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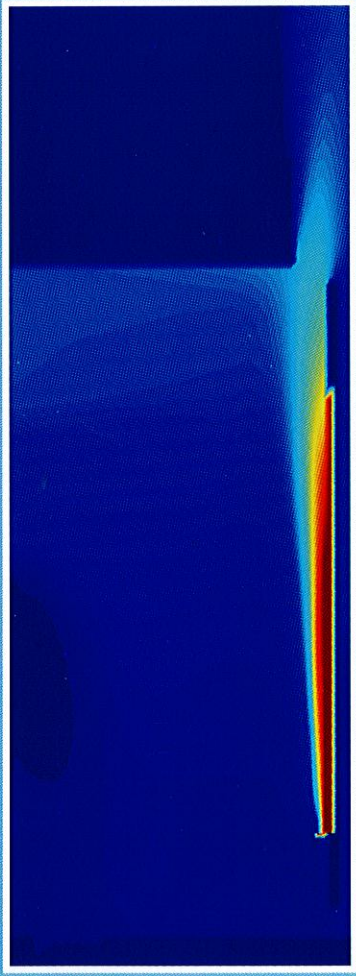
Implementation of a Physical Flame Spread Model in the SOFIE CFD Model

Brandforsk Project 307-971



SP Swedish National Testing and Research Institute
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Abstract

This report describes the work performed by SP within a joined project between Lund University and SP. The project, called "Development of engineering tools for the prediction of flame spread", increased the knowledge of flame spread modelling both with respect to thermal flame spread models and pyrolysis models. The implementation of a physical flame spread model developed by Yan inside the SOFIE CFD model has been described. Moreover an extensive sensitivity study of the pyrolysis model has been performed and a vertical stand-alone flame spread model has been developed using this pyrolysis model. Both items were performed as validation work for the pyrolysis model. The possibility of the use of a flame spread model inside SOFIE will enlarge the future application areas for CFD modelling within fire research and fire engineering. For this reason some future feasibility studies and guidelines are given in the conclusions of the report.

The work has been sponsored by Brandforsk (Swedish Board for Fire Research) with project number 307-971.

Key words: Fire modelling, flame spread, CFD models, pyrolysis models

Sökord: Brandmodellering, flamspridning, CFD modeller, pyrolysmodeller

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Preface

The use of flame spread models has increased substantially during the last years. Mainly two types of models have been developed. The first ones are thermal flame spread models which either can be used as stand-alone models or incorporated in zone models. Their application is mainly restricted to specific well defined scenarios. The second type of models are pyrolysis models which are developed within CFD (computational fluid dynamics) codes. The latter models will allow a more flexible calculation of the flame spread in a wide variation of scenarios. By increased computer capacity these types of models will become more and more realistic for use in the future.

The work has been sponsored by Brandforsk (Swedish Board for Fire Research) with project number 307-971 and was a joined collaboration between SP and LTH (Lund Technical University). A reference group monitored this project. The group is Jan Blomqvist, Staffan Bengtson, Bengt Hägglund, Göran Holmstedt, Bror Persson, Birgit Östman, Björn Karlsson, Patrick Van Hees, Heimo Tuovinen, Örjan Thorné, Tomas Kemeny and Susanne Hessler. Their assistance is acknowledged.
It should also be noted that a large part of this work was possible in conjunction with the FIPEC project. This project was sponsored by DGXII of the EU with additional funding at SP from cable manufacturers (Draka Sverige, Alcatel, Ericsson, Habia, Helkama, NK Cables, Reka), cable material manufactures (Borealis, Norsk Hydro), cable users (Barsebäck Kraft, Forsmarks Kraftgrupp, OKG, Statens Vattenfall AB Ringhalsverket, Telia Nättjänster), governmental research support bodies(NUTEK and Räddningsverket) and Brandforsk (Brandforsk project 280-961).

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Summary

A physical flame spread model for the prediction of flame spread has been studied and implemented for use inside the CFD code SOFIE. Before this implementation a sensitivity study of the pyrolysis model which formed the main body in the physical flame spread model was performed varying different input parameters for the model. This revealed that parameters such as thermal conductivity, pyrolysis temperature, and heat of pyrolysis seemed to have most influence on the prediction results. It was observed that caution should be taken when choosing to use either the charring or non-charring mode of the model.

The project also developed a simple procedure to obtain the material parameters as input to the physical flame spread model by means of cone calorimeter data. It is concluded that a more automatic calculation module is necessary and the possibility of use of other methods such as TGA (Thermogravimetric analysis) should be investigated in order to facilitate the determination of the input parameters when setting up an automatic input parameter determination.

The physical model has been validated by means of cone calorimeter test results, a newly developed stand-alone vertical flame spread model and a simple run inside the CFD code SOFIE.

It is observed that more extensive work for optimising the implementation of the physical flame spread model is necessary. This work will be performed within the SOFIE consortium with the latest version of SOFIE. In addition, a number of future feasibility studies are suggested which are necessary in order to validate and further develop the flame spread routines.

Sammanfattning

En fysikalisk flamspridningsmodell för prediktion av flamspridning har studerats och implementerats i CFD-koden SOFIE. Innan implementeringen utfördes en känslighetsstudie på pyrolysmodellen som utgör kärnan i den fysikaliska flamspridningsmodellen. Studien utfördes genom att variera de olika indata parametrarna till modellen och visade att parametrar som värmekonduktivitet, pyrolystemperatur och pyrolysvärme verkade ha störst inverkan på simuleringarna. Det noterades att viss försiktighet bör iakttagas vid valet av förkolnande eller icke förkolnande material i pyrolysmodellen.

I projektet utvecklades även en enkel procedur för att med hjälp av konkalorimeterdata erhålla de materialparametrar som är indata till den fysikaliska flamspridningsmodellen. En slutsats är att det behövs en mer automatiserad beräkningsmodul samt att möjligheter att använda andra metoder som TGA (Thermogravimetric analysis) borde undersökas för att förenkla framtagandet av indata parametrar vid en automatisk procedur för att ta fram data.

Den fysikaliska flamspridningsmodellen ha validerats med resultat från tester i konkalorimetern, en nyligen utvecklad fristående modell för vertikal flamspridning samt med en enkel körning i CFD-koden SOFIE.

