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THERMAL MODELS FOR FIRE SAFETY – CALCULATION OF FLAME SPREAD ON SURFACES AND HEATING OF STRUCTURES

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Abstract

The studies presented in this thesis under the title "*Thermal models for fire safety – calculation of flame spread on surfaces and heating of structures*" consist of two parts: flame spread on combustible surfaces and calculation of heating of structures.

This work consists of the development of *thermal models* for Fire Safety purposes. The main objective of the present thesis work is to produce new information for fire safety related to the development of models for flame spread on surfaces and to develop engineering calculation methods in heating of structures.

In the context of Fire Safety, the word "fire" means accidental unwanted fires. The primary goal in Fire Safety is to protect life and property. The research field is relatively young and multi-disciplinary.

The growth rate of a fire depends on how fast the flame will spread and involve more burning surfaces. In an enclosure, the burning rate is enhanced due to feedback effects but it is still the increasing area of the fire that affect the flame size. In fully developed fire, as in enclosures, the availablilty of air limits the rate of heat release. Fire growth rate and the rate of heat release depend highly on how rapidly the initialized fire propagates on surfaces. Thus, it is the flame spread that controls the rate of heat release in large or open spaces. This shows the importance of modeling flame spread, due to its direct impact on fire safety.

This first part of the work discusses upward surface flame spread on a combustible solid surface. The flame spread is a process of a moving flame in the vicinity of a pyrolysing region on the surface which acts as a fuel source. The flame itself results from the combustion in the atmosphere of the pyrolysed gases leaving the surface. The oxygen and fuel concentrations together with the heat transfer phenomena between the flame and the solid phase affect strongly the process. Flame spread models of various levels of complexity are developed. A novel thermal pyrolysis upward flame spread model is also developed to predict the fire growth of combustible charring wall linings.

Heat release rate in fires is of primary importance. When a structure is present, a part of the calorific energy dissipated in the fire is fed back to the structure via thermal radiation and convection with consequence of raising its temperature. As the performance of structures decrease with the increasing of temperature, knowledge of temperature distribution within the structure it is important to estimate the safe-escape time for occupants, safe-operational time for firemen and fire resistance. It is therefore essential to model heat transfer in structures. In the second part of the thesis heating of structures and temperature calculations in solids are addressed.

Efficient engineering temperature calculation algorithms for various fire heated structures are developed.

Chapter 1

Preface

The publications included in this thesis work have been carried out under the auspices of the Fire Research Group of VTT, Building Transport, Finland, during my full-time work as researcher scientist during the period 1989 – 2002 at VTT. The synthesis of the thesis has been carried out under the financial support of the Finnish National Graduate School in Engineering Mechanics for the period 2006-2007.

Professors Jukka Aalto and Juha Paavola both from the Laboratory of Structural Mechanics at HUT (Helsinki University of Technology) deserve my warmest thanks for making the needed administrative and financial arrangements for me to write the synthesis of this thesis at HUT (Finland) and during my stay in France. Their encouraging words and their trust in me are more appreciated than the obtained necessary material support.

Thanks again to my supervisor Prof. Juha Paavola for patiently reading and constructively commenting the text of this synthesis. I should not forget to re-thank him since he was the one who introduced me to Professor Matti Kokkala from VTT (Technical Research Centre of Finland) for my first *summer job* in Fire Safety in 1989. Before 1989, I did not know at all that there is a multidisiplinary field called Fire Safety Science! Now I know.

I thank sincerely Prof. Matti Kokkala from VTT who first firmly introduced me to the exciting and endless field of Fire Safety Science during my first job at VTT as a research assistant in 1989 at the *ex. Laboratory of Fire Technology* (palotekniikka) – for his perseverance in encouraging me to continue my post-graduation studies and in agreeing to supervise this thesis. Thank you Matti, for finding time to read and to concisely comment this synthesis.

Thanks from the heart is deserved by my colleague Dr. Tuula Hakkarainen from VTT who with patience and preciseness read, commented, re-read and re-commented until convergence. I also appreciate her words of encouragement during the process of writing.

In a word, thank you to my tireless supporting *Finnish troika*: M. Kokkala, J. Paavola and T. Hakkarainen, for all that and more.

I thank Dr. Vytenis Babrauskas, actually head of Fire Science and Technology Inc. in the USA, for his encouraging words and for directing me to Dr. Indrek Wichman to obtain valuable information. I express my gratitude to Dr. Indrek Wichman, Professor at Michigan State University in Mechanical Engineering, for kindly replying to my literature request with his commented review on heat conduction solid and related topics.

I thank also my ex-colleagues Mr Simo Hostikka and Dr. Timo Korhonen both from VTT for providing me by e-mail all the publications I needed.

My sincere thanks go to my pre-examinators: Dr. Björn Karlsson (Director General, Iceland Fire Authority and Associate Professor, Department of Environmental and Civil Engineering, University of Iceland) and Professor Yuji Hasemi (Department of Architecture, Faculty of Science and Engineering, Waseda University, Tokyo, Japan), for accepting to evaluate and to comment this work.

Thanks from heart deserves Professor Ulf Wickström, heads of the Department of Fire Technology at the Swedish National Testing and Research Institute (SP), for accepting to opponent and evaluate this dissertation.

I use this opportunity to thank again all the co-authors of the publications composing this thesis for their invaluable contributions in the materialisation of this thesis.

I dedicate this work to the memory of my father and to my mother who were my library of kindness and wisdom in my childhood. It is now, with humble and sadness, that I am rediscovering this lost library with its endless and unbounded treasures of the oral culture of Humanity.

Djebar BAROUDI
Helsinki, November 2007

Chapter 2

List of publications

This dissertation consists of an overview and of the publications listed below:

I Kokkala, M., Baroudi D. and Parker W. Upward flame spread on wooden surface products: experiments and numerical modelling. *Fire safety science: Proceedings of the 5th international symposium.* Melbourne, AU, 3 - 7 March 1997. Hasemi, Y. (ed.). *International Association for Fire Safety Science.* Melbourne (1997), 309–320.

II Baroudi D. and Kokkala, M. Flame spread and heat release rate model for a burning mattress. *Proceedings of the Interflam '96 Conference.* University of Cambridge, England, 26 - 28 March 1996. *Interscience Communications.* London (1996), 37–46.

III Babrauskas, V., Baroudi, D., Myllymäki J. and Kokkala, M. The cone calorimeter used for predictions of the full-scale burning behavior of upholstered furniture. *Fire and materials.* Vol. **21** (1997) No: 2, 95–105.

IV Baroudi, D. A discrete dynamical model for flame spread over combustible flat solid surfaces subject to pyrolysis with charring — an application example to upward flame spread . *Fire Safety Journal.* Vol. **38** (2003), 53–84.

V Myllymäki, J. and Baroudi, D. Simple method to predict fire resistance of composite columns. *Fire safety science: Proceedings of the 6th International Symposium.* Poitiers, FR, 5 - 9 July 1999. Curtat, Michel (ed.). International *Association for Fire Safety Science* (2000), 879–890.

VI Myllymäki, J. and Baroudi, D. A method to determine thermal conductivity using boundary temperature measurements. *Fire safety science: Proceedings of the 6th International Symposium.* Poitiers, FR, 5 - 9 July 1999. Curtat, Michel (ed.). *International Association for Fire Safety Science* (2000), 349–360.

VII Myllymäki, J., Baroudi, D. and Ptchelintsev, A. Experiments and numerical simulation on lightweight steel balconies exposed to natural fire. *Fire and Explosion Hazards. Proceedings of the 3rd International Seminar.* Preston, UK, 10 - 14 April 2000. Bradley, D., Drysdale, D. and Makhviladze, G. Centre for Research in Fire & Explosion Studies, University of Central Lancashire. Preston (2001), 611–620.

Chapter 3

Author's contribution

The publications included in this thesis have been part of research work carried out at the Fire Research Group of VTT Building and Transport, Finland, during my full-time work as a research scientist in the period 1990–2002. The studies presented consist of the development of *thermal models* for Fire Safety purposes which are gathered in two parts *flame spread on surfaces* (Papers I – IV) and *heating of structures* (Papers V – VII).

In the synthesis part of this thesis, these papers will be referenced to as Papers I . . . VII.

Paper I includes the development and application study of a thermal upward flame spread model to predict the heat release rate using cone calorimeter data. The experimental research programme and the physical flame spread model was developed jointly by all the three authors. Mr Baroudi participated in the reduction of the measured data into physical quantities. He also developed the numerical model, wrote the computer programme and made the calculations to compare the experimental and theoretical results and wrote the respective parts of the paper.

Paper II deals with model development and application study to predict flame spread rate and heat release rate of a mattress ignited by a burner at the centre of its upper surface. The physical model developed is a novel extension of thermal flame spread theory. The work presented was part of the CBUF (Combustion Behaviour of Upholstered Furniture) research programme which was initiated by the European Commission to provide scientific and technical support for assessing the burning behavior of upholstered furniture. The authors jointly developed the physical model. Mr Baroudi participated in the reduction of the measured data into physical quantities. He also developed the numerical model, implemented it into a computer programme made the calculations to compare the experimental and theoretical results and wrote the respective parts of the paper.

Paper III presents model development and application studies. Three models of different complexity are developed for predicting full-scale burning of furniture by using cone calorimeter data. Model I is a correlation-based model developed mainly by Dr Babarauskas. Model II developed jointly by Mr Baroudi and Mr Myllymäki is based on area-convolution model with the functions derived by solving an inverse problem. Model III is a thermal flame spread model and was developed jointly by Mr Baroudi and Prof. Matti Kokkala and described in more detail in Paper II. In the case of Model II, Mr Baroudi and Mr Myllymäki jointly developed the formulation of the inverse problem used. In the case of Model III, Mr Baroudi applied the physical model, made the numerical simulations, and compared the experimental and theoretical results in collaboration with Prof. M. Kokkala. Mr Baroudi also participated in the reduction of the measured data into physical quantities. Kokkala and Baroudi also derived new results concerning untenability time predictions and formulated explicit conditions for propagating/non-propagating fires. Both of them contributed to writing the paper.

Paper IV presents a novel thermal pyrolysis upward flame spread model and an application study. The model is developed to predict the fire growth of combustible charring wall linings in an open configuration. The model accounts for preheating and includes an in-depth pyrolysis submodel to calculate local 'charring' depths and fuel mass fluxes of the pyrolysing solid combustible to calculate, *via* a simplified combustion model, feed back wall flame heat flux.

Paper V is an application study. A numerical method to predict the fire resistance of concrete filled tubular composite columns is developed. The model calculates the temperature field in a composite section and computes the respective load-bearing capacity of the column. Mr Baroudi developed the non-linear transient finite element thermal analysis algorithm and implemented it into a computer programme. The fire resistance part is developed by Mr Myllymäki who made the calculations to compare the experimental and theoretical results. Each author wrote the respective parts of the paper.

Paper VI includes an application study. An inverse method to estimate thermal conductivity of insulating material using boundary temperature measurements is developed. Mr Myllymäki and Mr Baroudi have jointly developed and implemented the direct and the inverse formulation methodolgy. The direct problem consisted of temperature field computation by a finite element numerical algorithm developed in the work. In the inverse problem, thermal conductivity as a function of temperature is extracted based on boundary temperature history. The theoretical part of the paper was written jointly by Mr Myllymäki and Mr Baroudi. Mr Myllymäki carried out

the comparison of the experimental and theoretical results and wrote the respective part.

Paper VII presents an application study to calculate transient heating of lightweight steel balconies installed in front of a facade and exposed to flames emerging from a window-opening under the balcony. The experimental research programme was developped and carried out by several VTT researchers including the authors of the paper. The physical problem was jointly developed by all the authors. Mr Baroudi developed the simplified finite element heat transfer model for the balcony including a model for the stratified slab with internal radiation cavities. He also implemented the algorithm into a computer program. The theoretical derivation and the computer implementation of the simplified radiative part of the heat transfer were done jointly by Mr Myllymäki and Mr Baroudi. The paper was jointly written by all the authors.

Contents

Chapter 4

Nomenclature

A	pre-exponential factor
D	fuel characteristic length
E_{A}	activation energy
L_{p}	pyrolysis length
$\dot{Q}(t)$	total heat release rate
$\dot{Q}'$	heat release rate per unit width
R	universal gas constant
T	temperature
T_{ig}	ignition temperature
V_{p}	flame spread velocity
c_{p}	specific thermal capacity
k	thermal conductivity
m, n	reaction exponents
$\dot{q}_{\mathrm{f}}'', \dot{q}''$	flame heat flux
t_{ig}	ignition time
w	width
x_{p}	ignition/pyrolysis front
x_{f}	flame height
δ_{f}	preheating length
ρ	mass density
ρ_{O}	oxygen concentration
ρ_{F}	fuel concentration
ω	chemical rate of reaction
t, τ	time
Δh	enthalpy change per unit mass
$\mathbf{C}$	capacitance matrix
$\mathbf{f}^i$	vector of nodal heat flux
$\mathbf{K}^i$	conductance matrix
$\mathbf{T}^i$	vector of nodal temperatures

Part I

Flame spread on surfaces

Chapter 1

Introduction

In the context of *Fire Safety*, the word 'fire' means *accidental unwanted fires*. The primary goals in Fire Safety are to protect life and property. The research field in *Fire Safety Science and Engineering* is relatively young and multi-disciplinary. The *SFPE Handbook of Fire Protection Engineering* [1] is a monumental condensate of the current knowledge of fire science and engineering. The book [2] by Babrauskas is a major and explicit thorough contribution on ignition phenomena including theoretical treatments and a vast amount of experimental data. Classical textbooks on Fire Safety and Fire Protection Engineering are those by Drysdale [3] and Karlsson and Quintiere [4]. Emmons [5] makes a review listing many aspects of Fire Science. Hirano [6] summarizes the various physical fundamental aspects of combustion in fires. In [7], Cox reviews the current state of the disciplines of fire safety science and engineering and also exposes research requirement and directions for the next century. An interesting reading on fire science and fire safety engineering, are reflexions of P. Thomas [8]. Reference [9] by McGrattan et al., provides an overview with illustrative applications to various full-scale real cases on the use of modern physics-based computational models in Fire safety problems (Fire Dynamics Simulator (FDS)). A fresh full-scale application example of using such computational code, is the simulations of the criminal fires in the World Trade Center [10] and [11], in order to estimate the behavior of the fires in the twin towers on September 11, 2001. Mc Grattan [12] discusses current trends in CFD modeling of fire and gives suggestions to develop better fire models. The paper [13] by Olenick and Carpenter, presents an international survey of computer models in use in fire safety engineering. One can even find a song about a *Fire Protection Engineer* as reported by Drysdale in [14].

Combustion is an exothermal chemical reaction of combustible species with oxygen. Combustion (burning) can be flaming or flameless. Smouldering is a flameless combustion sustained by heat generated by oxidation on a solid surface directly attacked by oxygen. A familiar example is a burning cigarette.

Simultaneous presence of next three elements is required for burning: *a combustible (fuel), oxygen and energy.* The supply of energy is needed to activate the reaction. This set of three requirements is known from firefighting science as the 'fire triangle' or briefly the 'triangle'. It illustrates that the three elements are simultaneously needed for sustained burning. However, there is an essential fourth element: *sustained chemical reaction.* Instead of a triangle, a *fire tetrahedron* is developed. The four faces correspond to : the three original elements from the triangle plus the *sustained chemical (chain) reaction.* In most fires, if one element is removed, the fire fails to ignite, or it extinguishes. The meaning of the fire tetrahedron can be understood by inspecting the expression of the chemical rate ω of reaction in burning as given by the Arrhenuis formula

$$\omega = A \cdot \underbrace{\rho_{\mathrm{O}}^{m}}_{\text{Oxygen}} \cdot \underbrace{\rho_{\mathrm{F}}^{n}}_{\text{Fuel}} \cdot \exp(- \underbrace{E_{\mathrm{A}}}_{\text{Sustainted chemical reaction}} /(R \cdot \underbrace{T}_{(Heat)\ energy})). \quad (1.1)$$

Lavoisier [15] was the first to demystify the fire (combustion) as a chemical exothermic reaction of oxidation in which oxygen and a fuel combine. He offered scientific experimental facts to support his new theory of combustion and threw away the phlogistic theory which postulated that materials release a mysterious substance called *phlogistic* when they burn.

