P_{\text{max}}} \right)^2}
\]  
(6.2)

where \(N\) is the total number of particles in the horizontal direction, \(P_i\) and \(P_{i,\text{theoretical}}\) are the numerical and analytical pressure of the \(i^{\text{th}}\) particle respectively, and \(P_{\text{max}}\) is the maximum pressure.

Figure 6.5 shows the \(L_2\) norm error measures calculated based on Equation (6.2) and plotted for different levels of resolution refinement. For this simple validation case with water-water, the agreement is satisfactory with convergence to the analytical solution and the \(L_2\) norm error follows a convergence line of between first and second order, which is typical of SPH (Vacondio et al., 2012).
Figure 6.2 Comparison of pressure between theoretical and SPH results (water-water interface using $\Delta x/R = 0.25$)

Figure 6.3 Comparison of pressure between theoretical and SPH results (water-water interface using $\Delta x/R = 0.2$)
Figure 6.4 Comparison of pressure between theoretical and SPH results (water-water interface using $\Delta x/R = 0.1$)

Figure 6.5 $L_2$ norm pressure error against first and second order convergence for water-water bubble test case
6.2.3.2 Water – air bubble

Figures 6.6 to 6.8 present the results for water-air phase surface tension validation with three different resolutions $\Delta x/R = 0.25$, 0.2 and 0.1. The theoretical pressure drop from the air phase to the water phase is 3.5 Pa. Although the differences between theoretical and SPH results appear especially just at the interface, this can be acceptable for multi-phase simulations as the density ratio is large (1000:1.25) and there is no gravity force acting in the simulation.

With the resolution increases (smaller $\Delta x/R$), closer agreement for the predicted pressure with the theoretical solution for the outer fluid and the inside of the air bubble has been obtained. This is also proven by calculating an $L_2$ error norm of pressure shown in Figure 6.9. The error decreases with increased resolution ($\Delta x/R$). The overshoot near the interface is typical of SPH surface tension models using these resolutions.

Provided that a sufficiently fine resolution is used, this demonstrates that the Hu and Adams (2006) model is appropriate for predicting the pressure fields in 3-D bubbles for the density ratios encountered in intumescent coatings.

**Figure 6.6** Comparison of pressure between theoretical and SPH results (water-air interface $\Delta x/R = 0.25$)
Figure 6.7 Comparison of pressure between theoretical and SPH results (water-air interface $\Delta x/R = 0.2$)

Figure 6.8 Comparison of pressure between theoretical and SPH results (water-air interface $\Delta x/R = 0.1$)
6.2.4 Discussion

Overall, satisfactory agreement between SPH and theoretical results has been obtained using $\Delta x / R = 0.1$ for the water-water phase and water-air phase simulations. However, surface tension dominates any flow problem including bubble growth modelling. In order to predict the surface tension correctly, the curvature of the interface ($\kappa$) in Equation (5.59) has to be calculated correctly. Figure 6.10 shows the pressure magnitude of contours with regard to surface tension simulations of water-air multi-phase using ParaView visualisation software.

**Figure 6.9** $L_2$ norm pressure error against first and second order convergence for water-air bubble test case
Figure 6.10 Pressure magnitude contours of surface tension simulation of water-air interface for almost 150,000 particles using $\Delta x/R = 0.1$ (a) 2-D slice from 3-D view (b) 3-D view
6.3 Test Case 2: Bubble Formation and Rise through Submerged Orifice

6.3.1 Introduction

Bubble formation at a submerged orifice, its growth and finally its departure from the orifice mouth has been an attractive interest in fluid mechanics besides its hydrodynamic processes. This process is used in a wide range of application such as for chemical and process equipment. For the purposes of this work, the case is useful to demonstrate the expansion process for a non-spherical bubble evolution.

The evolution of the bubble can be divided into two different steps, namely initial forming and the final growth and movement period. Due to the pressure differences between lower (air phase) and upper chamber (liquid phase), the air flows through the orifice and eventually forms the bubble as a sphere shape and grows further as time progresses. At the final stage, the bubble becomes stretched and its shape is no longer spherical.

The formation, growth and detachment of the bubble from the orifice are governed by inertia, buoyancy and viscous forces. Therefore, a number of parameters such as density, viscosity and surface tension have direct influence on the bubbling process.

6.3.2 Model Description

With the complexity of the test case, the computational domain needs to be selected carefully. Gas and fluid chambers should be large enough compared to the orifice diameter to neglect drastic (i.e. sudden) fluid chamber pressure change due to the bubbling and gas particles’ movement (Das and Das, 2009). Pressurised air occupies the bottom compartment whereas the top compartment comprises the water with free surface. A 3-D domain consists of a liquid pool at atmospheric pressure over a circular orifice. The flow of air from the bottom compartment into the liquid pool passing through the orifice occurs due to high pressure. The schematic diagram is shown in Figure 6.11.

Figure 6.12 shows the 3-D computational domain with water particles having a density of 1000 kg/m$^3$, air particles having a density of 1.225 kg/m$^3$ and boundary particles at the four sides of the domain to bound the liquid and gas phase. The sheet
boundary, which has an orifice, has been created between the chambers. To model the fixed boundary particles, the dynamic boundary condition has been used (Crespo et al., 2007). Two layers of boundary particles are placed in a staggered manner, which follows the continuity equation (Equation (5.42) in Section 5.3.3.5) and momentum equation (Equation (5.43) in Section 5.3.3.5). However, they remain fixed in position. All boundary particles including sheet boundary have been assumed to be water particles such that the interaction between an air particle and a boundary particle follows the normal air-water particle interaction. The diameter of the orifice under consideration is 6 mm (see Figure 6.13), and the dimensions of both chambers are 45 mm × 45 mm × 45 mm. The pressures of the lower and upper chamber are 2.5 atm and 1 atm respectively. The variation of temperature is not modelled.