Det konstateras att det behövs ett mer omfattande arbete för att optimera implementeringen av den fysikaliska flamspridningsmodellen. Detta arbete kommer att genomföras inom SOFIE konsortiet, i den senaste versionen av SOFIE. Utöver detta föreslås ett antal framtida genomförbarhetsstudier som är nödvändiga för validering och vidare utveckling av flamspridningsrutinerna.

1 Objectives of the study

The aim of the proposed project was mainly twofold:

- to improve the existing calculational models so these can be used by engineers and researchers
- to investigate which bench scale data should be used as input to these models.

The long term goal of the work was to bring forth easy to use engineering models, needing straight forward material input data from as few as possible small scale test methods. The models should be of use in practice for several basic ignition scenarios.

Two types of calculational tools are developed:

- one based on relatively simple thermal theories, resulting in a computer program to be used in performance based design by engineers.
- one based on a CFD modelling technique mainly for testing and research purposes and product development.

The results can be used in the following areas:

- performance based fire safety engineering,
- product development for manufacturers,
- material testing
- fundamental research purposes.

The project was a collaboration between SP Swedish National Testing and Research Project (SP) and Lund Technical University (LTH).

2 Background of the study

The growth of a fire in a room is to a considerable extent controlled by the energy released from the burning material and the velocity at which a flame spreads over it. The difficulty of predicting this velocity and the resulting fire growth is a fundamental problem in fire research.

Mainly two types of methods for such predictions have been proposed in the literature in recent years. Firstly, thermal theories for upward flame spread have been used, with input data from the Cone Calorimeter, to predict flame spread and the resulting heat release rate. This work is based on the methodology proposed in an earlier BRANDFORSK project [1], [2] where thermal theories were used together with Cone Calorimeter data, to successfully predict fire growth in several variations of the ISO 9705 Room Corner test. Secondly, more fundamental work has been carried out using CFD models and pyrolysis models to predict fire growth in the same full-scale scenario [3].

2.1 State of the art and ongoing work

Table 2-1 summarises the ongoing international work in the field. The list of institutions is not complete, but several institutions are named and the work being carried out is divided into three categories, namely

- the bench scale work
- the full scale work
- the modelling work

The table has not to be seen as being complete in any way, but should give an indication of the state of the art and the type of work being carried out.

Bench scale work

The bench scale work being carried out is mainly Cone Calorimetry and LIFT apparatus work. The main aim is to determine which material parameters are needed to categorise and to model material behaviour. This can be done in a multitude of ways.

Full scale work

The full-scale work is often concentrated on the ISO full scale Room Corner test, but also smaller scales of that room. In addition, work is being done in several other scenarios; walls; stacks; parallel plates; etc.

Modelling

The modelling work can be divided into two approaches; fundamental work using CFD codes and work on thermal theories, following Saito, Quintiere and Williams [4] and Thomas and Karlsson [2].

Institute	University of Lund	University of Edinburgh	University of Maryland	BRI, Japan	Worchester Polytechnic Institute
Bench scale experiments	Cone, LIFT	Cone, LIFT	Cone, LIFT	Cone, LIFT	Cone, LIFT
Full scale experiments	ISO, 1/3 ISO	Industrial storage, parallel walls	ISO, 1/3 ISO	ISO, intermediate scale room	ISO, Walls
Modelling	TT, TT + zone models, CFD + cone, CFD + pyrolysis	TT	TT, TT + zone models	TT, TT + zone models	TT, TT+ CFAST
Institute	VTT, Finland	FRS, England	SP, Sweden	University of Gent	Factory Mutual Research Co.
Bench scale experiments	Cone, LIFT	Cone, LIFT	Cone, LIFT	Cone	Cone, LIFT and other measurement
Full scale experiments	ISO, Walls	ISO	Cables, ISO, storage racks	Floor coverings	Various industrial applications
Modelling	TT, TT + zone models	CFD + cone, CFD + pyrolysis	TT	TT	TT, TT + zone models, CFD + cone, CFD + pyrolysis

Table 2-1 Summarised overview of ongoing international work

Key to symbols:

Cone = Cone Calorimeter
LIFT = Lateral ignition and flame spread test
ISO = ISO 9705 Room Corner test
1/3 ISO = 1/3 scale of the ISO 9705 Room Corner test
Intermediate scale room = a smaller room that the ISO 9705 Room Corner test, used in Japan
TT = Thermal theories for upward flame spread
TT + zone models = Thermal theories for upward flame spread incorporated into zone models
CFD + Cone = CFD models using Cone data as input
CFD + pyrolysis = CFD models with pyrolysis and combustion models incorporated

The CFD work either uses data from the Cone Calorimeter to predict pyrolysis and calculate heat release rates or uses fundamental material properties to calculate these. There is a considerable difference in the two approaches with regards to bench scale data needed. The full scale scenario being simulated is mainly the ISO room and 1/3 scale of the ISO room.

The thermal theories used are all based on the work presented by Saito, Quintiere and Williams [4] and Thomas and Karlsson [2], where Cone Calorimeter data is used as input to equations developed from thermal theories for upward flame spread. There are several different approaches being used; some use the thermal theories directly, others link them to zone models of various degrees of sophistication. The input to the models varies greatly; some use a single result from the cone calorimeter to indicate flame propensity or to roughly simulate flame spread and heat release rate; others use multiple data from both cone calorimetry and LIFT apparatus; still others use results from these bench scale tests (and other tests) to derive material parameters that are used as input to the models.

The methods used are of various degrees of sophistication and complexity. Some give approximate answers to specified end use scenarios, can be used by non-expert and require simple input. Others are more general, but may require expert knowledge and large amount of input data.

In order to develop sound engineering procedures for calculating flame spread and fire growth, work must be carried out on improving the models and examining needed input data in a systematic way.

2.2 Further details on some international work

A very brief description of the ongoing or planned work at some of these institutions is given below. This project has followed closely the mentioned research areas.

The University of Edinburgh is currently carrying out experimental and theoretical work on flame heights and heat transfer from various types of gas burners, of various areas, below and contiguous with instrumented walls [5].

The Building Research Institute in Japan has an ongoing experimental and theoretical research program in this field. They have carried out bench scale and full scale experiments (ISO 9705 as well as intermediate scale tests) under the leadership. They plan to use several models in their theoretical evaluations, but do not propose to carry out any model development work [6].