A combustible mixture of gases and oxygen can burn directly. To burn, solid and liquid fuels should be first converted into the gaseous phase. For solid combustible, the thermal decomposition (pyrolysis) produces volatiles which are a complex combustible mixture of gases and vapors. Most combustible liquids evaporate in open atmosphere directly from the surface and mix with air. This is a phase change. In burning the evaporation rate depends on the liquid temperature and the concentration of the fuel vapour above the liquid surface. The Clausius-Clapeyron equation governs the saturated vapour pressure which is reached by the fuel vapour above the surface at equilibrium. Some polymers are decomposed by heat into new volatile products. Inside a flame, thermal radiation is emitted and absorbed by the hot gas-soot mixture. It is mainly the radiation from hot soot particles which forms the visible flame by acting as minute carbonaceous black bodies at high temperatures[1] [3]. (Thermal radiation spectrum range is $0.4 - 100$ μm [3] and [1].)

In a premixed flame, the fuel and the oxidizer are thoroughly mixed with appropriate relative concentrations prior to burning as is in an internal combustion engine, for instance. This process is known as *premixed burning.* Combustion will not occur if there is too much or not enough oxygen in the mixture for given temperature and pressure. These conditions are known as flammability limits.

[1]The visible colors of hot objects: 500℃–first visible red glow, 700℃–Dull red, 900℃–Cherry red, 1100℃–Orange, 1400℃–White, [3].

In a diffusion flame, the fuel and the oxidizer are initially separated and combustion takes place in regions where the gases mix. A classical Bunsen burner is a simple example of such a diffusion flame. The stream of the fuel leaving the burner chimney mixes with air by diffusion When there is a sufficient heat source to ignite, the mixture burns where the relative concentrations of fuel and oxygen are within appropriate flammability limits. Burning of gas jets and of combustible solids and liquids gives rise to diffusion flames. In fires, the rate of combustion depends on the mixing rate of the pyrolysed or evaporated gaseous fuels. Buoyancy and turbulence mix the available gaseous fuels with air and the combustion occurs. Drysdale [16, Chap. 5] wrote an excellent chapter containing a condensed essential of chemistry and physics of fire.

A natural fire, as opposite to "premixed controlled combustion", as in *combustion technology*, is a process where the *fire itself*, *via* feedback effects, supplies itself with heat, gaseous fuel, oxygen and momentum as it spreads and grows. Therefore, the fire is *a self supplying combustion phenomenon.* This definition for 'fire', joins the one suggested by Philip H. Thomas in a recent IAFSS[2] newsletter [17]. This is this kind of 'fire' which is meant in *Fire Technology* and *Fire Safety Engineering.* Evolution of a fire is depends highly on the spread of the flames. Premixed fire is related to artificially controlled combustion as, for instance, what happens in the combustion chambers of combustion engines.

The appropriate scientific definition of the word 'fire' is not trivial. It should be put in the right context of Fire Safety Science and apprehended as a phenomenon not an event. P. Thomas, in his article "What is "fire"? [17], pointed to such problem in the terminology. The new definitions as given in ISO 13943 "Fire Safety – Vocabulary" in English, French and German:

- Fire (controlled), "feu" in French and "Feuer" in German: "Self supporting combustion which has been deliberately arranged to provide useful effects and which is controlled in its extent in time and space."

- Fire (uncontrolled), "incendie" in French and "Brand" in German: "Self supporting combustion which spreads uncontrolled in time and space."

This standardized separation of 'fire' into controlled and uncontrolled *combustion* does not seem satisfactory. P. Thomas [17] suggests that the right definition should encompass the idea that :

> ... fire includes a gaseous combustion zone which has no taps, is self sustaining until the fuel or the oxygen runs out or the links in the triangle[3] are broken.

[2]International Association for Fire Safety Science: `http://www.iafss.org`.

[3]The "Fire Triangle": Heat, fuel and oxidant.

The flame spread is a process of a moving flame in the neighborhood of a pyrolysing surface which acts as a fuel source. The flame itself results from the combustion of the pyrolysed fuel leaving the surface. Flame spread will be treated in more detail in Chapter 2. The growth rate of a fire depends on how fast the flame will spread and involve more burning surfaces. As the gaseous pyrolysed or evaporated fuels become available, they burn in regions where they mix with air when appropriate limits of flammability are reached. During burning, heat and combustion products are generated. In an enclosure, the burning rate is enhanced due to feedback effects but it is still the increasing area of the fire that affects the flame size [3]. However, the burning is limited by available ventilation. Fire growth rate and the rate of heat release depend highly on how rapidly the initialized fire propagates on surfaces. The rate of heat release is a primary fire loading in Fire Safety Engineering (beside smoke and gas emissions during a fire). This variable affects directly the performances of structures, their fire resistance, safe-escape time for occupants, safe-operational time for firemen and loss of property. In large spaces and in open configurations, the spread of the flame mainly "controls" the rate of heat release making modeling of the flame spread phenomenon important as it has a direct impact on fire safety. (In fully developed fires, the availablity of air limits the rate of heat release). In addition to the thermal effects of a fire, there are other important aspects influencing fire safety, such as the toxicity of combustion products, visibility, the sufficient number of escape routes and doors, escape route visibility and accessibility, the presence of smoke control systems, fire detectors and alarms, and the operation time of fire fighters.

Chapter 2

Upward flame spread

This work treats upward surface flame spread; *wind-aided flame spread* on a combustible solid surface. Flame spread in the direction of the mean flow (wind or buoyancy) is called wind-aided (also called concurrent flow flame spread). When, on the contrary, the spread occurs in a direction opposite to that, we speak about *opposed-flow spread*. The flame spread is a process of a moving flame in the vicinity of a pyrolysing region on the surface which acts as a fuel source. The flame itself results from the combustion in the atmosphere of the pyrolysed gases leaving the surface. The oxygen and fuel concentrations together with the heat transfer phenomena between the flame and the solid phase affect strongly the process. In this part of the thesis, it is the upward flame spread which is of our concern. For readers interested in opposed-flow flame spread, an extensive literature review is provided by Wichman in [18]. Analyses of the solid phase together with analysis of phase change effects are studied in detail by Zheng, Wichman and Benard [19], [20] and [21] for flame spread on melting polymers.

Figure 2.1 is a schematic view of a possible scenario where a flame propagates on a lining of an external wall. In the next fire scenario a) – a garbage can be, accidentally or in criminal purpose, ignited and pushed close to a wooden facade of a building – which may ignite the combustible lining and initializes the fire spread. In this situation, the upward flame spread b) and c) is very important due to its velocity on the vertical surface. The buoyancy forces are significant and they form the upward "wind". A facade fire may also propagate inside the rooms of the building through windows, balconies and other openings by igniting combustible items *via* thermal radiation and convection. This is already an example of another fire scenario. Most of the problems encountered in Fire Safety Science and Engineering are complex physical and chemical phenomena involved in fires. What makes Fire Safety analysis laborious is the huge number of possible scenarios to be considered.

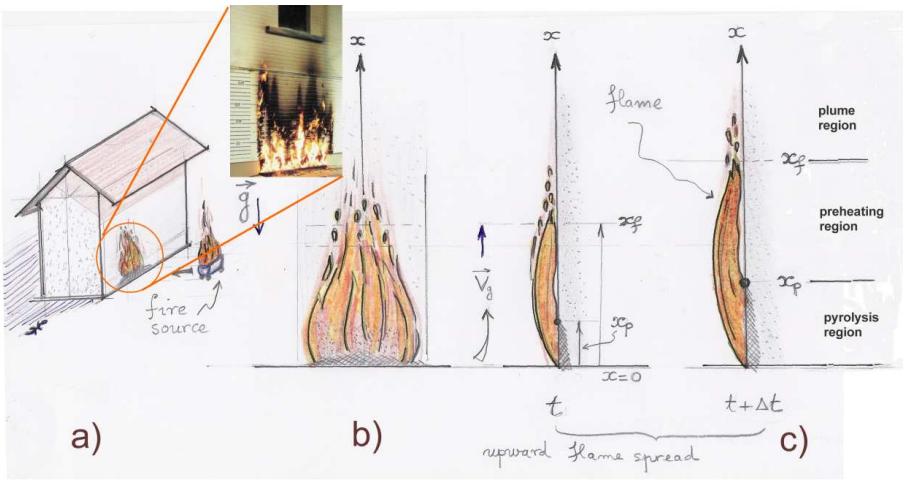

Figure 2.1: The physical problem of upward flame spread. a) A possible fire scenario of initialization of a façade fire. b) and c) scheme of upward flame spread on combustible lining. In c) burning front $x_{\mathrm{p}}(t)$ has propagated into a new location $x_{\mathrm{p}}(t + \Delta t)$ in a time Δt. The flame height is noted by x_{f}. The buoyancy forces act as upward wind. (The photography over a) and b) is slightly adapted from Hakkarainen et al. [22]).

2.1 Literature review

Williams [23] presents a review of flame spread controlling mechanisms. Quintiere [1, Chap. 12] gives a detailed review on surface flame spread phenomena. Thomas and Karlsson [24] used an analytical approach to analyse the behaviour of the upward flame problem by Laplace transforms. Baroudi and Kokkala [25] give in a revised form the basic concepts used to describe upward flame spread originally presented by Saito et al. [26] and investigated further the behaviour of upward flame. Hakkarainen [27] and Baroudi [28] (Paper IV) provide a detailed literature review on upward flame spread and fire growth modeling.

A large number of flame spread and fire growth models with a varying level of complexity has been developed. The choice of the appropriate level of description is guided by the purpose of the model and the available resources. Most simple models are in the form of *empirical correlations* for the evolution of the burning area [29]. The next level is represented by a class of phenomenological models having simple empirical correlations as submodels. This class is known as *thermal upward flame models*; [30], [26], [31], [29], [32], [25], [24], [33], [34], [35], [36], [37] (Paper I) and [38]. In these models, the burning front is seen as a propagating ignition front and the mass flux or heat release rate per unit area of the pyrolysed fuel is taken from experimental results, typically from the cone calorimeter measurements [1, Chapter *The Cone Calorimeter*]. Thermal upward flame models use cone calorimeter data and transient burning rate obtained from cone calorimeter experiments at appro-

priate irradiance levels corresponding approximately to flame heat flux levels prevailing in the upward flame configuration. Paper I includes development and application study of a thermal upward flame spread model to predict heat release rate. The developed numerical model, *THIMES* [39] (Paper I), uses directly measured cone calorimeter data as local heat release curve and an arbitrary relationship between the flame height and the total heat release rate. Traditionally, in the field of fire safety, this kind of models are formulated as a non-linear Volterra equation. Diffrent methods are then used to solve this integral equation. In Paper I, Kokkala, Baroudi and Parker, proposed for the first time, a new and simpler approach to solve the problem: instead of solving the Volterra equation the authors integrated numerically directly the original non-linear initial value problem of their model. Gojkovic and Hultquist [40] incorporated the *THIMES* algorithm into a compartment computational fire zone model (the WPI/Fire Code). More recently, the numerical model *THIMES* (Paper I) was also applied successfully by Hakkarainen and Kokkala [41] to predict heat release rate in the Single Burning Item (SBI) tests. Details are given in Paper I.

Baroudi and Kokkala [42] (Paper II) and Babrauskas, Baroudi, Myllymäki and Kokkala [43] (Paper III), developed and implemented novel flame spread models for assessing the burning of upholstered furniture. This work was part of the CBUF (Combustion Behaviour of Upholstered) research programme which was initiated by the European Commission to provide scientific and technical support for assessing the burning behavior of upholstered furniture. A flame spread model for a burning mattress is developed in [42] (Paper II) and in [43] (Model III of Paper III). These models are a physically based novel extension of thermal fire spread theory with many extensions and adaptations to convert it into a furniture fire model to calculate flame spread and heat release rate history. Refer to Papers II and III for details.

An extension to previous class of thermal models based on measured local heat release rate uses submodeling of in depth-pyrolysis [44], [45], [46], [47], [48, paper 7], [49], [50], [51] and [52], in the solid, to predict mass loss flux of the pyrolysing fuel escaping the solid and burning rate. In that way, they account more correctly for transient preheating from the flame in the actual upward flame configuration. These models can be labeled as *thermal pyrolysis upward flame models*; [53], [54], [55] and [28] (Paper IV). In these models, various in depth-pyrolysis submodels are coupled to upward flame spread models to calculate transient wall flame reradiation heat flux generated by the burning of the gasified fuel in order to take into consideration the transient preheating in actual upward spread configuration to calculate local temperatures and ignition times. More recently, Baroudi [28] (Paper IV) developed a novel discrete dynamical upward flame spread model using in depth-pyrolysis submodeling. The flame spread model consisted of a two-dimensional upward flame spread model coupled with an in depth-pyrolysis model. The model calculates the transient preheating at different locations

and depths, variable local pyrolysis times (times to ignition), the transient pyrolysis in depth direction, the transient local pyrolysis mass fluxes, and the re-radiation from flames generated by the burning of gasifed solid fuel *via* a simplified burning model. The model was able to describe the transient evolution of pyrolysing area, flame spread patterns and total mass loss rate. Details are given in Paper IV.

The most sophisticated and "universal" models solve the conservation equations governing fluid dynamics, heat transfer and combustion in the gas-phase, coupled to the energy equation in the solid-phase (or liquid-phase) and to solid (or liquid surface) pyrolysis. The coupling of the gas and solid phase is achieved through jump terms of the conservation equations at interfaces and accounting for pyrolysis kinetics at solid or liquid surfaces [56], [57], [58], [48], [59] and [60]. These models, generally, also account for soot formation and combustion, as this is a crucial feature in thermal radiation calculations. Some new implementations in the FDS, Hostikka and McGrattan [61] account even for the interaction of thermal radiation with water sprays.

Opstad [56] developed a numerical model which uses cone calorimeter data and a CFD model to predict thermal upward flame spread on solid surfaces. This model includes, turbulence *via* the $k - \epsilon$ approximation, soot formation model, a discrete transfer model for radiative heat transfer, eddy dissipation concept for combustion. A one-dimensional thermal model is used for thermal conduction in the solid lining to calculate ignition surface temperature.

Yan and Holmstedt [57] developed a CFD model to study fire spread over combustible surface lining material and fire growth in the room corner configuration. The CFD model includes modeling of turbulent heat and mass transfer, combustion, radiation in absorbing-emitting medium. A simplified soot formation model was used. The burning of the solid linings is accounted for in two ways: a) use of cone calorimeter data as input. Ignition of wall-elements was obtained by solving one-dimensional heat conduction equation in the depth-direction of the lining and by choosing an ignition temperature. Once ignition occurs, the burning wall-element is assumed to release fuel mass flux as in the cone calorimeter test. b) the second method (way) is more versatile and uses a pyrolysis submodel to calculate the mass flux of the prolysing solid fuel.

Jia et al. [58] developed an integrated fire spread model including many submodels representing different phenomena of gaseous and solid combustion. The model is used to simulate a fire spread experiment in a compartment. Jia et al. integrated to a general purpose CFD software (CFDS-FLOW3D) many submodels including submodeling of gaseous combustion utilizing the eddy dissipation concept, empirical soot formation, thermal radiation including effects of soot and pyrolysis for charring combustible solids.

The SOPHIE (Simulation of Fires in Enclosures) CFD model [59] integrates different flame spread models. The mass flux of the pyrolysing solid fuel is obtained either from small-scale experiments or given by a pyrolysis

submodel. SOPHIE is developed by a consortium of several European fire laboratories, coordinated by Cranfield University.

The Fire Dynamics Simulator (FDS), developed at The Building and Fire Research Laboratory (BFRL) at the National Institute of Standards and Technology (NIST) is used to predict fire spread in compartments of various sizes. FDS is a physics-based mathematical and computational model [62] and [63]. Paper [64] by Rehm and Baum, presents basic equations of thermally driven buoyant flows; this paper can be regarded as the "progenitor" of the FDS. Actually, the FDS represents the state-of-the-art in fire simulation computing technology [9].

Hostikka et al. [65] made FDS simulations to calculate the rate of heat release of wooden samples in the cone calorimeter. Hostikka and McGrattan [60] introduced a wood pyrolysis submodel into FDS to perform eddy simulations of wood combustion to predict full-scale fire spread in a room partially covered with wood linings (part of walls and ceiling). The eddy simulation of the gas phase flow is combined with a combustion model using a flame sheet approximation and a finite volume thermal radiation model. A reasonable agreement between experimental and computational results has been found. VTT researchers, Hietaniemi et al. [66], performed many case studies comparing experimental data with those obtained using the Fire Dynamics Simulator (FDS) for the fire spread. The experiments ranged from the cone calorimeter to the full-scale. The objective of this extensive work was to validate the FDS especially for fire spread, to provide parameter values for engineer use, and to spot further needs in the development of the FDS program.

In the present synthesis, we will concentrate on thermal upward flame spread modeling.