Three different particle resolutions have been used: $\Delta x/R = 0.66$, 0.5 and 0.33 corresponding to particle sizes of $\Delta x = 2$ mm, 1.5 mm and 1 mm respectively. For the finest resolution, $\Delta x/R = 0.33$, the total number of particles used for this multiphase simulation is approximately 250,000 with approximately 20,000 time steps using the variable time step approach explained in Section 5.3.5. The CPU used to run this simulation is Intel i7-2600 with 8GB of RAM and a clock speed of 3.40GHz. The simulation duration is almost 2 days.

![Schematic diagram of the problem domain](image)

**Figure 6.11** Schematic diagram of the problem domain
Figure 6.12 3-D domain and initial model particle representation for SPH simulation

Figure 6.13 Representation of the orifice with diameter of 6 mm at $z = 46$ mm, $\Delta x/R = 0.33$
6.3.3 Results

The pressure change from bottom compartment to top compartment drives the flow due to the pressure difference. The water particles’ pressure is predicted according to the Equation of State explained in Section 5.3.4.1 while the pressure is kept constant for all air particles at 2.5 atm to represent the effect of a reservoir. With the nature of the meshless method, all fluid particles including water and air are allowed to take their own position according to the continuity (Equation (5.42)) and momentum equation (Equation (5.43)).

At the initial movement of the simulation, air particles move towards the orifice. The resolution effect has a significant influence on the air particles’ movement and therefore bubble formation at the orifice mouth. The simulation has been performed with the three resolutions ($\Delta x/R$) with 0.33, 0.5 and 0.66. No movement for the air particles has been observed with the resolution of 0.66 where the distance between the particles is 2 mm whereas a very slow movement occurred with the resolution of 0.5 (the distance between the particles is 1.5 mm). This is shown in Figure 6.14.

The air particles that are close to the water particles rise further with time. This will result in gas particles passing through the orifice and entering into the upper compartment containing the water phase as shown in Figure 6.15 for different instants in time for the simulation using $\Delta x/R = 0.33$. The no-penetration force here (Equation (5.86)) prevents the unphysical mixing of the two phases.

Figure 6.15 shows that the air mass above the orifice continues to enlarge gradually with the arrival of more air particles from the lower partition. This results in forming the bubble shape as hemispherical. As the simulation moves forward in time, the bubble expands further and the centre of the bubble shifts up from the orifice mouth. This physical behaviour transforms the hemispherical bubble into a mushroom shape.

The present simulation has run up to 0.4 seconds of physical time. The artificial viscosity formulation (Equation (5.50) in Section 5.3.4.3) has been considered in the implementation for this simulation to compare with Das and Das (2009). However, surface tension implementation has not been considered in this study but this case exhibits rapid evolution and is therefore less significant. Figure 6.15 shows snapshots
of the particles using vertical 2-D slices at $y = 23$ mm through the 3-D domain.

Figure 6.16 shows the comparison of bubble contour with Das and Das (2009) at different times above the submerged orifice of 3 mm radius. Dots represent the new SPH simulation results. With the exception of consideration of the surface tension in the bubble forming model with submerged orifice, the obtained results have good agreement with the results of Das and Das (2009). As the surface tension has not been considered herein, the exact shape of the interface (see Figure 6.15) in the flow situations has not been obtained whereas this has been observed in Section 6.2. Davidson and Schüler (1997) reported, in one of the experimental studies related to bubble formation at an orifice in a viscous liquid, that surface tension has a negligible effect at constant higher flow rates compared to the viscous and pressure forces. This is also seen in this study (see Figure 6.16). However, the surface tension has a significantly important effect on the pressure inside the bubble when the flow rate is low. This is examined in the modelling of bubble growth in polymer fluid in Section 6.4.

Figure 6.14 Effect of resolution on bubble formation at time $t = 0.005$ s (2-D slice at $y = 23$ mm from 3-D simulation)
**Figure 6.15** Bubble formation from a submerged orifice – snapshots from 3-D simulation using 2-D slices at $y = 23$ mm, $\Delta x/R = 0.33$
It should be noted that boundary particles are not shown in Figure 6.15. Red colour donates the liquid particles and blue colour donates the gas particles.

![Figure 6.16 Comparison of bubble growth](image)

**Figure 6.16** Comparison of bubble growth – Dots represent the current model, lines represent Das and Das (2009)

### 6.3.4 Discussion

The modelling technique of SPH is employed herein to simulate the bubble growth with two different phases. The present model has given an opportunity to study the details of the movement of gas through liquid with a high flow rate and of a non-spherical shape. It also helped to understand the effect of high air pressure on the bubble growth. Neither the corrected SPH (kernel correction) method nor shifting algorithm have been used in this study, the obtained results from the SPH simulation have a better agreement with Das and Das (2009). There is no movement towards the orifice seen for air particles with the coarse resolution. Therefore, the resolution has a great effect on the bubble formation. As the pressure from the bottom chamber is the main driving force for the physical phenomenon, the pressure of the fluid (water) particles on the top compartment is evaluated according to their change of density using an equation of state (Equation (5.44)). The penetration of the particles of one
fluid into the other is restricted using no penetration force. This test case has shown that SPH can simulate the growth of a 3-D bubble of non-hemispherical shape. The test case has shown that realistic pressures can also be used.

### 6.4 Test Case 3: Gas Bubble Growth

#### 6.4.1 Introduction

As mentioned earlier in Chapter 2, one of the main objectives of this research project is to demonstrate the feasibility of simulating the expansion of the bubbles in 3-D using a multi-phase SPH model and to identify the main challenges for this kind of detailed numerical simulation. With this aim, the growth of a single bubble has been modelled using the meshless SPH method with the consideration of surface tension between phases and viscosity effect of the polymer melt. The predicted results from the numerical study have been compared with the well-known analytical solution for single bubble growth developed by Patel (1980).