Factory Mutual Research Corporation (FMRC) in Massachusetts has for many years been the leading research institution with respect to flammability properties of materials. Their work has been of a fundamental nature as well as being applied to practical problems in industry. FMRC has, through Dr. John de Ris, had a rewarding co-operation with Lund University and SP in this area. FMRC has an ongoing research program where flame spread and fire growth experiments are carried out in several large-scale scenarios [7].

Worchester Polytechnic Institute has in recent years carried out mainly theoretical work in the field. They have incorporated the model proposed by Karlsson [1] into the well-known zone model CFAST [8].

VTT in Finland have in recent years carried out experimental and theoretical work on upward flame spread and fire growth. The theoretical work is based on the above mentioned thermal theories and the experimental work concentrated on flame spread and fire growth on a vertical slab of material ignited by a line burner. This resulted in a computer code for upward flame spread, which is probably the most comprehensive and numerically stable code of its type available [9].

3 Description of the project

This chapter gives an overview of the complete project. As the project is a collaboration between SP and LTH, reference will be made in this paragraph where the different results are reported.

The project was divided into five work packages.

The first two work packages involved refining and preparing the calculation tools needed for estimating flame spread and fire growth. These tools are:

- a simple flame spread and fire growth model (based on the so called thermal theories), mainly intended for use of engineers for performance based calculations in relatively simple scenarios
- a CFD code with an incorporated flame spread and fire growth model, which is mainly intended for product development, material testing and fundamental research purposes

Both work packages analysed which bench-scale input data should be used as input to these tools. Several options are available and the most feasible options are identified.

The third work package included for both tools (thermal and CFD tool) the verification by means of the following:

- comparison of different input data models.
- simulation results versus real scale data for both tools

The fourth work package investigated the possibility for using the models with real scale data in more complex scenarios and recommends further work to be carried out in these areas.

The fifth work package gives guidelines and recommendations. A more detailed description of the different work packages and corresponding reports is given in the next subchapters.

3.1 Work package 1: Refinement of thermal theories model

Several workers have developed computer codes where thermal theories are used for calculating upward flame spread. One of the most recent and most comprehensive efforts is the one by Baroudi and Kokkala [10] at VTT in Finland. The numerical solution of the problem are especially well treated in their code. VTT has been contacted and will contribute to the project with this code.

Workers at Factory Mutual Research Corporation have shown that the flame heat flux, which is dependent on the type of material burning, will need to be quantified for each material and taken account of in the models. There are strong indications that results from the Cone Calorimeter can be used to give a rough value of the flame heat flux. This was investigated and included in the model wherever possible.

Similarly, the thermal feedback from the room boundaries and smoke layer can in a simple way be taken into account in the model. This was also incorporated if deemed feasible.

The model is developed for use in certain relatively simple scenarios, for which experimental data already exists. The scenarios treated include ignition in a corner in a relatively small room, ignition in a corner of a relatively large room, ignition along a wall in a relatively large room.

The input to these flame spread and fire growth models varies greatly. Some models use a single result from the Cone Calorimeter to calculate flame spread and heat release in full scale. Other models may use multiple data from both the Cone Calorimeter and LIFT apparatus or even data from several different types of bench-scale apparatuses.

There was a considerable need to investigate which combination of input data will give the best results. A multitude of input data which may require added bench-scale testing and will add to the complexity of the model. A simple set of input data offers clarity and economy, while the results may be more approximate.

The following options were examined:

- using a single heat release rate curve from the Cone Calorimeter, taken at a certain radiant flux
- using multiple heat release rate curves from the Cone Calorimeter, taken at different radiant flux levels
- using Cone Calorimeter results to determine material flammability parameters

The result from this work package is a thermal flame spread computer model that can be applied to a limited number of flame spread scenarios in a compartment, with recommendations for which bench-scale data are needed for each scenario.

Lund University was the responsible for this work package and the results are given in reports called "Analytical and Numerical Techniques for Modelling Flame Spread on Solids"(G. North, B. Karlsson, D. Gojkovic, P. Van Hees) and "Incorporating Flame Spread and Fire Growth Algorithms into a Computational Zone Model" (D. Gojkovic, H. Hultquist).

3.2 Work package 2: Implementation of flame spread model into SOFIE

Yan and Holmstedt [3] have developed a flame spread model for use in CFD codes, but this model has not yet been implemented into the CFD code SOFIE. In this work package the flame spread model is implemented into SOFIE and a limited model evaluation is carried out. Similarly to work package 1 input data and its reduction is investigated in this work package and also the sensitivity of the model for different input parameters. The type of input data can vary also from directly accessible data from the cone calorimeter to data, which have to be reduced with help of cone calorimeter results to fundamental material characteristics.

The result from this work package is that a flame spread model is incorporated into SOFIE code, which will allow use in a wider range of scenarios. At the same time routines and procedures are developed obtain the input data needed for this model.

SP was responsible for this work package and the results and achievements are described in this report.

3.3 Work package 3: Verification of the simulation results

This work package was divided into two different sub packages dealing with the following:

- the selection of the most appropriate input data routine for each tool by comparing the simulation results from each input data routine with a selected limited set of real scale data.
- the verification of simulations with the chosen input data routine for a wider selection of real scale test data.

For both model types each sub package selected the available data in order to cover most building products and simple scenarios.

3.3.1 Verification of the thermal flame spread model

This sub package verified the thermal flame spread model as described above.

LTH was the responsible for this work package and the results are given in reports called "Analytical and Numerical Techniques for Modelling Flame Spread on Solids"(G. North, B. Karlsson, D. Gojkovic, P. Van Hees) and "Incorporating Flame Spread and Fire Growth Algorithms into a Computational Zone Model" (D. Gojkovic, H. Hultquist).

3.3.2 Verification of the CFD model

This sub package verified the flame spread within a CFD code as described above with a simple geometry. SP was responsible for this work package and the results are described in this report.

3.4 Work package 4: Feasibility studies for future work

There is a need to address flame spread and fire growth in geometries which are more complex than those considered in WP1- WP3 above. Experimental data exist for several other scenarios of interest. The feasibility of modelling such complex scenarios will be investigated by listing and discussing a number of available data sets. Also recommendations for future work in this area will be given.

SP was responsible for this work package and a discussion is given in chapter 8.