2.2 Formulation of flame spread as a propagation ignition front

In thermal theory, the ignition front $x_{\mathrm{p}}(t)$ (Figure 2.2) is seen as a successive ignition front $x_{\mathrm{p}}(t_{\mathrm{ig}})$, solution of the ignition condition,

$$t_{\mathrm{ig}} = \mathrm{sol.}\{T(t_{\mathrm{ig}}; x_{\mathrm{p}}) = T_{\mathrm{ig}}\}, \tag{2.1}$$

obtained by scanning different values of $x_{\mathrm{p}} \in [0,\ x_{\mathrm{max.}}]$ on the exposed surface and updating appropriately the contribution of the flame heat flux $\dot{q}_{\mathrm{f}}''$. The surface temperature is $T(t; x)$.

Consider, for instance, one-dimensional heat conduction in the semi-infinite half space $y \in]0, \infty[$. This is an approximation for thermally thick case where y is the thickness direction. Assume that, heat transfer by conduction in

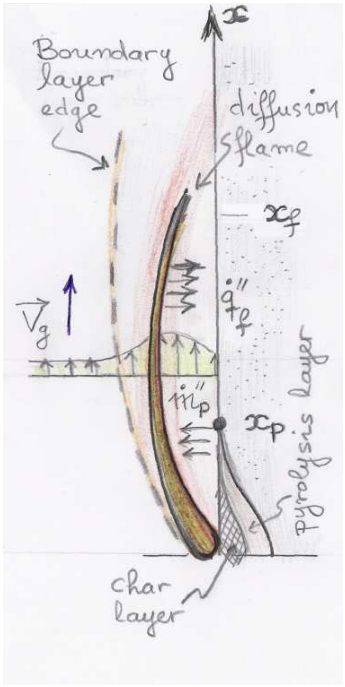

Figure 2.2: A schematic view of upward flame spread on combustible charring lining. The burning front is $x_{\mathrm{p}}(t)$, the flame height is x_{f} and $\dot{m}''_{\mathrm{p}}$ is the pyrolysed fuel mass flux at the surface. The buoyancy forces act as the upward wind.

direction x is small (a rough approximation; but the radiative heat flux is dominant on the preheating surface), the evolution of the surface temperature is obtained as

$$T(t;x) - T_0 = \int_0^t \frac{\dot{q}_{\mathrm{f}}''(\tau;x)}{\sqrt{\pi k \rho c_{\mathrm{p}}}} \frac{1}{\sqrt{t-\tau}}\,\mathrm{d}\tau, \tag{2.2}$$

[67]. By considering different temporal and spatial distributions for the flame heat flux $\dot{q}''_{\mathrm{f}}$ in (2.2), expressions for the flame spread velocity can be derived by solving this ignition equation.

2.3 Fundamental equation of fire spread

Williams [23] made an extensive review on various flame spread processes and identified the controlling mechanisms. *Via* energy balance considerations and quasi-steady assumptions, he arrived at the so called *fundamental equation of spread*

$$\rho V_{\mathrm{p}} \Delta h = \dot{q}''_{\mathrm{f}}, \tag{2.3}$$

where ρ is the density of the solid medium, V_{p} the spread rate, $\Delta h = c_{\mathrm{p}}(T_{\mathrm{ig}} - T_{\mathrm{s}})$, the enthalpy change per unit mass of medium from initial surface temperature T_{s} to ignition temperature T_{ig}, and $\dot{q}''$, the net heat flux ahead of the advancing ignition front to heat combustible from T_{s} to T_{ig}. The specific

heat of the solidis c_{p}. The ignition temperature is understood as the smallest surface temperature causing a sufficient production of pyrolysed fuel in order to sustain a piloted ignition. This temperature is controlled by the chemical kinetics of the pyrolysis. A review on piloted ignition of wood can be found in [68]. Reference [69] discusses the pyrolysis of solid wood in detail. Delichatsios [70] studied the effects of reduced oxygen atmospheres on piloted ignition times. In his paper [71], Babrauskas provides an extensive review on charring rates of wood. ("charring rate" means approximately pyrolysis rate.)

Williams identified the flame spread rate as the principal factor of interest and noted the importance of time-dependent flame height x_{f} in modeling upward flame spread.

2.4 Flame height correlations

Combustion reactions take place in the visible flame above a fire source. Typically, the lower part of a flame has a steady luminosity while the upper part is intermittent. Usually flame height is determined based on visual observations of luminous flames. The mean flame height, shortly flame height, is defined as the height above the source having intermittency of 0.5 [72]. This delimits the region where the level of combustion reactions is practically complete. Intermittency at an elevation is the fraction of residence time that at least part of the flame is above that elevation There are other definitions based on "chemical" flame height. The flame length is determined based on a critical value of the ratio of CO to CO_2 yields or mole fraction of fuel, or of other combustion products. This critical value delimits the zone of complete combustion and leads then to the concept of the chemical flame length. Newman and Wieczorek [73] showed that a "chemical" flame height defined from the ratio of CO to CO_2 yields is practically identical with previous results based on flame luminosity.

It is generally known that the length scale of the pre-heating region is defined by the flame height. The height of a wall flame is generally expressed in terms of the heat release rate as

$$x_{\mathrm{f}} = k_{\mathrm{f}}(\dot{Q}')^n \tag{2.4}$$

where k_{f} is an empirical factor which depends on ambient atmosphere. Such empirical correlation is observed experimentally as shown, for instance, in Figure 2.3.

Empirical correlations of the form (2.4) have been derived by Delichatsios [53] and Eklund [74] for an ideal line source. They obtained

$$x_{\mathrm{f}} = k'(c_{\mathrm{p}}T_\infty\rho_\infty\sqrt{g})^{-2/3}(\dot{Q}')^{2/3}, \tag{2.5}$$

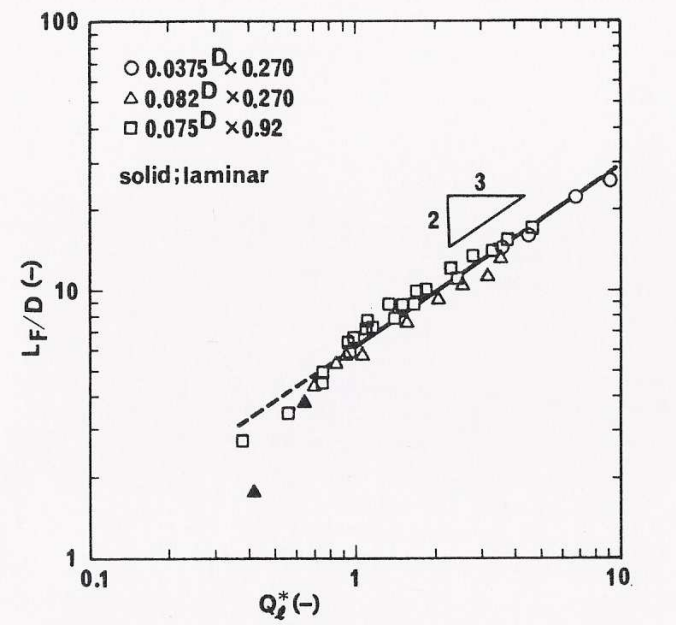

Figure 2.3: Experimental data of scaled heights L_f/D of wall flames versus scaled heat release rates; a correlation with $n = 2/3$. $\dot{Q}^*_\ell \equiv \dot{Q}'/(c_\mathrm{p} T_0 \rho_\infty \sqrt{g}) D^{2/3}$ and D is the fuel characteristic length (after Hasemi [31]).

with $n = 2/3$. For turbulent conditions, the empirical constant k' has the values 4.65 in the model of Delichatsios and 5.0 in that of Eklund.[1] For upward flame on a flat wall and turbulent flow conditions, Tu et al. [75] give value $k_\mathrm{f} = 0.0666\ \mathrm{m}^{1/3} \cdot \mathrm{kW}^{-2/3}$ and Delichatsios $k_\mathrm{f} = 0.0433\ \mathrm{m}^{1/3} \cdot \mathrm{kW}^{-2/3}$, respectively. Various available experimental results give values of the same order of magnitude for k_f and n. In upward turbulent spread, it is believed that n has values between $\frac{1}{2}$ and 1.

In his study, Hasemi [31] found that the flame height x_f correlates with the dimensionless group $\dot{Q}_\ell{}^*$ as follows:

$$x_\mathrm{f}/D = \gamma \dot{Q}^{*^n}_\ell, \tag{2.6}$$

where $n = 2/3$ and $\gamma = 6.0$ for $\dot{Q}^*_\ell \geq 1$, as shown in Figure 2.3.

In tests with line burners with power output up to 300 kW, Kokkala et al. [37] have found $k_\mathrm{f} = 0.043\ \mathrm{m}^{1/3} \cdot \mathrm{kW}^{-2/3}$ for $n = 2/3$ and $k_\mathrm{f} = 0.0058\ \mathrm{m}^2 \cdot \mathrm{kW}^{-1}$ for $n = 1$, respectively. They also noted that linear fit agrees better with their data. Newman and Wieczorek [73] reviewed reported values for γ and n [73, Table 1].

Tsai and Drysdale [76] found experimentally that flame height conforms to the classical correlation (2.4), however, boundary condition at the lower edge

[1]Eklund arrived at his correlation using a two-dimensional vortex model to describe flames on burning walls.

of the wall and the width of the burning area have an effect on the parameters of the correlation. For burning PMMA samples, they found $n = 0.98$–1.25.

Thomas [34] suggests that for wall flames, the fractional power n would tend to unity because wall friction appears to lengthen the flame. This qualitative conclusion will linearize the relationship between the heat release and the flame length. This linearisation is important since it enables analytical approach to analyse the upward flame problem, as done in references [24], [25] and [35], and gives key insights in investigating limiting behavior of wall fires. This linearisation enabled the development of diagrams to analyse limiting behavior of upward flame spread as applied in various studies [36], [77], [25], [35] and [78].

2.5 Flame spread velocity

A simple qualitative relation for flame spread velocity can be already derived from the Williams fundamental equation of spread [23] as

$$V_{\mathrm{p}} \propto \frac{1}{\rho}, \tag{2.7}$$

which means that, materials with low density spread flames faster than the heavier ones.

Orloff et al. [79] studied turbulent fire spread and they wrote the simple but interesting *delayed equation*

$$x_{\mathrm{f}} = x_{\mathrm{p}}(t + \tau), \tag{2.8}$$

where $\tau(x)$ is the surface heat-up time at position x, *i.e.*, the time elapsed between arrival of x_{f} at x. The time increment $\tau(x)$ depends on flame heat flux $\dot{q}_{\mathrm{f}}''$ and material properties of the solid combustible slab. In fact, this equation describes flame spread velocity. Since, if we suppose that $\tau(x)$ and $|\ddot{x}(t)|$ are small quantities[2], then (2.8) can be developed into Taylor series as

$$x_{\mathrm{f}}(t) = x_{\mathrm{p}}(t) + \dot{x}_{\mathrm{p}}(t)\tau + O(\tau^2), \tag{2.9}$$

which already implies that flame spread velocity can be expressed as

$$V_{\mathrm{p}}(t) \equiv \dot{x}_{\mathrm{p}}(t) = \frac{x_{\mathrm{f}}(t) - x_{\mathrm{p}}(t)}{\tau} + O(\tau). \tag{2.10}$$

[2]These are assumptions for a quasi-steady flame spread.

Sibulkin and Kim, in their paper [30], investigate the propagation of upward burning on a combustible wall. Based upon a thermal flame spread theory, they derived flame spread rate expressions for both thermally thin and thick combustible linings when expressions for surface flame heat flux distribution are specified (exponentially decreasing flux distribution ahead of the burning front and constant below that). They defined steady flame spread rate V_{p} as the velocity of the moving ignition front on the combustible surface. They found that for thin combustible slabs a steady velocity is reached when an empirical *forward heat transfer parameter* ϕ is less than a critical value; $\phi < \phi_{\mathrm{crit.}} \equiv c_{\mathrm{p}}(T_{\mathrm{p}} - T_{\infty})/h_{\mathrm{c}}$, where the fuel heat of combustion being h_{c} and the empirical parameter $\phi \equiv \dot{q}_{\mathrm{F}}/\dot{q}_{\mathrm{c}}$ is the ratio of forward heat transfer rate to rate released by combustion. Sibulkin and Kim found that the rate of the flame spread (considered as an ignition or pyrolysis moving front) is given by

$$V_{\mathrm{p}} = \frac{\dot{q}_{\mathrm{f}}''^{2}\delta_{\mathrm{f}}}{k\rho c_{\mathrm{p}}(T_{\mathrm{ig}} - T_{\mathrm{s}})^{2}} \tag{2.11}$$

and

$$V_{\mathrm{p}} = \frac{\dot{q}_{\mathrm{f}}''\delta_{\mathrm{f}}}{d\rho c_{\mathrm{p}}(T_{\mathrm{ig}} - T_{\mathrm{s}})}, \tag{2.12}$$

for thermally thick and thin case. The maximum heat flux at the pyrolysis front is $\dot{q}_{\mathrm{f}}''$ and the effective flame heat transfer extension distance δ_{f} which is essentially the extent of the pre-heating region; $\delta_{\mathrm{f}} \approx x_{\mathrm{f}} - x_{\mathrm{p}}$ (Figure 2.1). The thickness of the thin slab is d.

Quintiere et al. [80] based on kinematic arguments and assuming a quasi-steady burning front velocity, wrote an approximation for the flame spread velocity as

$$V_{\mathrm{p}} = \frac{\mathrm{d}x_{\mathrm{p}}}{\mathrm{d}t} \approx \frac{x_{\mathrm{f}} - x_{\mathrm{p}}}{t_{\mathrm{ig}}}, \tag{2.13}$$

where t_{ig} is the time for the pyrolysis front to move across the flame heat transfer region (ignition time). This expression is equivalent to (2.10).

Hasemi, in his awarded paper of the First International Symposium on Fire Safety Science [31], derived the basic expressions for upward flame spread on both thick and thin materials. The starting point of Hasemi is the thermal ignition theory stating that ignition surface temperature is given as

$$T_{\mathrm{ig}} - T_0 = \int_0^t \dot{q}_{\mathrm{f}}''(x, t-\tau)\phi(\tau)\mathrm{d}\tau \tag{2.14}$$

and that the location of the pyrolysis front x_{p}, as a function of time, is obtained by solving this ignition equation (2.14) for the variable x. The impulse response of surface temperature to heat flux application is $\phi(\tau)$ [67].

By neglecting heat losses and effects of charring on the surface prior to ignition and assuming that flame heat flux is independent of spread velocity, Hasemi, replaced time-integration in (2.14) with space-integration *via* the relation $\mathrm{d}x_\mathrm{p} = -V_\mathrm{p}\mathrm{d}\tau$. He assumes that heat flux distribution is known implicitly without making explicit assumptions on its functional form. The contribution of the burning rate of the material is accounted for through correlations of the flame heat flux with heat release rate [31, Fig. 4].

For thermally thick (semi-infinite) case, the flame spread velocity is

$$V_\mathrm{p} = \frac{\left(\int_0^\infty \dot{q}_\mathrm{f}''(\xi + L_\mathrm{p})/\sqrt{\xi}\,\mathrm{d}\xi\right)^2}{\pi k\rho c_\mathrm{p}(T_\mathrm{ig} - T_0)^2}, \tag{2.15}$$

where $\xi = x - x_\mathrm{p}$ is the height above the pyrolysis front and L_p is the pyrolysis length. If the flux is approximated in (2.15) by the exponentially decreasing expression $\dot{q}_\mathrm{f}'' = \dot{q}_\mathrm{f}''(0)\exp(-\xi/\delta_\mathrm{f}')$ with constant $\dot{q}_\mathrm{f}''(0)$ and δ_f', one will rediscover essentially equation (2.11) by Sibulkin and Kim [30] as

$$V_\mathrm{p} = \frac{\dot{q}_\mathrm{f}''^2\delta_\mathrm{f}'}{\pi k\rho c_\mathrm{p}(T_\mathrm{ig} - T_0)^2}. \tag{2.16}$$

For a constant flame flux over $x_\mathrm{p} < x < x_\mathrm{f}$ and zero above x_f, one obtains

$$V_\mathrm{p} = \frac{4\dot{q}_\mathrm{f}''^2(x_\mathrm{f} - x_\mathrm{p})}{\pi k\rho c_\mathrm{p}(T_\mathrm{ig} - T_0)^2}. \tag{2.17}$$

If now one identifies, in (2.11), the length of the preheating region δ_f with $\frac{4}{\pi}(x_\mathrm{f} - x_\mathrm{p})$, then (2.17) reduces to the earlier result by Sibulkin and Kim [30].

