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Konrad Wilkens Flecknoe-Brown

DOCTORAL DISSERTATION

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Abstract

In this research, both experimental test methods and computer models were used to characterise the thermal decomposition processes of selected upholstered furniture component materials, namely; flexible polyurethane foam and a range of different fabric coverings. This was first done at some of the smallest, simplest levels available, and how these materials were tested and the methods chosen to investigate them, was examined. Results here already showed the importance of thorough material characterisation and how sensitivity analysis on the chosen research tools can give the researcher a much better knowledge base to begin further studies. A direct result of this was the production of one of few full factorial analyses within fire research used to characterise the influence of test input on the experimental outcomes.From there, the obtained material characterisation parameters were used to move up the scale in both size and material complexity and investigate how this acquired knowledge from a previous lower scale can be used to predict the fire behaviour as the complexity was increased. Modelling was used to simulate material fire behaviour at a larger scale based on the model input parameters obtained at a previous simpler scale. Additionally, extended experiments, at the larger scales, were performed to act as validation for the models, but were also used to investigate the effects of increasing complexity. One of the outcomes from this work was the development of new or modified testing methods that were designed to provide new knowledge on smoke development, and improve the ability to use fire test outcomes as a means of model validation for the scaling process. Furthermore, investigations at the middle scale highlighted complex interactions when different materials (e.g. foam core and fabric cover) were combined to form a composite product. The form of interaction was also dependent on the type of fabric used, and these interactions were found to be unpredictable based on previous lower scale data.Finally, the larger scales were investigated experimentally through a series of large-scale, multi-dimensional test series. These test series, aimed to be the last rung in the scaling ladder for this study, andhighlighted a number of weaknesses or limitations in the scaling methodology. These limitations were predominately about influencing factors that could not be investigated through lower scale research, thus highlighting the need in fire science for both bottom-up (i.e. scaling methods) and top-down (i.e. large scale experiments) research methods in order to get a more comprehensive knowledge base on material fire behaviour and contribute to increasing the overall fire safety of our world.

Key words: Fire, Upholstered furniture, Polyurethane foam, Fabric, Scaling, Experimental, Modelling

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Well, I must stop somewhere, but before I do, I must give the biggest thanks, love and gratitude to my families, both in Australia and in Sweden. Especially, to my Linda and our Oliver and Otto that came into our lives and forever changed them during this research.

Summary

The overarching goal of this thesis was to investigate the fire behaviour of upholstered furniture component materials at different scales. Upholstered furniture materials were chosen for this research since furniture comprises a large portion of the fuel load within buildings, is often considered as one of the ‘first items ignited’ and is a significant factor in fire related deaths. According to the National Fire Protection Association (NFPA), upholstered furniture accounts for the largest share of fire deaths of any first item ignited in US home fires. If this is expanded to include fires where upholstered furniture is not the first item ignited but the primary contributor to the fuel load, the estimates for losses (e.g. death and damage) increase significantly.

In the context of this thesis, the term “different scales” has two intertwined meanings; the first follows the physical definition of scale, beginning with small and moving up to the large – for example, starting with a small piece of foam and ending in a large foam mattress. The second, which is inherently linked with the physical scale, is about complexity - moving from the simple to the more complex, an example of this may be going from a single material to a composite product.

In this research, both experimental test methods and computer models were used to characterise the thermal decomposition processes of selected upholstered furniture component materials, namely; flexible polyurethane foam and a range of different fabric coverings. This was first done at some of the smallest, simplest levels available, and how these materials were tested and the methods chosen to investigate them, was examined. Results here already showed the importance of thorough material characterisation and how sensitivity analysis on the chosen research tools can give the researcher a much better knowledge base to begin further studies. A direct result of this was the production of one of few full factorial analyses within fire research used to characterise the influence of test input on the experimental outcomes.

From there, the challenge was to use the obtained material characterisation parameters and move up the scale in both size and material complexity and investigate how this acquired knowledge from a previous lower scale can be used to predict the fire behaviour as the complexity was increased. This was achieved with modelling work – trying to simulate material fire behaviour at a larger scale based on model input parameters obtained at a previous scale. Additionally,

extended experiments, at the higher scales, could not only act as validation for the models, but were also used to investigate the effects of increasing complexity. One of the outcomes from this work was the development of new or modified testing methods that were designed to provide new knowledge on smoke development, and improve the ability to use fire test outcomes as a means of model validation for the scaling process. Furthermore, investigations at the middle scale highlighted complex interactions when different materials (e.g. foam core and fabric cover) were combined to form a composite product. The form of interaction was also dependent on the type of fabric used, and these interactions were found to be unpredictable based on previous lower scale data.

Finally, the larger scales were investigated experimentally through a series of large-scale, multi-dimensional test series. These test series, aimed to be the last rung in the scaling ladder for this study, ended up highlighting a number of weaknesses or limitations in the scaling methodology. These limitations were predominately about influencing factors that could not be investigated through lower scale research, thus highlighting the need in fire science for both bottom-up (i.e. scaling methods) and top-down (i.e. large scale experiments) research methods in order to get a more comprehensive knowledge base on material fire behaviour and contribute to increasing the overall fire safety of our world.

List of Publications

This thesis is a compendium of the work presented in six publications. The publications are included in Annex A at the end of the thesis. The author's contribution to each of the publications is described in the following table.

Paper I	Wilkens Flecknoe-Brown, K. and van Hees P. (2018). "Sensitivity analysis on the microscale combustion calorimeter for polyurethane foam using a full factorial design methodology", *Journal of Fire Sciences. Vol 36(6) pp. 453-471. DOI: 10.1177/0734904118798603*
Paper II	Wilkens Flecknoe-Brown, K., Hostikka, S. and van Hees P. (2016). "Pyrolysis modelling of composite fabrics based on individual fabric properties using micro combustion calorimetry". *Interflam 2016, Proceedings of the 14th International Conference.4-6 July 2016, Nr Windsor, UK, pp. 131-142. Interscience Communications Ltd.*
Paper III	Wilkens Flecknoe-Brown, K. and van Hees P. (2015). "Obtaining additional smoke characteristics using multi-wavelength light transmission measurements", *Fire and Materials 2015 Proceedings of the 14th International Conference.2-4 February 2015, San Francisco, US, pp. 136-148. Interscience Communications Ltd.*
Paper IV	Wilkens Flecknoe-Brown, K., Livkiss K., and van Hees P. (2017). "Experimental and numerical investigation on fire behaviour of foam/fabric composites", *Fire and Materials 2017 Proceedings of the 15th International Conference.2-4 February 2017, San Francisco, US, pp. 240-253. Interscience Communications Ltd.*
Paper V	Wilkens Flecknoe-Brown, K. and van Hees P. (2021) "Experimental investigation into the influence of ignition location of flame spread rates of polyurethane foam slabs", *Fire and Materials. Vol 45(1) pp. 81-96.* DOI: 10.1002/fam.2921

Paper VI	Wilkens Flecknoe-Brown, K. and van Hees P. (2021) "Geometrical and environmental effects on fire behaviour of flexible polyurethane foam slabs", *Manuscript (submitted)*

PAPER	AUTHOR'S CONTRIBUTION
I	The author developed the test methodology and performed the tests. The author performed the data analysis and wrote the paper.
II	The author developed the concept, performed the tests and the majority of the simulations. The author wrote the majority of the paper.
III	The author developed the concept, and wrote the calculation software. The author performed the data analysis and wrote the paper.
IV	The author co-designed the experimental procedures and performed the experiments with co-authors. The author performed the majority of the simulations and wrote approximately half of the paper.
V	The author designed the experiments and performed the tests with colleagues. The author performed the data analysis of results and wrote the paper.
VI	The author designed the experiments and performed the test with colleagues. The author performed the data analysis of results and wrote the paper.

Other publications not included in the thesis

- McLaggan, M. Wilkens Flecknoe-Brown, K., Dragsted, A., van Hees, P., Heat release and flame spread assessment of insulation in External Thermal Insulation Composite System (ETICS) facades, 3rd European Symposium on Fire Safety Science 12–14 September 2018, Nancy, France.
- van Hees P., Wahlqvist J., Andres B., Wilkens K., Bhargava A., and Livkiss K., "Analysis of fire barriers with respect to fires with combustible gases and liquids". *Fire and Materials, San Francisco USA, February 2017.*
- van Hees P., Andersson B., Guay F., Lauridsen D., Barghava A., Livkiss K., Andres B., Vermina Lundstrom F. and Wilkens K. , "Simulation of

fire technical properties of products and construction barriers to support efficient product development in industry”. *Interflam, Windsor UK, June 2013.*

Table of Contents

1 Introduction

Defining what a fire actually is, is a much harder task than at first glance, and through the work enclosed in this thesis, I find myself having more questions than answers. However, establishing that the consequences of fire can be incredibly serious, is not difficult. Everybody learns this as a child, and we see its impacts in all scales of life, from the smallest candle flame to the largest forest fire. Thus, it stands to reason that we need to know more about this phenomenon so that we can better prepare ourselves for when it jumps into life again – as it surely always will.

So, what to investigate? This is the next question once we have established that it is an important phenomenon to study and this too, is an extremely difficult question. I find Michael Faraday put it best:

"*There is not a law under which any part of this universe is governed which does not come into play and is touched upon… there is no better, there is no more open door by which you can enter into the study of natural philosophy than by considering the physical phenomena of a candle*."

Michael Faraday, Chemical History of a Candle - Christmas lectures at the Royal Institution.

We can extend this passage even further, as the study of fire not only encompasses the realms of natural philosophy, but extends into human philosophy as well. How we behave in a fire event, especially when we are considering the approach of "fire safety", plays a huge role in such considerations. Although not discussed further within this thesis, the importance of the "human factor" in determining the consequences of a fire should never be underestimated.

Returning to the research encompassed in this thesis, a quote from the author Johan Goudsblom below provides a seed from which some of the work in this thesis has grown:

"By far the greatest number of fatal fire incidents around the world occur in the single-family home - According to the simplest definition (although not entirely correct) fire is a process of combustion, manifested in heat and light. Its immediate effect is destructive. It reduces the highly organised structure of organic substances, to ash and smoke. A process that is self-perpetuating, irreversible and serves no obvious purpose other than to destroy."

Johan Goudsblom, 1992.

The subsequent sections of this first chapter endeavour to explain in more detail, why, from this seed, the work for this thesis was undertaken. Chapter 2 then provides a brief summary of the background knowledge that was acquired from the literature, and Chapter 3 turns this knowledge into a set of research objectives to strive for. The subsequent chapters then attempt to explain how these objectives were achieved through the research methods and both experimental and computational studies at the various scales. From this, the learnings of all this work are highlighted and the thesis concluded. A discussion about work that still needs to be done is provided and a list of references, that I am grateful to for imparting much of their knowledge and wisdom to me, follow behind. Finally, the appendix provides copies of the scientific papers which represent the core of this thesis, in case the reader wants to dive deeper.

1.1 The FIRETOOLS project

The second seed for the work that lead to this thesis was its connection to a much larger project: the FIRETOOLS project. Hence, it is important to give a brief summary of that project here for context. The FIRETOOLS project was an EU program, funded through the Marie Skłodowska-Curie Initial Training Network (FP7-PEOPLE-2012-ITN). The consortium behind FIRETOOLS – the Danish Institute of Fire and Security Technology (DBI) and the Division of Fire Safety Engineering from Lund University (LTH) along with associated industry partners, aimed to provide a training network for five Early-Stage Researchers (ESRs), who were to carry out research on fire safety, with a particular focus on the use of fire modelling and scaling, to increase the knowledge obtained from fire tests conducted on materials involved in the built environment.

The research activities within FIRETOOLS were organised through seven work packages, which comprised five individual ESR research projects, structured around three different designated scales and three different application areas as illustrated in Figure 1. The scales were:

- **Bulk material or micro scale**: at this scale, only the fire behaviour of individual materials in very small amounts (<1g) was investigated through the use of both lab scale experimentation and detailed modelling approaches.
- **Composite materials scale:** most real materials and products within the built environment are a composition of multiple component materials, at this scale the interaction and fire behaviour of these composites was to be investigated through both experimental and modelling research.

- **System scale:** this scale represents the largest studied scale, and takes into account not only the materials but also the geometrical and environmental context of how these materials are used in the “real world”.

Research within these scales was applied in three different areas, designated as:

- **Building Content:** interior and objects that are added after a building has been completed, e.g. furniture, TV, etc.
- **Building Products:** products used in the construction of a building, e.g. gypsum and wood wall panels, paints, insulating materials, etc.
- **Building Barriers:** the boundaries of a room or fire compartment, i.e. the combination of various building products used to create fire compartments to inhibit the spread of fire to other parts of the building.

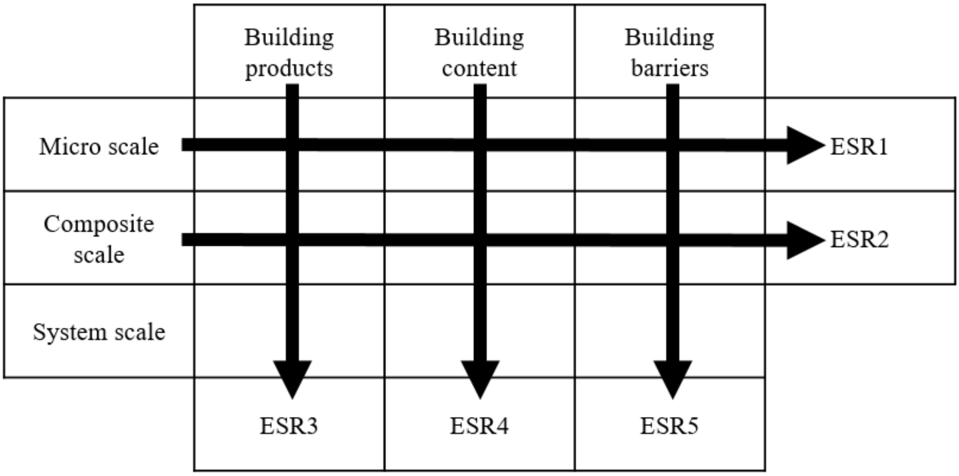

Figure 1 – FIRETOOLS project structure

Each ESR was designated either as an application area using all scales, or centred on a specific scale across all application areas. The focus of this thesis is *Building Content* (ESR4) through all scales as illustrated in Figure 2.

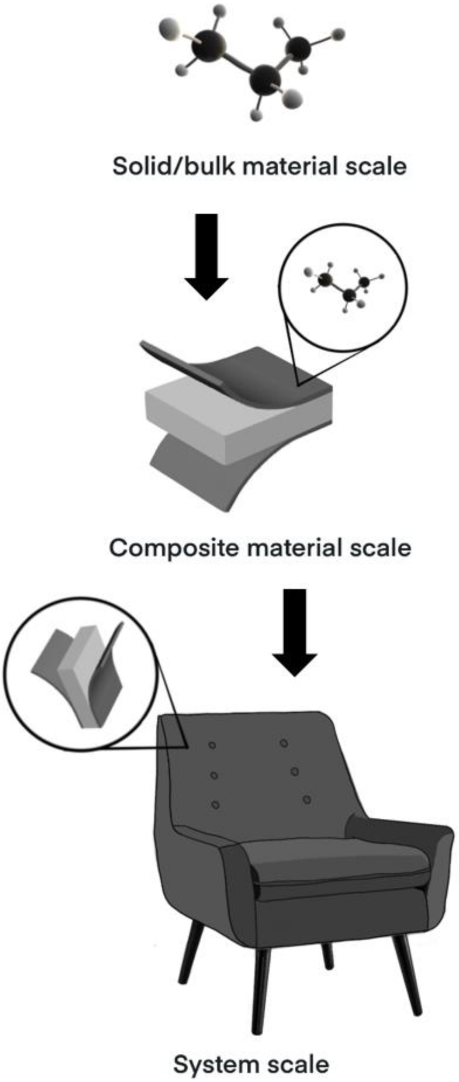

Figure 2 – FIRETOOLS methodology for ‘building content’ (ESR4)

1.2 Building Content

Building Content is defined in this thesis as: An object(s) that can be moved and/or is mobile that is placed within a building, which is not a part of the building's construction and/or internal infrastructure (e.g. lighting, doors etc.).

Some examples include but are not limited to: Furniture (e.g. sofa, chairs), Electrical equipment (e.g. TVs, computers) or other (movable) internal furnishings (e.g. curtains). Building content is usually a composition or assembly of numerous materials, and is predominately of a combustible nature.

1.2.1 Why is building content important?

One of the first tasks that fire engineers must undertake in many new projects is to define and develop fire scenarios. Fuel load density, the burning characteristics and the properties of the enclosure are generally the dominating quantities that will define this task. Fuel loads quantify the amount of energy available as fuel to the fire, and the burning characteristics or fire behaviour of the fuel (e.g. how easily it ignites and how quickly a fire spreads) designate how that energy and the products of combustion will be dispersed into the space and over time.

Building content is an important subject as this is generally where a significant portion of the fuel for a space is contained (Elhami-Khorasani et al., 2019) and thus, it will, in many cases, be a defining factor in the initial fire development and design for a fire scenario.

When considering the fire behaviour of building content, it is most important to define 'what', within this broad definition, should be the focus of any study. The majority of previous research has focused on the fire behaviour of furniture, in particular upholstered furniture, (Babrauskas et al., 1982) and the CBUF project (Sundström, 1996) along with many others (e.g. Enright, 1999; Krasny et al., 2008; Valencia, 2009) demonstrate this. This preference is attributed to the fact that furniture comprises a large portion of the fuel load within buildings, is often considered as one of the 'first items ignited' and is a significant factor in fire related deaths (Ahrens, 2017, 2013; Fabian, 2013; National Fire Protection Association, 2013, 2011; Steen-hansen and Kristoffersen, 2007a; Sundström, 1996; Wong and Spearpoint, 2001; Young and Fleischmann, 2007). Examples include: a publication from the US National Fire Protection Association (NFPA), and the fact that upholstered furniture accounts for the largest share of fire deaths of any first item ignited in US home fires (Ahrens, 2017; National Fire Protection Association, 2013). If this is expanded to include fires where upholstered furniture is not the first item ignited but the primary contributor to the fuel load, the estimates for losses (i.e. death and damage) increase significantly, with deaths increased from 19% to 24% in the US (National Fire Protection Association, 2013). In the Netherlands, furniture accounts for 29% of the object of fire origin in fatal fires, and this increases to 39% with the inclusion of beds/mattresses (Kobes and Groenewegen, 2009), while in New Zealand this figure is reported as approximately 35% of residential fire deaths (without counting mattresses) (Wong and Spearpoint, 2001)[i].