3.5 Work package 5: Guidelines and recommendations

This work package gives guidelines and recommendations when using the different engineering tools documented in a final report. Lund University was responsible for this work package and the results are given in reports called "Analytical and Numerical Techniques for Modelling Flame Spread on Solids"(G. North, B. Karlsson, D. Gojkovic, P. Van Hees) and "Incorporating Flame Spread and Fire Growth Algorithms into a Computational Zone Model" (D. Gojkovic, H. Hultquist).

4 Description of the physical flame spread

The physical flame spread model used for this project is the model developed by Yan at Lund University. In this chapter a short description of the physical flame spread model is given. More detailed information can be found in [14].

The model is based on a one dimensional numerical heat transfer model which uses a standard numerical solver for the heat conduction equation. Each numerical heat conduction strip is then divided in a number of substrips to which a simple pyrolysis model is applied. The pyrolysis model is explained in paragraph 4.1. The input parameters with respect to thermal and pyrolysis model are:

- Ignition Temperature (K), only of interest for non charring materials
- Pyrolysis Temperature (K)
- Heat of Pyrolysis (J/kg)
- Heat of Combustion (J/kg)
- Virgin Density (kg/m^3)
- Char Density (kg/m^3)
- Specific Heat (J/kg K)
- Thermal Conductivity (W/mK)

The next paragraph will explain more in detail the model while the last paragraph of this chapter discusses the changes made in order to be able to use the model efficiently for future use.

4.1 Description of model

One of the possibilities of implementing a flame spread model into a CFD code is the direct use of cone calorimeter data for each cell at the surface of the material. However the problem here is that the net heat flux input will vary substantially during the simulation because of the fire growth or decay. It is hence difficult to change the mass loss rate in each cell depending on the actual net heat flux into the cell calculated within the CFD code. For this reason Yan developed a flame spread code that allows a more flexible approach. A brief explanation is given in this paragraph. For further details one is referred to the corresponding literature in [14].

This method differs from the Cone data input method mainly in its way of providing the heat release rate for the elements of the solid fuel. The one-dimensional transient heat conduction equation is solved numerically here, but with pyrolysis and charring included. The heat conduction equation can now be written as

$$\frac{\partial(\rho H)}{\partial t} + \dot{m}'''(H_{py} + H) + \frac{\partial\left[\dot{m}''\left(H_{G,T} - H_{G,T_p}\right)\right]}{\partial x} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) \quad (1)$$

where

$$\dot{m}''' = -\frac{\partial \rho}{\partial t} = \frac{\partial \dot{m}''}{\partial x} \geq 0$$

representing the mass-loss rate of the pyrolysing material per unit volume. The third term is the energy required to heat the vaporised gas as it flows to the solid surface. This term will be zero for non-charring material and has no important effect in this study, and thus it is ignored here (but it can be very easily included). H_{py} is the heat of reaction of the pyrolysis process, and can be calculated by the difference in total enthalpy of virgin material and volatile products, i.e.

$$H_{py} = H^*_{vol,Tp} - H^*_{vir,Tp} = H^*_{vol,Tp} - \left(H^*_{vir,To} + \int_{To}^{Tp} c_p \, dT \right) \qquad (2)$$

It is worth pointing out that H_{py} is a material constant and is different from the heat of gasification:

$$H_g = \dot{q}_{net} / \dot{m}_{total} = \frac{\left[h_c (T_g - T_{x=0}) + R_{flux} \right]}{\dot{m}_{total}} \qquad (3)$$

which is a local and transient value and changes considerably during the pyrolysis process. For the thermally thick vaporising material, at steady state,

$$H_g = H^*_{vol,Tp} - H^*_{vir,To} = H_{py} + \int_{To}^{Tp} c_p \, dt \qquad (4)$$

Equation (1) can be rewritten as

$$\rho c_p \frac{\partial T}{\partial t} + \dot{m}''' H_{py} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x} \right) \qquad (5)$$

The material will start to pyrolyse only when its temperature reaches the pyrolysis temperature, T_p, and it will then keep this temperature until completely pyrolysed. Thus we have

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x} \right) \quad \text{when} \quad T \le T_p \; or \; \rho \equiv \rho_{char} \qquad (6)$$

$$\dot{m}''' H_{py} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x} \right) \quad \text{when} \quad T \ge T_p \; and \; \rho > \rho_{char} \qquad (7)$$

The following is the detail of the numerical solution of equation (5), which can be discretised as

$$\rho c_p \frac{T_n - T'_n}{\Delta t} \delta x + \dot{m}''_{\delta x} H_{py} = k \left(\frac{T_{n+1} - T_n}{\delta x} - \frac{T_n - T_{n-1}}{\delta x} \right) \qquad (8)$$

Where the prime indicates the previous time step and $\dot{m}''_{\delta x}$ is the mass loss rate per unit area of the δ_x thick strip.
If we define

$$A_c = \frac{K}{\delta x}; \qquad A_w = \frac{k}{\delta x} \qquad (9)$$

$$A_p = A_c + A_w + \rho c_p \delta x / \Delta t \qquad (10)$$

$$S_u = \rho c_p \delta x T'_n / \Delta t - \dot{m}''_{\delta x} H_{py} \qquad (11)$$

then equation (8) becomes

$$A_p T_n = A_c T_{n+1} + A_w T_{n-1} + S_u \qquad (12)$$

Since the conductivity, k, is generally a function of temperature, it is consequently a function of x and it is not necessary for A_c to be equal to A_W.

It was found by Yan [14] in order to obtain a reasonable result for the mass loss rate, a very fine grid was required. However, this very fine grid is unnecessary and very expensive for the temperature solution. This inconsistency is overcome by defining a reasonably coarser grid for temperature solution and refining the grid into a second grid to determine the mass loss rate, as shown in Figure 4-1.