For a thermally thin wall with Newtonian cooling, Hasemi obtains

$$V_\mathrm{p} = \frac{1}{\rho c_\mathrm{p} d(T_\mathrm{ig} - T_0)}\int_0^\infty \dot{q}_\mathrm{f}''(\xi + L_\mathrm{p})\exp(-h\xi/\rho c_\mathrm{p}V_\mathrm{p})\mathrm{d}\xi, \tag{2.18}$$

where h is the heat transfer coefficient. However, to solve for V_p, iterations are needed. For adiabatically insulated wall Eq. (2.18) reduces to

$$V_\mathrm{p} = \frac{1}{\rho c_\mathrm{p} d(T_\mathrm{ig} - T_0)}\int_0^\infty \dot{q}_\mathrm{f}''(\xi + L_\mathrm{p})\mathrm{d}\xi. \tag{2.19}$$

For the exponentially decreasing heat flux distribution one obtains

$$V_\mathrm{p} = \frac{\dot{q}_\mathrm{f}''\delta_\mathrm{f}'}{\rho c_\mathrm{p} d(T_\mathrm{ig} - T_0)}, \tag{2.20}$$

and for the constant case,

$$V_\mathrm{p} = \frac{\dot{q}_\mathrm{f}''(x_\mathrm{f} - x_\mathrm{p})}{\rho c_\mathrm{p} d(T_\mathrm{ig} - T_0)}, \tag{2.21}$$

respectively. Equations (2.17) and (2.21) are the basic equations of upward flame spread.

2.6 SQW-equations

Saito, Quintiere and Williams [26] studied upward propagation of a flame along a thermally thick charring and non-charring combustible materials. Assuming that flame heat flux $\dot{q}_{\mathrm{f}}''$ remains roughly constant over the preheating zone $x_{\mathrm{p}} < x < x_{\mathrm{f}}$, zero elsewhere and that $x_{\mathrm{f}} - x_{\mathrm{p}}$ remains quasi-constant during the spread, they obtained based on thermal ignition theory the expression of the velocity of the spread as

$$V_{\mathrm{p}} = \frac{4}{\pi} \frac{\dot{q}_{\mathrm{f}}''^2 (x_{\mathrm{f}} - x_{\mathrm{p}})}{k\rho c_{\mathrm{p}} (T_{\mathrm{ig}} - T_{\mathrm{s}})^2}. \tag{2.22}$$

Note that, when equations (2.22) and (2.11) are compared, one may found that there is a difference of a factor $4/\pi$. This means that the effective length δ_{f} of the pre-heating region used in [30] extends by $4/\pi$ over the pre-heating length $x_{\mathrm{f}} - x_{\mathrm{p}}$ used now; in other words $\delta_{\mathrm{f}} \equiv \frac{4}{\pi}(x_{\mathrm{f}} - x_{\mathrm{p}})$. Recognizing in (2.22), the characteristic ignition time t_{ig} associated with the flame heat flux as $t_{\mathrm{ig}} \equiv \frac{\pi}{4} k\rho c_{\mathrm{p}} (T_{\mathrm{ig}} - T_{\mathrm{s}})^2 / \dot{q}_{\mathrm{f}}''^2$ (thermally thick case), they obtain the first order ordinary differential equation

$$V_{\mathrm{p}} \equiv \frac{\mathrm{d}x_{\mathrm{p}}}{\mathrm{d}t} = \frac{x_{\mathrm{f}} - x_{\mathrm{p}}}{t_{\mathrm{ig}}}, \tag{2.23}$$

which is the starting point for many upward flame spread models.

For illustration purposes, experimental ignition time data for different thermally thin and thick materials obtained in cone calorimeter tests are shown in Figure 2.4. We have $1/\sqrt{t_{\mathrm{ig}}} \propto \dot{q}_{\mathrm{e}}''$ and $1/t_{\mathrm{ig}} \propto \dot{q}_{\mathrm{e}}''$ for thick and thin cases, respectively, at constant heat flux irradiance level $\dot{q}_{\mathrm{e}}''$.

The total heat release rate per unit width including the contributions of the burner and the material is calculated as

$$\dot{Q}' = \dot{Q}'_{\mathrm{b}}(t) + \int_0^{x_{\mathrm{p}}} \dot{q}''(x,t)\mathrm{d}x, \tag{2.24}$$

where $\dot{q}''$ is the heat release rate per unit area of the burning combustible surface. *Via* change of integration variables, the total heat release rate is expressed as

$$\dot{Q}(t) = \dot{Q}_{\mathrm{b}}(t) + w x_{\mathrm{p}}(0)\dot{q}''(t) + \int_0^t w\dot{q}''(t-\tau)V_{\mathrm{p}}(\tau)\mathrm{d}\tau. \tag{2.25}$$

Further, Saito et al. used the empirical flame height correlation

$$x_{\mathrm{f}} = k_{\mathrm{f}} \dot{Q}'^n \tag{2.26}$$

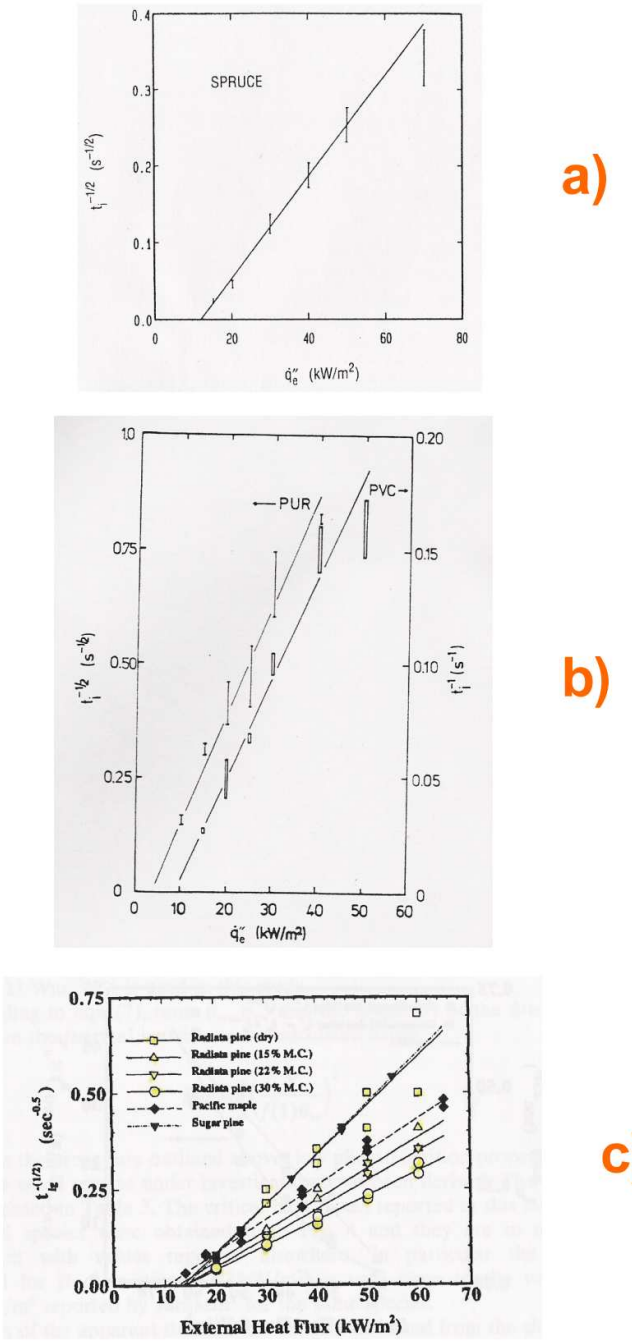

Figure 2.4: Experimental ignition time data; time to ignition *versus* irradiance heat flux level. a) thermally thick spruce [81], b) thermally thick polyurethane and thermally thin PVC [82], and c) thermally thick Radiata pine, Pacific maple and Sugar pine [83] .

and the expression of the total heat release rate (2.25) to finally derive, for the velocity of spread, the classical Volterra type integral equation

$$V_{\mathrm{p}}(t) = \frac{1}{t_{\mathrm{ig}}}\left[k_{\mathrm{f}}\left(Q_{\mathrm{b}}(t) + wx_{\mathrm{p}}(0)\dot{q}''(t) + \int_0^t w\dot{q}''(t-\tau)V_{\mathrm{p}}(\tau)\mathrm{d}\tau\right)^n\right] + -\frac{1}{t_{\mathrm{ig}}}\left(x_{\mathrm{p}}(0) + \int_0^t V_{\mathrm{p}}(\tau)\mathrm{d}\tau\right). \quad (2.27)$$

Equation (2.27) is known as the SQW-Equation, after its developers Saito, Quintiere and Williams. The flame spread velocity can be obtained by solving it as done, for example, in [24], [35] and [33]. The total heat release rate is finally calculated by Equation (2.25). For instance, Karlsson [35], used empirical burning area correlations to calculate total heat release rates in room corner tests. The flame spread rate equation (2.23) is the basic equation for many upward flame spread models [24], [25] and [37].

In their upward flame analysis, Saito et al. assumed further a linearized flame height correlation and with the help of (2.27), they discussed propagation and non-propagation of flame spread for both temporally constant and square root local pyrolysis mass fluxes having finite burning times.

2.7 Heat fluxes from flames

In thermal upward flame spread models, the cone calorimeter is usually used to provide material data, such as time to ignition, and to derive appropriate $\dot{q}''$ at irradiance levels corresponding approximately to those prevailing in the flame spread configuration. This is an approximation, since the flame heat fluxes prevailing in upward flame configuration are not necessarily the same as in the cone calorimeter configuration. Figure 2.5 shows experimental wall flame heat distribution, with for example, a heat flux range of approximately 10–30 kW/m^2 under the flame.

Lattimer [1, Chap. 14] provides an extensive well documented and quantitative review on heat fluxes from fires to surfaces. The review regroups the wide international up-to-date experimental data on the subject.

Quintiere et al. [80] present an extensive wall flame heat flux data for various materials; PMMA, particle board, rigid foam, flexible foam, carpet and aircraft panel. The measured flux maxima were in the range 15–37 kW/m^2 with observed flame height in the range 39–167 cm.

Kokkala et al. [84] in their laboratory tests, measured wall flame heat fluxes in the range of 10–40 kW/m^2 with a burner of 100 kW at the base of a wall and 10–60 kW/m^2 for 300 kW, respectively. Azhakesan et al. [85] made a critical review concerning derived flame heat flux data and flame heat flux measurements and estimated values for upper bounds for common combustible linings. For upward turbulent flames of moderate size ($x_{\mathrm{f}} < 1.4$ m), the flame heat flux ahead of the pyrolysis region is approximately 25 kW/m^2.

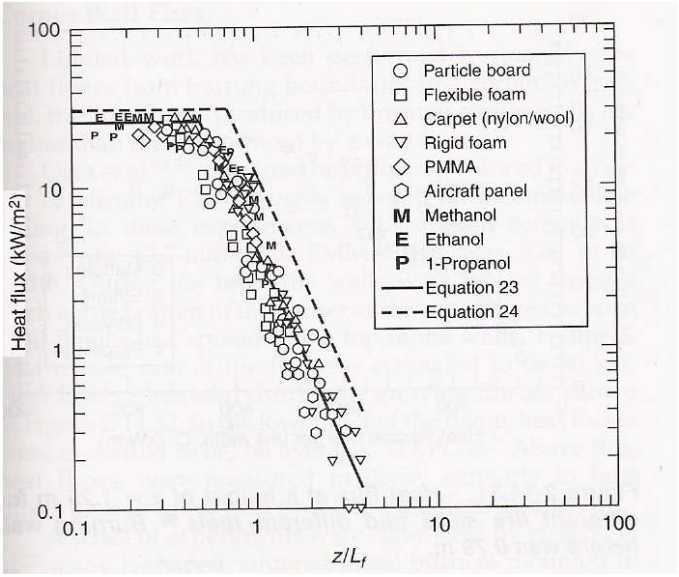

Figure 2.5: Experimental wall flame heat fluxes (as presented in [1, Chap. 14, Fig. 2-14.26]) .

2.8 Analysis of the SQW-equations

Thomas and Karlsson [24] and Baroudi and Kokkala [25] extended further the work on the SQW-Equation started by Saito, Quintiere and Williams [26]. Based on a linearized flame height relation, they derived analytical solutions obtained for various expressions of local heat release rates and discussed limiting behavior of such solutions. One of the main results was the identification of the regions of acceleration and non-acceleration of the flame front on a phase space representation. Extending the work started by Saito et al. and continued by Thomas and Karlsson, Baroudi and Kokkala developed further these "limiting diagrams" and their applications. (Figures 2.6 and [86, Fig. 3]).

Based on simple empirical expressions for local heat release rate curve and a linearized flame height correlation, Karlsson [32], [86]) and [35] obtained solutions for the Volterra-type integral equation (SQW-Equation) when applied to model the growth of a fire in a standard room corner test with combustible lining materials. Data derived from standarised bench-scale tests were used as input. Karlsson obtained, in a closed form, expressions for heat release rate and pyrolysing area. Heat release rate computation results from the model corresponded reasonably well the test results for most materials.

In the following, the behavior of the SQW-Equation is investigated analytically following and partially reproducing some key points from reference [25]. The flame spread rate equation (2.23) is the starting point. Assuming

$n = 1$, in (2.4) and rewriting it in the form

$$x_{\mathrm{f}} = \frac{\dot{Q}'}{\dot{E}''}, \tag{2.28}$$

where $\dot{E}'' = 1/k_{\mathrm{f}}$, Baroudi and Kokkala [25] wrote SQW-Equation (2.27) in non-dimensional form

$$V_{\mathrm{p}}(\epsilon) = \int_0^{\epsilon} V_{\mathrm{p}}(\epsilon')F(\epsilon - \epsilon')\mathrm{d}\epsilon' + G(\epsilon), \tag{2.29}$$

where $\epsilon = t/t_{\mathrm{ig}}$ and $V_{\mathrm{p}}(\epsilon) = V_{\mathrm{p}}(t)/V_{\mathrm{p}}(0)$. The functions $F(\epsilon)$ and $G(\epsilon)$ are known functions of dimensionless time. The initial dimensionless velocity is

$$V_{\mathrm{p}}(0) = \frac{\dot{Q}'_{\mathrm{b}}}{\dot{E}''\tau} + \frac{x_{\mathrm{p}}(0)[\dot{q}''(0)/\dot{E}'' - 1]}{\tau}. \tag{2.30}$$

The function $F(\epsilon)$ is defined by

$$F(\epsilon) = \frac{\dot{q}''}{\dot{E}''\tau} - 1, \tag{2.31}$$

and $G(\epsilon)$ by

$$G(\epsilon) = \frac{\dot{Q}'_{\mathrm{b}}(\epsilon)/\dot{E}'' + x_{\mathrm{p}}(0)[\dot{q}''(\epsilon)/\dot{E}'' - 1]}{\dot{Q}'_{\mathrm{b}}(0)/\dot{E}'' + x_{\mathrm{p}}(0)[\dot{q}''(0)/\dot{E}'' - 1]}, \tag{2.32}$$

respectively.

Thomas and Karlsson showed that SQW-Equation can be solved for flame spread velocity by Laplace transform techniques [24]. Taking Laplace transform of (2.29) one gets

$$\mathcal{L}\left(V_{\mathrm{p}}(\epsilon)\right) \equiv \hat{V}_{\mathrm{p}}(s) = \frac{\hat{G}(s)}{1 - \hat{F}(s)}, \tag{2.33}$$

where $\hat{F}(s)$ and $\hat{G}(s)$ are Laplace-transforms of known functions. The velocity of flame spread is obtained by taking inverse Laplace-transform of Equation (2.33) as

$$V_{\mathrm{p}}(\epsilon) = \mathcal{L}^{-1}\left(\frac{\hat{G}(s)}{1 - \hat{F}(s)}\right). \tag{2.34}$$

Baroudi and Kokkala [25] discussed various analytical expressions for the local heat release rate $\dot{q}''(\epsilon)$. They obtained most interesting results when using the model

$$\dot{q}''(\epsilon) = \dot{q}''(0)\exp(-\gamma\epsilon), \tag{2.35}$$

where $\dot{q}''(0)$ and γ are the parameters of the model. The SQW–Equation (2.33) becomes

$$\hat{V}_{\mathrm{p}}(s) = \frac{1}{a-1}\frac{(a-1)s - \gamma}{s^2 + (1 + \gamma - a)} \equiv \frac{P(s)}{Q(s)}, \tag{2.36}$$

where $a \equiv \dot{q}''(0)/\dot{E}''$. Finally, they obtained

$$V_{\mathrm{p}}(\epsilon) = C_1(s_1)e^{s_1\epsilon} + C_2(s_2)e^{s_2\epsilon}, \tag{2.37}$$

where s_1 and s_2 are the simple roots of the denominator in (2.36). By inspecting the asymptotic behavior of the solution, criteria for flame spread velocity to grow continuously or to stop have been derived. Figure 2.6 presents the graph where these different behaviours are shown. Some authors have called this diagram the *Baroudi-Kokkala diagram* [36] and [87].