Upholstered furniture, in this case, refers to furniture items that in their simplest forms, have soft padding (e.g. foam), surrounded by a fabric cover (e.g. cotton, polyester), some examples include a sofa or armchair. The consequence of these statistics means that the majority of the research within this thesis continues the tradition of, and focuses on, the investigation of the materials involved in upholstered furniture.

1.2.2 What fire behaviour is important with regards to building content?

When considering the fire behaviour of building content, and how to begin searching for relevant research questions (which are outlined in chapter 3), there are four initial points to consider:

- Which phenomena should be considered under the umbrella of “fire behaviour”.
- How such phenomena contribute to: the development of the fire, its spread, the safety of occupants and the effect on other building components.
- Which phenomena within the term “fire behaviour” would be the most useful to others within relevant fields (e.g. practising fire engineers, product developers, etc.).
- What has previous research investigated and achieved within these topics.

To begin, consider point 1 - What phenomena come under the topic of fire behaviour? Here it is important to separate out the term *fire behaviour* in more detail to help define, and then refine the topics worthy of further investigation. In this thesis, *fire behaviour* has been separated into two distinct areas represented by the following questions:

a) how does the material/product begin to undergo thermal decomposition?

This question pertains more to fundamental material properties – the chemical makeup of the material and how it reacts when exposed to heat, the thermal

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[i] Statistics mentioned here are based solely on residential fires, and do not include e.g. mattresses. For statistics on mattresses the reader is referred to (Krasny et al., 2008) or other building types.

degradation process (e.g. kinetics and pyrolysis), heat transfer through the material (e.g. thermal conductivity, specific heat) and any associated material transformations (e.g. phase changes, char formation). This also includes the process of ignition.

b) what are the results of the combustion process?

This question refers to what happens to the materials/products after ignition occurs. Relevant considerations here are fire growth, energy release, smoke and toxic gas production and how the fire spreads across the material and extinguishes.

In point 2, we must not only look at the phenomena, but also consider how these are affected by the surrounding environment, e.g.: geometry, transportation of combustion products, spread to other materials and heat feedback are all important phenomena in this context.

Points 3 and 4 define the target audience of the research, ensures it is relevant, has not already been addressed previously and helps to refine what the research objectives for this thesis should be.

2 Background

The specific research project this thesis encompasses has a focus on fire behaviour of building content from the material to the system scale. Much of the theoretical background on the fundamental material properties is considered insensitive to the “application area” (i.e. building content, product or barriers). The background theory for how materials begin to undergo thermal decomposition was covered within the FIRETOOLS reports (Bhargava et al., 2016) and theses of ESR1: Abhishek Bhargava (Bhargava, 2020) and ESR 2: Karlis Livkiss (Livkiss, 2020). Hence, in this section, focus is on providing some background knowledge on the broader processes that occur after ignition, namely fire growth, its spread, and smoke production.

2.1 Fire growth

Studies for both building content and building products have traditionally focused on fire growth. In fact, for building products, the Euroclass system given in EN 13501-1 was developed for classifying building products in terms of fire performance. The major test method for the Euroclass system; the SBI (Single burning item) method – EN13823 (Technical Committee CEN/TC 127 “Fire safety in buildings,” 2020), is based on the concept of fire growth being the most important factor to consider. Both the testing apparatus and the parameters for the major classification obtained from it – the FIre GRowth RAte (FIGRA) index and Total Heat Release (THR), were designed as a means to quantify how quickly a fire develops (Sundström, 2007) and how much energy is produced. The fire growth process is composed of three main mechanisms; ignition, heat release rate (HRR) and flame spread. Depending on preference, fire growth may also be defined by an increase in mass loss rate (MLR) rather than HRR. However, both define an increasing rate as a key parameter (Babrauskas and Peacock, 1992; Quintiere, 1997).

Mechanisms affecting fire growth are now briefly described and a general discussion on sensitivity with regards to how these parameters affect growth is conducted in subsequent paragraphs.

2.1.1 Ignition

Ignition can be defined as an exothermic process in which a chemical reaction takes place that requires the combination of fuel (e.g. volatiles), oxygen in the correct proportions (i.e. within the flammability limits for a given fuel) and heat (Babrauskas, 2003; Torero, 2016). This is what is commonly known as the “fire triangle” – which has subsequently been updated to the “fire tetrahedron” with the additional requirement of a chemical chain reaction to sustain the combustion process (Babrauskas, 2003). Ignition is accompanied by the production of energy in the form of heat and light, and the conversion of volatile gases into the by-products of the combustion process. Ignition of fuel can occur in two ways:

- Piloted ignition, by which an external source of heat is used to ignite the fuel (e.g. spark) and initiates combustion
- Non-piloted ignition/Auto-ignition, which usually requires much higher temperatures, increased oxygen or higher pressures (Huth and Heilos, 2013) in order for the fuel to receive the required energy to initiate combustion

One commonly used simplification of ignition phenomena used in the testing and modelling communities, is the semi-empirical parameter known as the ‘ignition temperature’. This term refers to a specific temperature at which a fuel is certain to ignite. This is however based on a broad assumption, as the influence of the local fuel/air mix, that must be within the required flammability limits for ignition to occur, is not explicitly considered (Janssens et al., 2003). Hence, this methodology is technically valid only for the specific experimental conditions under which this parameter was determined (Bowes, 1952). However, Janssens et al. (2003) state that surface temperature at ignition of thermoplastic materials and some charring materials, such as wood, is reasonably constant, although when the time to ignition is greater than a few minutes the surface temperature of some charring materials can increase significantly with lower imposed heat fluxes. Much research has been focused on the “ignition problem” and the reader is referred to the thesis of ESR3 – Frida Vermina Plathner (Plathner, 2020) for a more detailed account and investigation of this topic.

The critical radiant heat flux to the surface has also been used as a measure in determining piloted ignition propensity. This parameter is also considered to be sensitive to environmental and geometrical changes (i.e. material orientation). However, it can be useful in modelling, as a minimum imposed heat flux is deduced, under which ignition is unlikely to occur.

The method predominately used to obtain the above-mentioned parameters is to undertake numerous time to ignition measurements (t_{ig}) with a range of different applied heat fluxes (i.e. using a radiant heat source, e.g. the Cone calorimeter (ISO 5660-1). By measuring the t_{ig} at a number of incident heat fluxes, at slowly decreasing values, until no ignition occurs (within a reasonable time), an estimate of the critical heat flux (Drysdale, 1998) can be obtained. Ignition temperature may also be calculated from these plots (Janssens, 2004).

The critical mass flux for solid materials may be quite hard to determine. While a number of methods have been proposed, none has been shown to demonstrate widely applicable results. However, critical mass flux has been seen as a way forward in terms of specifying a more ‘fundamental’ ignition parameter; for more information and novel research on this topic, the reader is referred to Plathner’s thesis (Plathner, 2020).

Ignition is considered a central phenomenon in both modelling and experimental studies. In the context of the full-scale fire behaviour of materials (i.e. system scale), it is known that the choice of ignitor and location of ignition point can have a large impact on the outcomes and consequences of a fire scenario (Söderbom et al., 1996). Even so, relatively few studies (Cleary et al., 1994; Janssens, 2012; Mitler and Tu, 1994; Robson et al., 2014; Söderbom et al., 1996; Wang et al., 2011; Yoshioka, 2014) were found that experimentally investigated how large of an impact these types of small changes can have. Some additional examples highlighting this are presented in the studies performed in the CBUF project (Sundström, 1996). In these studies, the location or type of the ignition source on an item of upholstered furniture is the varied parameter. Measured outputs show large variations in the peak HRR and the overall HRR curves differ significantly.

2.1.2 Heat Release Rate

The heat release rate (HRR) is defined as the rate (time) at which energy (in the form of heat) is released by the material undergoing combustion and has the units of Watt (joule per second). Often in fire science, kilowatt (kW) is the commonly used unit of measurement. The HRR is often quoted as “*the single most important variable in fire hazard”*(Babrauskas and Peacock, 1992). Fire growth, by definition, is the growth of the fire after ignition, this implies an increasing production of energy (heat), which is more commonly referred to as a “rate”. This rate increase can occur in two ways; by an increase in heat to the burning surface e.g. through heat flux contribution from the fire itself, or by an increase in the area of volatilization, pyrolysis and burning due to the spread of flame. Both of them can occur individually or simultaneously and subsequently increase the rate of heat release (and the rate of the overall production of species).

When considering a well-ventilated scenario (i.e. when there is excess oxygen to sustain the combustion), heat release is largely associated with fuel consumption. Hence, it may be said that fire growth is closely connected to the nature of the fuel, i.e. the material (Torero, 2013). However, the assumption that the fuel itself governs the fire growth, may only be considered in a free burning environment. In many cases (often the more realistic cases) HRR is dependent not only on the fuel, but similarly on the geometry of the fuel, the spreading rate and the external environmental factors (Poulsen and Bwalya, 2011; Van Hees et al., 2017; Zeinali et al., 2021).

2.1.3 Flame Spread

The aim of this section is to give a basic overview of flame spread, present the basic equations and highlight some of the important factors that can affect it. It is not the intention to cover all aspects and detailed theories of flame spread in this work but to highlight those points used in this thesis. For a more in-depth review the reader is referred to one of the many comprehensive texts on the topic, such as the review by Williams (1977). In this thesis, the focus is on flame spread over combustible solid materials. Flame spread in this context can be described as an advancing ignition front through the processes of heat transfer, where the released volatile gases from the material are ignited by the flame, which in-turn heats the unburnt material ahead of the flame, ensuing further pyrolysis, and moving the flame front onward as illustrated in Figure 3 below.

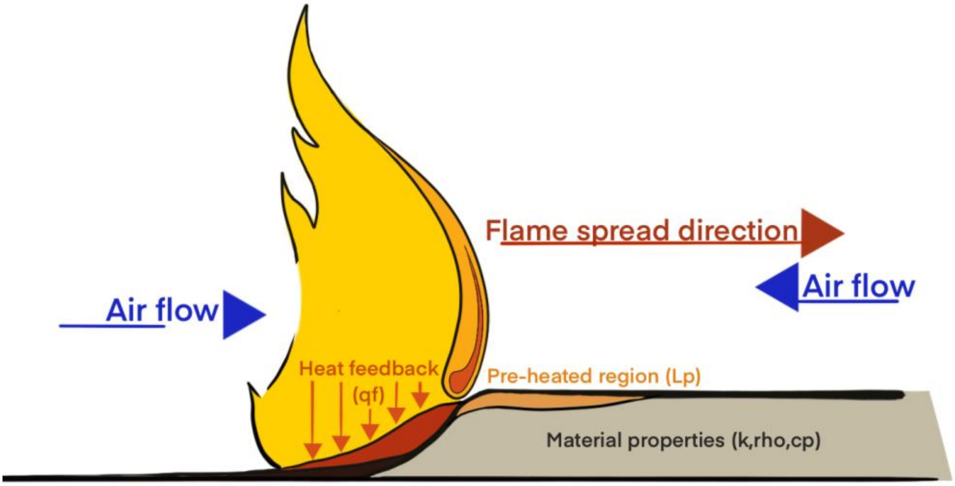


Figure 3. Simplified illustration of fire spread processes

The flame front may either spread in the direction of the air flow (i.e. concurrent) or opposed to the entrained air (i.e. opposed). Concurrent spread is usually the case for upward flame spread whereas opposed is usually assigned to downward spread. In real fires and especially in the case of horizontal spread (where the mode may be dependent on where the point of ignition occurs, the geometry of the burning object and the ventilation conditions) both forms of spread (concurrent and opposed) are likely occurring simultaneously as spread tends towards all regions of unburned fuel (Huang and Gao, 2021).

Flame spread in its most basic mathematical form is a velocity function (V_f), and can broadly be defined as the change in area (dA_b) of the burning region over the perimeter of the burning area (p) and the change in time (dt) (Huang and Gao, 2021):

Equation 1

$$V_f = \frac{dA_b}{p \cdot dt}$$

Translated into physical properties, the spread rate is governed by the ratio of heat transfer to the fuel and the thermal inertia of the fuel (Williams, 1977):

Equation 2

$$V_f = \frac{\dot{q}_f''^{\,2} L_P}{\rho_F k_F c_F (T_{ig} - T_0)^2} = \frac{heat\ transfer\ to\ fuel}{material\ properties\ of\ fuel}$$

Where $\dot{q}_f''$ is the effective heat flux from the fire and L_P is the pre-heating region respectively, ρ_F, k_F, c_F are density, thermal depth and specific heat of the fuel and $(T_{ig} - T_0)$ represent the difference between the ignition and ambient temperatures.

Equation 2 is still a simplified description of flame spread, as there are many other factors that can impact flame spread that are not accounted for. Table 1 lists examples of some of the material and environmental factors affecting flame spread.

Table 1. Processes that affect flame spread (Drysdale, 1998)**.**

Chemical Material Factors	Physical Material Factors	Environmental Factors
Composition of fuel. Presence of retardants or other chemical additives.	Initial temperature. Surface orientation. Direction of propagation. Thickness. Thermal capacity. Thermal conductivity. Density. Geometry.	Composition of atmosphere. Humidity. Pressure of atmosphere. Temperature. Imposed heat flux (re-radiation). Air velocity.

These processes may be interdependent or dependent on factors not included in the table, and other phenomena such as *delamination, melting* and *charring* may also change the behaviour of the fuel and the flame spread mechanisms.

2.2 Smoke production

The topic of smoke production pertains to how smoke develops during thermal decomposition. Important factors related to smoke production include: what can affect its production, and the visual perception through smoke, i.e. how smoke affects a building occupant or person's ability to 'way find' (i.e. see exit signs and use escape routes) through smoke. The visual perception through smoke in this manner is often defined by the term *visibility*.

Smoke production is an important, but in the opinion of the author, a somewhat overlooked phenomenon within the topic of "fire behaviour". Referring to the questions outlined in Section 1.2.2 as a guide, in some cases it should be considered one of the most important issues. Some arguments for this position include:

- it impacts significantly on occupants' life and safety – inhalation of smoke is often highlighted as one of the actual causes of death in a fire scenario over the fire itself (Harland and Woolley, 1979).
- More knowledge of it would be extremely useful for fire safety engineers (FSEs) – ask a FSE doing computational fluid dynamics (CFD) modelling of fire scenarios which tenability criterion usually governs when an area is no longer deemed "safe", undoubtedly they will reply "visibility" (which is a direct outcome of smoke production).
- There is a definite lack of research on the topic in the scientific literature compared to other subjects such as HRR and flame spread.

2.2.1 Factors affecting the production of smoke

The definition of smoke for this section follows that of G.W. Mulholland in the SFPE handbook: *a smoke aerosol or condensed phase components (excluding gases) of the products of combustion outside the combustion zone* (Mulholland, 2008).

The production of smoke is one of the basic features we associate with fire. There are many factors within the fire environment that can affect the production and characteristics of smoke; materials, combustion conditions (flaming or smouldering), ventilation (under-ventilated or not) and the surrounding environment are a few examples of these factors. Smoke emission outside the combustion zone represents a divergence, away from ideal combustion. Therefore, by definition, smoke is comprised of the products from an incomplete combustion process.

Though it is not possible at this stage, to predict smoke emission in detail based on fuel chemistry and the conditions of combustion, several factors that influence smoke production and composition are known (Mulholland, 2008). Some examples of influencing factors are briefly described below:

- Material structure – Materials may be more or less inclined to produce smoke when burning, depending on their chemical structure. For hydrocarbons, a higher number of carbon-carbon bonds generally indicates a higher smoke production potential compared to materials with fewer or single carbon-carbon bonds (Rasbash and Drysdale, 1982). It is thought that aromatics undergo gas-phase condensation within the flame to produce higher yields of polyaromatic species (e.g. PAHs), which are the precursors of soot, and thus, smoke. In contrast, the presence of chemically bound oxygen within the materials may reduce the smoke production potential of materials by increasing the available oxygen for combustion (Bras et al., 2004). A ranking of smoke production potential for hydrocarbons taken from Rasbash and Drysdale (1982) is shown in Table 2:

Table 2 Smoke Production Potential for Hydrocarbons (Rasbash and Drysdale, 1982)

Rank of Smoke Production Potential	Hydrocarbons
Highest	Naphthalene
	Benzene series
	Alkynes
	Alkenes
	iso-alkanes
Lowest	n-alkanes

- Ventilation conditions – As smoke is generally considered a product of incomplete combustion, ventilation conditions will affect the completeness of combustion by limiting the available air or oxygen required by the combustion process, therefore affecting the smoke production (Ukleja, 2012). The effects of ventilation may be quantified in various ways; one method is by using the equivalence ratio (Φ) which is defined as the ratio of actual fuel/air to the ratio of stoichiometric fuel/air. If this value is <1 combustion is lean, with excess air, if >1 combustion is rich with insufficient air to complete the process hence products of incomplete combustion remain.

- Modes of combustion – The mode of combustion can significantly affect the composition of unburned products of which the smoke is composed. Smoke from smouldering combustion tends to be formed by aerosolised droplets of condensed, partially oxidised products, similar to that found in unburned pyrolysed material, and is usually light in colour. In contrast, flaming combustion is typically (though not always) characterised by darker smoke (Putori, 1999), which may predominately be composed of unburned carbon particles. Modes of combustion can also affect the mean particle sizes and smoke yields (i.e. gram of smoke produced per gram of fuel burned), with flaming combustion tending to create smaller mean particle sizes and smouldering combustion generating high smoke yields (Fabian and Pravinray, 2007).