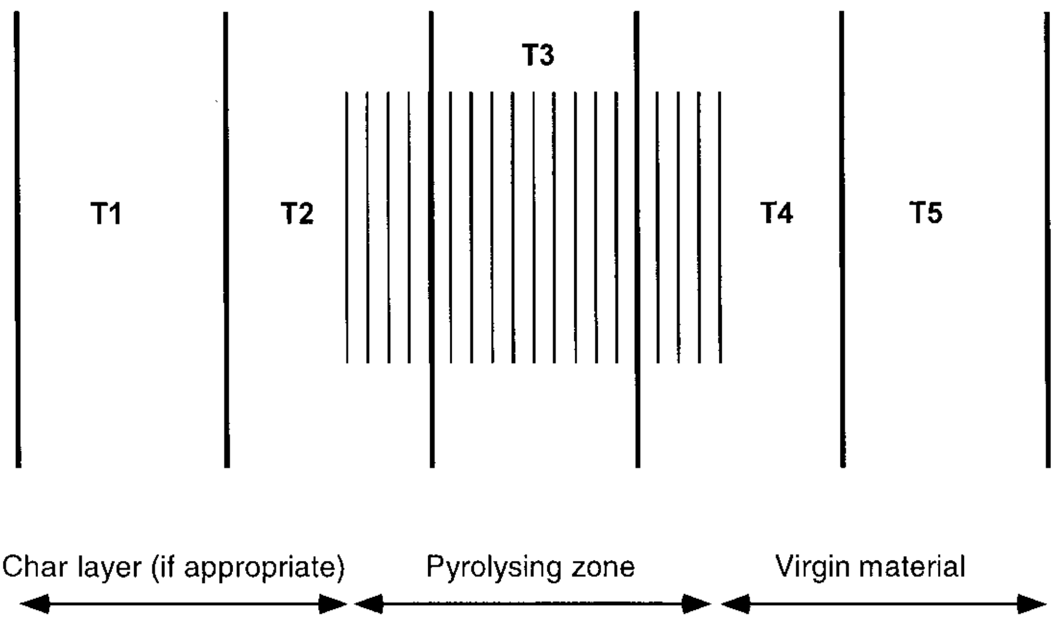

Figure 4-1 Temperature solution node and grid refinement (N=5, M=10)

The temperature of the refined node, m, of the coarser node, n [we will denote this node as node (n, m) later], $T_{n,m}$ is obtained by interpolation, as shown in Figure 4-1, assuming a linear distribution between T_n and T_{n+1}.

From eqn (12), for an arbitrary small node (n, m), the energy available for pyrolysis can be approximated as

$$H_{n,m} = \max\left[0.0, A_p\left(T_{n,m} - T_p\right)/M\right] \qquad (13)$$

On the other hand, the mass of the volatisable material remaining in the node (*n*, *m*) which may have been completely, partially or not at all pyrolysed, is generally given by

$$mass_{vol} = \frac{\delta x}{M} \min\{\rho_{vir} - \rho_{char}, \max[0.0, (\rho_{n,m} - \rho_{char})]\} \qquad (14)$$

where

$$\rho_m = M\rho' - (m-1)\rho_{char} - (M-m)\rho_{vir}$$

The mass loss rate from node (*n, m*) is thus finally determined by

$$\dot{m}_{n,m} = \min\{H_{n,m} / H_{py}, mass_{vol} / \Delta t\} \qquad (15)$$

The overall pyrolysis rate can be obtained by summation over all the nodes and expressed as

$$\dot{m} = \sum_n \sum_m \dot{m}_{n,m} = \sum_n \sum_m \min(H_{n,m} / H_{py}, mass_{vol} / \Delta t) \qquad (16)$$

The heat release rate is represented by

$$Q = \dot{m} H_c \qquad (17)$$

where H_c is the heat of combustion related to the gaseous fuel produced. Generally, during flaming combustion, it has been shown that H_c is approximately constant.

4.2 Changes in the model

The model developed by Yan was mainly written for the use of PMMA and particleboard. One of the disadvantages was the difficulty with the model when using composite materials. As the model is also being used in the FIPEC project [16] involving cables and composite material tests it was necessary to modify and improve the programme so that both multiple combustible and non combustible materials could be used. Also a flexible input routine was written to facilitate the input of the material data and the numerical properties. The changes allowed us to improve the results as can be observed in chapter 7.

5 Implementation of the model in the CFD code SOFIE

The main problem of implementing a physical flame spread model applicable in a wide range of scenarios is still the problem of solving the grid at the flame spread surface. Due to the still limited calculation power it was decided to implement the model first in a simple configuration. While still limited in its application it would give us the possibility to extend it later more generally. Also it appeared that more knowledge of the pyrolysis model itself was necessary to understand fully the physics behind it. An extended sensitivity study was hence performed which is described in the next chapter. Also a stand-alone flame spread model was developed to understand and to verify the physics of the model. The flame spread code was then introduced in SOFIE by using so called transpiring wall boundaries. The corresponding heat flux into the pyrolysis model is the heat transfer mode of SOFIE used for in the boundaries conditions of the model.

6 Sensitivity analysis of the physical flame spread model

In order to understand the model as good as possible a number of sensitivity analyses were performed. This is extremely important for later use of the model within the CFD code. In the following paragraphs different graphs give an overview of the influence of specific material parameters on the modelling results for a specific material. Time and HRR scales are adapted to show more clearly the changes observed. It should be noted that this sensitivity analysis has been performed on a specific set of input data and that only specific trends are shown.

The material simulated for this study was a 3 mm PVC plaque with a heat flux level of 75 kW/m^2. This plaque was simulated as a composite of two 1.5 mm plaques and with a copper plate underneath the combustible material. As mentioned earlier the original model of Yan had to be adapted substantially in order to deal with composite materials. In addition, a flexible input routine was written by SP to facilitate the change of the different parameters without compiling the programme each time one single parameter had to be changed. The standard input levels are given in Table 6-1. The table also gives an example of the new developed flexible input file.

PARAMETER(S)	VALUE
Number of Faces and Number of Materials (-)	4/3
Flux levels (kW/m^2)	75
Time steps, Iterations and number of strips (-)	1000/25/10
Number of combustible layers and Number of non combustibles layers (-)	2/1
Ignition temperature* (K)	650
Pyrolysis temperature Material 1 (K)	593
Pyrolysis temperature Material 2 (K)	593
Heat of Pyrolysis Material 1 (MJ/kg)	3.0
Heat of Pyrolysis Material 2 (MJ/kg)	3.0
Heat of Combustion Material 1 (MJ/kg)	14
Heat of Combustion Material 2 (MJ/kg)	14
Density char Material 1 (kg/m^3)	100
Density char Material 2 (kg/m^3)	100
Virgin Density Material 1 (kg/m^3)	1000
Virgin Density Material 2 (kg/m^3)	1000
Virgin Density Material 3 (kg/m^3)	9000
Thickness Material 1 (m)	0.0015
Thickness Material 2 (m)	0.0015
Thickness Material 3 (m)	0.0007
Specific Heat Material 1 (J/kg/K)	1000
Specific Heat Material 2 (J/kg/K)	1000
Specific Heat Material 3 (J/kg/k)	380
Thermal Conductivity Material 1 (W/m/K)	0.5
Thermal Conductivity Material 2 (W/m/K)	0.5
Thermal Conductivity Material 3 (W/m/K)	400

** It should be noted that the ignition time in the model is only taken into account for non charring materials and determines the change in the boundary conditions on the surface. Hence changes in the ignition temperature were not studied for this case.