#### 6.4.2 Model Description

A single bubble expansion case has been simulated with slightly different properties from the properties presented in Table 6.1. Instead of air density ($\rho_{\text{air}} = 1.25$ kg/m$^3$), the density of CO$_2$ ($\rho_{\text{CO}_2} = 1.9$ kg/m$^3$) has been used for the gas phase. To link the density and pressure, a compressible equation of state formulation (Equation (6.3)) first introduced in SPH by Morris et al. (1997) has been used since it is computationally faster than Tait’s equation of state (Equation (5.44)) without resulting in large pressure fluctuations. The large value of polytropic index $\gamma$ (7 for the water phase) in Tait’s formulation leads to very sensitive simulations such that a small density variation can cause large pressure fluctuations, and unstable simulations which were not apparent for the static bubble cases of Section 6.2. The Morris equation of state, $\gamma = 1$, is used in both phases:

$$
P_l = c_{s_l}^2 (\rho_l - \rho_{0l}) \quad \text{liquid}
$$

$$
P_g = c_{s_g}^2 (\rho_g - \rho_{0g}) \quad \text{gas}
$$

where subscripts $g$ and $l$ denote liquid and gas phases respectively.

As explained in Section 6.2, the surface tension effects are critical for bubble
modelling and growth in microscale engineering problems especially for multi-phase problems with low flow. Running the SPH model at microscale (1 \( \mu \)m) proved to be unstable numerically. This is due to several factors, most notably that the denominator of \( \alpha_d \) in Equation (5.10) is proportional to \( h^3 \) in 3-D. As \( h \) decreases to the microscale, this dependence on \( 1/h^3 \) proves to be prohibitively unstable and is recommended for further study in Chapter 7. Hence, simulations were performed at the millimetre scale to investigate the feasibility of modelling bubble growth. Surface tension effects should be scaled according to the Buckingham theorem with six dimensionless groups: namely Reynolds number, Froude number, Bond number, Weber number, Capillary number and Marangoni number given by Bush (2013). Multi-phase bubble growth for intumescent coating in isothermal conditions is dominated by viscosity effects so that capillary number scaling is the preferable option since it is based on the viscous and curvature forces given in Equation (6.4).

\[
Ca = \frac{\rho \nu U}{\sigma_s} \quad (6.4)
\]

where \( \nu \) is the viscosity of polymer, \( U \) is a characteristic speed as:

\[
U = \sqrt{gR} \quad (6.5)
\]

The Capillary number represents the ratio of viscous effects to surface tension (curvature) effects.

The surface tension coefficient \( (\sigma_s = 0.028 \text{ N/m}^2) \) given in the model parameters of Elshereef et al. (2010) is for the bubble growth model of which the initial bubble radius is 1 \( \mu \)m. At the micrometre scale, the Capillary number is \( Ca = 447 \). Therefore, the surface tension coefficient has been scaled by keeping the Capillary number constant, that is \( (Ca)_{\mu m} = (Ca)_{mm} \), to simulate the bubble growth process at millimetre size. Table 6.2 presents the properties used for the simulation.
Table 6.2 The properties of the 3-D bubble growth model

<table>
<thead>
<tr>
<th>Properties of the model</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Box dimension – $L$ (m)</td>
<td>0.05</td>
</tr>
<tr>
<td>Radius of Fluid 1 – $R$ (m)</td>
<td>0.01</td>
</tr>
<tr>
<td>Density of Fluid 1 (kg/m$^3$)</td>
<td>1.9</td>
</tr>
<tr>
<td>Density of Fluid 2 (kg/m$^3$)</td>
<td>1000</td>
</tr>
<tr>
<td>Speed of Sound of Fluid 1 (m/s)</td>
<td>30</td>
</tr>
<tr>
<td>Speed of Sound of Fluid 2 (m/s)</td>
<td>5</td>
</tr>
<tr>
<td>Surface tension coefficient - $\sigma_s$ (N/m)</td>
<td>0.5</td>
</tr>
<tr>
<td>Gravity – $g$ (m/s$^2$)</td>
<td>0</td>
</tr>
<tr>
<td>Laminar viscosity</td>
<td>0.01 (water)</td>
</tr>
<tr>
<td></td>
<td>0.01 (air)</td>
</tr>
</tbody>
</table>

In Section 6.2, artificial viscosity was sufficient and convenient to maintain a stable solution for a static bubble. In a low Reynolds number flow, such as this case, laminar viscosity is appropriate to represent the processes in a physically more appropriate manner.

As mentioned previously in Section 2.6, the mass conversion from polymer melt to gas (mass loss) due to heat such as fire drives the expansion process of the intumescent coating by increasing the pressure inside the bubble. If the pressure inside the bubble is maintained, the volume of the bubble would have to increase as the mass of the gas phase increases (see Equation (3.1)). This mass transfer has been represented in SPH by increasing the number of gas particles inside the bubble during the simulation. The amount of the mass and the number of new gas particles have been estimated. The simulation of the single bubble growth model has been run up to 0.05 seconds. For an isothermal simulation duration of 0.05 s, the predicted expansion of a single bubble of initial radius 10 mm is 11 mm according to the model properties of Elshereef et al. (2010) based on the analytical solution of Patel (1980). This analytical solution is presented in Appendix B. This expansion is driven by a mass transfer across the interface of $m_{\text{transfer}} = 2.74 \times 10^{-6}$ kg of gas from
the polymer melt into the bubble over a period of 0.05 seconds. In this simulation, it is assumed that the mass transfer occurs continuously throughout the simulation duration such that a certain number of new gas particles have been inserted into the bubble at regular intervals. For example, for a resolution of \(\Delta x/R = 0.2\), the mass of a SPH gas particle, \(j\), is \(m_j = 1.52 \times 10^{-8}\) kg. Hence 180 \(= m_{\text{transfer}}/m_j\) new SPH gas particles need to be added to the bubble throughout the simulation. The rate of insertion of these particles is presented in the next section. This newly developed approach or idea is similar to the bubble growth with orifice test case presented in the previous section (Section 6.3) where air particles move and enter into the water phase in the upper compartment due to the pressure difference.