- Size of the fire – Various studies, (e.g. Mulholland, 2008), have shown that the amount of smoke produced can also depend on the fire size. Generally, up to a point, smoke yields have been shown to increase with fire diameter. Studies on crude oil fires (Mulholland et al., 1996) show that up until an approx. fire diameter of 10m, smoke yields increased, after which they began to decrease. Other research shows a decrease in the overall soot yield from larger experimental fires compared to smaller ones (Gottuk et al., 2008).
- Agglomeration and residence time – As smoke particles are produced and escape the combustion zone, they interact with each other. Non-reactive collisions between particles take place, and agglomeration may occur when colliding particles fuse together, forming new, larger particles. Hence, agglomeration affects the number density and size distribution of particles within the smoke. Residence time, i.e. the time in which the smoke resides in a certain volume, also affects number density and size distribution as longer residence times lead to increased opportunities for collisions and hence, further agglomeration to occur (Floyd et al., 2014) This overall phenomenon is often called smoke aging.

2.2.1.1 Soot yield

The soot yield (Y_s) or otherwise known as the smoke conversion factor (ε) and in this thesis also defined as *Smoke yield*, is designated as the mass of smoke produced ($\dot{m}_S$) per mass of fuel burned ($\dot{m}_F$):

$$Y_S = \frac{\dot{m}_S}{\dot{m}_F}$$

Caution should be exercised when assessing this parameter as the definitions of smoke and soot can be different. Smoke may be defined as at the beginning of this section which can include various products of incomplete combustion, such as; carbon particles, tars and other aerosolised liquid particles, and in some cases gases are also lumped into this definition. Soot on the other hand, is usually defined only as unburned carbon particles, though this is not always the case, hence, caution is needed. Therefore, values given in references such as Mulholland (2008) not only depend on the conditions in which they were measured, they may also depend on the authors' definition of smoke/soot and how it was measured.

Smoke yield is an important property for modelling purposes, as currently, this parameter is a critical component for determining how much smoke should enter the calculation domain in a simulation (McGrattan et al., 2015a). In FDS (Fire Dynamics Simulator), soot yield, which in this case refers to the more general smoke case, is used in conjunction with burning rate calculations, to determine the amount of smoke produced from a designated fire and transported through the computational domain (McGrattan et al., 2015b). This in turn can be used to assess the level of risk to occupants (usually by the determination of visibility) in a building, by fire safety engineers.

2.2.2 The Visual Perception of Smoke

Smoke, as defined above, consists of particulate matter and aerosolised liquid droplets from incomplete combustion. These constituents of smoke, generally being in the same size range as the wavelengths of visible light (electromagnetic radiation with a frequency of ≈390-700nm), interfere with, and obscure the passage of this light. The consequence of this effect is the reduction of our vision through smoke, thereby hindering the visibility of exits and our ability to escape from fire (Gann and Bryner, 2008).

Particles within the smoke interfere with light via scattering and absorption, this can be a highly complex process, dependent on the particle size, shape and composition as well as the wavelength of the light (Bohren and Huffman, 2004). Simplified, as shown in Figure 4, the action of scattering and absorption results in a reduction of the light beams intensity, a process known as light extinction.

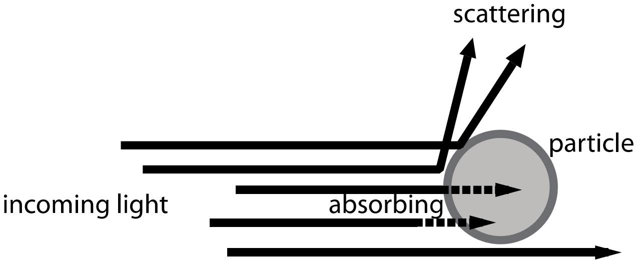


Figure 4 – Light scattering by smoke particles

2.2.2.1 The Extinction Coefficient

Light extinction is used as a method to measure smoke from fires; most techniques are based on measuring what is known as the extinction coefficient. The extinction coefficient of the aerosol equates to the fractional loss of light intensity per unit path length associated with an elemental thickness *dL* (Hinds, 1982).

For a parallel beam of light, such as that in Figure 4, the extinction coefficient (k_e) is related to the ratio of the intensity of light (I) after traversing a set distance (L)

and the intensity of the incident light (I_0) via what is known as Bouguer's, or the Beer-Lambert law (Hinds, 1982):

Equation 3

$$\frac{I}{I_0} = e^{-k_e \cdot L}$$

Equation 3 means practically, that the extinction coefficient can, with relative ease, be determined experimentally by using light transmission measurements. The extinction coefficient can then be used to determine smoke production rates and the perceived visibility of persons through smoke e.g. in an evacuation scenario.

2.2.2.2 Visibility

The visibility of exit signs and escape routes is an important criterion with regards to occupants attempting to escape from fire. In order for objects (e.g. signs, doorways) to be seen, there must be a certain level of contrast between the background and the object being viewed. The level of contrast can be determined using various methods, however, these usually involve measuring the intensity of the luminance from the object and the background and comparing them in some way (Hinds, 1982; Mulholland, 2008). In fire engineering however, the most common method is instead to use empirically determined constants for illuminated or reflective signs, and the extinction coefficient as follows:

Equation 4

$$S = \frac{C}{K_e}$$

where S is the determined visibility (m), C is the visibility constant and K_e is the extinction coefficient. The issue with this method is the use of these generic constants, which may not accurately characterise the scenarios in which they are being used, and that the extinction coefficient is highly dependent on the scenario (Gottuk and Lattimer, 2016), the wavelength of light (Widmann et al., 2003), and the material (Hurley et al., 2016).

2.3 Research gaps

Fire growth in particular, is a largely studied area in fire science, however there are aspects that still require much research. Some of these aspects identified during this research include:

The scalability of material property data.

- Material property data retrieved at a small scale may not necessarily be viable for full-scale modelling. This is due to many factors, for example: boundary conditions of the small-scale test being incorporated into the retrieved properties, dependencies (e.g. temperature) of the property itself, or the use of similar (but not the same) material data acquired from the literature.

Composite performance and material properties at elevated temperatures or at various heat exposures and material-material interactions.

- How materials react at elevated temperatures can be highly complex and dependent on the type of exposure, however when materials are put together to form composite products (e.g. foam and fabric combinations used in upholstered furniture) they do not act independently and are not only influenced by the type of exposure, but will impact each other and interact.

Influence of environmental and geometrical factors.

- Despite the fact that well-defined small-scale experiments are perfect tools for screening, product development and property estimation, they cannot capture all effects involved at a large scale. Environmental effects, geometrical effects and the interaction between solid and gas phase can be highly influential in fire development at larger scales. However, due to the complex requirements of large-scale experiments needed to investigate these factors, much remains open for further study.

Smoke production and its measurement

- Predominant methods used to measure smoke within fire research are largely primitive compared to other fields (e.g. environmental monitoring). How smoke is modelled within applied fire safety engineering is often very basic, hence much more research needs to be done in this area to build up our basic knowledge and data. Finding practical means in which this can be done, will encourage more studies and data to be obtained, and hence better methods for modelling can then also be developed.

3 Research Objectives

The core aim of this work was to decide on a given material, relevant to the topic of “building content” and take it through the generalised FIRETOOLS methodology shown in Figure 2 at the beginning of this thesis. This can be summarised as: to characterise a chosen material, at different complexity scales, using both experimental and modelling approaches with the aim of understanding what happens at the “large-scale” based predominately on information obtained at simpler scales. In addition, given the ubiquity of previous work using similar approaches, an important objective of this thesis was to investigate some of the limitations of this approach, i.e. important aspects of fire development that may be less applicable to a generalised scaling methodology. These are summarised in the following 4 key research objectives below:

RO1. Characterise a chosen material/product, using both experimental means and numerical modelling at all the given scales outlined in the FIRETOOLS methodology.

RO2. Investigate the interaction between experiment and model, by analysing the sensitivity of experimental and model outcomes to changes in prescribed inputs.

RO3. Investigate and develop new measurement and analysis techniques that may improve the characterisation of materials and the scaling process.

RO4. Exemplify limitations in the scaling methodology by investigating phenomena that are integral to the fire development process but are less amenable to the concept of scaling.

3.1 Limitations

1. Materials investigated were limited to one main material – basic, non-fire retarded flexible polyurethane foam. Supplementary materials e.g. fabrics, are also included, in specific cases to investigate specific aspects of the research reported in this document but are not investigated at all scales.

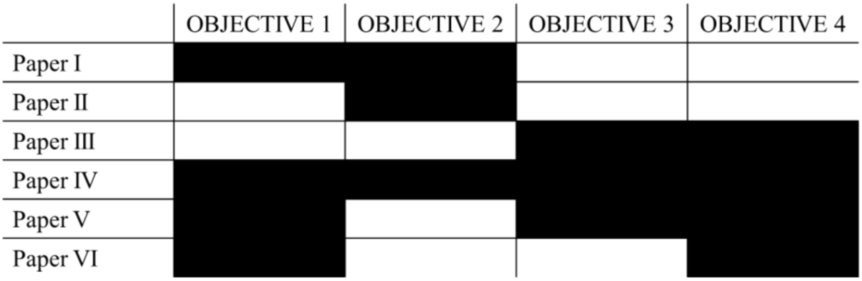
2. No complete upholstered furniture products were tested during this work.
3. The findings are limited to the test methods and material used.
4. Testing methodologies and apparatuses developed during this work, should be considered prototypes, and likely further studies are required in order to more thoroughly verify and validate their repeated use.
5. Some of the investigations described within this thesis, should be considered case studies, used to illustrate a larger concept, and thus generalising from them without further work may be ill-advised.

3.2 Overview of publications

This thesis is composed of a collection of 6 papers in total. Each of the papers is the outcome of research performed and Figure 5 shows how these publications are linked to the 4 objectives stated at the beginning of this chapter.

- Paper I – Sensitivity analysis on the microscale combustion calorimeter for polyurethane foam using a full factorial design methodology
- Paper II – Pyrolysis modelling of composite fabrics based on individual fabric properties using micro combustion calorimetry.
- Paper III – Obtaining additional smoke characteristics using multi-wavelength light transmission measurements.
- Paper IV – Experimental and numerical investigation on fire behaviour of foam/fabric composites.
- Paper V – Experimental investigation into the influence of ignition location of flame spread rates of polyurethane foam slabs.
- Paper VI - Geometrical and environmental effects on fire behaviour of flexible polyurethane foam slabs.

The links between the above publications and the defined research objectives is discussed in detail towards the end of this thesis in chapter 6. However, a brief illustration is provided in Figure 5.



	OBJECTIVE 1	OBJECTIVE 2	OBJECTIVE 3	OBJECTIVE 4
Paper I	■	■		
Paper II		■		
Paper III			■	■
Paper IV	■	■	■	■
Paper V	■		■	■
Paper VI	■			■

Figure 5 – Connections between papers and research objectives

4 Research Methods and Materials

4.1 Research approach

The general research approach followed in this project is that of a bottom-up method, i.e. starting from the small scale, using simple materials, and then gradually increasing the level of complexity. Increasing complexity is defined here in three different ways:

- Chemically, or in a material sense – e.g. from basic materials to more complex materials or combinations of materials
- Geometrically – increasing size (scaling) or going from 0D to 3D
- Environmentally – going from very controlled test conditions and environment to less controlled and more complex interactions

The terminology used in this thesis to describe these levels of complexity more intuitively takes inspiration from the terms commonly used to describe the size of the fire testing apparatuses (see Figure 6) applied in the experimental side of fire research:

- Micro-scale – Low level of complexity: individual materials, very small sample sizes (milligrams), lumped summed (0D) assumption with regards to heat transfer, highly controlled test environment.
- Bench-scale – Medium level of complexity: individual, combined or layered materials, sample sizes of the order of ten centimetres, simple geometry, defined incident heat fluxes, simplified heat transfer (approx. 1D), moderately controlled environment conditions.
- Large-scale – High level of complexity: multiple materials/components interacting, scale of the order of metres, more complex geometries, non-uniform heat fluxes, 3D heat transfer, turbulence and less controlled environmental conditions.

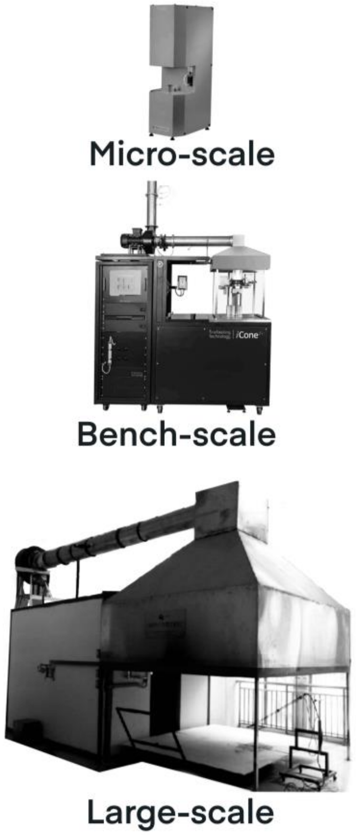


Figure 6 – Scaling of complexity with fire testing apparatus size (exemplified by the micro combustion calorimeter, the cone calorimeter and a large calorimeter)

The testing apparatus shown in Figure 6 are all used within the research contained in this thesis and are outlined in section 4.3.

As discussed previously, this thesis predominately describes a bottom-up or 'scaling' approach to the research starting with micro-scale up to large scale. Undertaking this process, involves both an experimental side and a numerical modelling side. The overall aim is to define and validate models with experimental data as the level of complexity is slowly raised. This overall concept and process is outlined in more detail in Figure 7.

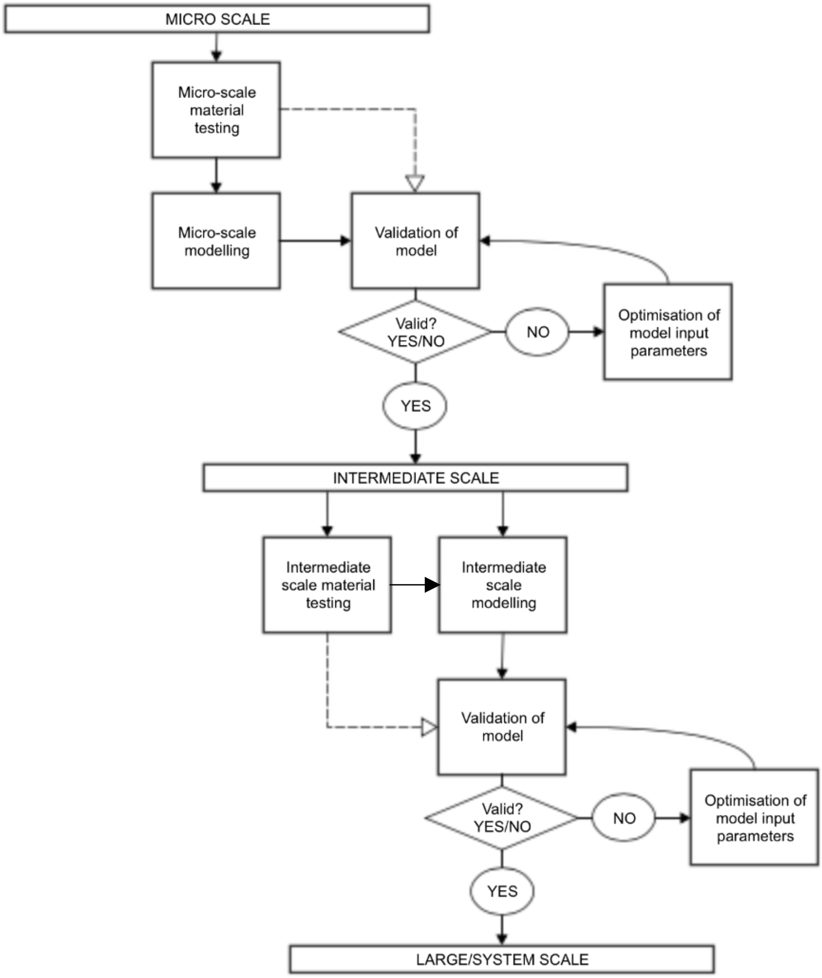


Figure 7 – Scaling process including both experimental and numerical work

However, at the largest scales, experiments performed had a dual purpose: 1) to act as the end goal of the scaling process outlined in Figure 7; and, 2) as research objective #4's purpose was to investigate factors that the scaling process may not consider, their purpose was also to investigate what these factors may be and how they affect the overall outcomes of a fire scenario. This secondary purpose is considered to be more of a "top-down" research approach. In a top-down approach to research, parameters of interest can only be considered at a system-level are investigated (e.g. effects of environment or geometry) through large-scale experiments in order to understand how sensitive the overall system performance is to such factors.

Both these methodologies are important. While the bottom-up approach progresses the field towards more efficient methods to quantify fire behaviour, top-down approaches help to highlight where knowledge is lacking and set the goals for future bottom-up methods.

4.2 Materials

4.2.1 Flexible polyurethane foam

Flexible polyurethane foams (FPUF) have a wide range of applications. Most familiar is FPUFs use as a cushioning agent for a wide variety of consumer and commercial goods, e.g. upholstered furniture and bedding. Due to its wide use and potential fire risk, understanding FPUF fire behaviour has been a priority within the fire community, as observed by the many previous studies (Chattopadhyay and Webster, 2009; Krämer et al., 2010; Lefebvre et al., 2004; Parker, 1997; Pau, 2013; Sundström, 1996; Valencia, 2009; Vanspeybroeck et al., 1992a). However recent studies such *as: Revisiting flexible polyurethane foam flammability in furniture and bedding in the United States* (Morgan, 2021) highlight the fact that there is still much work to do with this material.

Within this thesis, FPUF is considered the primary material investigated. The FPUF used was a basic, commercially available, non-fire retarded polyether polyurethane. Non-fire retarded FPUF was chosen for two main reasons; the first being that the majority of countries have little or no requirements on the fire performance of upholstered furniture, excluding the UK and USA. This means fire retarded FPUF used for upholstered furniture has limited use in most of the world. The second reason was to reduce complexity – fire retardants add a significant additional layer of complexity to the fire behaviour of this material, and as the focus of this research is on the development of methodologies rather than the material itself, use of “simplistic” materials was deemed more appropriate. The FPUF samples were donated by the research team at Laboratoire National de Métrologie et d'Essais (LNE) France as part of a previous project (Valencia, 2009) which also gave valuable input data, or they were ordered directly from the supplier (see Table 3).