Table 6-1 Overview of standard input parameters for the sensitivity analysis

6.1 Influence of the pyrolysis temperature on the results

As can be seen in Figure 6-1 a reduction of the pyrolysis temperature results in a delay of ignition time and peak heat release time and a reduction of the peak heat release.

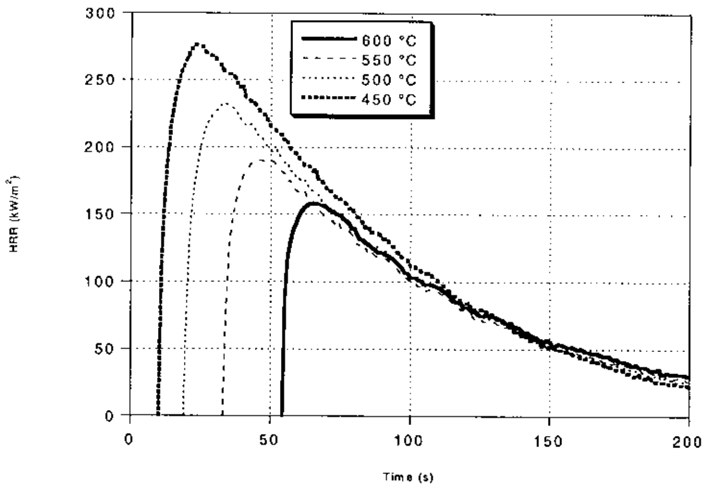

Figure 6-1 Analysis of the influence of the pyrolysis temperature on the results

6.2 Influence of heat of pyrolysis on the results

In Figure 6-2 it can be seen that the heat of pyrolysis mainly affects the peak HRR. An increase of the heat of pyrolysis reduces the peak HRR and flattens the curves. Rather limited influence on ignition time is observed as the temperature governs this one.

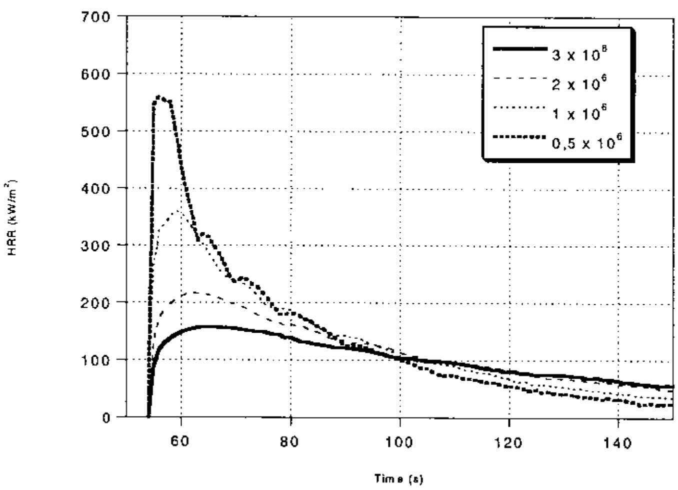

Figure 6-2 Analysis of the influence of the heat of pyrolysis on the results

6.3 Influence of the heat of combustion on the results

As can be expected a change in heat of combustion results only in a linear change of the actual HRR output as it is directly linked to the mass loss rate.

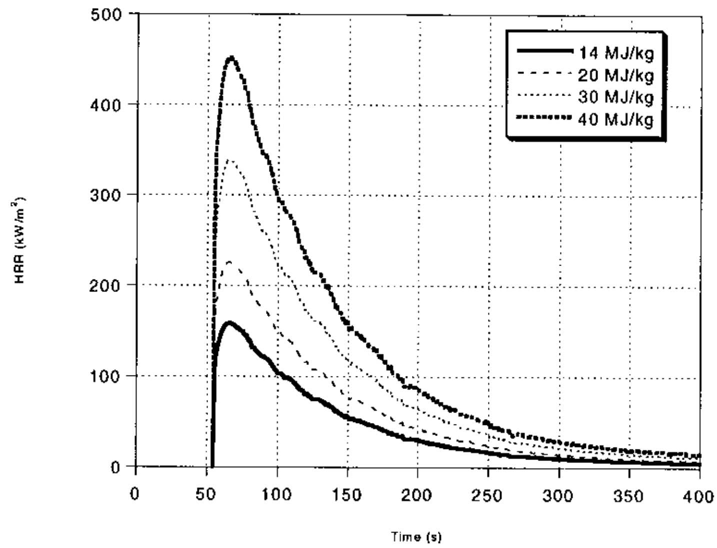

Figure 6-3 Analysis of the influence of the heat of combustion on the results

6.4 Influence of the char density on the results

Varying the char density results in a small change of the peak HRR and also a transposition of the decay period of the HRR curve. The values of char densities are those which can be expected as realistic with the corresponding virgin density.

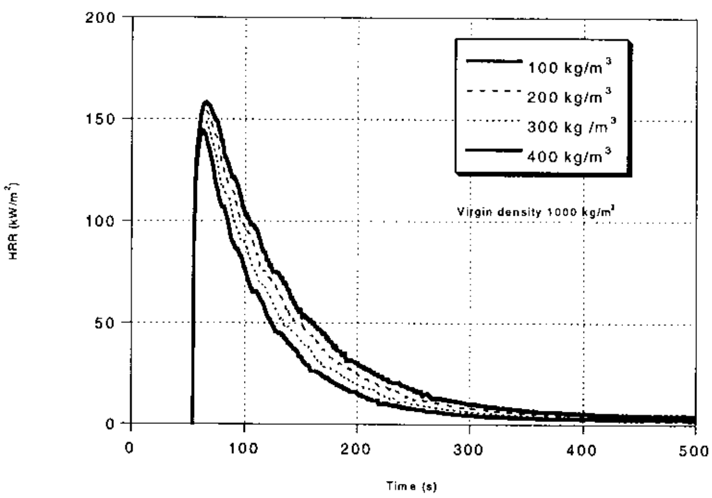

Figure 6-4 Analysis of the influence of the char density on the results

6.5 Influence of the specific heat on the results

Even with a considerable change the main influence of the specific heat is the ignition time.