### 6.4.3 Results

The bubble growth model has been run with two different resolutions with \((\Delta x/R) = 0.2\) where the distance between the particles is 2 mm and \((\Delta x/R) = 0.1\) where the distance between the particles is 1 mm. Figure 6.17 shows the particle distribution of the bubble growth model, with the finer resolution \(\Delta x/R = 0.1\), before and after conduction of the particle insertion method. In this simulation, 45 new gas particles have been inserted into the area close to the centre of the bubble every 0.01 seconds. Even though mass transfer takes place at the interface, adding particles at the centre of the bubble is satisfactory since the hydrodynamic conditions within the bubble for the timescales of this problem are uniform and steady. Identifying the location for new particles is not straightforward and is recommended as part of further research in Chapter 7. Special care has been taken not to generate a new gas particle at a position another gas particle has already occupied so as to prevent particle clumping. This is achieved by giving a random position to new gas particles using the FORTRAN RAND function. This function and position of a new gas particle in x, y and z-directions have been given as:

\[
\begin{align*}
xp_{\text{new}} &= x_c + 0.25dx_0 + \text{rand}(0) \times 0.2dx_0 \\
yp_{\text{new}} &= y_c + 0.25dy_0 + \text{rand}(0) \times 0.2dy_0 \\
zp_{\text{new}} &= z_c + 0.25dz_0 + \text{rand}(0) \times 0.2dz_0
\end{align*}
\]  

(6.6)

where \(xp_{\text{new}}, yp_{\text{new}}\) and \(zp_{\text{new}}\) are the positions of the new particle in three coordinates and \(x_c, y_c\) and \(z_c\) are the positions of the bubble centre while \(dx_0, dy_0\)
and $dz_0$ are the distances between the particles. $rand(0)$ represents the RAND functions in FORTRAN which have a value between 0 and 1.

As new gas particles are introduced into the bubble, a slight expansion has been obtained at $t=0.01 \text{s}$ as shown in Figure 6.17 (b). Therefore, the pressure inside the bubble increases while the outer pressure remains almost zero at 0.01 s.

![Figure 6.17](image)

**Figure 6.17** Particle distribution of the bubble growth model, (a) just before particle insertion at $t = 0.00996 \text{ s}$ (b) after particle insertion at $t = 0.01 \text{ s}$ (2-D slice at $y = 25 \text{ mm from 3-D simulation}$)
Due to presence of the surface tension force, the shape of the bubble remains spherical as shown in Figure 6.18, which shows the final particle arrangements for the two resolutions. As the number of new gas particles increases further, the radius of the bubble increases as the air particles at the surface of the bubble push the water particles away at the surface. After the new particles’ insertion, the particle distribution has been arranged according to the shifting algorithm explained in Section 5.3.4.5. However, the $D$ (diffusion) parameter in Equation (5.66) has a significant effect on the shifting distance. Xenakis et al. (2015) proposed a slightly modified shifting (diffusion) parameter to eliminate particle clumping in regions of low velocity, and this was implemented in the current code. However, it was found necessary to modify the proposal of Xenakis et al. (2015) for the current application, to be given by:

$$
\delta \mathbf{r}_s = \begin{cases} 
-A_s h \| \mathbf{u} \| \Delta t \nabla C_i, & D \geq D_0 \\
-D_0 \nabla C_i, & D < D_0 \\
-D_{\text{min}} \nabla C_i, & D < D_{\text{min}} 
\end{cases}
$$

Therefore, the $D$ parameter has been defined as a low threshold diffusion coefficient which takes a value of $D_0 = 0.01 h^2$ and a minimum value of $D_{\text{min}} = 0.001 h^2$ for this bubble expansion problem. In general for this model, particle shifting works satisfactorily herein and is also necessary for these kinds of multi-phase simulation where non-uniform deformations appear.
As mentioned earlier, the simulation of the bubble modelling and expansion has been performed by insertion of new gas particles into the bubble at certain times. This particle insertion has been performed at regular intervals up to 0.05 seconds. Three simulations have been performed to identify the effect of the time period of particle insertion by inserting particles every 0.0025, 0.005 or 0.01 seconds. The radius of the bubble has been predicted using an algorithm tracking the surface.

**Figure 6.18** Expansion of the single bubbles at the end of the simulation (a) - Low resolution ($\Delta x/R = 0.2$) (b) - High resolution ($\Delta x/R = 0.1$)
particles by considering a threshold value of 2.5 for the divergence of particle positions (Equation (5.71)). The radius is given by the average distance of the gas particles at the liquid-gas interface.

\[
R(t) = \frac{1}{N} \sum_{i=1}^{N} r_i
\]

(6.8)

where \( r_i := \) all \( N \) gas particles where \( r = \sqrt{(x_i - x_c)^2 + (y_i - y_c)^2 + (z_i - z_c)^2} \) for which \( \nabla \cdot r_i < 2.5 \).

However, as the bubble was not entirely spherical due to the resolution, the initial radius of the bubble was not exactly 10 mm. The initial value is approximately 8.9 mm for low resolution (\( \Delta x/R = 0.2 \)) and 9.5 mm for high resolution (\( \Delta x/R = 0.1 \)) simulations.

The comparison of the SPH bubble expansion with the analytical solution has been shown in Figure 6.19. The predicted radius of the bubble has been shifted in time to have a comparison with the analytical solution of Patel (1980) given in Section 2.5.3. There is no bubble growth observed until the new particle insertion algorithm performed at either 0.0025 s, 0.005 s or 0.01 s. Although there is a difference between the predicted bubble growth and analytical solution, this quite complex multi-phase algorithm presented the feasibility of bubble modelling and expansion using the SPH method.

Figure 6.19 shows a qualitatively appropriate expansion of the bubble with a difference due to the initial stages and particle insertion of the SPH simulation.