The basic properties of the FPUF used in this research are summarised in Table 3. FPUF is generally composed of two main components that react to form the polyurethane; a polyol, and an isocyanate (Witkowski et al., 2015). These may come in many forms according to the desired properties of the final product. The polyol, an organic compound, is the base component of an FPUF and generally comprises the largest portion of the composition. The isocyanate used in FPUF is generally a diisocyanate (compound with two isocyanate groups) and in flexible polyurethanes, toluene based diisocyanate (TDI) is most commonly used. However, methylene diphenyl diisocyanate (MDI), is also used (Vanspeybroeck et al., 1992b).

Table 3 – Basic foam properties

Property	Basic properties	Additional information
Type	White Polyether polyurethane – supplier: Sherlock foams UK, material reference number: 21/130	No added fire retardants No fillers Approx. 32% TDI and 68% polyol. TDI: toluene Diisocyanate: Type 1 composed 80% from 2,4 Isomer TDI and 20% 2,6 Isomer TDI Polyol: Polyoxyalkylene triol
Density	According to the manufacturer: - 22kg/m3 Previous study of Bustamante (Valencia, 2009): - 20.9kg/m3 This study - 20.88±0.2 kg/m3*	*The density was obtained by taking the average of 12 separate sample measurements and masses.

Properties in Table 3 were taken from three sources; the manufacturer, the previous LNE research project (Valencia, 2009), and from measurements taken as part of this study. For further material properties, including conductivity and specific heat measurements, the reader is referred to the work by LNE (Valencia, 2009).

Thermal decomposition of FPUF is generally accepted to occur in two stages (Pitts, 2014). Heating of the FPUF first results in the release of the isocyanate, which manifests itself in the structural collapse of the foam, and a pooling of the yet-to-be-volatilised material that is predominately composed of the polyol. The polyol subsequently gasifies upon further heating. In air, this leads, in addition, to the production of CO_2 and H_2O, to the formation of various CN-containing structures such as HCN and results in nearly no char formation (Döring et al., 2021).

4.2.2 Textile fabrics

Textiles are an important addition to the FPUF, as they give the upholstered furniture its desired look and feel, and protect the FPUF from external damage. Textile fabrics are considered secondary materials involved in this research. The textiles used in the current research were basic, commercially available fabrics that were used in a Master's thesis at Lund University (Leisted, 2014), Cotton, Polyester and a Cotton/Polyester blend. They were purchased 'off-the-shelf', thus there is a level of uncertainty in their composition and manufacturing process. These fabric materials were chosen as they comprise a large portion of the upholstered fabrics market (Willbanks et al., 2015) and are used in a wide range of other products, including: bedding, clothing and other household furnishings. Table 4 lists the fabrics used in this research and their basic linear densities.

Table 4 – Fabric materials tested in this thesis

Material/Fabric	Composition	Approx. Density [kg/m^2](Leisted, 2014)
Cotton	100% Cotton	0.160
Polyester	100% Polyester (composition not specified)	0.400
Polyester/cotton blend	25% Polyester 75% Cotton (mass based)	0.183

Cotton is a natural fibre, primarily composed of cellulose. Cellulose decomposition is generally accepted to occur via two main mechanisms, the first being dehydration of cellulose producing char (plus gases such as CO, CO_2 and water), and the second being depolymerisation with formation of levoglucosan (Lédé, 2012) which in-turn breaks down into low molecular weight products which are flammable (Zhu et al., 2004). Temperature of pyrolysis and ignition occurring at around 350°C with a heat of combustion of approximately 19kJ/g (Horrocks, 1983).

Polyester is a synthetic fibre and goes through softening and melting stages before pyrolysis. Temperatures of these stages are approximately 85°C, 255°C and the pyrolysis temperature ranging between 420-450°C respectively (Horrocks and Kandola, 2021). Volatilization of light aliphatic fragments make polyesters easily ignitable polymers and it is believed that carbon dioxide, benzoic acid and aromatic esters are evolved in the initial stage of decomposition, however the subsequent thermal decomposition pathway still seems to be debated in the literature (Levchik and Weil, 2004).

4.2.3 Additional materials

4.2.3.1 Poly-Methyl Methacrylate (PMMA)

The material used for some of the smoke tests conducted in this research was standardised black PMMA (supplier: Fire Testing Technology). It was used in this research as a benchmark material, as it is a widely studied and well characterised material within fire science (Bal, 2012; Jiakun et al., 2013; Korobeinichev et al., 2017; Rhodes and Quintiere, 1996; Xu et al., 2016).

4.2.3.2 Wall materials

For some of the large-scale experiments, a corner wall configuration was needed. This consisted of a steel frame structure, filled with 45mm thick Rockwool stone wool, and skinned with either 9.5 mm thick gypsum plaster boards, manufactured by KNAUF, or 12 mm standard particle board product (manufactured by Kronospan).

Table 5 – Corner wall material properties

Material	Manufacturer/supplier	Properties	
Gypsum plaster board – GPB (Clima boards)	KNAUF, SAP no. 10302	Thickness [mm]	9.5
		Density [kg/m3]	789 (from manufacturer)
Particle board - PB	Kronospan - Novopan Spaandex EN 312 P1	Thickness [mm]	12
		Density [kg/m3]	~704 (as measured)

All materials used in the research were either donated from previous research studies or bought directly from suppliers.

4.3 Experimental tools

In this section. an overview of the experimental tools used throughout this research project is given. Tools are split into the different scales illustrated in Figure 6 and consist of both physical apparatus and methodological tools.

4.3.1 Micro-scale

4.3.1.1 Micro Combustion Calorimeter (MCC)

The micro combustion calorimeter (MCC) is an apparatus developed by the US Federal Aviation Administration (FAA). Its primary use is as a flammability assessment-screening tool for new materials with potential applications in the airline industry (Lyon et al., 2013). The MCC was designed to fill a perceived gap in material flammability testing. Common flammability tests in use today require relatively large sample sizes in comparison to the MCC (e.g. the cone calorimeter requires a 10 x 10 cm plate), or provide less detailed information on the fire performance of the tested material than the MCC (e.g. UL94 test). The sample sizes required in the MCC are in the order of milligrams (approx. 1-10mg), allowing efficient testing of newly synthesized material compounds, e.g. new polymer formulations. In addition, because of the small sample size, thermal gradients within the material samples may, in some cases be ignored, and thus output data extracted from the MCC may be considered close to fundamental material properties.

The MCC is based on the principles of pyrolysis and combustion analysis via oxygen consumption calorimetry (Janssens, 1991), employing pyrolysis-combustion flow calorimetry (PCFC) (Lyon et al., 2007). PCFC relies on the ability to separate the two governing processes observed in flaming combustion - solid-phase pyrolysis (i.e. generation of fuel gases from the material) and gas-phase combustion. This is achieved via the MCC's two-stage reactor, as illustrated in

Figure 8, the first stage is the pyrolysis section of the chamber, and the second stage is where combustion of the pyrolysis gases takes place. Due to this separation, each 'chamber' may be individually controlled, allowing users to adjust various input conditions e.g. heating rate, pyrolysis atmosphere, or combustor temperature. This also permits researchers and material developers to study the effects these changes may have on the flammability of their chosen materials (Lyon and Walters, 2002).

The MCC allows material samples to be exposed to a wide range of heating rates, something that is less common in other micro-scale apparatus, from as low as 10°C/min potentially up to 180°C/min (Lyon et al., 2013). The combustor temperature may also be varied; however, the temperature must be high enough to fully combust all the evolved gases in the second combustion chamber, as the measurement output relies on the reduction of oxygen that occurs through the combustion process. Material flammability may be investigated under two atmospheric conditions: anaerobic pyrolysis conditions, and aerobic or oxidative conditions. In anaerobic mode, the samples are heated in an inert (nitrogen) atmosphere, thus excluding solid-phase oxidation reactions. In the aerobic mode, oxygen is added to the pyrolysis atmosphere, hence, samples may also react with oxygen whilst being heated. In both conditions, the evolved gases from the pyrolysis chamber are completely combusted with excess oxygen in the second stage combustion chamber. The use of the MCC has been standardised under ASTM 7309 (ASTM International, 2011).

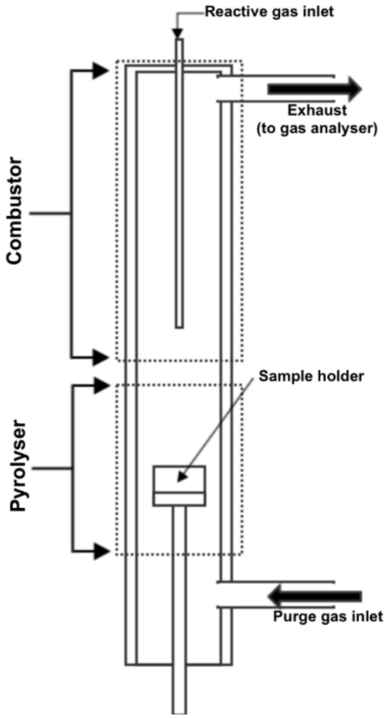


Figure 8 - The Micro Combustion Calorimeter (simplified schematic)

The MCC has predominately been used as a method to study and test new materials and different methods of flame retardation (Joseph and Tretsiakova-McNally, 2012; Snegirev et al., 2012; Tretsiakova-McNally and Joseph, 2015; Yang et al., 2010). However, the MCC may also be used to obtain properties useful in material fire behaviour modelling, specifically in the research for this thesis; peak reaction temperature(s) and the material's heat of combustion are investigated. Kinetic parameters (A, E_a), used in pyrolysis modelling may also be obtained from the MCC outputs (Lyon et al., 2013), which are traditionally obtained by using thermo-gravimetric analysis (TGA) apparatus (Wolska et al., 2012).

4.3.1.2 Design of Experiments (DoE)

In order to analyse the effects of changes in test parameters in a systematic way, an experimental procedure implementing the theory of design of experiments (DoE) was formulated and a full factorial experimental design (FFED) (Öivind, 2012) was executed. The goal of DoE is to maximise the amount of useful information gathered from an experimental test series, while still keeping the number of experimental runs required to a manageable level (Suard et al., 2013). In most cases, implementing a FFED is not feasible, as the number of required experimental runs increases significantly with each input factor that is tested. As an example; for a 2-level FFED, the number of required tests increases to the power of the number of input factors (k) to be tested, i.e. number of tests = 2^k. The advantages of performing a FFED however, are worthwhile if the number of tests is still manageable. An FFED not only allows the experimenter to investigate how changing each of the input factors affects the experimental output individually, it also allows for the investigation of potential interaction effects between the different input factors.

Due to the relative ease and speed of performing tests in the MCC, it was deemed feasible to perform a full factorial analysis in this case. Extending the FFED to a 3-level-3-factor design was chosen to be the most valuable with regards to the objectives of this study. A full factorial 3^3 design implies 27 factor-treatment combinations. A model for analysing this experimental design is expressed as Equation 5 (National Institute of Standards and Technology, 2013):

Equation 5

$$\boldsymbol{Y_{ijk} = \mu + A_i + B_j + C_k + AB_{ij} + AC_{ik} + BC_{jk} + ABC_{ijk} + \varepsilon_{ijk}}$$

where *A*, *B* and *C* are the input factors tested, and *i*,*j*,*k* the treatment levels, where *i*=1,2,3 and similarly for *j* and *k*. The combined letters, e.g. *AB*, denote the 2-way and 3-way (*ABC*) interaction terms, and epsilon is the error term. For more details on DoE and regression modelling, the reader is referred to National Institute of Standards and Technology (2013) and Öivind, (2012).

4.3.2 Bench-scale

4.3.2.1 Cone Calorimeter

The cone calorimeter (Babrauskas, 1984), shown in Figure 9, is widely considered the work horse of bench-scale fire testing apparatuses used in fire science research. In this apparatus, a conical shaped heater emits electrically induced radiant heat via an induction coil to a sample which, if following ISO 5660 standards (ISO, 2020) is positioned 25 mm below the bottom surface of the cone. The heat exposure (designated in kW/m^2) is defined before the start of a test and remains constant. A spark ignitor may be used to ignite combustible gases being released from the sample surface and when there are sufficient combustible gases, ignition will occur and is recorded.

Gases from the thermal decomposition processes are captured, collected and measured in the exhaust hood and duct system above to enable calculation of the heat released by a material via oxygen consumption calorimetry (Janssens, 1991).

Smoke is measured using the ISO 5660 standard protocol via light transmission/extinction measurement, using a single HeNe laser (wavelength ~633nm) positioned along the horizontal duct section before the exhaust fan.

The mass loss rate of a specimen is also recorded using a load cell.

Specimens of dimensions 100 x 100 mm and of varying thickness are placed under the cone heater, generally in a purpose build sample holder, in the horizontal orientation. Vertical testing is also possible but was not performed in this research.

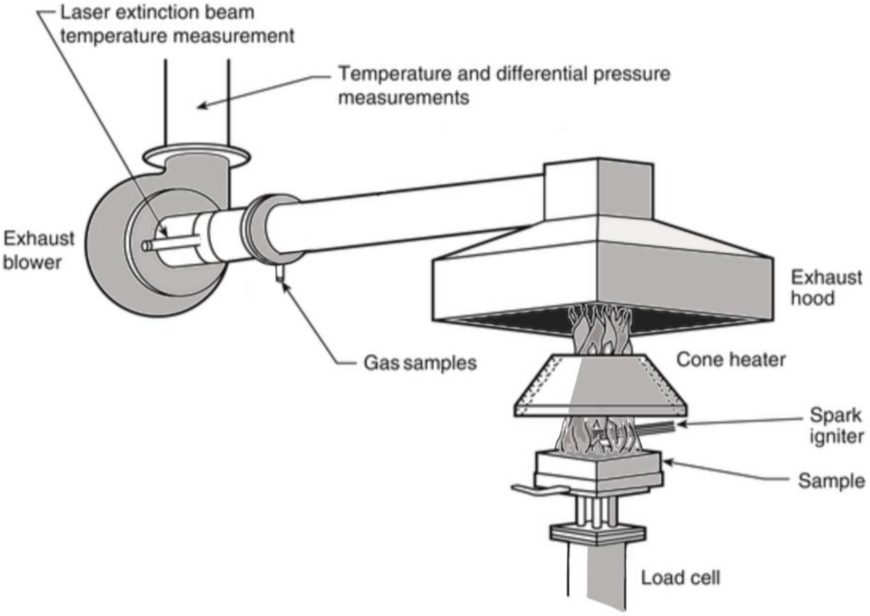


Figure 9 – schematic of cone calorimeter apparatus

4.3.2.2 Novel light extinction method using diode lasers

In addition to the standard smoke measuring system via the cone calorimeter, as part of this research, a new system for measurement of smoke was developed. This setup also used the cone calorimeter, but replaced the standard single HeNe laser measurement section of the duct with a new duct section that allowed for 5 different light sources to simultaneously measure smoke produced from a cone test.

Three diode lasers of varying wavelengths, a white light source and the HeNe laser were used in this study as shown in Figure 10.

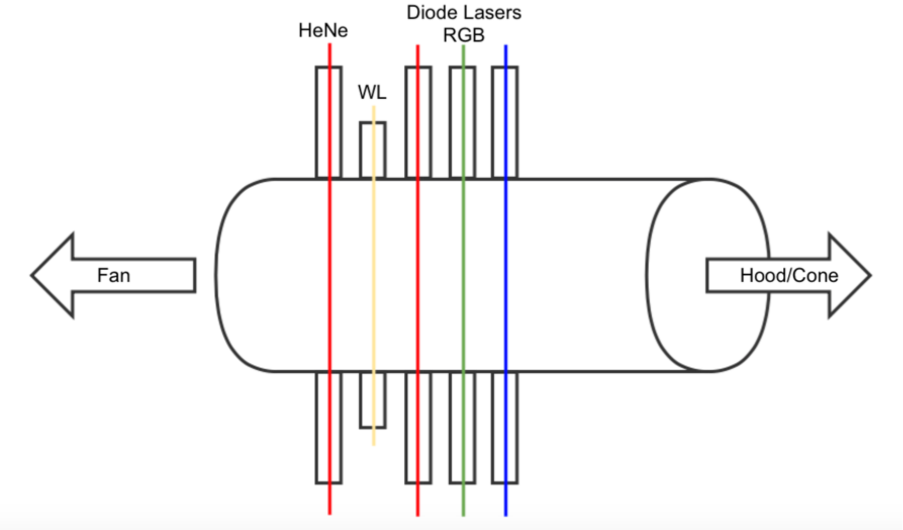


Figure 10 – schematic of the new duct section with the multiple light sources

The diode lasers used in this system were 1mW diode lasers (product numbers: FP-D-405-1-C-F, FP-D-532-1-C-F, FP-D-650-1-C-F from lasercomponents.se). The wavelengths were 405nm, 532nm and 650nm respectively, and were chosen to represent the approximate range of the visible spectrum. The white light setup was built according to DIN 50055 (DIN, 1989) (manufacturers: Fire Testing Technology, UK). The HeNe laser was as per ISO 5660 (ISO, 2020). A photo of the actual fabricated duct section is provided in Figure 11

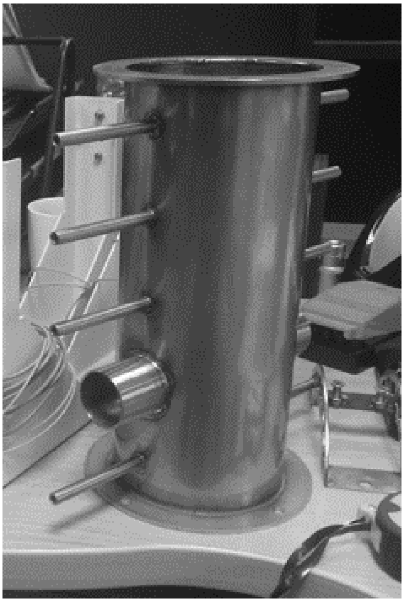


Figure 11 – Photo of modified duct section.