Under certain conditions, the basic solution family (2.36) anticipates oscillatory behaviour. Strictly speaking, such solutions are valid as long as flame spread velocity remains positive or null. However, experimentally, cyclic flame spread behaviour has been reliably observed by Kokkala et al. [84] and Hakkarainen et al. [88] in large-scale upward flame spread tests on wood products at VTT.

In these tests, 3-4 successive cycles of "accelerating-decaying-stopping-regain-of-propagation" phase of the upward flame spread have been observed [84, Fig. 11a and Chap. 5.1, 5.2 and 5.5] and [88, Fig. 8 and 1st Chap. of Sec. 2.2.2]. In [84], the cyclic behaviour was observed in the tests with particle board and solid wood (height 2.4 and 7.5 m), in an open configuration. Figure 11a shows measured flame height as function of time for paricle board on mineral wool backing. In [88], such cyclic behaviour has been also observed for wood and plywood in intermediate- and large-scale facade tests. Figure 8. represents measured heat release rate of painted pine boards.

It is interesting to note that Grant and Drysdale [33] have observed, numerically, oscillating behaviour for the pyrolysis front velocity and the RHR contribution from the burning of linings when solving numerically an extended form of the classical SQW-equation accounting for the burnout.

The diagrams of Figures 2.6 – 2.8, illustrate flame spreading characteristics of lining materials [25], [35], [3], [36] and [77]; they show what material properties are essential to explain upward flame spread. The diagrams try to answer the question: *does the material spread fire or not*? (see Figure 2.7 for an application.) The burning parameters a and γ are derived from bench-scale cone calorimeter tests. In addition, this diagram answered, for the first time, the question how the results obtained in testing wall and ceiling products in one scenario relate to the results obtained from another scenario (bench-scale Cone Calorimeter data)? Hasemi pointed to sensitivity of flame spread to “material properties” in the vicinity of the limiting curves on the diagrams [38].

However, there are materials, especially charring ones, for which a more appropriate model for measured local rate of heat release is

$$\dot{q}''(\epsilon) = \dot{q_0}'' \exp(-\gamma\epsilon) + \dot{q_1}'' \equiv \dot{q_{0,4}}''[r + (1-r)\exp(-\gamma\epsilon)], \tag{2.38}$$

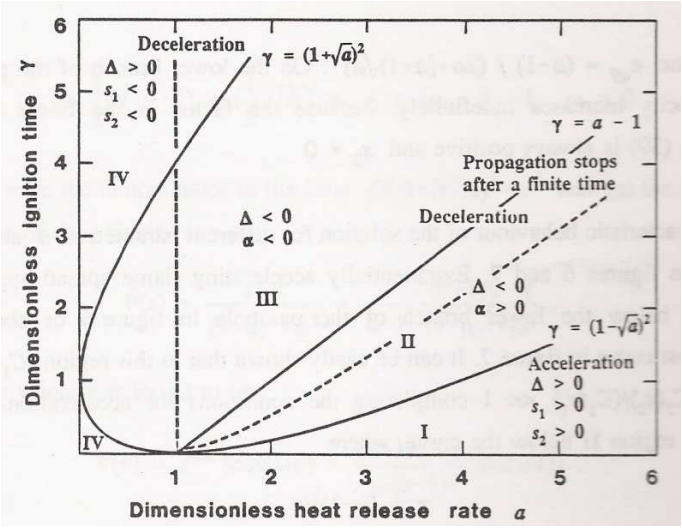

Figure 2.6: The flame spread limiting diagram (as presented originally by Baroudi and Kokkala [25]). Regions of various type of flame spread. The discriminant $\Delta = (1 - a + \gamma)^2 - 4\gamma$ and $\alpha = 1/2(a - \gamma - 1)$.

where $r = \dot{q}_1''/(\dot{q}_1'' + \dot{q}_0'')$. When $r = 0$, model (2.35) is obtained. Materials which burn longer have $r \neq 0$.

Using this extended model, Baroudi and Kokkala [25] showed that the limiting curves on the diagram are ellipses, Figure 2.8,

$$\left(\frac{a' - \frac{\sqrt{2}}{2r}}{\rho_x}\right)^2 + \left(\frac{\gamma'}{\rho_y}\right)^2 = 1, \tag{2.39}$$

with principle axes a' and γ' of the rotated coordinates at a 45^o angle with respect to the original coordinate axes. The semi-axes in the coordinate system $(0, a', \gamma')$ are $\rho_x = \sqrt{(1-r)/(2r^2)}$ and $\rho_y = \sqrt{1/(2r)}$. The coordinates of the center (of coordinates) of the ellipses in the original coordinate system is $(1/(2r), 1/(2r))$. For $r = 0$, the limiting curve is a parabola (the diagram of Figure 2.6).

The type of sensitivity, pointed to in [38] by Hasemi and Yasui, can be partially explained, at least for one material parameter as the limiting curve; a parabola, in the original limiting diagram (for $r = 0$ in diagram 2.8), becomes rapidly an ellipse for $r = 0.1$. The right branches of the parabola and the ellipse limit acceleration-deceleration regions. Indeed, we see that the region enclosed between the two branches is not negligible, even though r changed only by 10%. It is thought that this extended diagram can be more appropriate than the original one as guidance for evaluating flame spread behavior based on small-scale material data.

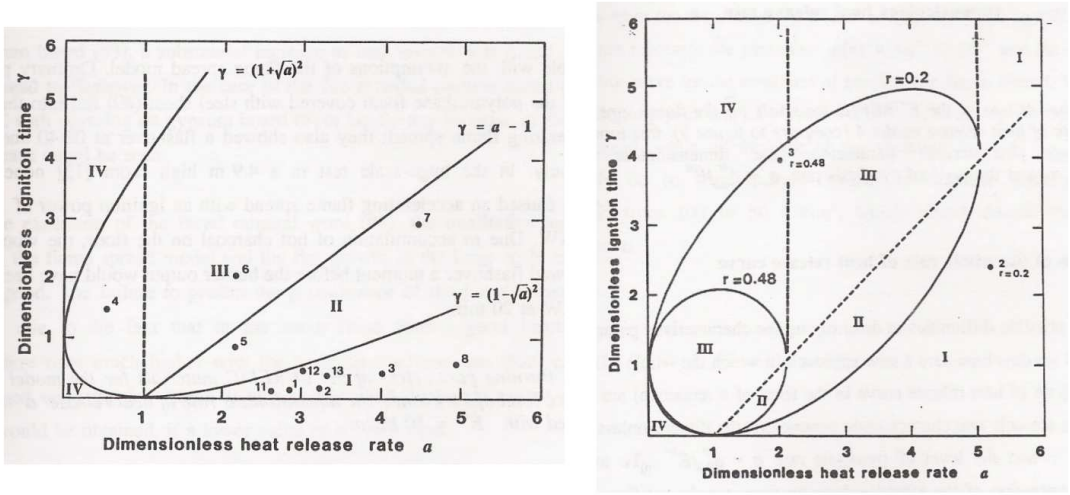

Figure 2.7: Limiting diagrams (as presented in [25]). Location of various lining materials. a) on original diagram: 1: insulating fibreboard, 2: medium density fibreboard, 3: particle board, 4: gypsum plasterboard, 5: PVC cover on gyps. pl. board, 6:paper cover on gyps. pl. board, 7: textile on gyps. pl. board, 8: textile cover on mineral wool, 9: melamine-faced particle board, 10: expended polysteren, 11: rigid foam polyurethane foam, 12: wood panel (spruce) and 13: paper cover on particle board (numbered symbols from 1–13) on the flame spread diagrams; and b) on extended diagrams; symbol 2: ordinary plywood and 3: textile wall covering on gypsum board.

2.9 Numerical formulations of the SQW–equation

In thermal upward flame spread theory, the flame spread problem is considered solved once flame heat flux, flame length and material data such as characteristic time to ignition and local mass flux are provided for that particular configuration.

Different variation of solution algorithms for the SQW-equation are applied to calculate turbulent flame spread with success [32], [35], [89], [37] (Paper I), [33], [42] (Paper II), [43, *Model III*] (Paper III) and [41].

In modeling flame spread in warehouse fires, Grant and Drysdale [33] solved numerically the non-linear Volterra equation (2.27) using local heat release rate curve from cone calorimeter directly as input. Their formulation accounts also for burnout. They developed a computer program which incorporates a non-linear root finding scheme within the basic solution algorithm for Volterra equations allowing solutions for non-linear flame height correlations.

Instead of solving the complicated non-linear Volterra equation (2.27), as is traditionally the case, Kokkala, Baroudi and Parker [37] (Paper I) and [89], solved directly the original non-linear initial value problem (2.23) using

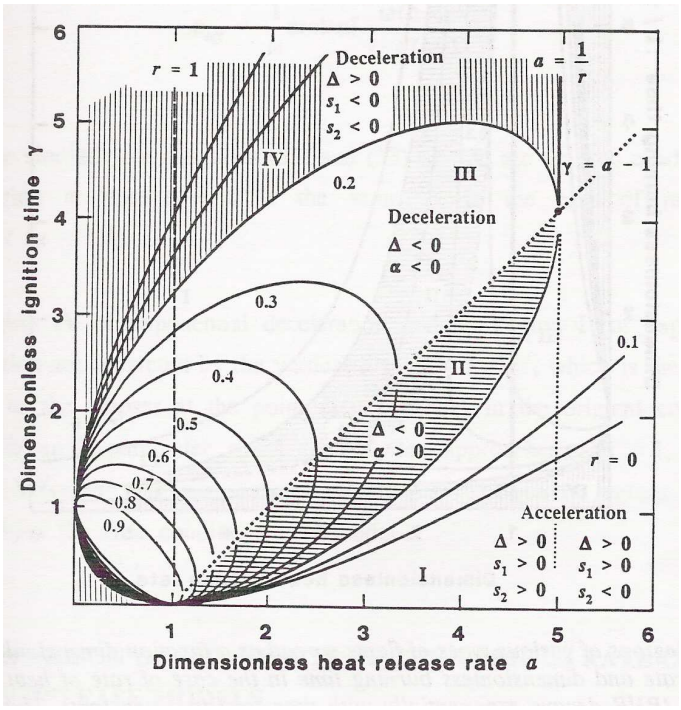

Figure 2.8: Extended limiting diagrams (as presented in [25]). Regions of various type of flame spread. The shaded area shows the different regions for $r = 0.2$. The discriminant $\Delta = (1 - a + \gamma)^2 - 4\gamma(1 - ra)$ and $\alpha = 1/2(a - \gamma - 1)$.

conditionally stable explicit Euler first order quadrature scheme

$$\frac{\mathrm{d}x_\mathrm{p}(t_{\mathrm{i}+1})}{\mathrm{d}t} \approx \frac{x_\mathrm{p}(t_{\mathrm{i}+1}) - x_\mathrm{p}(t_\mathrm{i})}{\Delta t_{\mathrm{i}+1}} = \frac{x_\mathrm{f}(t_\mathrm{i}) - x_\mathrm{p}(t_\mathrm{i})}{t_\mathrm{ig}}, \tag{2.40}$$

with appropriate initial conditions. (Both solutions are naturally equivalent but solving initial value problems is much easier than finding solutions to non-linear Volterra-type equations.) The location of the pyrolysis front is obtained as

$$x_\mathrm{p}(t_{\mathrm{i}+1}) = (1 - \Delta t_{\mathrm{i}+1}/t_\mathrm{ig})x_\mathrm{p}(t_\mathrm{i}) + (\Delta t_{\mathrm{i}+1}/t_\mathrm{ig})x_\mathrm{f}(t_\mathrm{i}), \tag{2.41}$$

where the time step $\Delta t_{\mathrm{i}+1} \leq 2t_\mathrm{ig}$ and $x_\mathrm{f}(t_\mathrm{i}) = k_\mathrm{f}(\dot{Q}'(t_\mathrm{i}))^n$. The total heat release rate is calculated by evaluating the convolution integral (2.25) using trapezoidal quadrature rule (Equation 6 in [37]).

$$\dot{Q}'(t_{\mathrm{i}+1}) = \dot{Q}'_\mathrm{b}(t_\mathrm{i}) + \sum_{n=1}^{n=i} \dot{q}''(t_i - \tau_n)[x_\mathrm{f}(\tau_\mathrm{n}) - x_\mathrm{p}(\tau_\mathrm{n})]w_\mathrm{n}/t_\mathrm{ig} \tag{2.42}$$

with integration weights as given in [37] (Paper I). This numerical model was implemented in reference [37] (Paper I) as a computer program called

THIMES [39]. In a further research work, Gojkovic and Hultquist [40] incorporated the *THIMES* algorithm into a compartment computational fire zone model (the WPI/Fire Code).

The flame spread model for a burning mattress developed in [42] (Paper I) and Model III in [43] (Paper III), is a physically based novel extension of thermal fire spread theory with many extensions and adaptations to convert it into a furniture fire model to calculate flame spread and heat release rate history (HRR). The numerical algorithm used for flame spread calculation is essentially an adaptation of that of reference [37] (Paper I) accounting for the finite size of the mattress. The prediction of the early phase of the HRR-curve was reproduced numerically with success. Detailed presentation of the model can be found in the cited papers. The numerical model developed in [37] (Paper I) was also applied successfully by Hakkarainen and Kokkala [41] to predict heat release rate in the Single Burning Item (SBI) tests.

Part II

Calculation of heating of structures

Chapter 3

Introduction

This part of the thesis synthesis addresses heating of structures and temperature calculations in solids.

Heat release rate in fires is of primary importance. When a structure is present, part of the calorific energy dissipated in the fire, is fed back to the structure *via* thermal radiation and convection with consequence of raising its temperature. As the performance of structures decrease with increasing of temperature, knowledge of temperature distribution within the structure is important to estimate safe-escape time for occupants, safe-operational time for firemen and fire resistance. (Fire resistance is the ability of a structure or its element to maintain its function as structural component or a barrier in a fire.) There are many other aspects influencing fire safety, *i.e.*, toxicity of combustion products, incapacitation by heat exposure, visibility, sufficence of escape paths and doors and escape-path visibility and accessibility, presence of smoke control systems, fire detectors and alarms and also the time it takes for firemen to intervene, to cite only few factors. (Smoke control systems are necessary to prevent lethal concentrations of smoke accumulation.)

To determine the fire resistance of a structure, using calculation methods, three basic aspects should be at least considered [1, Chap. 9]; fire exposure, heat transfer and structural response. Fire exposure should be first characterized. Then, using principles of heat transfer, the heat response can be evaluated. Temperature field is calculated by solving the heat conduction equation with appropriate boundary and initial conditions (typically radiation and convection boundary conditions). And finally, structural response is addressed. For instance, a complete calculation example exposing the three phases mentioned above can be found in the paper by Quintiere et al. [90] in which fire-induced collapse of the World Trade Towers was investigated.

Chapter 4

Heat transfer

Thermal energy is transferred from one object to another *via* three mechanisms: radiation, conduction and convection.

When two objects at different temperature are brought in contact, heat is transferred from the hot to the cold one. Consequently, the hot object cools down and the cold one is heated [91]. Heat *diffuses* from a hot to a cold medium. This energy transfer process associated with solids is known as *heat conduction*, Carslaw and Jaeger [67], Eckert [92], Luikov [93], and Lienhard IV and Lienhard V [94]. Rockett and Milke [1, Chap. 2] provide a thorough review on heat conduction in solids. Heat transfer and especially the heat conduction will be treated in more detail in Chapter 5.

Fundamentally, *convection* is not a basic a heat transfer mechanism but rather a practical macroscopic heat transfer model for heat transfer processes between a fluid layer and a solid surface involving movement of the fluid medium, [3] and [94]. Atreya [1, Chap. 3] gives an extensive review on convective heat transfer. In fires, a significant amount of heat released in combustion is "transported" by convection *via* the motion of hot gases (buoyancy-induced convective flow). Heat transfer between a solid surface and a surrounding fluid by convection can occur in two prevailing flow conditions. The fluid region close to the surface where the heat transfer occurs is known as the *boundary layer*. An important engineering parameter quantifying the amount of convection between two objects is the *convection coefficient* (heat transfer coefficient usually denoted by h) which is the ratio of the transferred heat flux between the boundary layer and the surface to the gradient of temperature within that boundary layer. *Forced convection* is associated with heat exchange when a continuous fluid flow stream passes the solid surface. An example would be the cooling of a burned finger by a continuous flow of cold faucet water. In such case, heat is evacuated from the hot surface of the skin by the forced water flow. In *natural* or *free convection*, the motion of the fluid is due to the buoyant flow of the warm (or cold) fluid next to the surface. The heat exchange between a naked skin (hands, face, body) of a person in an unwindy room and the surrounding air occurs mostly through

natural convection. In this case the heat exchange by radiation is comparably small. Another example is the cooling of a hot pizza in air. In addition, when the flow occurs inside or outside the considered body, we speak of *internal* or *external* convection, respectively.