Figure 6.20 shows a comparison of the rate of the bubble expansion \( dR/dt \) predicted by SPH compared with theory. The theoretical bubble expansion rate is initially non-zero. The SPH results take a short period but reach close agreement with theory by the end of the simulation. This agreement of the numerical results with the bubble expansion rate clearly demonstrates the potential of using SPH for intumescent coatings. Figure 6.20 also shows that the rate of particle insertion has a limited effect, particularly for simulations longer than 0.05 seconds that are simulated here.
Figure 6.19 Comparison of the bubble growth between SPH modelling and analytical solution

Figure 6.20 Comparison of bubble growth rates
In order to show numerical stability for the single bubble growth simulation, a time step analysis has been performed with a change of time. Figure 6.21 shows the change of time step \((dt)\) with respect to time \((t)\) when gas particles are inserted every 0.01 s. This demonstrates that the time step remains unchanged, being controlled by surface tension (Equation (5.84)) until the new particles’ introduction. With the new gas particles, the interaction and the forces between the particles increases as the distance between the particles would be less than the particle distance before insertion of new gas particles so that the time step is now controlled by Equation (5.83) where interparticle distance is in the denominator, reducing \(\Delta t_{CV}\) in Equation (5.82). Therefore, the time step reduces at 0.01, 0.02, 0.03 and 0.04 seconds based on the forces according to the variable time step explained in Section 5.3.5.2.

Following the introduction of new particles, for example at \(t = 0.01\) s, the shifting algorithm of Section 5.3.4.5 gradually rearranges the particles to have a more uniform distribution, which is demonstrated in the recovery of the time step by \(t = 0.015\) s.

![Figure 6.21 Change of time step \((dt)\) with time \((t)\)](image)
To demonstrate the need for the new particle shifting routine, Figure 6.22 represents a particle distribution after performing the mass transfer without using the particle shifting. Even though the mass inside the bubble has been increased by particle insertion, shrinkage of the bubble can be observed. The newly inserted gas particles remain almost at the same positions where they are generated while the other gas particles move according to the momentum equation (compare to Figure 6.18a). Therefore, the shifting methodology is significantly important for simulating bubble growth in multi-phase problems.

![Particle distribution at t = 0.05 s without particle shifting (Δx/R = 0.02)](image)

**Figure 6.22** Particle distribution at $t = 0.05$ s without particle shifting ($\Delta x/R = 0.02$)

The main challenges of bubble growth modelling will be explained in the following section.

### 6.5 Discussion on Challenges of SPH Bubble Growth Modelling

As demonstrated in the previous sections in this chapter, SPH is a promising method for bubble modelling that can be used to simulate the expansion process of intumescent coating. Steady bubble modelling (surface tension test cases in Section 6.2), and dynamic and non-spherical bubble modelling which have a nonlinear multi-phase behaviour (bubble formation in Section 6.3) have been developed using the SPH method. Numerical convergence and comparisons have been obtained in those studies which will help the future studies explained in Section 7.3.2. The physics of multi-phase problems such as bubble expansion in intumescent coatings contains
complex processes since they involve different phases with different properties such as the density ratio of around 1000 in gas bubble modelling. For instance, this high density ratio between fluids can be problematic with SPH multi-phase approaches and needs extra care to minimise the density and pressure fluctuations for running stable simulations. However, the results of Section 6.4 demonstrate that multi-phase SPH has the potential to simulate the behaviour of intumescent coating. There are still significant challenges for bubble growth modelling with the SPH method. They are mainly:

- A better description of the physical processes of the bubble growth mechanisms in intumescent coatings.
- The mathematical formulation of this physics, such as mass transfer into the bubbles (conversion of mass from liquid to gas) should be developed in a Lagrangian energy, mass and momentum conserving scheme.
- An appropriate SPH discretisation scheme is employed or developed.
- In this thesis, the mass transfer algorithm has been developed by estimation of the mass and converting this mass to the number of new inserted gas particles needed. However, this representation of the mass transfer can be done in a more accurate way by taking the current newly developed algorithm and improving it with better description of the physical process for intumescent coating expansion.
- The current developed particle insertion algorithm is computationally expensive with serial SPHysics FORTRAN code as it runs on a Central Processing Unit (CPU). Hence, the new algorithm should be implemented on Graphic Process Units (GPUs) to accelerate the simulations in a quick and efficient way (hardware accelerations).
- During the expansion process of the intumescent coating, thousands of bubbles are generated throughout the expanded thickness. The simulation of multiple-bubble growth, possible coalescing and bursting of bubbles pose significant challenges to using SPH, since bubble-bubble interaction needs to be considered to capture the physics of the expansion of the intumescent coating.
- Finally, more validation needs to be carried out providing all physical parameters such as viscosity, surface tension, etc. with this current developed SPH algorithm (particle insertion method with SPH).
6.6 Concluding Remarks

This chapter has presented the feasibility of using the smoothed particle hydrodynamics (SPH) method to model the bubble growth process in intumescent coating expansion.

Close agreement with analytical solutions was obtained for static bubbles with typical convergence rates for SPH obtained for the surface tension modelling. The modelling of hemi-spherical bubble forming with an orifice helped to understand the influence of high pressure on the bubble growth and also the details of the movement of the gas phase through liquid with a high flow rate resulting in non-linear multi-phase deformations. The comparison of predicted bubble growth for this study was satisfactory.

A single gas bubble’s growth in surrounding liquid has been developed and the main challenges in terms of the SPH approach have been identified and discussed. For the new approach, particle insertion to represent the mass conversion showed that this new SPH model can be applicable for the bubble expansion simulations with further improvements required for efficient, accurate and stable multi-phase simulations.
CHAPTER 7 CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE RESEARCH

7.1 Introduction

This thesis has explored using two different methods to quantify the behaviour of intumescent coatings: (1) extending the analytical solution of Amon and Denson (1984) to predict the global expansion process of intumescent coatings and to investigate the influences of different design parameters including the coating thickness, the steel section factor and the fire exposure condition on the protection performance of intumescent coatings; (2) detailed numerical simulation using the Smoothed Particle Hydrodynamics (SPH) method, taking advantage of its meshless and Lagrangian nature.