The new duct section was fabricated as per the standard cone calorimeter duct section with the additional measurement ports added. Two small diameter tubes (O.D. ~8.1mm) for each laser were welded onto each side of the exhaust duct to serve as part of the light baffling for the purging air and also allow for any smoke that may enter, despite the purge flow, to be deposited on the tube walls before reaching the optical elements as per recommendations in ISO 5660 part 1 and 2 (ISO, 2020). The laser cradles and detector setups were also as per ISO 5660 and were supplied by Fire Testing Technology (FTT) with a slight modification so that the diode lasers could be fitted in lieu of the standard HeNe laser. Two larger diameter tube sections (O.D~38.3mm) were welded to the duct in a similar manner to accommodate the white light setup. Spacing between centres (CC) is 60mm.

4.3.3 Large-scale

4.3.3.1 Open Calorimeter

The open calorimeter used in this research is part of the large-scale testing facility located at the Danish institute of Fire and Security Technology (DBI) designed according to ISO 24473 (ISO, 2008) standard. Heat Release rate is measured in a similar manner as in the cone calorimeter via oxygen consumption calorimetry. Smoke is measured using DIN 50055 (DIN, 1989) standard white light system.

4.3.3.2 Thermocouple bed

As part of the large-scale experiments performed during this research, a thermocouple (TC) bed or measurement tray was fabricated from calcium silicate boards (CSB) in order to perform some additional measurement within the experiments to track flame spread. The bed comprised of a single CSB measuring approximately 600x1200mm with additional sections of CSB fasten to the outside of the horizontal board in order to create a lip around the perimeter of the tray.

TCs were positioned by drilling very small holes (approx. thickness of the TC wire) through the CSB, then pushing the TCs through each hole so that each TC stuck out approximately 3 mm from the surface of the CSB. TCs were then fastened from the backside of the board with aluminium tape and staples. The temperature measurements were performed using 0.5 mm diameter wire type-K thermocouples. The TC array was set out in a grid of 5 by 10 (total of 50). The grid was positioned, with spacing of 120 mm between each TC, as illustrated in Figure 12. Temperatures were logged at 2-second intervals using data loggers.

Each TC location was uniquely identified based on its position in the grid, rows were named A-E and columns were designated numbers from 1 to 10. The TC bed sat on top of a load cell (Sartorius M-177 with a sensitivity of 0.001 kg). The load cell was protected from heat by the base frame and the insulation that was sandwiched in between the base frame supports, which did not touch the load cell.

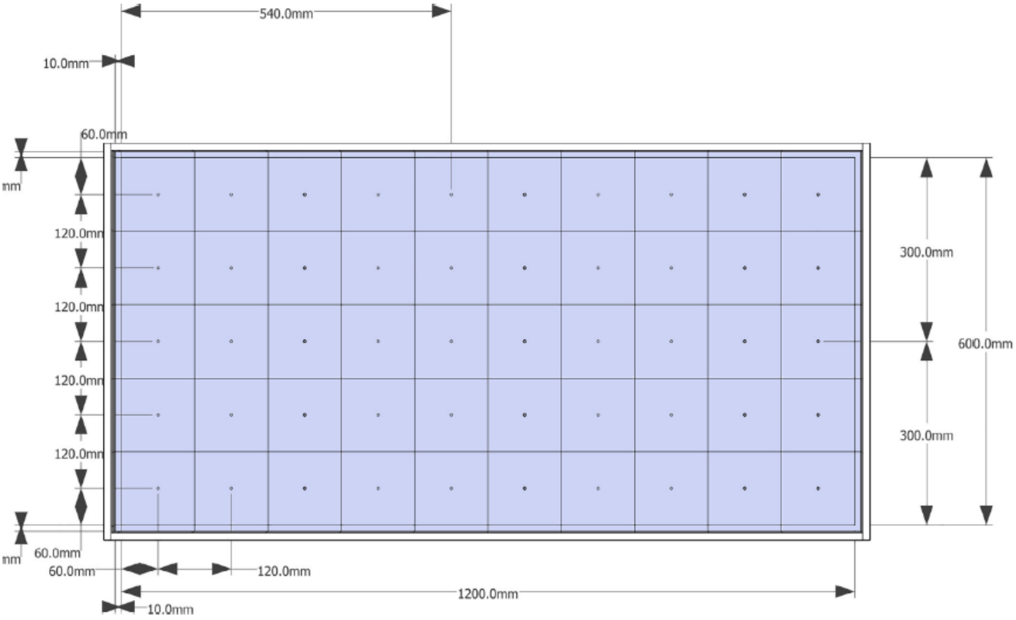


Figure 12 – Thermocouple bed schematic

4.4 Numerical tools

In this section a brief overview of the modelling tool and the relevant underlying mathematical equations used in this thesis are presented.

4.4.1 Fire Dynamics Simulator

Fire Dynamics Simulator (FDS), is a computational fluid dynamics (CFD) model of fire-driven fluid flow. FDS solves numerically a form of the Navier-Stokes equations appropriate for low-speed (Ma < 0.3), thermally-driven flow with an emphasis on smoke and heat transport from fires. The theoretical background, numerical implementation and verification and validation of the various models and sub-models are contained in the FDS Technical Reference Guide (McGrattan et al., 2015a) and the FDS Verification and Validation Guides (McGrattan et al., 2016; McGrattan et al., 2016).

The most common applications of the model have been for fire safety engineering purposes, undertaking performance-based design approach for the design of smoke handling systems, sprinkler/detector activation studies and risk/consequence and comparative analysis. However, FDS is also a tool to study fundamental fire dynamics and combustion and has embedded a series of complex sub-models that can be used to study material fire behaviour (McGrattan et al., 2015a).

FDS is implemented in a variety of ways throughout this thesis, at the micro-scale level only the solid-phase, 0D pyrolysis modelling was implemented. The aim of this was to investigate the capability of pyrolysis modelling to predict single and composite material behaviour at the smallest possible scale.

The procedure followed was based on the guidance found in the FDS user guide (McGrattan et al., 2015b). In FDS, pyrolysis simulation is calculated via numerical integration of Equation 6 for each, user defined, material component specified within the input file (McGrattan et al., 2016).

Equation 6

$$\frac{dY_\alpha}{dt} = -A_\alpha {Y_\alpha}^{n_\alpha} \exp\left(-\frac{E_\alpha}{RT}\right) \quad ; \quad Y_\alpha(0) = Y_{\alpha,0} \quad ; \quad \alpha = 1, N$$

where Y_α is the mass fraction of component α, calculated as a material mass concentration divided by the *initial* layer density of the material layer.

The material specific parameters for Equation 6 can be determined in a number of ways. Commonly, the user specifies input parameters, such as the activation energy (E_α) and the pre-exponential factor (A_α) which are usually determined via mass loss measurements performed in a thermo-gravimetric analyser (TGA). In this research, the parameters are determined from the MCC data, in which case, the mass-based reaction rate must be calculated from the heat release rate data using the method described below.

The two main parameters required for this method are named: *reference temperature*, and the *reference rate*.

- REFERENCE_TEMPERATURE ($T_{\alpha,p}$) (in the nomenclature of FDS), is the temperature at which the peak HRR for each reaction occurs, and may be determined via inspection of the MCC data.

- REFERENCE_RATE is calculated from MCC data using Equation 7 (McGrattan et al., 2016).

Equation 7

$$\text{REFERENCE\_RATE} = \frac{r_{\alpha,p}}{Y_{\alpha,0}}$$

where:

$r_{\alpha,p} = \frac{\dot{q}_{\alpha,p}}{\Delta h'}$ and $Y_{\alpha,0}$ is the initial mass fraction of the component, with $\Delta h' = \frac{1}{\beta}\int_0^\infty \dot{q}(T)dT$

These parameters are then used by FDS to calculate the respective component activation energy (E_α) and the pre-exponential factor (A_α) based on Equation 8 and Equation 9 (Lyon, 2000):

Equation 8

$$E_\alpha = RT_{\alpha,p}^2 \frac{A_\alpha}{\beta} \exp\left(-\frac{E_\alpha}{RT_{\alpha,p}}\right) = \frac{RT_{\alpha,p}^2}{\beta} \frac{r_{\alpha,p}}{Y_{\alpha,p}} \approx \frac{RT_{\alpha,p}^2}{\beta} \frac{er_{\alpha,p}}{Y_{\alpha,0}}$$

Equation 9

$$A_\alpha = \frac{r_{\alpha,p}}{Y_{\alpha,p}} \exp\left(-\frac{E_\alpha}{RT_{\alpha,p}}\right) \approx \frac{er_{\alpha,p}}{Y_{\alpha,0}} \exp\left(\frac{E_\alpha}{RT_{\alpha,p}}\right)$$

Equation 6 then calculates the mass loss rate of each material component.

To obtain the MCC result of heat release rate, this calculated mass loss rate must then be multiplied by the user specified heat of combustion for each component ($\Delta h'_{\alpha}/(1-Y_c)$), via Equation 10 (McGrattan et al., 2016) where Y_c denotes the char yield.

Equation 10

$$\dot{q}_{\alpha} = \frac{dY_{\alpha}}{dt}\,\Delta h'_{\alpha}/(1-Y_c)$$

At the *bench-scale*, a 1D model is implemented with multi-layered material components in an attempt to simulate the experimental results from the cone calorimeter testing. At this stage, simulations differ from the previous *micro-scale* stage by the inclusion of heat transfer properties. At the *micro-scale,* heat transfer is assumed to be insignificant since due to the sample sizes tested, chemical reactions govern the thermal decomposition process only. At the *bench-scale,* this assumption can no longer hold as thermal gradient through the sample significantly affect the material's thermal degradation behaviour. In particular, properties such as the material density, conductivity and specific heat are expected to play an important role in accurately predicting the cone calorimeter experiments.

In FDS this means that a 1D heat transfer model is now coupled with the pyrolysis model outlined previously, however the model is still only solid-phase, hence no gas-phase physics are yet included.

FDS allows solid materials to consist of multiple layers, with each layer allowing multiple material components that can undergo multiple thermal degradation reactions. Heat conduction is assumed only in the direction normal to the material surface using Equation 11 (McGrattan et al., 2015a):

Equation 11

$$\rho_s c_s \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x}\left(k_s \frac{\partial T_s}{\partial x}\right) + \dot{q}_s'''$$

where ρ_s, c_s, k_s are the component-averaged material properties, density, specific heat and conductivity respectfully and $\dot{q}_s'''$ is the heat source term consisting of the chemical reactions (i.e. the pyrolysis model in equation 10) and radiative absorption terms. To mimic the cone calorimeter, an external heat flux is imposed to the outer node of the model as a boundary condition.

5 Research Outcomes

In this chapter, an overview of the research outcomes is presented. Section 5.1 first provides an overview of the six appended papers included in this thesis, and how they interact with the three scales introduced in section 4.1. The research papers are then split into the three different scales and presented as a brief summary, with the main outcomes of each paper provided in sections 5.2 to 5.4. Chapter 6 then discusses these research outcomes in relation to the research objectives of this thesis.

5.1 Overview of the appended research papers

Figure 13 provides a pictorial overview of the six papers (represented as P1-P6) and their relationship to the scales and complexity of the models included in this thesis. The aim of this figure is to illustrate how each of the papers interact (by use of the different coloured shapes) with the different complexity scales and to show what research methods were used in them (e.g. was the paper an experimental paper or modelling paper or did it include both methods).

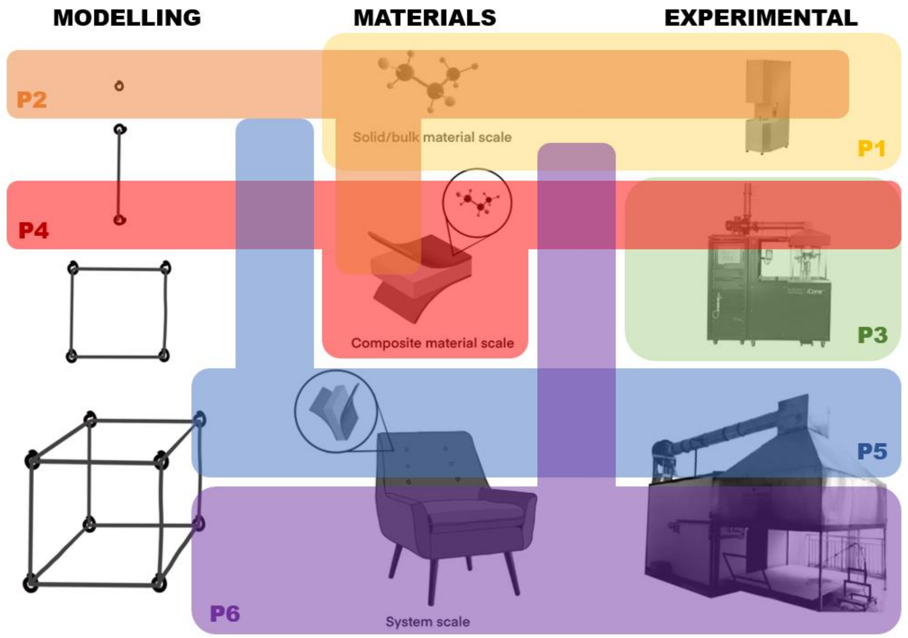


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Figure 13: Diagram showing the content of the papers included in this thesis and how they interact with the research methods and complexity scales.

5.2 Micro-scale

Two separate but connected studies were undertaken as part of this research that may be classified as micro-scale studies. The first investigated the primary material, FPUF, in an extensive experimental test series. The second study involved both experimental and numerical work, investigating the thermal decomposition behaviour of the secondary textile materials described in section 4.2.2.

5.2.1 Paper I – Sensitivity analysis on the microscale combustion calorimeter for polyurethane foam using a full factorial design methodology

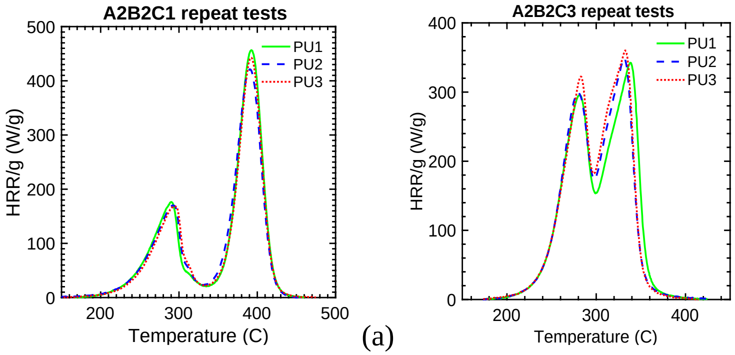
The aim of this study was to investigate the use and the sensitivity of results coming from the microscale combustion calorimeter (MCC) for the primary FPUF material. Characterising the sensitivity of experimental apparatuses used in fire research is essential. This informs researchers about the material’s behaviour under different conditions; but just as importantly, it also provides information on the dependency of the experimental outcomes on the chosen test conditions and the apparatus itself. This is important information to consider when data obtained from these experiments is used for material development and classification purposes. It is also important when data obtained is used for modelling purposes.

The experiments in this study were set up according to the principles of Design of Experiments (DoE) (Öivind, 2012). Three input factors were investigated, and each factor had three treatment levels as summarised in Table 6. A full factorial design was implemented identifying 3^3 factorial designs requiring 27 unique tests. A total of 39 tests were performed as part of this study, i.e., 27 unique tests and 12 repeats.

Table 6 – Factors and Treatments used in FFED

Factors	ID	Treatment levels		
		1	2	3
Sample preparation	A	2.5mg (in original foam state)	2.5mg (compressed state)	5mg (compressed state)
Heating rate	B	15°C/min	60°C/min	180°C/min
Atmosphere in pyrolysis chamber	C	0% Oxygen (inert, nitrogen atmosphere)	10% Oxygen 90% Nitrogen	20% Oxygen 80% Nitrogen

Results from the MCC showed good repeatability in most cases as exemplified in Figure 14. Sample inhomogeneity especially in the uncompressed samples was suggested as a possible explanation for the variation observed in the test results of Figure 15.



(a) (b)

Figure 14: example of MCC test results of compressed FPUF samples tested in a Nitrogen (a) and 20% Oxygen (b) atmosphere (PU1,2,3 represent repeated tests)

After the results were collected, statistical analysis was performed to quantitatively assess how each input factor affected the test results.

The outcomes of this analysis showed that heating rates and pyrolysis chamber atmosphere were the most influential factors in regard to the analysed output quantities. Sample preparation was split into two categories – mass and form. The sample mass showed very little influence, while the sample form (i.e. whether left in its original uncompressed state, or ground and compressed into the sample cup), was found to have some influence, especially on repeatability of the uncompressed samples as shown in Figure 15. Interestingly, the consistent plateau or dip observed in the first reaction for the uncompressed samples may be explained by the structural collapse of these at this point of the tests. Structural collapse of FPUF generally occurs at this stage of the thermal decomposition process (Krämer et al., 2010) and this physical change in the sample will affect the heat transfer rate through the material and thus the temperature measurement the MCC uses to control the heating rate. This in turn will affect the mass flow rate of volatiles to the combustion chamber and thus the measured heat release rate.

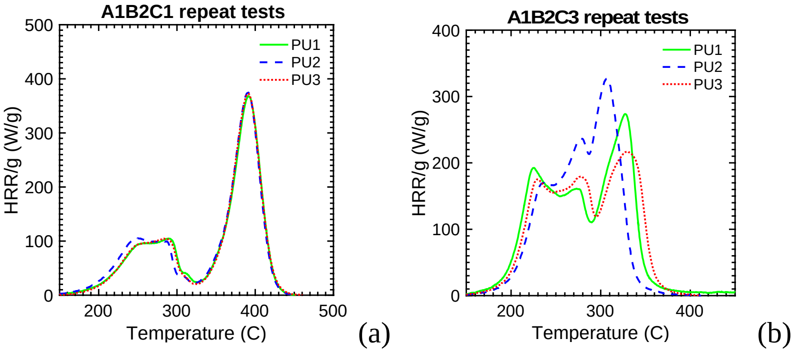


Figure 15: example of MCC test results of uncompressed FPUF samples tested in a Nitrogen (a) and 20% Oxygen (b) atmosphere

The complex behaviour observed in the uncompressed samples tested in oxygen has been observed in many studies using also TGA (Bilbao et al., 1996; Garrido and Font, 2015; Pau, 2013; Valencia, 2009), and has been used to develop more complex reaction mechanisms for modelling (Valencia, 2009). However, this behaviour is not observed in the compressed samples, suggesting that this added complexity might not be attributed to additional material reactions, but may be an artefact from some physical changes in the sample during the test, e.g. collapse, occurring in the sample.