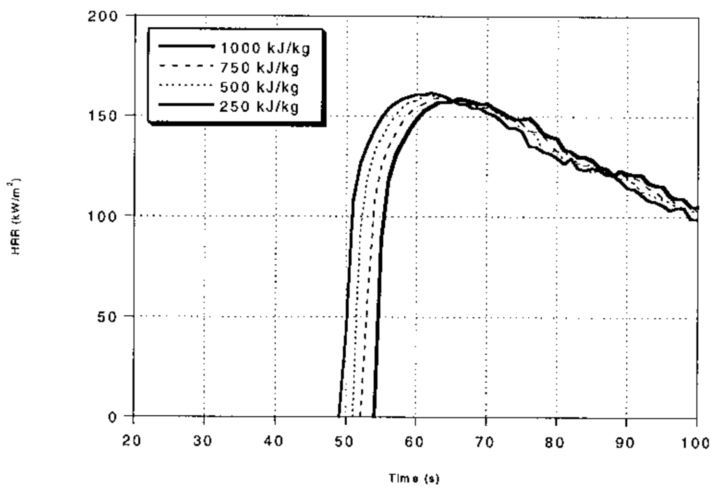

Figure 6-5 Analysis of the influence of the specific heat on the results

6.6 Influence of the thermal conductivity on the results

The parameter mostly influencing the HRR curve is the thermal conductivity. An example of this is given in Figure 6-6. A reduction of this parameter results first in a shorter ignition time and higher peak HRR. At very small numbers of thermal conductivity the ignition time is still reduced but the peak HRR decreases again. Unfortunately the thermal conductivity is one of the parameters which is very difficult to determine in fire simulations as it is strongly temperature dependent and changes considerably if the material undergoes transformations such as intumescing, charring, melting, etc.

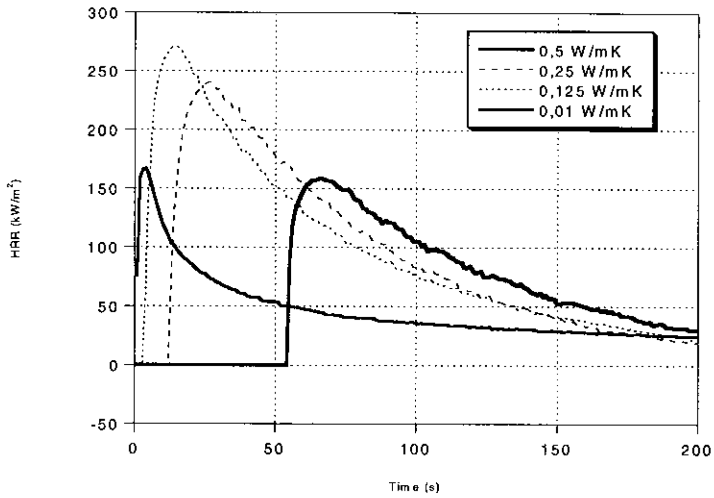

Figure 6-6 Analysis of the influence of the thermal conductivity on the results

6.7 Influence of the number of iterations and thickness of numerical strips on the results

With a separate analysis the influence of the number of iterations on the numerical model and the thickness of the strips was investigated. In the discussion of his thermal flame spread model Yan only mentions the importance of time steps and number of sub-strips. However it could be observed that the number of strips and the number of iterations can have an influence especially when using small numerical strips for the numerical thermal heat conduction solver. From experience it is advised not to reduce the thermal strips to less than 0.5 mm. With this value a number of iterations about 20 are more than sufficient (case of n=10 in Figure 6-7). When the thickness of the strip for the thermal heat conduction solver is less than 1mm, the number of iterations needs to be increased to 100. Some more study is required to investigate this phenomenon and to determine an automatic convergence criterion. This is not clear in the code for the moment and should in the future not be left to the personal knowledge of the user.

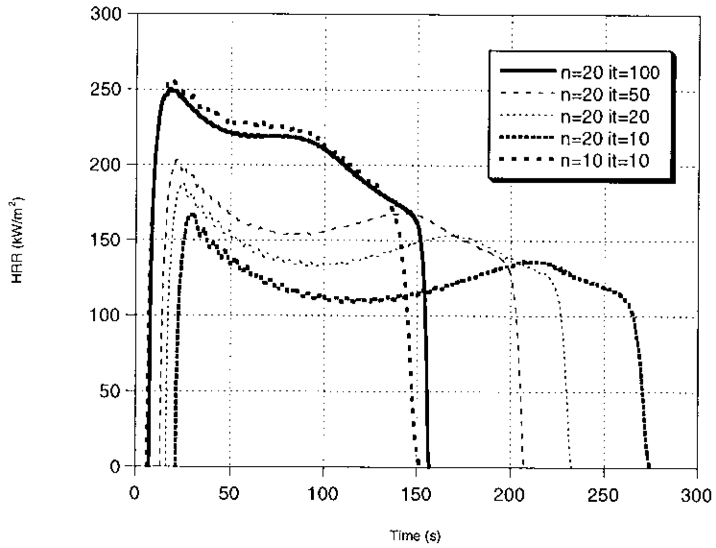

Figure 6-7 Analysis of the influence of the number of iterations and thickness of numerical strips on the results

6.8 Influence of ignition temperature for non-charring materials

Another important input parameter for the model is the change in addressing the boundary conditions from charring to non-charring materials. It was observed that for non-charring materials the ignition temperature is used for the change in boundary conditions. This means that before the ignition temperature is reached, the net flux to the surface is composed of the incident heat flux minus radiation and convection losses. At the moment of ignition, the convection losses are zero while the total heat flux is increased by the flame heat flux. Radiation losses are equal to the radiation losses from a surface at a temperature equal to pyrolysis temperature. This means that the pyrolysis temperature should be chosen equal or lower to the ignition temperature or else a sudden change in boundary conditions results in an abrupt change of heat release as can be seen in Figure 6-8. Some caution is hence appropriate and a further investigation of this change in boundary condition is desirable.