The detailed work of this research includes:

- Extending the multi-cell model of Amon and Denson (1984), originally derived to predict the speed of bubble expansion due to increasing internal bubble pressure in viscous fluid at ambient temperature with constant properties, to intumescent coatings at high temperatures with temperature dependent viscosity, surface tension and mass conversion.
- Checking the accuracy of the extended analytical approach against the test results of Zhang et al. (2012a; 2012b) for intumescent coating protected steel plates under cone calorimeter heating and in furnace fire tests.
- Using the analytical method to examine in more detail the effects of various design conditions (fire temperature-time curve, intumescent coating thickness and steel section factor) on the behaviour and thermal conductivity of intumescent coatings, and to assess the conditions under which the thermal properties extracted under the standard fire condition may be used to predict steel temperatures under other fire conditions.
- Derivation of a set of equations that describe the three-dimensional evolution of bubbles.
- Implementation of the equations in the multi-phase SPH model SPHysics FORTRAN open-source code.
• Comparison of the new SPH model results with available test cases for static bubbles, bubble growth including analytical solutions.
• Exploiting the feasibility of using SPH to simulate intumescent coating expansion and identifying the challenges as well as suggesting possible solutions.

The following sections present detailed conclusions pertaining to the above research studies.

7.2 Detailed Conclusions

7.2.1 Extension of the Analytical Model of Amon and Denson (1984)

7.2.1.1 Modelling the Expansion Process of Intumescent Coatings

The main extensions of the Amon and Denson (1984) model to allow it to predict intumescent coating expansion were: (1) non-uniform temperature field with temperature-dependent viscosity; (2) internal bubble pressure coming from mass conversion of the intumescent polymer melts to gas. An incremental approach was taken: within each time step, the Amon and Denson equation for calculating the bubble expansion rate was directly used on the assumption that equilibrium was instantaneously achieved. The modified analytical solutions were compared against the test results of Zhang et al. (2012b) under different cone calorimeter heating conditions and Zhang et al. (2012a) under different furnace fire conditions. The main conclusion is that the modified Amon and Denson equation is suitable for predicting intumescent coating expansion.

7.2.1.2 Assessment of the Behaviour of Intumescent Coatings under Different Conditions

The modified Amon and Denson model can be used to predict the expansion process of intumescent coatings. From the calculation results, the effective thermal conductivities of the intumescent coatings can be calculated for different temperatures and different rates of heating. The thermal conductivity values can then be used to calculate the intumescent coating protected steel temperatures using the steel temperature calculation equation in Eurocode (EN 1993-1-2) (CEN, 2005). In order to allow the steel temperature calculation equation to deal with the non-uniform temperature field in the intumescent coating, the intumescent coating was
divided into several layers, each having its own thermal conductivity (and hence thermal resistance) according to its temperature and rate of temperature rise. To calculate the intumescent coating temperatures, steady state heat conduction was assumed because the heat storage within the intumescent coating was considered negligible due to the very small amount of coating used. The calculated steel temperatures were compared against the measured steel temperatures by Zhang et al. (2012a). The main conclusions are:

- The maximum expansion ratio of the intumescent coating decreases as the rate of heating increases. Therefore, when other conditions are the same, a faster fire exposure would render the intumescent coating less effective than a slower fire exposure.
- Following from above, the effective thermal conductivity values extracted from the Standard fire exposure cannot be used for faster fires since this would produce unsafe results. In contrast, the same effective thermal conductivity values can be used for slower fires.
- The smothering phase of a fire has minor effects on the intumescent coating behaviour.
- When using the EN 1993-1-2 equation to calculate steel temperatures, it is necessary to divide the intumescent coating into multiple layers to accurately deal with the non-uniform temperature field in the intumescent coating. Using one single layer cannot accurately represent the significantly wide range of expansions and thermal conductivities within the intumescent coating thickness.

### 7.2.2 SPH Modelling of Bubble Expansion

A smoothed particle hydrodynamics (SPH) multi-phase model using a central processing unit (CPU) and serial open source FORTRAN code (SPHysics) has been developed in three dimensions to present the feasibility of bubble modelling and expansion in intumescent coatings. In order to simulate the bubble expansion, the SPH multi-phase model has been developed and validated against available theoretical solutions or other simulation results.

The major advantage of using SPH to simulate the multi-phase models compared to other mesh-based computational methods is that the highly non-linear
and non-uniform behaviour of the motion at the interface (e.g. interface between polymer melt and gas in this project) can easily be captured without any requirement to generate a mesh.

However, one major limitation of the SPH method is the large amount of computational resources and time needed for complex multi-phase simulations. This is related to the small time step and the number of neighbour particles of a particle, which must be increased to a large number of particles (high resolution) to achieve sufficient accuracy for applications, especially in 3-D. The open-source FORTRAN code SPHysics is not accelerated (using parallelisation or using novel hardware such as graphic processing units). Simulations have been run as a single-thread execution such that large simulations with 100,000 particles take a long time, with runs on the order of several days. Due to these problems, mainly high computational time, the SPH model in this project has been run for a short time (less than 1 second). However, the actual expansion process of the intumescent coating may take more than 30 minutes.

The SPHysics code has been significantly modified in order to tackle the multi-phase simulations for bubble modelling with necessary implementations. Those implementations and some general guidelines were:

- The code has been modified to simulate liquid-gas encountered in intumescent coatings.
- As surface tension is the key effect controlling the bubble behaviour and growth, this has been implemented in 3-D for the particle interactions.
- In order to solve the unphysical penetration or mixing of two different particles of the phases, implementation of no-penetration force has been performed in the necessary subroutines.
- For the bubble growth modelling with SPH, newly developed implementation of the mass transfer has been proposed to represent mass conversion from liquid to gas, which resulted in pressure increase inside the gas bubble. In other words, increasing the number of gas particles inside the bubble has been performed in this research.
- This thesis has used shifting particle algorithms for multi-phase bubble simulations modified by Mokos et al. (2013) based on Lind et al. (2012) and
Skillen et al. (2013). This has been implemented and modified with new threshold volumes for activation.