Increasing the heating rate from 15°C/min to 180°C/min illustrated the effects of thermal lag, even in these very small sample sizes. This was observed as an increase of the temperatures at which the sample reactions took place (i.e. a shift of the curves to the right on the HRR/g vs Temperature plots).

The pyrolysis chamber atmosphere, either inert or oxidative, was observed to have the largest effect on the tested output parameters. Most interesting was the observation that increasing the oxygen levels produced a drop in the peak reaction temperatures, which was consistent for all tested atmospheres (from 0% to 10% and 10% to 20% Oxygen).

This study illustrated that outcomes from this apparatus for materials such as flexible polyurethane foam, are highly dependent on the user's choice of test input conditions and that these choices may significantly affect the use and interpretation of test outputs. Hence, performing studies such as this are important when test outputs are to be used further.

5.2.2 Paper II – Pyrolysis modelling of composite fabrics based on individual fabric properties using micro combustion calorimetry.

The main aim of paper 2 was to take the data obtained from MCC testing and use it for modelling purposes as per the proposed scaling concept outlined in section 4.1. Two areas were explored in this research:

1 – to investigate the ability of the pyrolysis model outlined in section 4.4.1 to simulate a simple material pyrolysis reaction from MCC data, and

2 – to extend this, by taking the first step in scaling up, to investigate whether the models created for the individual materials could then be added together to simulate the pyrolysis of a composite material made from the two individual materials without modification to the model parameters.

Materials used were the textile fabric materials outlined in section 4.2.2. The individual materials tested and subsequently modelled were cotton and polyester fabrics as described in Section 4.2.2, and the composite material was a blended polyester-cotton (PC) fabric supposedly containing 25% polyester and 75% cotton based on mass. MCC tests were performed in a nitrogen atmosphere.

Test results from the MCC again (as in paper 1) showed good repeatability for all three materials tested as shown in Figure 16.

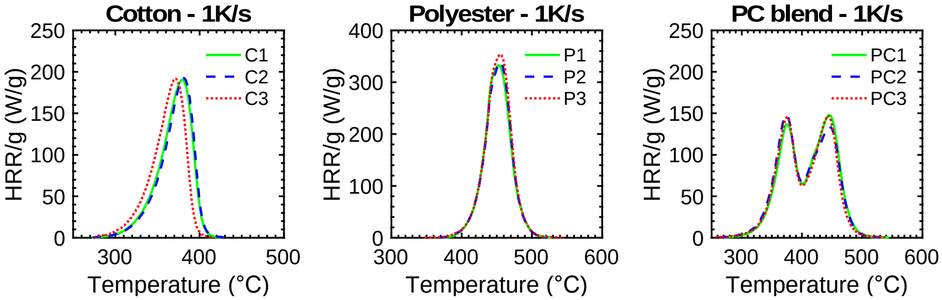


Figure 16 – repeated MCC test in nitrogen at 1K/s for Cotton, Polyester and Polyester-cotton blend

With regards to point 1, the simulations of both the individual cotton and polyester materials gave a respectable likeness to the experimental results highlighted in Figure 17. Peak HRR values were within the experimental uncertainty limits for the MCC (ASTM International, 2011). With the percentage error in the simulated peak HRR, values for both fabrics being approximately 5% when compared to the mean values for the peak HRR from the replicate experiments without any input optimisation, after some optimisation of the input parameters this result was reduced below 0.1% error.

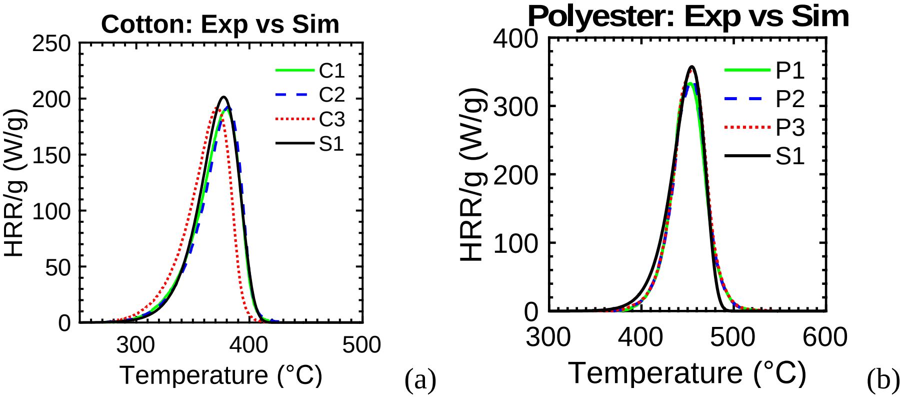


Figure 17 –Experiment vs Simulation (S1): (a) Cotton (C=experiments, S=simulation) (b) Polyester

Initial outcomes for point 2 in this study gave mixed results. The first peak in the HRR curve (attributed to the cotton decomposition) was reproduced well, however the second peak (i.e. the polyester decomposition) was significantly under predicted by the model for both the original inputs and the optimised versions as shown in Figure 18.

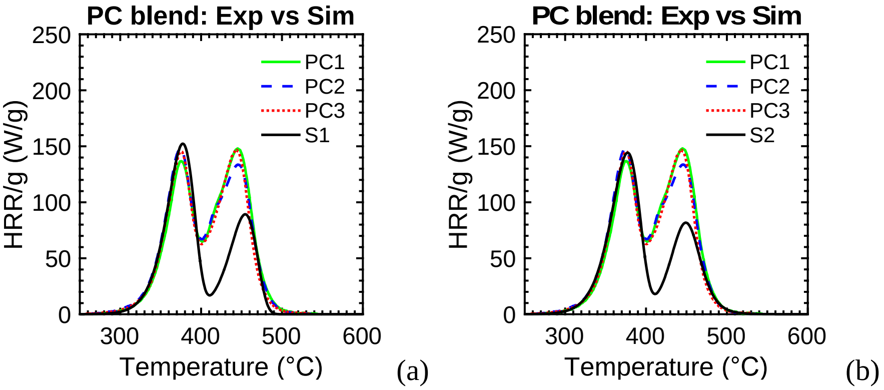


Figure 18– PC Blend: Experiment vs Simulation (a) original inputs, (b) optimised inputs

When analysing the data from these second stage simulations and experiments, it was noted that although the initial PC simulations proved unable to fully predict the experimental behaviour seen in the experiments, the modelling results were consistent with the initial assumptions made in the modelling stage. However, as the model predictions were inadequate, scrutiny of these assumptions and further investigation was required. The main assumptions made include:

1. The mass fractions of each component in the PC fabric equates to 75% cotton and 25% polyester as stated from the manufacturer.
2. The compositions of the material components in the PC fabric are indistinguishable for the single component fabrics.
3. Material component reactions are independent of each other (i.e. no material-material interaction).

Based on the investigation of these assumptions, additional MCC tests were performed with a self-synthesised PC blended material made from the single material fabrics. Tests were performed with approximately 3:1 ratio of cotton and polyester fabric, replicating the 25-75% spilt of the original blended fabric. A total of 4 replicate tests were performed using this material, and results were then compared to simulations with both the original (S1) and optimised input data (S2) in Figure 19.

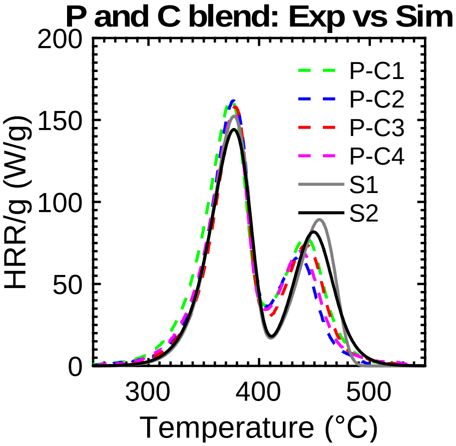


Figure 19 - Additional testing of semi-PC blend (P-C) vs original (S1) and optimised (S2) simulations

Interestingly, the additional testing of the semi-blend PC fabric provided results that were much closer to what was expected based on the simulations. This hints that some of the assumptions made in the previous modelling stage may not have been valid and highlights the fact that caution needs to be taken as it should not be assumed that one material ‘with the same name’ will behave similarly to another.

This is especially true when information on detailed material composition is not available.

Finally, analysis of these second round results hinted at the possibility of potential material-material interactions having some effect on the test results, leading to a hypothesis that the cotton reaction may be acting as a form of catalyst to stimulate the polyester reaction, speeding up its rate of reaction. However, further investigation would be required to confirm this.

5.3 Bench-scale

Two separate studies were performed at this scale. The first investigated the current state of smoke measurement and proposed a novel method to obtain more detailed information on smoke characteristics. The second followed the main scaling methodology of this thesis and can be seen as the combination of the previous work at the microscale, and the next steps in both size and complexity, using both modelling and experimental techniques.

5.3.1 Paper III – Obtaining additional smoke characteristics using multi-wavelength light transmission measurements.

Through the literature research performed for this thesis, it was evident that there is a need for increased information on the composition and properties of smoke in order to further develop, validate and extend the fire safety engineering community’s knowledge and ability to model smoke and visibility in fire scenarios. The main objective of the research in paper 3 was to critically review the current methods used to measure smoke and to investigate methods that could improve upon them in order to move towards gaining more knowledge.

Current measurement methods were classified into three groups:

- Dynamic or static – real-time measurements or time-averaged/single point measurements.
- In-situ or ex-situ – measured in smoke flow or collected and taken elsewhere for subsequent analysis.
- Intrusive and non-intrusive – interrupt the flow of smoke by taking samples or not.

The classifications and measurement methods all have their advantages and disadvantages, and choosing one method normally involves a trade-off in some regard. Static methods may give more accurate measurements, however; they are limited to time-averaged measurements. Static methods may also be more prone to smoke aging issues. Dynamic methods typically are the opposite of this, offering less accurate, but real-time measurements that allow fluctuations in smoke production over time to be better measured.

In-situ measurements offer the opportunity to study smoke in a more natural environment, allowing for easier or simultaneous comparison with other measured properties (e.g. HRR measurements). In contrast, ex-situ measurement may have increased precision, however, are more laborious and removing the smoke may have unknown consequences on the smoke composition. This can also be said for intrusive sampling methods. Nonintrusive methods offer significant benefit as they allow measurements to be performed without affecting the smoke itself.

It was also noted that within the field of fire research, light transmission, which is a dynamic, in-situ and non-intrusive method is by far the most common form of smoke measurement. Thus, a method that can take advantage of this fact but provide some more refined information on the measured smoke would have many advantages – ease of implementation being one important such advantage.

With this knowledge, a theoretical methodology, and requirements for a measurement apparatus using a multi-wavelength light transmission technique, were developed based on previous work (Cashdollar et al., 1979; Dobbins and Jizmagian, 1966). This involved the application of Equation 12 and the ratio of the logarithms of the transmissions, T, where T = $\frac{I}{I_0}$, for different wavelengths of light:

Equation 12

$$\frac{I}{I_0} = \exp\left(-\frac{3 \cdot C_m \cdot \overline{Q_e} \cdot L}{2 \cdot \rho \cdot d_{32}}\right)$$

Equation 12 is the Beer-Lambert or Bouguer’s law expressed in terms of particle mass concentration (C_m) (Hinds, 1982) and for polydispersed aerosols such as smoke, $\overline{Q_e}$ is the average extinction efficiency, ρ is the particle density and d_{32} is the volume-to-surface mean particle diameter (Dobbins and Jizmagian, 1966).

The ratios of $\overline{Q_e}$ are calculated using Mie theory (Bohren and Huffman, 2004) for the wavelengths of light used experimentally. The computed values are then compared to experimentally determined log-transmission ratios measured using the same wavelengths. If the chosen input parameters used in the theoretical Mie calculations are correct, the values of the log-transmission ratios should align and the mean particle diameter can be determined,

Using this knowledge, a parameter estimation code was developed for performing the calculations involving Mie scattering and an optimisation routine. This code was verified and the results were compared to the previous data (Cashdollar et al., 1979) shown in Table 7 below:

Table 7 – Results from comparative analysis

Parameters	(Cashdollar et al., 1979)	Parameter estimation routine
Fitting Residual	1.8E-3	8.7795E-5
Best fit Refractive Index ($m+mi$)	1.8+0.3i	1.85+0.55i
Estimated mean diameter (d_{32})	0.12µm	0.1489µm

The outputs showed similar results to the previous work (Cashdollar et al., 1979), however, with a significant reduction in the *fitting residual*, suggesting that in fact the parameters estimated by this code were actually a better fit with the data than the original paper's results. This is likely due to the age (1979) of this original research and the advancement in optimisation algorithms available.

This method provided an additional benefit, as the refractive index is determined based on the optimisation techniques and not taken from literature. This could provide a benefit for modelling, as it provides a method to experimentally obtain these values from actual tested materials or in certain environments, rather than requiring the use of literature data, that may not be comparable.

The second part of this research then outlined the design requirements for an apparatus involving multi-wavelength measurements, that are essential for this technique to be possible.

5.3.2 Paper IV – Experimental and numerical investigation on fire behaviour of foam/fabric composites.

The research performed in paper 4 can be thought of as the next level up the scaling ladder, using much of the data obtained in paper 1 and 2. It investigates the fire behaviour of materials at a bench-scale level, both as individual materials and as composite, multi-layered samples, from experimental and modelling perspectives. This research had a number of objectives, the first was to test the performance of the bench-scale 1D model outlined in section 4.4.1 using the kinetic parameters obtained from individual material experiment/modelling performed at the micro-scale level and heat transfer properties obtained through literature and/or optimisation methods. The second objective, which rose out of a need to get the validation experiments for the 1D model closer to what was actually being modelled, was to propose and test a novel specimen preparation method for the composites samples.

The materials used were a combination of the previous materials used in the micro-scale work, FPUF and the three textile fabric types described in section 4.2. All materials were first tested individually in the cone calorimeter three times. Modelling of these results was then undertaken, using the so-called "*double* *optimisation*” method outlined in Figure 7. Once results were deemed acceptable, the process was moved to the composite level.

Each composite (consisting of foam covered by one of the three fabrics - simulating an upholstered furniture arrangement) was then tested three times in the cone at the same incident heat flux as the individual materials. Cone calorimeter test results at this level were then to act as a validation step for the modelling results. Also at this stage, a new sample preparation method was introduced as shown in Figure 20. This method was developed in order to make the experiments “more 1D” as other suggested methods for testing foam fabric combinations such as ASTM E1474 were not so conducive to this requirement of the model.

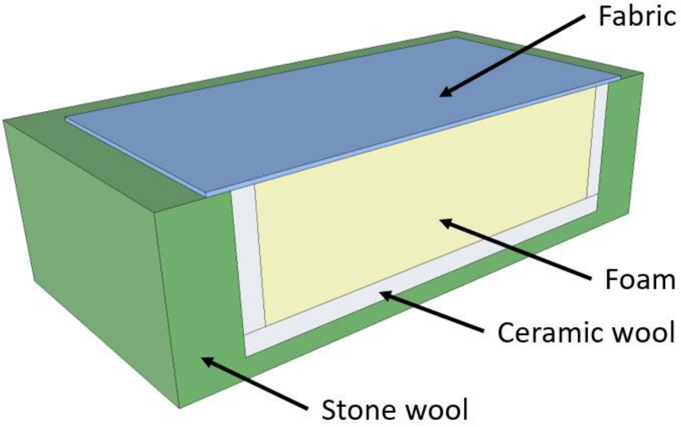


Figure 20 – novel sample preparation method developed for this study

Simultaneously to this, these composite products were also modelled by combining the input parameters obtained from the 1D modelling of the individual materials. Two different approaches to modelling the composite product were taken; the first modelled the materials as different layers, i.e. 1st layer was fabric, 2nd layer was FPUF as per the experimental setup. The second approach came after the experiments were performed and was based on observations in the experiments about how the materials interacted with each other. In this case the composite was modelled as one bulk material, with multiple components (i.e. fabric = component 1 and FPUF=component 2), each with mass fraction representing the amount of material.

The results from the two rounds of modelling showed mixed performance. Individual materials, once the heat transfer properties had been optimised, showed reasonable agreement with the experimental results. However, this was not re-created in the composite model results, with simulation performing poorly when compared to the experimental results. The principal reason for this is likely due to "model limitations", especially in accounting for the material-material interactions that occurred in composites testing stage. A prime example of this for the cotton-FPUF tests was that after the initial burn off of volatiles from the cotton, a char-type fabric layer remained in place, and acted as a partial barrier to the volatiles flowing from the FPUF underneath. This type of observation is far from the current modelling capabilities, so it should not be surprising that the models performed poorly.

5.4 Large-scale

Two connected papers were produced at this scale. Both papers present studies on a set of large-scale experiments performed on FPUF slabs. In the first, the influence of ignition location on the fire behaviour of the FPUF slabs is examined for slabs in a free-burning condition. In the second, the complexity of this experimental setup is increased by adding a corner wall configuration of either gypsum plaster board or particleboard.

5.4.1 Paper V – Experimental investigation into the influence of ignition location on flame spread rates of polyurethane foam slabs.

This study represents the first step into the final scale proposed in section 4.1 – the *large scale*. The purpose of the study was to investigate the influence of the ignition location on the fire behaviour of FPUF slabs measuring 600x1200x50mm in a free-burning scenario. Five different ignition locations were chosen for investigation, all resided in one quadrant of the FPUF slab, due to the slab's symmetrical nature and the free-burn conditions as shown in Figure 21.