Thermal radiation transport occurs *via* electromagnetic waves, confined to a narrow wavelength window in the electromagnetic spectrum between 0.4 and 100 μm (including visible light and extending towards infra-red) Siegel and Howell [95], Drysdale [3] and [94]. Tien et al. [1, Chap. 4] have reviewed thoroughly radiative heat transfer. All objects radiate – except those which the temperature is at the absolute zero. Radiative transfer does not need medium to occur. The total amount of thermal energy flux emitted by a black body within a narrow band of wavelength λ and $\lambda + \mathrm{d}\lambda$ is given by the *Plancks's distribution law* [95]. The net radiative heat flux for a single frequency ν, across an arbitrarily oriented surface, is given by the spectral radiative energy flux $q_\nu = \int_0^{4\pi} I_\nu \vec{n} \cdot \vec{R}\mathrm{d}\Omega$, where $\vec{R}\mathrm{d}\Omega$ is the oriented solid angle element, I_ν the radiation intensity expressed as energy per unit area per unit solid angle within a unit frequency interval. In fires, thermal radiation is involved in heat exchange between various surfaces, in absorption and emission by different gases (water vapor and carbon dioxide, etc.) and soot particles generated by the fire. A more familiar example of radiative heat transfer would be the heating effect of the sun on the naked skin.

4.1 Measurement of temperature

For Aristotle and ancient Greek philosophers heat and cold were fundamental properties of matter. In Aristotle's matter theory the qualities *dry* and *wet*, *heat* and *cold* are *mixed* with prima materia to obtain the 4 elements: *earth, water, air* and *fire*. It is the ratio in which they are *tempered* which confers the matter its property. For instance, fire has the properties dry and hot, and the earth, wet and cold. These qualities are *tempered* in an element conferring it its *temperament*. The word *temperature* is derived from the Latin word *temperamentum*.

The first thermoscope (a thermometer without a scale) appeared late 16th century [96]. This invention is attributed to Galileo Galilei (1592). Galileo Galilei (1592), Santorre Santorio, Galilei and Galilei's friend Sagredo and others developed the thermoscope to include a numerical scale. Already in the 1630's, the liquid in a glass thermometer was conceived. However, there was no universal scale division. Universal temperature scales based on specified points appeared in the early of 18th century.

Around 1724, Fahrenheit constructed thermometers in which he fixed 32^{o}F as the ice freezing point and 212^{o}F as the boiling point of water (in normal atmospheric conditions). This scale was adopted in England. The first al-

cohol[1] thermometer was constructed by Réaumur in 1730. He proposed a different scale: 0^o for the melting point of water and 80^o for the boiling point of water. This type of thermometer was used in France and central Europe. Celsius developed in 1741 a thermometer with the scale of 100^o for the normal boiling point of water and 0^o for the freezing point. The systems of Celsius and Fahrenheit are still in use. The system of Celsius has been extended to become the standard absolute temperature scale (Kelvin scale). About nineteen different scales were known during the 16th century. In all these devices, the measurement is based on the thermal expansion of a gas or a liquid. Note that a thermometer measures only its own temperature. This temperature is the same as the contacting body temperature only at thermal equilibrium. See Wisiak [96] for a detailed chronological review on history of the thermometer. Dreyer et al. [97] provide an interesting reading about the history of thermometry and the concepts of temperature, heat and entropy.

There are other temperature measuring devices based on electrical and electromagnetic phenomena; thermocouples, resistance thermometers and optical pyrometers [98, Chap. 8: *Thermometry*] and [16, Chap. 5: *Chemistry and physics of fire*]. The thermocouple consists of a closed electric circuit composed by two conductors made of different materials with two small junctions: a hot junction and a cold junction kept in known reference temperature. The hot junction is immersed in a medium whose temperature is to be measured. The typical precision of such measurement is about 0.1–0.2 degrees. The measurement is based on the Seebeck effect: an electric current flows in the closed circuit when the junctions are at different temperatures. The resistance thermometer is based on the change of the electric resistance of a metal wire with temperature. The platine resistance thermometer was developed in 1888. In infrared pyrometry, temperature measurement is based on thermal radiation. There are also measurement techniques based on laser beam tomography. However, these techniques are too expensive instrumentation in many cases. Baroudi and Somersalo [99], Kaipio et al. [100] and Hietaniemi et al. [101] developed a novel robust and inexpensive measurement technique for temperature field in a hot gas based on impedance tomography. They constructed an operational device prototype consisting of a planar grid assembled in a defined way using a relatively small number of thin metallic wires. The total electric resistance changes are measured. Based on this, the temperature field is reconstructed using inverse methods.

4.2 Literature review

(Short review on Heat Transfer:) Newton was probably the first who published studies on heat exchange between objects and surrounding air; *Newton's law of cooling* [102]. Newton postulated that: *The rate of loss of the*

[1]He used spirit of wine diluted with certain amount of water.

temperature of a hot object in a blowing flow of cold air is proportional to temperature itself. This can be written appropriately using modern notation as

$$\mathrm{d}\Delta T/\mathrm{d}t \propto -\Delta T. \tag{4.1}$$

Heat transfer textbooks often use the notation $q/A = h\Delta T$ or $q \propto \Delta T$ when referring to this law. This notation, can be misleading since one can think that heat transfer textbooks credit Newton for the discovery of the concepts of "convection coefficient" h and of heat flux.[2] In Newton's article the word "heat" means the intensive thermal parameter known as temperature. Newton did not use equations at all nor defined a heat convection coefficient. Newton was however, the first one who postulated the cooling law. Find here the exact Newton's words in his translated paper *Scale of Degrees of Heat* [102] :

> This Table was constructed with the help of a Thermometer and a piece of a red hot Iron. ... if the Times of cooling are taken equal, the Heats will be in a Geometrical Ration, and therefore are easily found with a table of Logarithms.

Newton published his work in 1701 in Latin in a brief paper "Scala graduum Caloris. Calorum Descriptiones & Signa." in the *Philosophical Transactions of the Royal Society of London.* This work[3] concerns the construction of a scale of temperature on his thermometer and a method to measure high temperatures. For example, Newton used two fixed reference points for this thermometric scale: "melting point of ice" as 0 degree and "external heat of a human body" as 12 degrees Newton [102]. Wisiak [96] made a review on the historical development of the thermometer.

Based on the Newton's law of cooling, the French physicist Biot [105] addressed the problem of heat conduction (in a thin bar heated at one end). However, he seemed to incorporate external convection in the analysis and believed that the temperature at a point is influenced by all the points in its vicinity [94].

Fourier [106] studied further heat transfer phenomena and arrived to completely quantify and solve the heat conduction problem. His book [106] is a complete presentation of the theory of heat conduction. Note that, there was not a clear distinction between heat and temperature until the middle of the 18^{th} century. A detailed review on heat conduction will be given in Chapter 5 (*Heat conduction in solids*) of the present synthesis.

[2]There is a controversy saying that, Fourier is the conceiver of both h and "Newton's cooling law", see papers [103] and [104] by Adiutori on the origins of the heat transfer coefficient.

[3]The first English translation of this work was included as Newton's *Scale of Degrees of Heat* in the *Hydrostatical and Pneumatical Lectures, (1738, London).* Another translation into english can be found in *The Philosophical Transactions (from year 1700, to year 1720) Abridged* by Henry Jones [102] in 1749 (London).

In the following, a short review on heating of structures in fires is presented. The textbook, "Structural Design for Fire Safety" by Buchanan [107], introduces explicitly the structural design of buildings and their elements exposed to fire. It also gathers a large amount of literature and data related to the fire resistance of building structures. The textbook is intended for structural engineers and students and for all those practicing fire safety. To evaluate the fire performance of a structure, various methods are in use: experimental testing, tabulated data, simple calculation methods and advanced calculation methods [108]. The performance of structural elements can be assessed through fire testing. Tabulated data summarise the results of a significant number of testing on similar elements in tables, graphs or simple best fits. Physical interpolation can be best performed by using appropriate models or by approximating by linear interpolation. However, the question of possible extrapolations is complex[4] and remains open. Pettersson [109] gives various design charts for steel members under fire exposure. Simple calculation methods are simple equilibrium and conservation of energy equations. Usually, they include few degrees of freedom (or unknowns) rapidly tractable by hand or implemented in MS Excell-like calculus spread sheet or in Matlab. For instance, lumped heat capacity formulae are usually used in temperature calculation of unprotected or protected steel sections when the steel temperature can be assumed spatially constant. Typical equations are provided by Pettersson [109] and Milke [1, Chap. 9], for instance.

Advanced calculation methods are used to gain details in the response of complex structures. In these methods, the equations form a set of partial differential equations or/and integro-differential equations which can be coupled, so one have to use numerical methods to solve them. Such methods are Finite Elements Method (FEM), Finite Difference Methods (FDM), Finite Volume Methods (FVM) and so on. Reviewing literature on fire resistance is beyond the scope of this synthesis. Usually, such papers, as for instance, [110], [111], [112], [113], [114], [115] and [116] deal with development of calculation methods to predict structural response of structures or structure members at elevated temperatures. In structural modeling, it is primordial to account for degradation of material properties with increase of temperature and for thermal restraints and displacements. A concise and complete writing on experimental and calculation methods for determining fire resistance methods of various constructions with worked examples are provided by Milke [1, Chap. 9] for steel, Fleischmann and Buchanan [1, Chap. 10] for concrete and White[1, Chap. 11] for timber members, respectively.

In order to make temperature calculations, heat flux boundary conditions should be known (in the conjugate heat transfer problem, boundary conditions at the fluid-solid interface are part of the unknowns [93]). In other words, to solve a heat conduction problem, appropriate boundary conditions

[4] 1) because of possible and unpredictable bifurcations in the evolution paths. 2) the evolution may be unstable in the neighboring of these points.

should be imposed. These are, for instance, given temperature on part of boundary and heat flux on the remaining part. For references to experimental work dealing with flame heat flux to surfaces, please refer to Part I of this document. Modeling of heat transfer from flames is still under development, however experimental data and empirical correlations have been developed to calculate flame heat transfer for various common geometries; [1, Chap. 14], [117], [118], [119], [120] and [121]. Kamikawa et al. [121] performed recently new heat flux and temperature measurements on a square steel column in a fire adjacent or surrounding the column. They obtained vertical heat flux distributions on front and side of exposed surfaces with heat sources ranging from 52 kW to 255 kW (source heat release rate). They concluded that the "localized fire" concept does not apply for columns surrounded by fire. In fires, in most complex cases, heat transfer boundary conditions can be obtained through numerical full-scale 3-D field model simulations. For instance, in the FDS-simulation of the fires in the WTC towers [10], one can extract heat fluxes to boundaries if thermal and structural response calculations (in implied structures) are to be performed further [11] and [122]. This was, for instance, part of NIST WTC-investigation (`wtc.nist.gov`) where the detailed heat transfer to solid structures have been done by the finite element software ANSYS. In general, heat flux and temperature boundary conditions can be extracted from FDS or equivalent CFD fire simulations as field values at solid-fluid interfaces *via* for instance, the "Fire-Structure Interface" (FSI) [11]. After that, these boundary conditions can be used as input data for further temperature calculations in the solid. Such calculations can be made with a varying degree of details using simplified analytical and numerical models or more advanced finite element heat transfer software. FDS uses a simple 1-D heat transfer numerical model in the solid. (finite difference method). In [122] a complete and complex real world example is provided where the FSI [11] transfers the results of the FDS fire simulation to the commercial ANSYS finite element software to calculate the thermal response of a complex steel structure. The analysis can be continued or coupled to a structural analysis by a standard Finite Element software. For instance, in these papers, fire dynamics simulations are coupled to the heat transfer and structural analyses.

The most versatile numerical models are based on the finite element method; ABAQUS[5], ANSYS[6] and ADINA[7], for instance. These are universally used general purpose finite element analysis software. `ABAQUS` provides powerful tools to solve a wide range of engineering problems; static and dynamic analysis and complex nonlinear coupled physics analysis. `ABAQUS` solves also heat transfer problems and can couple between various physical phenomena among which, for instance, we can find thermo-mechanical and thermo-electrical

[5]http://www.abaqus.com (10.02.2006).
[6]http://www.ansys.com (10.02.2006).
[7]http://www.adina.com (10.02.2006).

modeling. ANSYS Multiphysics™ allows analysis of coupled effects of different interrelated physics; structural, thermal, CFD, acoustic and electromagnetic. On should not forget the emerging young COMSOL Multiphysics™, [8] which also allows to elegantly, interactively and efficiently model and solve numerically various coupled physical phenomena. ADINA is a Finite Element System for Structures, Heat Transfer and CFD. ADINA-T is a module for heat transfer analysis in solids. ADINA allows also coupling between fluid flow and structures. All these finite element softwares are able to couple heat transfer and structural analysis.

There is also a set of widely used finite element programs developed specially for fire design purposes like TASEF and Super TASEF [123], SAFIR [124] TEMPCALC. [125] Rockett and Milke [1, Chap. 2] give a complete review of computer models in use for computing the thermal response of a structure to a fire.

Temperature calculation methods can be divided into two classes: analytical and numerical. The classical textbook [67] on heat conduction in solids, by Carslaw and Jaeger, gathers a large number of analytical solutions to various problems with different boundary and initial conditions. However, the geometry and boundary conditions are rather limited. In addition, the analytical solution when computed may be less accurate than when it is directly obtained by numerically solving the heat conduction equation because the analytical solutions are often expressed as series which converge often very slowly. In practice, analytical approach is limited to linear problems. When the temperature inside a section is spatially approximately constant, lumped models can be used. This is the case for insulated or uninsulated thin steel sections. These models are usually expressed as one ordinary differential equation (ODE) describing the mean temperature evolution with respect to time. For arbitrary heat exposure, this ODE is numerically integrated. Myllymäki and Baroudi [126] showed, for an insulated steel (or metallic) section, *via* finite element formulation that using one element with two linear basis functions, one obtains most of the temperature calculation equations given in design codes. Traditionally, heat transfer to an insulated steel section is calculated using one ODE. These approximate equations have been derived by several authors assuming one dimensional heat conduction models with constant thermal properties [127], [128] and [129]. Many of these equations have been used in the design codes of steel structures in fire. Wickström [127] derived an exact analytical solution in a closed form for the temperature evolution of insulated steel structure when exposed to the ISO 834 standard curve. Wickström gives also approximate solutions using a lumped capacity model for the steel core to which one third of the capacity of the insulation is added. The accuracy of the approximation degrades, as expected, with heavy

[8] http://www.comsol.com (1.02.2007).

insulations. Milinek and Thomas [128] used Laplace transforms to derive an approximate differential equation similar to that derived by Wickström and confirming his earlier approximate results. McGuire et al. [129] gives some heat conduction scaling relations relating time and dimension to estimate fire resistance time of simple structural elements.

Advanced numerical methods are more versatile as geometry, boundary and initial conditions, can be arbitrary. They also account for nonlinearities. The heat conduction problems are usually solved using Finite Element Method (FEM) [130] or Finite Difference Method (FDM). In FDM, geometry is limited to simple cases. In FEM, the complexity of the geometry and of boundary conditions is not limited.

Examples of simplified engineering temperature calculation algorithms for fire heated structures are given in [131] (Paper V), [132] and [133].

Myllymäki and Baroudi [131] (Paper V) developed a semi-advanced engineering design tool to predict fire resistance of concrete filled tubular columns exposed to fire. The tool consists of a thermal and a mechanical part. In the thermal part a non-linear finite element algorithm is developed and implemented to solve the transient heat conduction problem. Computed temperature distributions and bearing capacities compare reasonably well with test results. Details are presented in the paper.