Three test cases (SPH simulations) have been presented in this thesis: namely surface tension models validation, bubble formation from an orifice and bubble expansion modelling. The general conclusions of each simulation will be given in the following sections.

7.2.2.1 Validation of Surface Tension Modelling

Surface tension forces are essential for accurately simulating the behaviour of the bubbles. Therefore, the current SPH multi-phase model has been validated and the validation of the surface tension has been performed with water-water and water-air bubbles, demonstrating numerical spatial convergence between first and second order. An overall satisfactory agreement between SPH and theoretical results has been obtained using a high resolution. Due to the nature of the Hu and Adams (2006) surface tension formulation, the pressure has not been well predicted in the surrounding fluid just at the interface. However, this thesis has shown that with an appropriately fine resolution, this can be acceptable for multi-phase simulations with a large density ratio (1000:1.25).

7.2.2.2 Validation of the Bubble Formation and Rise through Submerged Orifice

In order to demonstrate the expansion process of the bubble inside the intumescent coating due to the pressure increase (pressure difference between the phases), the formation, growth and detachment of the bubble from the orifice has been modelled. In addition, this presented model has given an opportunity to examine the details of the movement of gas into a liquid considering the effects of density and viscosity. It has been found that the resolution has had a great influence on the air particles’ movement and formation of the bubble at the orifice, thereby supporting the conclusion for a static bubble that a sufficiently fine resolution ($\Delta x/R = 0.1$) is required to capture the physical behaviour. As the actual model involved fixed water boundary particles, the penetration of air particles into the boundary particles (unphysical problem) has been prevented by employing the no-penetration force algorithm.
Although the surface tension was not considered in this bubble formation model, the obtained results using the SPH method had satisfactory agreement with the results of Das and Das (2009).

7.2.2.3 Bubble Growth in Polymer Liquid

Bubble growth in polymer liquids (melts) such as intumescent coatings mainly depends on the conversion of mass from liquid to gas, viscous and surface forces. Therefore, these forces have been considered to investigate the feasibility of bubble growth using the SPH method. A new SPH algorithm for representing the mass conversion has been performed to predict and simulate the single bubble expansion with and without shifting algorithm. It can be concluded that the shifting algorithm has a great influence on the bubble growth as shrinkage occurs without shifting. The comparison of the predicted bubble radius with this newly developed SPH approach showed that SPH is a potential method for these kinds of multi-phase expansion problem.

7.2.2.4 Challenges of Using SPH to Simulate Intumescent Coating Expansion and Possible Solutions

One of the main objectives of this research was to examine the expansion behaviour of intumescent coating under fire condition from different aspects including multi-bubble growth modelling in a nanometre scale rather than a millimetre scale. However, due to the complexity of the simulation and limitation of the computational resources, this global expansion model has not been simulated using SPH. On the other hand, simulating one bubble growth also presented some challenges such as the speed of sound for the gas phase and viscosity for the polymer melt phase in order to obtain similar pressure between the two phases in the interface.

One of the main challenges in simulating the process of expansion of intumescent coatings using SPH is to tackle the large expansion ratios, as the coating (the film thickness in mm size) expands to between 10 to 100 times the original thickness. This means that multiple bubbles should be modelled with a range of sizes using resolution less than 1 µm (generally the initial bubble radius is 10µm). However, due to the actual SPH formulation (Equation (5.10)) for kernel
calculations, this could not be done using SPHysics FORTRAN because of the precision error. This can be solved by changing the SPH formulation to a non-dimensional form.

Another challenge is the representation of the mass conversion in a more physically realistic manner. This thesis presented the mass conversion (increase in pressure inside the bubble) by increasing the number of air particles inside the bubble gradually at regular intervals during the simulation based on the assumption that the pressure inside the bubble is maintained. Increasing the number of particles using the SPH method is quite a sensitive and complex process, such that pressure fluctuations are possible. An alternative approach is to consider the variable resolution schemes that have recently been developed for SPH where particles are split or coalesced (merged) to provide automatically adaptive resolution for flow features of interest (Vacondio et al., 2013).

The actual expansion process of intumescent coating involves the merging and possible bursting of bubbles during the expansion and char process. These are the other challenges of simulating the whole expansion process using the SPH method. Investigations of coalescing of bubbles using the SPH method have recently been developing (Pengnan et al., 2014). Therefore, it would be worth investigating merging of bubbles within the context of application to intumescent coatings.

7.3 Recommendations for Future Research

This research has achieved its proposed objectives of exploiting the feasibility of predicting the expansion process of intumescent coatings and developing a method to quantify the global expansion process of intumescent coatings under different fire protection design parameters (coating thickness, steel thickness and fire condition involving smouldering fire). This research has identified a number of future research opportunities to further develop and improve the accuracy of the predictive methods. The following sections recommend possible future research studies.

7.3.1 Theoretical Modelling of Intumescent Coatings

- The present research used approximate rheological data for the studied intumescent coating. Matching rheological data and mass loss data should be obtained for the same intumescent coating.
To check the general applicability of the extended Amon and Denson model, further research studies should be conducted for different types of intumescent coatings.

The theoretical model allows the expansion of intumescent coatings to be calculated at different temperatures and for different rates of heating. To check the accuracy of calculating this fundamental property of intumescent coatings, a suitable experimental method that is capable of heating intumescent coatings uniformly at different rates of heating should be developed.

When calculating the thermal conductivity of intumescent coatings after expansion, the intumescent coating is treated as a porous material with an average bubble size. It would be useful to conduct direct thermal conductivity tests at high temperatures to check the accuracy of this assumption.