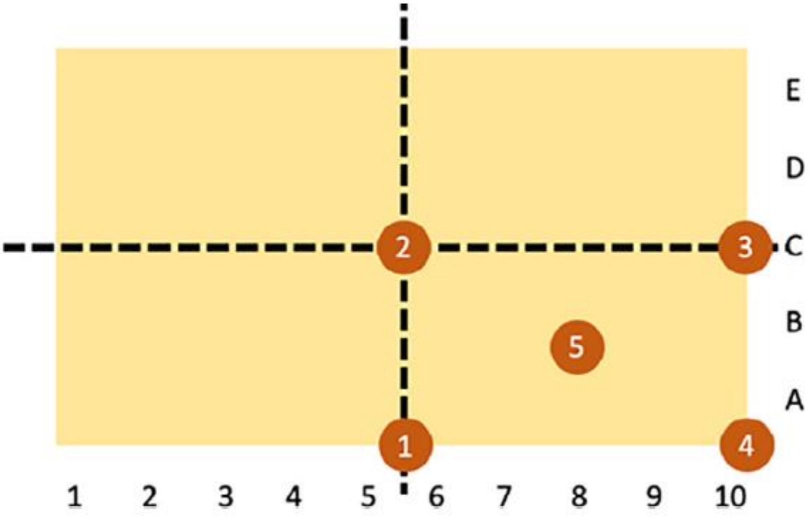


Figure 21 – ignition locations tested (dashed lines indicate lines of symmetry)

Experiments were performed under an open hood, with HRR measurement capabilities. A method for obtaining spatially resolved flame spread data was developed using the thermocouple bed outlined in section 4.3.3.2. HRR and the quantification of flame spread were used as representatives for investigating the sensitivity of fire behaviour to ignition location.

The HRR results showed that clear shapes formed that were dependent on the ignition location, with two distinct behaviours being observed between ignition locations 1-2 and 3-4, and with location 5 appearing to be a combination of the two. This was also observed in the flame spread data. Considerable variation in the peak HRR values was observed for the repeat tests, which lead to the conclusion that using peak HRR as a means to quantify the dependency of HRR on ignition location may not be appropriate and that other methods, such as calculating the correlation coefficient between tests of the complete time series data, may be a more robust approach.

Flame spread was quantified using three different methods of data interpretation: 1) Geometric flame spread visualisation—which simply mapped the TC measurements visually on the geometry of the foam slab over time; 2) Flame Spread Rate (FSR) maps—which visualise the calculated spread rate (i.e. velocity) at each measurement point; and, 3) Global FSR values—the mean, maximum, minimum and range of FSRs over the FPUF slab for each test.

Further analysis of the flame spread data also highlights that care should be taken here as well in deciding which values to use to investigate differences between test or studies. Using common methods such as the ‘mean FSR’ over the surface of the slab are not ideal, because much information can be lost. Even using mean and standard deviation may not be appropriate as this assumes a normal distribution of values over the surface of the slab, which is probably not a correct assumption. Instead, differences may be better resolved by using a metric such as the range instead.

Finally, results were seen to be classifiable into two primary types of behaviours. This may be useful information, for both fire scientists planning experiments and for fire safety engineers (FSEs) that may need to consider a fire scenario with a similar fuel source. In this case, FSEs may take a fire curve from each class to better cover the potential effects of that type of fuel source rather than picking one curve arbitrarily.

5.4.2 Paper VI - Geometrical and environmental effects on fire behaviour of flexible polyurethane foam slabs.

In this paper, the work from paper V was extended to include much more of the data obtained from the experiments performed in this part of the FIRETOOLS project. Paper V was limited to only investigating the influence of ignition location, in a free burning condition and with only one thickness of FPUF slab. The research in this paper, taking the learnings about ignition location influence from paper V, then investigated the influence of additional parameters, i.e. slab thicknesses and the effects of free burning conditions vs. restricted conditions.

A total of 23 large-scale FPUF slab tests were analysed. Four different slab thicknesses were tested, and the restricted burning conditions were comprised of a corner wall configuration made from either gypsum plaster board (GPB) or a more combustible particle board (PB), extending across two sides of the FPUF slabs as shown in Figure 22 and similar to that in EN13823 - SBI test (Technical Committee CEN/TC 127 “Fire safety in buildings,” 2020).

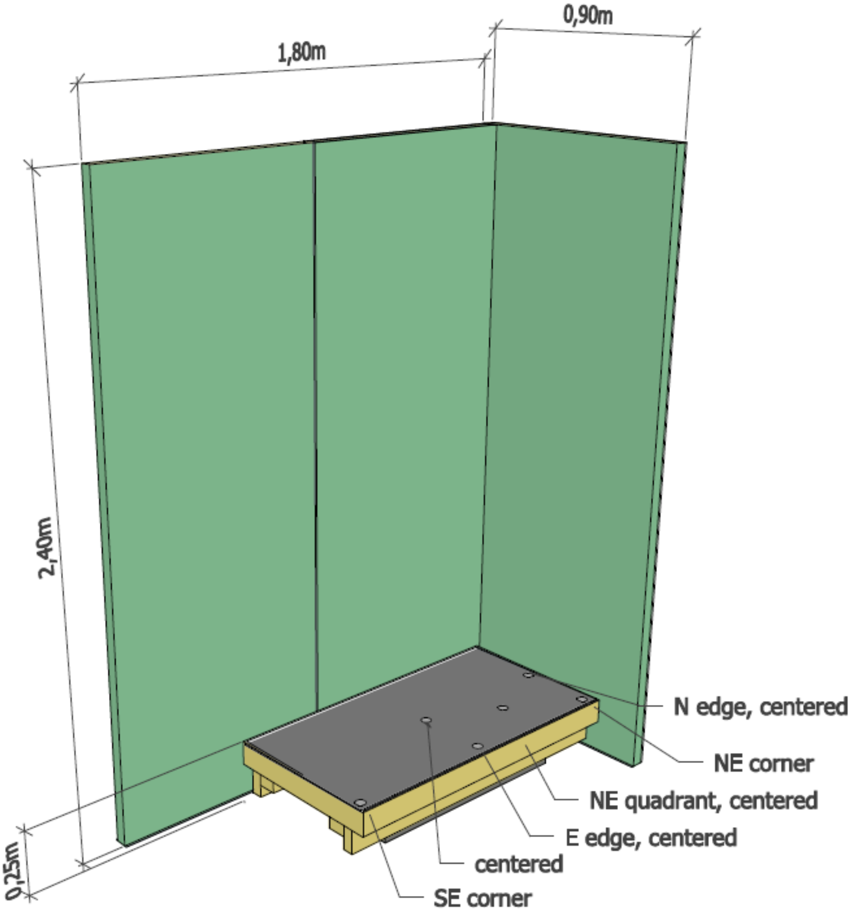


Figure 22 – corner wall configuration used in this study for both GPB and PB wall setups

As in paper V, HRR and flame spread were used to investigate the influence of the physical changes to the test scenario. Further, effects on smoke production were also investigated.

For changes in slab thickness, it was found that global values like total heat release and total smoke production correlated linearly with changes in material thickness as expected, although some other measured parameters did not. Peak values (peakHRR and peakSPR) increased more than expected, while the effective heat of combustion (EHC) remained approximately the same for all thicknesses. Interestingly, the specific extinction area (SEA), which could be considered the smoke-analogue to EHC, did tend to increase with slab thickness, although not enough data on this was obtained to draw a definite conclusion. Flame spread rates also increased with slab thickness, which may be counter-intuitive at first, and is not in line with observations for other materials (Chen et al., 2007). However this can be explained using classical flame spread theory (outlined in Section 2.1.3) by considering an increased burning area, due to material thickness in the z-direction.

For the comparative tests between *free burn, GPB wall, and PB wall*, see Figure 23, notable outcomes included: faster fire growth rates after initial incipient phase for both wall setups compared to free burn tests, with PB wall tests having the fastest growth rates, comparable to a classical ultra-fast alpha t^2 fire curve (Babrauskas, 1996). Significantly higher HRR and THR values were obtained for the PB wall test due to combustion of the wall products. However, this was not the case for smoke production, with no significant increase observed in the PB wall compared to the free burn tests.

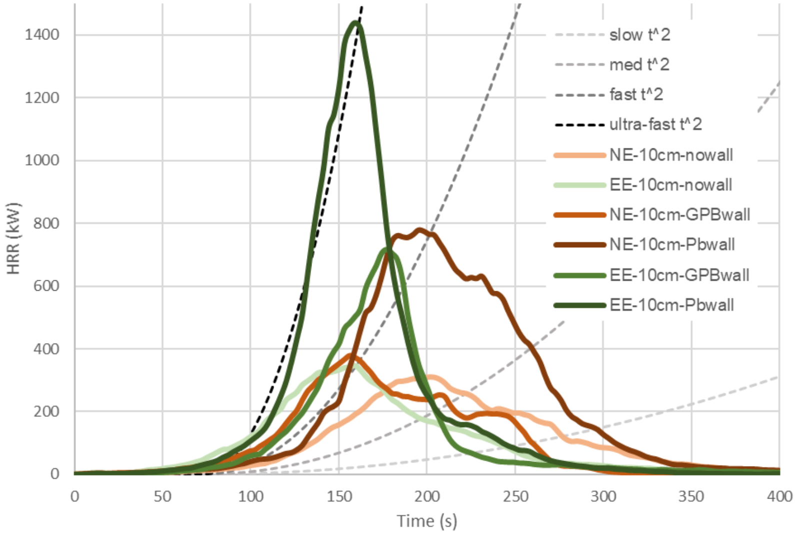


Figure 23 – alpha t^2 comparisons to FPUF slab tests (NE and EE refer to ignition location, 10cm refers to slab thickness tested)

Flame spread in general increased in the wall cases versus free burn tests and the highest rates were concentrated along the long side of the FPUF slab closest to the wall, highlighting the wall effects, likely through re-radiation from the wall back to the slab, which hastened the spread rate in this area.

6 Addressing research objectives and discussion

In this chapter, the results and learning outcomes obtained from papers I-VI, summarised in the preceding chapter, are discussed by reviewing the research objectives outlined in chapter 3 and relating how various papers contributed to addressing these specific objectives. Following this examination, a general discussion on learning outcomes from the work reported in this thesis is outlined.

The four key research objectives:

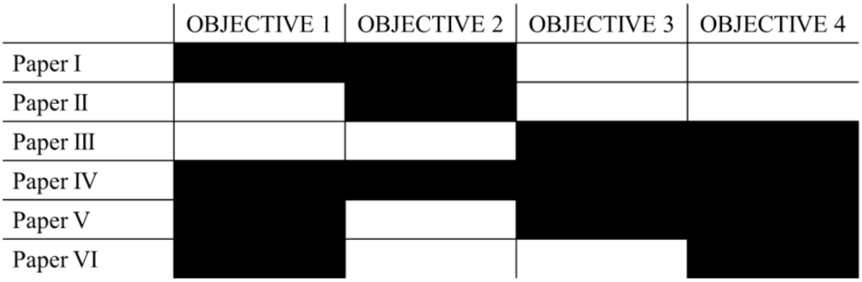
RO1. Characterise a chosen material/product, using both experimental means and numerical modelling at all the given scales outlined in the FIRETOOLS methodology.

RO2. Investigate the interaction between experiment and model, by analysing the sensitivity of experimental and model outcomes to changes in prescribed inputs.

RO3. Investigate and develop new measurement and analysis techniques that may improve the characterisation of materials and the scaling process.

RO4. Exemplify limitations in the scaling methodology by investigating phenomena that are integral to the fire development process but are less amenable to the concept of scaling.

Figure 5 is reproduced again to remind the reader of the connection between the papers and the research objectives.



	OBJECTIVE 1	OBJECTIVE 2	OBJECTIVE 3	OBJECTIVE 4
Paper I	■	■		
Paper II		■		
Paper III			■	■
Paper IV	■	■	■	■
Paper V	■		■	■
Paper VI	■			■

Figure 24 – Summary of connections between papers and research objectives

6.1 Addressing research objectives

RO1. Characterise a chosen material/product, using both experimental means and modelling at all the given scales outlined in the FIRETOOLS methodology.

This objective was addressed through a combination of papers I, II, IV, V and VI.

Paper I begins by investigating FPUF at the micro-scale level, from an experimental perspective. This paper provided the basis of the whole scaling concept and developed the data needed (i.e. kinetic parameters) to take the chosen material up the scaling ladder. Paper II goes on to extend the work of Paper I by extending to secondary materials (i.e. fabrics) and performing a similar set of experiments, building on the learnings from paper I with regards to the sample preparation and testing procedures. Paper II then takes the next step, by undertaking the first level of modelling using these materials. The results of this modelling showed that the chosen model could simulate the behaviour of these single materials with sufficient accuracy to give confidence in continuing. Added to this, paper II continues the scaling process by adding another layer of complexity to test the model – the first composite material. In terms of composites, the chosen material (polyester-cotton fabric blend) could be considered relatively simple, and model outcomes were still able to be validated at the micro-scale level through additional testing in the MCC.

Paper IV moves to the next level on the scaling ladder: the *bench-scale*. In this research, outcomes can be split into both experimental and modelling work, and from “simple” single material to a more complex composite. Results from the single materials were used in a second round optimisation process (as illustrated in Figure 7) to obtain viable input properties required for the step up in complexity of the model (i.e. inclusion of heat transfer phenomena). This method was chosen for two reasons:

(1) The required properties could not be easily obtained through separate experiments, partly due to scope considerations and partly due to the uncertainty in obtaining credible values for the materials involved, due to FPUFs complex behaviour under heating e.g. melting, structural collapse.

(2) From the learnings obtained in the previous research, and knowledge of the material complexities, using literature values was also deemed to be highly uncertain. Where literature values were valuable in this process, was to give estimations or order-of-magnitude for the given parameters; this helps to limit the

search space for the optimisation methods, so that determined values are still “within reason”.

Outcomes at this stage were varied, with results for the single materials getting to an acceptable level, however inclusion of composite product factors proved well beyond current modelling capabilities. Due to this experience, gained at the bench-scale level, paper V and VI represent a change in process – moving to solely experimental studies. They represent the final step in the scaling process outlined in the beginning of this thesis (i.e. the large-scale), however they may also be considered more as a representation of a top-down approach to research rather than bottom-up.

Modelling of this scale was not represented in this thesis, partly due to the experiences of modelling at the bench-scale level and partly due to scope/time restrictions involved. However, it should be noted, that as part of the overall FIRETOOLS project, a large-scale model of the scenarios and FPUF material tested in papers V and VI was made and compared to experimental results – this was a collaboration between all the team members of the project, and thus is not specifically included in this individual thesis, however the results were reported in the Work package 6 report submitted to the EU (Valiente et al., 2016). Briefly summarised here for completeness; the model failed to reproduce HRR curves of the experiments, and failed to represent the stark differences observed in HRR values when the ignition location was changed (refer Figure 25).

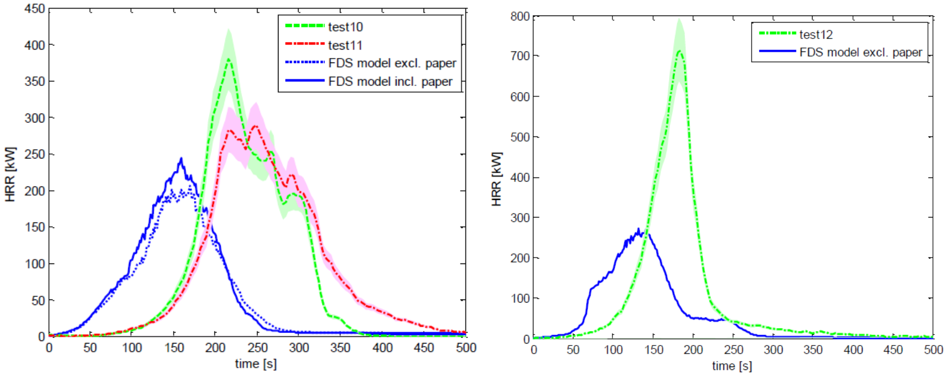


Figure 25 – model vs experimental results for ignition location 1 (test 10 and 11) and 4 (test 12) (Valiente et al., 2016)

Using global values such as peakHRR and Total Heat Release (THR) the model showed better performance compared to the experiments. However this reiterated the findings in papers V and VI i.e. that using such values to judge performance may be misguided. In general, the modelling approach used in this study indicated issues in resolving the heat transfer between flames and hot surfaces to the fuel bed, and modelling the initial incipient phase in the fire growth. As a result, flame spread was only managed with the addition of an artificial “baseline” heat flux applied directly to the FPUF slab material. This additional heat flux, however, may also have increased the ignition and flame spread resulting in the much faster burn out of the slabs in the model compared to the experiments (Valiente et al., 2016).

RO2. To investigate the interaction between experiment and model, by analysing the sensitivity of experimental and model outcomes to changes in prescribed inputs.

This objective was fulfilled through the combination of papers I, II and IV.

Paper I considers this objective by investigating the sensitivity of experimental apparatuses to changes in input variables. The major learning outcome from this paper was to highlight the importance of properly understanding the sensitivity of experimental apparatuses, and the importance of characterising this, rather than arbitrary choosing test conditions. As without this characterisation step, deeper analysis of any results is much harder to perform since it is not known what is an actual effect and what may be an artefact of the chosen test method, especially when the test results also have a large influence on the modelling. This was the case here, as these results were used to obtain the first key set of parameters (i.e. kinetics) needed for the scaling process. Thus, knowing how sensitive experimental results are, meant that we were better informed about the choice of data to use for modelling purposes. Paper II results in the context of objective 2 gave two important learning outcomes;

1. The importance of using identical materials for quantifying model performance and that just because a material is named the same does not mean it will perform the same. This also points out the level of caution that must be taken in using literature values of material properties.
2. Material-material interactions may play an important role in the fire behaviour of composite materials and should be taken more seriously than they seem to be, based on the lack of literature addressing the subject and current model limitations.

Paper IV built on these learnings and was important in building up an understanding of the complexities involved in both the experimental and modelling side of fire behaviour research. At this level, it was shown that for the single materials studies, modelling results could be achieved that were deemed acceptable when comparing to the experimental outcomes, but only after a certain level of optimisation was undertaken. Moving to composite results i.e. adding to the complexity level, here we see again that material-material interaction effects are observed to significantly affect the fire behaviour development. At this level (compared to the micro-scale), these effects are much more prominent and are suggested as the main reason for why the modelling performance drops significantly when compared to experimental results. Dependence of experimental results on the testing methods may be another reason for the inadequate model performance. For this reason, the new testing methodology was developed to attempt to get closer to the limitation of the model used, e.g. 1D heat transfer through the materials. However even with this improvement, model performance was not yet acceptable, and hence giving more credence to the suggestion that material-material interactions are likely governing the differences observed.