In paper [132] (Paper VII), Myllymäki et al. studied experimentally and numerically the heating of lightweight balconies on a facade exposed to flames emerging from a window under the balcony. This work is part of a research programm founded by the Finnish steel industry and National Technology Agency of Finland (TEKES) in which VTT Building Technology has been investigating fire exposure to lightweight steel balconies. In paper VII, an engineering temperature algorithm has also been developed to calculate temperatures within the structure and accounting for thermal radiation in internal cavities of the structure of lightweight steel balconies installed in front of a facade and exposed to flames emerging from a window-opening under the balcony. Comparison with ABAQUS results was satisfactory. This part of the project has been supported by the VTT Steel project. A new method to assist design has also been proposed. It allows transient gas temperature calculations under a balcony. It is based on an extension of Law's method [134] combined with the parametric fire exposure to account for transient flame temperature. For details, please refer to the paper.

An efficient and direct way to control and limit the growth of a fire is the use of sprinklers or water sprays. The passive approach to increase the fire resistance of structures is to insulate them. Knowledge of actual thermal properties of the insulation material is essential to make accurate temperature calculations. For insulation materials, the thermal capacity and conductivity are very often temperature dependent. Myllymäki and Baroudi Paper [133] (Paper VI) developed an inverse method to determine the thermal conductivity of a homogeneous insulation material as a function of temperature based

on boundary temperature measurements. It showed that the present method gives more accurate thermal conductivities for the whole temperature range when compared to the standard methods as for instance, the NT FIRE 021 and CEN Pr ENV YYY-4. The first part of the paper presents the direct non-linear transient heat conduction problem together with it discretisation by the finite element method. In the second part the inverse problem is formulated. In the formulation, optimal regularization is achieved by Tikhonov regularization [135] together with the Morozov discrepancy principle [135] and [136]. The developed algorithm was successfully used at VTT to determine thermal conductivities from measurements and to interpolate design tables for additional insulation thicknesses for ducts with internal hot gas flow (chimney test) based on these experimental results (thermal resistance tests). Full details are given in the cited paper.

In this second part of the dissertation synthesis, temperature calculation in structures is addressed briefly.

Chapter 5

Heat conduction in solids

Heat can be transferred from one body to another, by three mechanisms: conduction, convection and radiation. However, physically, heat is transferred only by conduction and radiation, whereas convection is only a macroscopic heat transfer mode used in modeling heat transfer between a fluid layer in motion and a solid surface.

In fire, all three mechanisms of heat transfer exist. Heat transfer in solids takes place by conduction. In addition to conduction, heat is transferred also by internal radiation and convection in porous and fibrous solid materials [92], [93] and [95]. Rockett and Milke [1, Chap. 2] present a concise review on heat conduction together with a historic development of heat conduction theory. The annual "Heat Transfer Review", founded by professor Ernst R. J. Eckert in 1954 and nowadays appearing in the International Journal of Heat and Mass Transfer, contains an extensive review covering the heat transfer literature in English. The first review contained 112 papers in 1954 and the last one [137] already 1700. In addition to review journal articles, the review presents important conferences and meetings and books on heat transfer. The aspects of heat transfer covered are reflected in the keywords of the review: conduction, boundary layers, internal flows, porous media, heat transfer, experimental methods, natural convection, rotating flows, mass transfer, bio-heat transfer, melting, freezing, boiling, condensation, radiative heat transfer, numerical methods, transport properties, heat exchangers, solar energy, thermal plasmas. The textbook *A heat transfer textbook*[1] by Lienhard IV and Lienhard V [94] covers a large domain of heat transfer with worked examples : Heat conduction, convection, thermal radiation and mass transfer. The classic textbook *Heat and mass transfer* by the academician Luikov [93] covers a wide domain : convective diffusional transfer, heat conduction, convective heat transfer, conjugate heat-transfer, transport phenomena in capillary-porous bodies and analytical heat and mass diffusion theory.

The classical textbook on heat conduction in solids by Carslaw and Jaeger

[1]Freely downloadable textbook of 749 pages from the internet! Thanks to the authors.

[67] provides a large amount of analytical solutions to various problems.

5.1 Introduction

The rate at which heat flows is determined by thermal conductivity. That is why, for example, touching a piece of metal feels cooler than touching wood, even though they are both at the same room temperature. The thermal conductivity of metals is much greater than wood, and therefore, less heat is transferred from your finger to a wood than to metal thus creating the sensation that metal is colder than wood. Conduction is important in problems related to ignition and flame spread over combustible solids, and to fire resistance. Exchange of heat between solid and fluid is called convective heat transfer. This involves motion of the fluid. In fires, this mode of heat transfer is important when the heat radiation level is low. Heat transfer by radiation is the transfer of energy by electro-magnetic waves [95]. It is the thermal radiation which determines the growth and spread of fires in compartments, forest fires, between buildings and in facade fires. Heat exposure raises the temperature of structures with the consequence of deteriorating material properties [107] and increasing thermally induced forces and displacements. These factors lead to the decrease of fire resistance performance. It is essential to model heat transfer in structures.

The temperature and the heat content of an object are related. For instance, an increase of heat content of one gram of water at zero Celsius by one calorie corresponds to an increase of its temperature by one degree Celsius. The heat content is associated with the mean kinetic energy of vibration of atoms. In metals, it is mainly the free electrons which transport the major part of heat flux. It is well known that good electrical conductors are also good conductors of heat [138] since it is the same electronic gas which is associated with the electronic flux (electric current) and the major heat flux. The thermal and electric conductivities of metals are closely related as shown by the Weidemann-Franz law: It is well known experimentally and theoretically that for metals not at too low temperatures the ratio K/σ of thermal conductivity K to electric conductivity σ is directly proportional to the temperature T, and that *the proportionality constant is the same for all metals* [138], *i.e.*,

$$\frac{K}{\sigma} = L \cdot T, \tag{5.1}$$

where $L = 2.45 \times 10^{-8}$ ($\mathrm{W}\cdot\Omega/\mathrm{K}^2$) is the Lorenz number. For other materials, the remainder heat content is due to atomic vibration within the crystal lattice. The quantized modes of vibrations in the atomic lattice of a solid are called *phonons*[2]. Phonons are the primary mechanism by which heat

[2]In solids sound is generated by the long-wavelength phonons (*voice* in Greek).

conduction takes place. The phonons confer the major physical properties of solids as thermal and electrical conductivities, for instance. In solids, thermal energy is transported by two mechanisms: the free electrons, and by the quanta of lattice vibrations (phonons). The temperature of a body is a measure of vibratory motions, the motions of molecules in a gas or the vibrations of a lattice in a solid. At the microscopic scale, heat is transported by near-neighbour excitation *via* change of momentum and energy which propagate as waves.

Therefore, transferring heat is equivalent to transfer kinetic energy of vibration. The temperature is defined through the mean kinetic energy of vibration of the atomic particles as

$$\langle K \rangle = \frac{1}{2}\langle mv^2 \rangle = \frac{3}{2}kT, \tag{5.2}$$

where $k = 1.38066 \times 10^{-23}$ (J/K) is the Boltzmann's constant [139].

5.2 On Fourier heat conduction

Fourier[3] conducted a series of experiments to discover the laws governing convective and conductive heat transfer. Jean-Baptiste Joseph Fourier [106] developed, for the first time, a complete scientific thermal theory to explain heat transfer in bodies in his "Théorie analytique de la chaleur" in 1816. He stated the empirical heat conduction law that bears his name : *the heat flux in thermal conduction is proportional to the opposite of the magnitude of the temperature gradient*

$$\mathbf{q} = -k\nabla T, \tag{5.3}$$

where k is the thermal conductivity.
It is well known that this law is only an approximation. Nevertheless, it leads to an excellent description of heat conduction physics [140]. Fourier derived the diffusion equation

$$\frac{\partial T}{\partial t} = \kappa \Delta T, \tag{5.4}$$

governing the diffusive propagation of heat (conduction) in solids. The parameter $\kappa = k/(\rho c)$ is the thermal diffusivity where k, ρ and c are themal conductivity, density and specific heat capacity.

To fix the ideas, some thermal conductivity values for many substances are shown in figure 5.2.

[3]In mathematics, FOURIER investigated partial differential equations and trigonometric series. Probably inspired by its scientific expedition in Egypt (Napoléon Egypte expidition (1798–1801)), he was interested in studying propagation of heat. He obtained a partial differential equation which he could solve only in the form of an infinite sum of terms in $\cos(nx)$ with n an integer. By looking into that heat problem he arrived to develop arbitrary functions into the later called the Fourier's series. This resulted in a new branch of mathematics called Fourier analysis which is still an active field of research and technological applications.

Figure 5.1: Joseph FOURIER (Auxerre 1768 – Paris 1830).

5.3 On non-Fourier heat conduction

In short-pulse laser heating of solids, for instance, the response time may be of picoseconds which is of the same order as the thermal relaxation time of the phonon-electron. In such short times, thermodynamic equilibrium cannot be reached by the metal lattice and the hot electron gas. This leads to the failure of the diffusion theory [141]. The classical heat diffusion equation is still a powerful tool for analysing dynamic motion of heat as well as for solving a wide range of diffusion-like physical problems, see Narasimhan [142] for a review on Fourier's heat conduction, influence and its history. However, the diffusion equation leads to the unphysical situation of infinite speeds of heat propagation. Fourier's law is still a good approximation of heat conduction applicable to a high accuracy even on the shortest time scales of our daily engineering applications [143]. To resolve the dilemma of infinite speed of heat propagation, Cattaneo [144] and Vernotte [145] proposed the constitutive equation known as Cattaneo's law

$$\tau \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} = -k\nabla T, \tag{5.5}$$

in solids, where τ is the thermal relaxation time[4]. This is a simple generalisation of Fourier's law leading to finite propagation speeds. This equation can be easily understood by accounting for the delayed response of the heat flux to a temperature gradient as $\mathbf{q}(\mathbf{r}, t+\tau) = -k\nabla T(\mathbf{r}, t)$ by using Taylor's expansion with small τ constitutive Equation (5.5) is obtained. Under some

[4]The build-up period for initiation of heat flow after application of a temperature gradient, *i.e.*, relaxation time associated with the communication time between phonon-phonon collision needed for the initiation of heat flow. It is a measure of thermal inertia of the medium. For instance, For metals at ambient temperature a typical value is $\tau = 10^{-10}$– 10^{-14} s and 10^{-3} s for a diamond at temperature 77 K. These times are reduced by impurities and imperfections. In metals, thermal waves have speeds are of order 10^5 m/s and 10^3 m/s in gases [141].

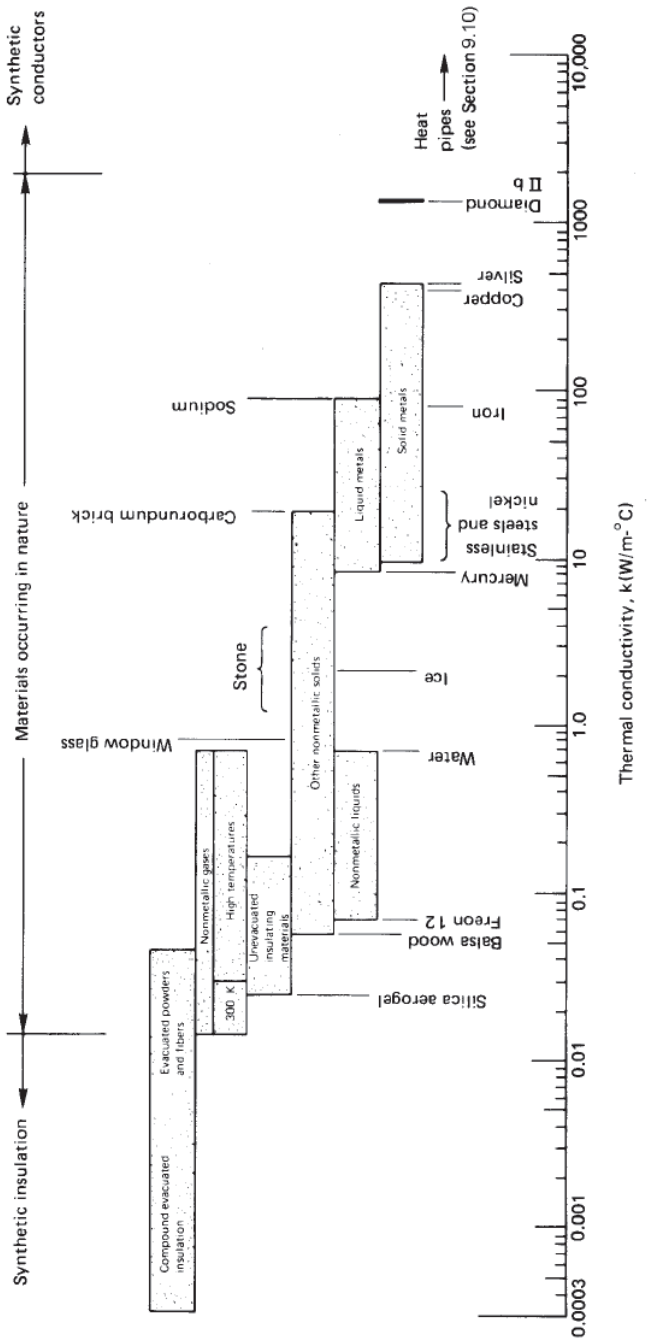

Figure 5.2: Thermal conductivities for various substances (reproduced from [94, Fig.1.6]).

assumptions [146], the heat-flux law can be written for a simplified conductor as

$$\mathbf{q} = -\left(k_1 + \frac{k_2}{\tau}\int_{\infty}^{t} \exp\left(-\frac{t-t'}{\tau}\right)\mathrm{d}t'\right)\nabla T, \tag{5.6}$$

in which an effective Fourier conductivity k_1 is recognised. The remaining constant in parentheses is called elastic conductivity.

For constant properties, the energy balance equation leads to the hyperbolic heat conduction equation known as the telegraph equation

$$\frac{\partial T}{\partial t} + \tau \frac{\partial^2 T}{\partial t^2} = \kappa \Delta T. \tag{5.7}$$

Now, internal thermal waves propagate at finite speed $v = \sqrt{\kappa/\tau}$. The development of thermal wave theory was influenced by the work of Maxwell [147] on the kinetic gas theory. Joseph [143] and Joseph and Preziosi [146] made a thorough and complete annotated chronological review on the literature on heat waves (non-Fourier behaviour). The paper [141] by Özişik and Tzou includes a review on wave theory of heat conduction and hotspots its many engineering applications. Ackerman et al. [148] observed thermal waves in solid helium.

The classical heat conduction equation in its local and global form will be briefly presented.

5.4 Local formulation

The local form, or the differential formulation, of the classical heat conduction equation is here derived using the energy-balance postulate of the first law of thermodynamics together with an additional equation of the state to relate internal energy to the state variable of interest (temperature) [149]. The energy-balance postulate says that

$$\dot{E} + \dot{K} = \mathcal{P}_{ext} + \dot{Q}_{cal}, \tag{5.8}$$

in words: the rate of change of the total energy, $\dot{E} + \dot{K}$, of an arbitrary closed system enclosed in a volume V is equal to the power of external forces $\mathcal{P}_{ext}$ plus the power of received heat $\dot{Q}_{cal}$ through the boundary $S = \partial V$. E and K stand for internal and kinetic energies, respectively. Using the equation of state $\dot{e} = c\dot{T}$, the rate of internal energy is written as $\dot{E} = \frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho c T \mathrm{d}V$. Ignoring the power of mechanical forces and the kinetic energy one obtains

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho c T \mathrm{d}V = \int_S \vec{n}\cdot\vec{q}\mathrm{d}S + \int_V \rho r \mathrm{d}V, \quad \forall V, \tag{5.9}$$

where $\vec{q}$ is the heat flux vector, $\vec{n}$ is the external normal to $S = \partial V$, r is the internal heat supply, ρ is the density and c is the specific heat capacity. ($\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \vec{v}\cdot\nabla$, is the total derivative. In the solid, the velocity $\vec{v} = 0$). Applying the divergence theorem for the surface integral one gets

$$\int_V \left[\rho c\dot{T} + \nabla\cdot\vec{q} - \rho r\right] \mathrm{d}V = 0, \quad \forall V, \tag{5.10}$$

for arbitrary choice of the volume V in the continuum. This means that the integrand vanishes, i.e.,

$$\rho c\dot{T} = -\nabla \cdot \vec{q} + \rho r. \tag{5.11}$$

Equations (5.9) and (5.11) are, respectively, the global and the local forms of the energy equation. Inserting the classical Fourier constitutive relation

$$\vec{q}(\mathbf{x}, t) = -k\nabla T(\mathbf{x}, t), \tag{5.12}$$

the heat conduction equation

$$\rho c\frac{\partial T}{\partial t} = \nabla \cdot (k\nabla T) + \rho r. \tag{5.13}$$

This equation was first derived in 1816 by Fourier [106] (for constant thermal conductivity k and without internal source). It is admitted that the classical heat Fourier law is valid for heat propagation relaxation times and time scales $\tau \geq 1\mu$s [150]. This covers most of practical cases in heat transfer. For smaller time scales non-fourier effects should be considered. Such cases can be for instance, ultra-rapid heating techniques, such as laser and microwave with extremely short duration or high frequency.