The analytical method quantitatively links the chemical behaviour of intumescent coatings with their fire protection performance. This is a powerful tool that can be used to help the intumescent coating manufacturers in their development of new intumescent coating products. Based on the analytical method of this research, a screening tool may be developed to judge the potential of different new intumescent coating formulations based on their chemical performance data (mass loss, viscosity, surface tension) without undergoing expensive fire tests.

### 7.3.2 SPH Modelling of Bubble Expansion in Intumescent Coatings

- This thesis only looked at a single bubble but the process of expansion of intumescent coatings involves bubble merging and bursting. Therefore, 3-D bubble SPH simulations of bubble coalescing and rising throughout the expansion process of intumescent coatings can be further investigated (Sun et al., 2015).

- As current SPH modelling of bubble growth has been performed in isothermal conditions, it is recommended that thermal effects to represent the fire conditions for intumescent coating expansion process should be considered with the SPH heat conduction modelling.

- The bubbles generated in the expansion process of intumescent coatings have expansion ratios in the order of 10-100. The methodology presented here would need to be further developed in order to capture these expansion rates.
• Alternative multi-phase formulations have recently been suggested (Szewc et al., 2014) in SPH and it might be worth investigating their suitability for intumescent coating expansion modelling. As mentioned earlier, the surface tension formulation has some drawbacks with sharp density and viscosity change at the interfaces. New surface tension approaches using SPH have been appearing in the literature. Therefore, it is recommended that an alternative and improved surface tension model should be chosen to handle the problem of accumulating density errors resulting in instable pressure at the interface and to simulate the multi-phase flows with high density ratios of 1000.

• The simulations presented were computationally expensive to run. More complex cases with more bubbles and their interaction would require many millions of particles. As mentioned previously, this is difficult and time consuming with SPHysics FORTRAN code. Therefore, it is highly recommended to develop some form of hardware acceleration such as Graphic Processing Units (GPUs) to run simulations quickly and efficiently (low energy use, etc.). It has already been proven that modelling SPH problems with GPUs presents a viable and highly accurate option (Crespo et al., 2010).

• As the main interest of this project using the SPH method lies in the bubble expansion process inside the intumescent coating. In other words, gas expansion is the main issue in the project. As mentioned previously, there should be a large number of particles in the simulation, especially for the gas phase, to obtain sufficient accuracy. The current project used a fixed resolution for all particles including gas and polymer liquid. It would be interesting to use variable resolution such as particle splitting or coalescing (Vacondio et al., 2013), (Bian and Ellero, 2014). This would help to increase the resolution for the gas phase, and therefore increase the accuracy while the resolution far from the bubbles remains fixed.
REFERENCES


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Appendix A  Comparison of steel temperatures between single layer and multi-layer calculation results and test results of Zhang et al. (2012a)

This Appendix presents the results for the comparison of measured steel temperatures by Zhang et al. (2012a) and predicted steel temperatures with single and multi-layer coating model. Details of the analytical prediction of steel temperatures are given in Section 4.5.

Figure A.1 Intumescent coating thickness: 0.4 mm, steel section thickness: 6 mm
Figure A.2 Intumescent coating thickness: 0.8 mm, steel section thickness: 6 mm

Figure A.3 Intumescent coating thickness: 1.2 mm, steel section thickness: 6 mm
Figure A.4 Intumescent coating thickness: 0.4 mm, steel section thickness: 10 mm

Figure A.5 Intumescent coating thickness: 0.8 mm, steel section thickness: 10 mm
Figure A.6 Intumescent coating thickness: 1.2 mm, steel section thickness: 10 mm

Figure A.7 Intumescent coating thickness: 0.4 mm, steel section thickness: 20 mm
Figure A.8 Intumescent coating thickness: 0.8 mm, steel section thickness: 20 mm

Figure A.9 Intumescent coating thickness: 1.2 mm, steel section thickness: 20 mm
Appendix B  Analytical solution for single bubble growth

This Appendix presents the analytical solution for a single bubble growth model based on Patel (1980). The detailed formulation is given in Section 2.5.3. In Equation (2.8), the gas pressure $P_g$ comes from the mass conversion of liquid intumescent coatings to gas and this gas pressure has been calculated using Equation (3.5). This analytical procedure is given as:

$$\frac{P_g}{P_a} = \frac{(m + \Delta m)}{m} = \frac{(V + \Delta V)}{V} \quad (B.1)$$

$$P_g = \left(\frac{\Delta V + V}{V}\right) P_a \quad (B.2)$$

where $\Delta m = 2.74 \times 10^{-6}$ kg is the amount of the mass transfer (mass conversion) into the single gas bubble of 10 mm radius with $m = 7.96 \times 10^{-6}$ kg initial mass and $4.19 \times 10^{-6}$ m$^3$ initial volume.

$P_g$ is calculated as 1.35 atm assuming that initial gas pressure ($P_a$) inside the bubble is 1 atm.

The bubble growth rate (Equation (B.3)) and the rate of change of gas pressure (Equation (B.4)) along with the initial conditions for the initial bubble radius $R_0 = 10$ mm and initial gas pressure $P_g(0) = P_{g_0} = 1.35$ atm have been solved simultaneously by using the fourth-order Runge-Kutta method implemented using MATLAB. The time step $dt$ is $1 \times 10^{-6}$ s.

$$\frac{dR}{dt} = R \left(\frac{P_g - P_a - 2\sigma_s/R}{4\eta_o}\right) \quad (B.3)$$

$$\frac{dP_g}{dt} = \left(\frac{(P_{g_0} - P_g)^2}{P_gR^3 - P_{g_0}R_0^3}\right) - 3P_g \left(\frac{dR}{R}\right) \quad (B.4)$$

where $\eta_o = 4000$ Pa.s and $\sigma_s = 0.028$ N/m$^2$.

Figure B.1 shows the radius-time relationship of the bubble.

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Figure B.1 Bubble radius-time relationship