RO3. Investigate and develop new measurement techniques that may improve the characterisation of materials and the scaling process

This objective is fulfilled through the combination of papers III, IV, V and VI.

The Paper III results came from literature research performed as part of the FIRETOOLS project, in which gaps in knowledge and techniques were investigated. Although not obviously part of the FIRETOOLS scaling concept, improved methods for the characterisation of smoke was deemed to be an integral but somewhat overlooked part of characterising the fire behaviour of materials. This was especially true for real-world fire research application in fire safety engineering. In addition to the theoretical and numerical work completed in this paper, a prototype of the apparatus was also designed and built by the author as described in section 4.3.2.2. This has since been tested as a proof of concept at facilities of Fire Testing Technology (FTT) UK, and in the laboratory at Lund University, showing encouraging results.

Paper IV saw the development of a novel sample preparation method with the specific aim of getting the experimental results closer to what could be modelled. This was undertaken due to model limitations of heat transfer calculations in a single direction, perpendicular to the exposed surface of the sample (i.e 1D). A review of previous testing of similar materials e.g. by Price et al., (2002), CBUF, (Sundström, 1996) and guidance from ASTM E1474, the majority of these suggested to wrap the foam entirely with the fabric and then test this “small pillow”-like sample. The issue with this method, when it comes to modelling, was that this creates a 3D product, without clearly defined layers, which increases the burning behaviour complexity. Another issue highlighted was that the standard sample holder used in the cone calorimeter is made of steel (ISO, 2020) and thus transfers heat to the sample sides that could induce thermal decomposition indirectly, again creating a non-1D behaviour that cannot be accounted for in the model. To counter these, the new method, shown in Figure 20 made sure that there was only one material per layer, and it was insulated around the sides of the sample to reduce the potential from side heating.

Papers V and VI partly aimed to investigate how fire spreads across a horizontal surface. Many previous papers had also investigated the phenomenon of horizontal flame spread, using a variety of techniques – from tracking video footage, using thermal imagery or placing thermocouples along the surface of the materials; all of these methods aimed at tracking the spread along the top surface. For the research in this thesis, a different approach was taken by using the knowledge of the FPUF material to an advantage. FPUF is a good insulative material and it was observed through previous investigations with the material and from the literature that the thermal wave closely tracks the structural collapse of the material. Using this knowledge and that of some of the issues associated with the other methods reported in the literature previously, a new method (outlined in section 4.3.3.2) was implemented as a means to track the fire spread – using temperature measurements from the backside of the material. This proved quite successful and provided a robust, novel and relatively simple way to obtain spatially resolved tracking of the spread, although technically, surface fire spread was not tracked, rather FPUF structural collapse spread. Therefore, this method may be limited to applications only with materials that behave in a similar manner, if proved an effective tool for quantifying differences in the fire spread behaviour described in these papers.

RO4. Exemplify limitations in the scaling methodology by investigating phenomena that are integral to the fire development process but are less amenable to the concept of scaling.

This objective is fulfilled through the combination of papers II, III, IV, V, VI.

Paper II results gave some first hints on the potential influence of materials' interactions, an aspect that has been somewhat overlooked in traditional scaling methodologies. Even at the micro-scale level, which is the simplest level of testing and modelling possible, as soon as the complexity level was stepped up to include composite or combined materials, the results of this study hinted that the assumption that individual materials still act independently of each other may not be adequate and hence a limitation. Paper IIIs topic came from the identified limitations found through the literature research. This showed "smoke" as a general term, had been conceptually left out of the entire scaling concept, even if it is a highly influential and important consequence of the fire. The very few studies found that had attempted to include smoke (e.g. (Myllymäki and Baroudi, 1999; Steen-hansen and Kristoffersen, 2007b) were all empirical in nature and relied on statistical correlations and cone calorimeter tests, likely due to the limited knowledge and ability to obtain any more detailed information on the smoke characteristics. Paper III was an attempt to begin delving into this issue by proposing a way to improve the measurements methods used today, as this must be the first step before more complex models can be developed. Paper IV continued to provide more evidence that material interactions can play a very important role in governing the overall fire behaviour of a product. It also exemplified the limitations of current models, which cannot account for the forms of material interaction observed in this study.

Finally, papers V and VI along with the additional modelling work briefly summarised in objective 1 of this chapter, highlight one of the major limitations with the scaling approach as it is currently – the effects on the fire behaviour of materials and products due to situational, geometrical and environmental changes. In many cases, as evidenced in these papers, these types of "large-scale" changes have a much more pronounced effect on the overall fire development and scenario than whether the pyrolysis model can simulate the thermal decomposition of a material to within e.g. 10% of the experimental values. This is a serious limitation of the scaling, demonstrated through the results provided in papers V and VI, and also through the poor model performance at this scale, even with only one material undergoing thermal decomposition. This issue is also part of a larger debate on model complexity, and is discussed further in section 6.2 below.

6.2 General lessons learned

In this section some general learnings obtained through the work described in this thesis and in the whole FIRETOOLS project are briefly discussed. These learnings are split into five general statements that I feel are some of the most important takeaways I have learned to appreciate through my Ph.D studies. These are some of the learnings that I will remember through the rest of my career, and will be the first things I would pass on to any new researchers starting their studies.

The importance of knowing your experimental apparatuses.

Understanding that every experiment and apparatus has its advantages and disadvantages, and knowing the limitations and the peculiarities of the tools you use in your research cannot be stressed enough. Blindly testing things without first considering what your testing, how you are testing it, what the purpose is, and what your tools can and cannot do, makes little sense. Making the effort and "playing around" with the tools you have at your disposal and getting a feel for them, but also doing rigorous sensitivity studies, and reading the work of others on this topic, makes the work you do afterwards much more meaningful, and useful to others.

Models are just that, models.

One of the major learning outcomes from this work, personally, is that the dependence or reliance on models to do everything is not feasible, it is also not helpful in terms of learning to become a good researcher. This is not to say models are not helpful, as they can be useful for many things, in all realms of fire research and engineering, however as with the experimental side, knowing the in-and-outs, their limitations and uses, that you understand what they are trying to do, and that you test them, and push them to get to know their limitations and idiosyncrasies, is the most important thing to learn in making models useful for further research purposes.

The importance of material interactions.

This became evident throughout this research work, and is discussed throughout the various sections of this thesis. How materials interacted and affect each other when combined is something within the fire research communities that is known but is not studied as much as it should be. One reason for this may be due to the sheer difficulty in undertaking these studies. However, in the authors opinion, improvement on the detailed modelling side of research, even at the bench-scale level, will not progress significantly without finding ways to address these types of material interaction issues.

Materials' fire behaviour is nuanced, not set in stone.

In the world of standardisation, materials are generally classified into simplified groups that may be deemed as “good” or “bad” materials, however with the move to more performance-based approaches in fire safety engineering, this classification method no longer holds true, and “context” must be taken much more into consideration. The results from papers V and VI give some good examples of this; take the combustible (PB) wall and a non-combustible (GPB) wall (except for the paper layer) that were tested, standard thinking would describe the combustible wall as the much worse choice, however considering the results in this study more carefully, this becomes much less clear-cut. The energy release was higher for the PB wall however, there was no added smoke production. How does this affect considerations of life safety for people outside the room of origin for example? Or looking at the differences in results based simply on changing the ignition location. Based on examples like these, making general rules about materials is in my view much harder to do, and requires that examination of the context or the environment be given much higher priority than it may have been given in the past, before being able to give a proper, considered response.

The importance of large-scale testing.

At least for me, at the beginning of my Ph.D. studies, I had a tendency to underrate the importance of large-scale experiments/testing. “That's what models are for, aren't they?” – especially coming from a background as a Fire safety engineer working in a consultancy. However, during my studies, my appreciation for the importance and the knowledge gained from large scale tests has only increased over time. Out of all the things I did during these last years through my studies, I think I have learned the most from the large-scale experiments I either performed as part of papers V and VI or participated/assisted in during my time at Lund university and at DBI for various other projects. It is only at the ‘large-scale’ where you get a full appreciation of fire – its power, and its complexity.

7 Conclusion

The general aim of this thesis was to investigate the scaling methodology outlined at the beginning of this document, and shown here again in Figure 26, from the perspective of “building content”. Beginning with investigations at the level of bulk/solid (i.e. ‘raw’) materials, the goal was to use both experimental test methods and computer models to characterise the thermal decomposition processes of the chosen materials. From there the challenge was to use the obtained characterisation parameters of the chosen materials to move up the ladder of complexity, in both scale and material composition and investigate how this predetermined knowledge can be used to predict the fire behaviour as the complexity was increased.

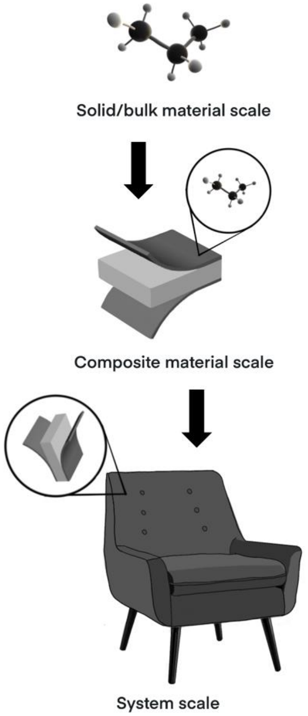


Figure 26 – FIRETOOLS methodology for ‘building content’

Two additional goals were added to this; to attempt to improve the process, and to investigate some of the limitations of this approach. These goals were summarised into 4 key research objectives:

RO1. Characterise a chosen material/product, using both experimental means and numerical modelling at all the given scales outlined in the FIRETOOLS methodology.

RO2. Investigate the interaction between experiment and model, by analysing the sensitivity of experimental and model outcomes to changes in prescribed inputs.

RO3. Investigate and develop new measurement and analysis techniques that may improve the characterisation of materials and the scaling process

RO4. Exemplify limitations in the scaling methodology by investigating phenomena that are integral to the fire development process but are less amenable to the concept of scaling.

These research objectives were fulfilled through the research papers presented in the appendix of this thesis, and how they were fulfilled was specifically addressed in the preceding chapter (chapter 6). These ‘hows’ are summarised briefly here as follows:

- RO1: a flexible non-fire retarded polyurethane foam material was chosen as the primary material investigated. This material was experimentally tested and numerically modelled at all three scales contained in the FIRETOOLS methodology: micro-scale, bench-scale and large-scale. Papers I, II, IV, V and VI all contributed to the fulfilment of this objective.
- RO2: Experiments and modelling of those experiments, as well as investigations into the sensitivity of both experimental apparatus and model helped to achieve this objective. Papers I, II and IV are considered the most relevant papers for this objective.
- RO3: three new or novel methods were developed as part of the research reported in this thesis, that are considered to satisfy this objective. These were outlined in Papers III, IV, V and VI.
- RO4: Papers II, III, IV, V, VI give a number of examples in which the standard scaling methodology was limited, however papers IV, V and VI are considered to exemplify this to a higher degree, by highlighting the importance of material interactions and the external influences such as geometry and environment.

In addition to the research objectives, to conclude this thesis, the major contributions of the appended papers and this thesis are now summarised as follows:

- Performance of a significant sensitivity study of the micro combustion calorimeter (MCC) using flexible polyurethane foam that highlighted how different decisions about input factors can impact the apparatuses output.
- Demonstrating how test results from the MCC can be successfully used to build and validate a pyrolysis model for polyurethane foam and fabric materials.
- Highlighting the significance of material-material interaction and their influence on composite materials' fire behaviour.
- Development of a calculation process and requirements for an experimental apparatus that could allow for more detailed smoke measurements to be obtained, without requiring a huge change in standard smoke measurement methods and practices.
- Development and testing of a novel method of sample preparation in the cone calorimeter, specifically designed in an attempt to improve the ability of the cone calorimeter to be used as a validation tool for material fire behaviour models.
- Investigation of the performance of models contained in the software FDS in simulating the material fire performance at a bench-scale level for both individual materials and composite constructions, and highlighting the need for further development that includes physical and material interaction effects.
- Development of a novel method by which fire spread over a polyurethane foam slab could be spatially tracked and measured quantitatively. Allowing spatially influence spread velocities to be calculated and investigated.
- Conducting a set of novel large-scale experiments that added to the scientific literature by quantifying the influence of ignition on foam slabs in terms of heat release, fire spread and other combustion parameters.
- Performing and analysing a set of novel large-scale experiments, that added to the scientific literature, on the influences of foam slab thickness and the addition of a corner wall configuration with both non-combustible and combustible wall materials.

This short summary should not be considered to be fully encompassing but aimed to provide an overview of the work described in this thesis from an external view point. The learnings, especially those discussed in section 6.2, have been an attempt to relay some of what has been gained by the author on an educational level, given the frame designated through the FIRETOOLS project. The last section of this thesis looks to the future.

8 Future Work

The final chapter in this thesis discusses future research. From the outset, one of the original aims of this research project was to investigate the possibility to predict “large-scale” fire behaviour of materials and products. Fire is an inherently complex phenomenon, and even the perfect model must be composed of many sub-models that could account for the many different processes involved in the thermal decomposition and combustion of materials. Based on the scaling concept, an ideal model would also be able to predict the fire behaviour of large-scale systems, based almost solely on the knowledge of fundamental material properties, which are measured at a micro-scale level. Through this research and that of the other ESRs involved in the FIRETOOLS project, one important conclusion could be that this is not yet possible, although, each thesis was an attempt to move the state-of-the-art slowly in this direction.

On the other hand, one could argue based on the findings in this thesis and others, that this idealised goal of creating the perfect deterministic model is unlikely to occur in the near future, if ever. There are a number of compelling reasons for taking this point of view, many of them due to the sheer level of complexity involved in just defining all the potential points that need to be considered in developing such a model and knowing how to describe these points in a concise deterministic way that would allow them to be implemented in such a model. The complexity of fire and all the processes involved around it, push this phenomenon in the author’s opinion into the realm of complexity and of complex systems, which are inherently difficult to understand using standard deterministic methods. In a common definition of a complex system:

- Complex systems are systems whose behaviour is intrinsically difficult to model due to the dependencies, competitions, relationships, or other types of interactions between their parts or between a given system and its environment. Systems that are "complex" have distinct properties that arise from these relationships, such as nonlinearity, emergence, spontaneous order, adaptation, and feedback loops.

The study of complex systems takes a wide-span approach, and considers the collective behaviour as the fundamental object of study. For this reason, complex systems research is considered as an alternative to the more classical approach or scientific method of *reductionism*, which attempts to explain a system’s behaviour in terms of the behaviours of its constituent parts, the sum of which can explain the system as a whole.

For a system to exhibit complexity means that the system's behaviour cannot be easily inferred from its properties (Bar-Yam, 2014). As I reflect on the work done and reported in this thesis, I think there is a good argument for taking a complex systems approach to fire research and something that should be looked into much more in the future.

From this broader view of interesting topics for future research, at a more practical level, there are also many areas of which the surface has only just been scratched in this thesis, and which could also prove worthy of future research by future researchers; some of these are outlined below:

- More emphasis and effort need to be put into research on smoke or "the products of combustion", both from an experimental and modelling view. Current models have a very simplified approach to modelling smoke production, however when you speak to practising fire safety engineers, it can be one of the most decisive factors in their engineering assessments, thus more knowledge in this area is very important.
- The study of material interactions is vital – both with other materials, but also the surrounding environment. These "interaction" factors can influence outcomes so significantly, that more work in this area must be done. At a detailed level, just from the experience gained in this research, interactions between core materials and their coverings (e.g. FPUF and fabric) need significant attention, and if the path for deterministic detailed material models is to be advanced, accounting for these types of interaction behaviours is of critical importance.
- Fire behaviour of fire retarded (FR) materials needs more study. In this thesis a lot of work is presented on FPUF. However, this was (on purpose) a non-fire retarded material. Using some of the processes developed in this research, and applying them to FR treated FPUF is one of the next steps in quantifying the fire risks of these types of materials. Some of the methods developed in this research could also be applied in the search for new methods for reducing the fire risks associated with these types of materials.
- Scaling is important. Although it has some limitations, scaling offers many benefits for many industries, including fire safety engineers and product developers and needs to be developed further and made simpler to use.

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10 Appended papers

Paper I	Wilkens Flecknoe-Brown, K. and van Hees P. (2018). “Sensitivity analysis on the microscale combustion calorimeter for polyurethane foam using a full factorial design methodology”, *Journal of Fire Sciences. Vol 36(6) pp. 453-471. DOI: 10.1177/0734904118798603*
Paper II	Wilkens Flecknoe-Brown, K., Hostikka, S. and van Hees P. (2016). “Pyrolysis modelling of composite fabrics based on individual fabric properties using micro combustion calorimetry”. *Interflam 2016, Proceedings of the 14th International Conference.4-6 July 2016, Nr Windsor, UK, pp. 131-142. Interscience Communications Ltd.*
Paper III	Wilkens Flecknoe-Brown, K. and van Hees P. (2015). “Obtaining additional smoke characteristics using multi-wavelength light transmission measurements”, *Fire and Materials 2015 Proceedings of the 14th International Conference.2-4 February 2015, San Francisco, US, pp. 136-148. Interscience Communications Ltd.*
Paper IV	Wilkens Flecknoe-Brown, K., Livkiss K., and van Hees P. (2017). “Experimental and numerical investigation on fire behaviour of foam/fabric composites”, *Fire and Materials 2017 Proceedings of the 15th International Conference.2-4 February 2017, San Francisco, US, pp. 240-253. Interscience Communications Ltd.*
Paper V	Wilkens Flecknoe-Brown, K. and van Hees P. (2021) “Experimental investigation into the influence of ignition location of flame spread rates of polyurethane foam slabs”, *Fire and Materials. Vol 45(1) pp. 81-96.* DOI: 10.1002/fam.2921
Paper VI	Wilkens Flecknoe-Brown, K. and van Hees P. (2021) “Geometrical and environmental effects on fire behaviour of flexible polyurethane foam slabs”, *Manuscript submitted*

Paper I

Paper II

Paper III

Paper IV

Paper V

Paper VI