Completing the partial differential equation (5.13) with appropriate boundary and initial conditions gives

$$\begin{cases} \rho c\dfrac{\partial T(\mathbf{x}, t)}{\partial t} = \nabla \cdot (k\nabla T) + \rho r, \quad \mathbf{x} \in V,\ t > 0, & (5.14) \\ \vec{n} \cdot \vec{q} \equiv -\vec{n} \cdot k\nabla T = \bar{q}_{\mathrm{n}}(\mathbf{x}, t), \quad \mathbf{x} \in \partial V_{\mathrm{q}},\ t > 0, & (5.15) \\ T(\mathbf{x}, t) = \bar{T}(\mathbf{x}, t), \quad \mathbf{x} \in \partial V_{\mathrm{T}},\ t > 0, & (5.16) \\ T(\mathbf{x}, 0) = \bar{T}_0, \quad \mathbf{x} \in V, & (5.17) \end{cases}$$

where $\bar{q}_n$ and $\bar{T}$ are imposed normal heat flux and temperature, respectively. The solid domain under consideration is V, its boundary $\partial V = \partial V_{\mathrm{T}} \cup \partial V_{\mathrm{q}}$ with no overlapping; $\partial V_{\mathrm{T}} \cap \partial V_{\mathrm{q}} = 0$. The system of equations above forms the heat conduction problem and is the starting point in temperature calculations in solids. Nonlinearities, arbitrary boundary and initial conditions together with geometrical complexity of the domain V make solutions in closed form impossible. Therefore, use of numerical solution methods as for instance, finite difference and finite elements method, is necessary to obtain practical solutions.

5.5 Variational formulation

Multiplying the local form of the energy equation, (5.14–5.17), by an arbitrary admissible smooth test function $w(x)$ and integrating by part leads to the

weak formulation:

$$\int_V \rho c \frac{\partial T}{\partial t} w \mathrm{d}V + \int_V k \nabla T \cdot \nabla w \mathrm{d}V = \int_V \rho r w \mathrm{d}V - \int_{S_\mathrm{q}} \vec{n} \cdot \vec{q} w \mathrm{d}S, \quad \forall w, \tag{5.18}$$

[130], [151] and [152]. Note that, for the choice $w = w(x,t)$ instead of $w = w(x)$, integration should be taken over time and space.

The variational formulation (5.18) is equivalent to the local formulation. This variational formulation is the starting point for the finite element method. This formulation has a well established theoretical basis which allows, for the discrete equations, error and convergence analysis.

5.6 Discretisation of the conduction equation

Traditionally, the domain V is discretised into finite elements V^e. This phase is called the *triangulation*. Following Galerkin method [130] and [151], the semi-discrete equations are obtained. To obtain the solution, these semi-discrete equations, should be time-integrated. This presentation follows partially the one in the author's paper [153].

The classical approximation of the temperature field as

$$T^{(e)}(\mathbf{x},t) = \sum_{i=1}^{N} \phi_i(\mathbf{x}) \Theta_i^{(e)}(t) \tag{5.19}$$

is made, where the local basis functions ϕ_i are piecewise functions over the element $e = 1 \ldots N_\mathrm{e}$ while $\Theta_i^{(\mathrm{e})}(t)$ being the nodal temperatures of the element. Inserting this approximation into the weak form and using the Galerkin method, one obtains the semi-discrete energy balance equations

$$\mathbf{C} \cdot \frac{\mathrm{d}\mathbf{\Theta}}{\mathrm{d}t} = -\mathbf{K} \cdot \mathbf{\Theta} + \mathbf{q}, \tag{5.20}$$

where, the elementary matrices and vector are

$$C_{\mathrm{ij}}^{(\mathrm{e})}(t) = \int_{V^\mathrm{e}} \rho c \, \phi_\mathrm{i} \phi_\mathrm{j} \, \mathrm{d}V^\mathrm{e}, \tag{5.21}$$

$$K_{\mathrm{ij}}^{(\mathrm{e})}(t) = \int_{V^\mathrm{e}} k \, \nabla\phi_\mathrm{i} \nabla\phi_\mathrm{j} \, \mathrm{d}V^\mathrm{e}, \tag{5.22}$$

$$q_i^{(\mathrm{e})}(t) = \int_{S^\mathrm{e} \cap S_\mathrm{q}} q_\mathrm{n} \, \phi_\mathrm{i} \, \mathrm{d}S^\mathrm{e} + \int_{V^\mathrm{e}} \rho r \, \phi_\mathrm{i} \, \mathrm{d}V^\mathrm{e}, \tag{5.23}$$

where $i, j = 1, M$ and $e = 1 \ldots N_\mathrm{e}$. ($N_\mathrm{e}$ is the number of elements and M is the number of degrees of freedom in an element.) These matrices are calculated by numerical quadrature. For instance, Gauss quadrature is usually used.

Often, the capacity matrix $\mathbf{C}$ is calculated using Newton-Cote like schemes to obtain a diagonal matrix. Assembling of the global matrices (from elementary contributions (5.21–5.23)) in (5.20) is made using standard FE-assembling methods. The essential boundary conditions should be accounted for.

The time-integration of the resulting system of nonlinear ordinary differential equations (5.20), can be performed using explicit or implicit schemes. Explicit methods are conditionally stable. Implicit schemes are unconditionally stable. This means that the time step is only limited by accuracy considerations. In the author's work, the implicit backward-Euler (BE) method [130] and [151], is used. The algorithm is

$$\mathbf{\Theta}_n^{(k+1)} = \mathbf{\Theta}_{n-1} + \Delta\mathbf{\Theta}_n^{(k)}, \tag{5.24}$$

where $\Delta\mathbf{\Theta}_n^{(k)}$ is solution of

$$\mathbf{C}_n^{(k)} \cdot \Delta\mathbf{\Theta}_n^{(k)} = \Delta\mathbf{q}_n^{(k)}, \tag{5.25}$$

where

$$\Delta\mathbf{q}_n^{(k)} = \left(-\mathbf{K}_n^{(k)} \cdot \mathbf{\Theta}_n^{(k)} + \mathbf{q}_n^{(k)}\right) \cdot \Delta t_n. \tag{5.26}$$

In (5.25) the column vector $\Delta\mathbf{\Theta}_n^{(k)}$ is solved using the Gaussian elimination scheme. The time step $\Delta t_n = t_{n+1} - t_n$. In solving (5.24)–(5.26), the Picard iteration scheme is used. The stopping convergence criteria for iteration step $k+1$ can be: stop if one of the two conditions, $\|T^{k+1} - T^k\|/\|T^{k+1}\| \leq RTOL$ or $\|T^{k+1} - T^k\| \leq ATOL$, holds for time t_n with chosen tolerances $RTOL$ and $ATOL$. Such temperature calculation algorithm is implemented by the author successfully, for instance, in [28], [126], [131], [133], [154] and [153].

Chapter 6

Concluding remarks

Flame spread has a direct impact on fire safety since it controls the rate of heat release of fires in open configurations as in facade fires and in large spaces. In Fire Safety, the rate of heat release is an essential fire loading. The fire resistance of structures deteriorate as they are heated and their temperature raised. This work consists of the development of *thermal models* for Fire Safety purposes. The main objective of the present thesis work is to produce new information for fire safety related to development of models for flame spread on surfaces and to develop engineering calculation methods for the heating of structures.

The flame spread modeling also provides the fire exposure, the heat release rate, needed in the determination of the fire resistance of a structure. To determine the fire resistance of a structure, by calculation methods, three basic aspects should be at least considered; *fire exposure*, *heat transfer* and *structural response*. Flame spread together with determination of the respective fire exposure is addressed in the first part of this work (Papers I ... IV). The second part addresses the heat transfer, Papers V ... VII. Paper V also addresses fire resistance.

Upward flame spread on wall linings has been analyzed theoretically with special emphasis on the application of the models to predict whether the flame spread will be decelerating or accelerating. It has also been shown which material properties are essential to explain upward flame spread.

Extending the work started by Saito et al. and continued by Thomas and Karlsson, Baroudi and Kokkala [25] developed a graphical representation, called by some authors "Baroudi-Kokkala diagrams", to characterize flame spreading properties of lining materials based on bench-scale cone calorimeter data. These diagrams answer the question: does the material spread fire or not? They showed, for the first time, how to relate results obtained in testing wall and ceiling products in one scenario to those obtained from another scenario. These diagrams have been used successfully to interpret test data

in the EUREFIC (EUropean REaction to FIre Classification) fire research programme.

In Paper I, an upward thermal flame spread model was developed to predict the fire growth rate of a burning wall lining based on direct use of measured local heat release rate curve from cone calorimeter tests. Based on the model, a computer program named *THIMES* [39] was also developed. This numerical model has proven to be able to calculate the rate of heat release as a function of time with reasonable accuracy. It has been incorporated by other researchers into a computational fire zone model with satisfactory results. This numerical flame spread model was also applied successfully by Hakkarainen and Kokkala to predict heat release rate in SBI test configuration.

In the EC-sponsored CBUF research programme, three models of various complexity have been developed to compute full-scale furniture burning based on cone calorimeter data (Papers II and III). Model III is a novel physically based extension of the thermal fire spread theory. This model gave reasonable predictions of the early phase of heat release rate history.

To overcome some of the limitations of thermal upward flame spread models, related to the used phenomenological description of local pyrolysis, a thermal pyrolysis model was also developed, including an in-depth pyrolysis submodel to calculate local pyrolysis mass loss fluxes in the upward flame configuration (Paper IV). This novel flame spread model consisted of a two-dimensional upward flame spread model coupled with an in depth-pyrolysis model. The model calculates transient preheating at different locations and depths, variable local pyrolysis times (times to ignition), transient pyrolysis in depth direction, transient local pyrolysis mass fluxes, re-radiation from flames generated by burning of gazified solid fuel *via* a simplified burning model. The model was able to capture very satisfactorily transient evolutions of pyrolyzing area, flame spread patterns and total mass loss rate (burning rate) as compared to full-scale tests carried out at VTT to investigate upward flame spread on walls when ignited by a propane diffusion burner at the base of the wall. This pyrolysis submodel can be incorporated into CFD codes since it computes local pyrolysis mass fluxes in actual configuration.

Two improvements concerning pyrolysis submodels for charring materials used to predict flame spread by CFD modelling can be suggested:

1. use of a two-step pyrolysis submodel (with the minimal set of requirements listed below)

2. procedure to determine the needed model parameters

Therefore,

1: Current one-step pyrolysis submodels are not able to predict the mass loss rate accurately enough when the incident heat flux is not constant, since the char yield is an input parameter to such models. This yield is usually determined under constant heat flux level. It is well know that this parameter depends, among others, on incident heat flux level. Because, in fires, wall flame heat flux is transient, the author thinks that in order to model correctly flame spreading on charring materials, the pyrolysis submodels to be used should account for at least: in depth pyrolysis including primary and secondary reactions (to account more correctly for effects of specimen thickness on residence time). Char surface oxidation for the actual oxygen concentration and surface regression with updating sample thickness should be accounted for. For instance, effects of different oxygen concentrations on char oxydationon of pyrolysis of wood are considered by Weng et al. [155] within their simple integral pyrolysis submodel. It is known that to predict product yields, a pyrolysis model with at least primary and secondary reactions should be used, Di Blasi [156], [157] and Bryden et al. [158]. A counter argument frequently given by others to not use such submodels is that the kinetic parameters are "difficult" to determine even for the classical one-step model. How then for the more complex submodel? This argument should not stop us from using more adequate pyrolysis submodels to gain in prediction accuracy of CFD models for flame spread. It is the determination procedure of these parameters that needs to be explicitely stated.

2: The author proposes the following approach to determine the parameters needed by the pyrolysis submodel:

Perform several cone calorimeter tests using test specimens having relevant representative sizes (with thickness as an *in situ* situation). The tests should be done at various parametrized constant and transient incident heat flux levels. The following measurements should be performed simultaneously: incident heat flux using a fluxmeter, inside temperature profile within the thickness of the sample using small thermocouples (at least one at the mid-thickness) and surface temperature with IR-camera. Temperature at the interface between the sample and the support insulation should also be measured. Total mass loss rate should also be recorded. Then use inverse methods with regularization based on all the recorded temperature and mass loss measurements to determine the parameters. The model used in the calculation of the residuals between observed and expected values for the parameter estimation should use heat conduction with internal convection and mass conservation equations together with the related constitutive relations. The whole data gathered should be used simultaneously in the extraction of the kinetic parameters (and other parameters such as thermal conductivity and capacity). Additional constraints on the expected interval of values should be imposed. It may be preferable to try to find the mean values for the set of the unknown parameters.

Before finishing with flame spread and related topics, we list below some important aspects which are, to cite Wichman [159], missed in the research field:

1. Theory of surface degradation

2. Analysis of surface regression effects (influences of surface consumption and regression)

3. Careful analysis that characterizes solids that may be grainy or stratified or composite or which may undergo thermal stresses under heating

4. Comprehensive theory of solids that undergo heating and then undergo thermal stresses and finally crack to expose internal surfaces to additional heating

The rate of heat release is a primary fire loading in Fire Safety Engineering (beside smoke and gas emissions during a fire). A part of the calorific energy developed in a fire is fed back to the structures present with the consequence of rising their temperatures. It is known that the performance of structures generally decrease with increasing temperature. It is then important to know the temperature distribution within the structure in order to estimate safe-escape time for occupants, safe-operational time for firemen and fire resistance. Therefore it is essential to model of heat transfer in structures since it has a direct impact on fire safety. In this part of the thesis, efficient engineering temperature calculation algorithms for various fire heated structures are developed.

In Paper V, a semi-advanced engineering design tool is developed to predict fire resistance of a concrete filled tubular and square composite column with or without reinforcement. The tool consists of a thermal and a mechanical part. In the thermal part a non-linear finite element algorithm is developed and implemented to solve the transient heat conduction problem. The load-bearing computation is based on the method given in Eurocode 4. This whole computer code is validated by comparing with experimental data. The computer code is fast enough and it provides automatically the results also in a graphical form allowing quick parameter studies and design.

It is essential to use measured thermal properties in numerical simulations to obtain the realistic thermal response of a structure in a fire. Paper VI presents an inverse method developed and implemented to determine the temperature dependent thermal conductivity of homogeneous insulation material using boundary temperature measurement history. Thermal conductivity is *a priori* an unknown function of temperature. The transient heat

conduction equation is solved using finite element method. The inverse problem is reduced to a Regularized Output Least-Squares Method (RLS) using Tikhonov and mesh coarsing regularisation. Morozov discrepancy principle is used to find the optimal regularization level. The method is validated using noisy synthetic data. It is shown that good estimates of thermal conductivity can be obtained without necessarily measuring temperature inside the insulation. Comparisons with the NT FIRE 021 and CEN Pr ENV YYY-4 of fire protected steel structures are performed. The present method gives more accurate thermal conductivities for the whole temperature range when compared to the standard methods. In the methods NT FIRE 021 and its CEN equivalent, the accuracy of the calculated thermal conductivity for low temperatures ($< 350\ ^oC$) is not sufficient. In addition, these two methods are limited to thin insulations. The inverse method developed in Paper VI applies for insulation with arbitrary thickness. Furthermore, the determined thermal conductivity can be used further the finite element simulations as such, since it is computed using a fine finite element mesh. The implemented computer algorithm was also successfully used by the authors at VTT to determine thermal conductivities from measurements and then to interpolate design tables for additional insulation thicknesses for ducts with internal hot gas flow (chimney test) based on these experimental results (thermal resistance tests).

In Paper VII, a method to predict the transient heating of lightweight steel balconies installed in front of a facade and exposed to flames emerging from a window-opening under the balcony was developed based on a series of full scale fire tests conducted in the facade rig of VTT. A finite element heat transfer model for the balcony including a model for the stratified slab with internal radiation cavities and a parametric transient fire method for the calculation of the time dependent gas temperature under the balcony was developed and implemented as a design tool to assist in preventing the fire spread through the balcony slab. In addition, a method to calculate hot gas temperature dependence under the balcony is proposed in this paper. In this method, gas temperature can be calculated as a linear interpolation between the parametric fire temperature of the burning room and the flame tip temperature using Law's method. Conventionally, a design method has been developed by Law et al. [134] and adopted in the Eurocodes [160]. These methods are based on a steady-state equation of lumped capacity model for bare steel structures, and they do not apply for balcony slabs constructed from several layers of lightweight steel and fire protection boards including cavities.

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