For charring material the actual calculated heat release is used as the trigger for a change in boundary conditions. Here the calculated surface temperature is used for the surface radiation losses during the whole simulation time.

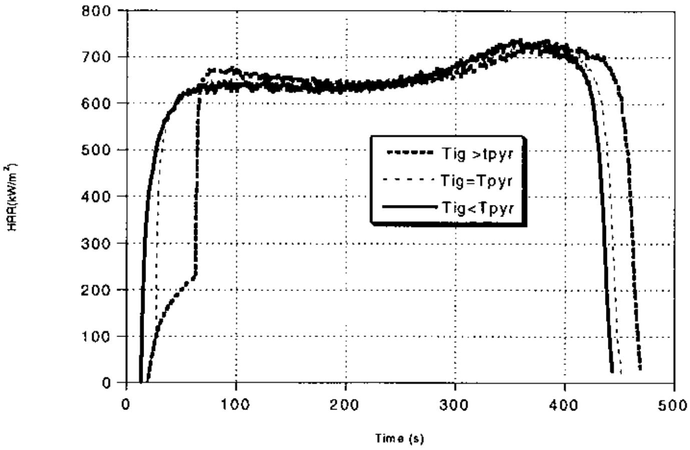

Figure 6-8 Influence of Ignition temperature for non charring materials

6.9 Final evaluation and procedure to define material parameters

From the previous subchapters it can be concluded that especially the thermal conductivity, heat of pyrolysis and pyrolysis temperature have a strong influence on the simulation results with respect to ignition time and heat release curve. The heat of combustion is only a linear parameter, which is used in the model for linking the mass loss and the heat release.

On the other hand the difference between charring and non-charring materials is also reflected in the change in boundary condition. While this is correct with respect to how the radiation losses are calculated it is more questionable by the way the ignition temperature is introduced in the calculation model for non-charring materials.

Since a char density of 5 kg/m^3 is used to make the difference between a charring and non charring material with respect to change of boundary conditions, the user of the model is warned for a big change in results if low char densities would be used. This can clearly been seen given in Figure 6-9.

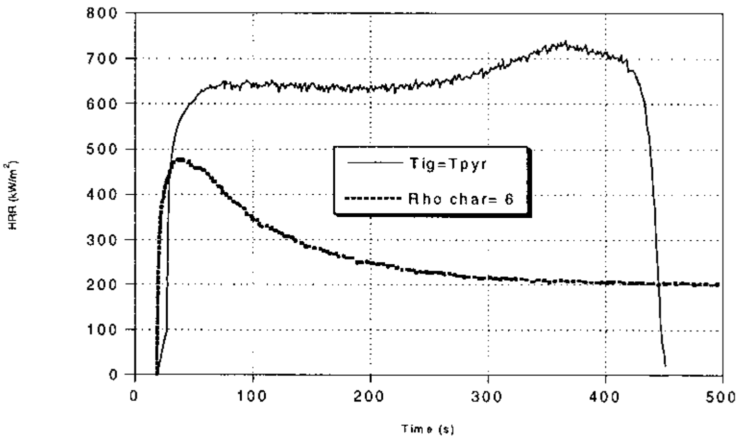

Figure 6-9 Difference between a simulation with small char density and a simulation as non charring material

While for many materials such as PMMA many of the input parameters can be found in literature a simple procedure was developed for this project by using mainly cone calorimeter test data.

The procedure is as follow:

1. Cone calorimeter tests on the material at specific heat flux levels to obtain the heat release curve as a function of time.

2. Cone Calorimeter ignition tests on some additional heat fluxes to determine the ignition times.

3. Determination of kρc and T_{ig} (ignition temperature) by means of ignition test results of the material at different heat flux levels. This is done by using thermally thin or thick ignition models e.g. the model developed by Janssens which can even be used for both cases. Then assume a specific heat value (the influence of c is rather limited why an estimated guess with help of literature data can be made). Then determine the density of the material and calculate the thermal conductivity. With the same ignition model a value for the ignition temperature can be obtained. As explained earlier this only has an influence for non-charring materials.

4. Determination of the char density (if appropriate) by checking the remaining mass after the cone calorimeter tests. When several flux levels are used an average value can be obtained.

5. Determine the heat of combustion as the effective heat of combustion obtained in the cone calorimeter tests.

6. Optimise by means of changing the pyrolysis temperature and heat of pyrolysis the HRR curve of the simulation so that it corresponds as good as possible with the measured data. As start values, literature values for the envisaged material can be used or data from other test methods can be used if available (e.g. Thermogravemetric analysis, TGA) for pyrolysis temperature. If necessary small changes in the other input parameter can be allowed to fine tune the heat release curve and the ignition time.

7. Checks should not only be performed at one heat flux level but also at different heat flux levels especially for the ignition time.

Experience with this rather simple procedure shows that about 10 to 15 simulations with the pyrolysis model of the cone calorimeter tests have to be performed in order to obtain the parameters needed for both the thermal and pyrolysis model. By means of the flexible input file this process can be performed simultaneously for different flux levels or for different changes in one specific input parameter when keeping the other input parameter constant.

An automatic process by means of curve fitting is mostly desirable in the future. Due to lack of resources this has not yet been performed. However this should be considered as a high priority item if a user-friendly technique is desirable.

7 Verification of the physical flame spread

7.1 Verification with cone calorimeter test data

7.1.1 Tests with PMMA

A check with PMMA has been performed with the modified code based on the material data given in Yan's PhD. However the simulation was performed with mineral wool under the PMMA simulating the exact thermal boundary condition as in the real test. Yan used namely adiabatic boundary conditions at the back. The test used for comparison was one of the PMMA tests in the pre RR within WP8 of the FIPEC project.

The results of the simulation are given in Figure 7-1. It can be seen that the ignition time and the constant HRR levels are predicted very well. The fact that the last peak is predicted less well can be explained as follows. PMMA burns as a liquid pool fire and at the end of the test the area is changing causing a different heat release curve. It can be concluded that the modified model predicts even better the cone calorimeter test on PMMA than the original code developed by Yan. This is mainly due to the fact that a more flexible composite input module is possible which allows introduction of the correct boundary conditions on the back of the PMMA.

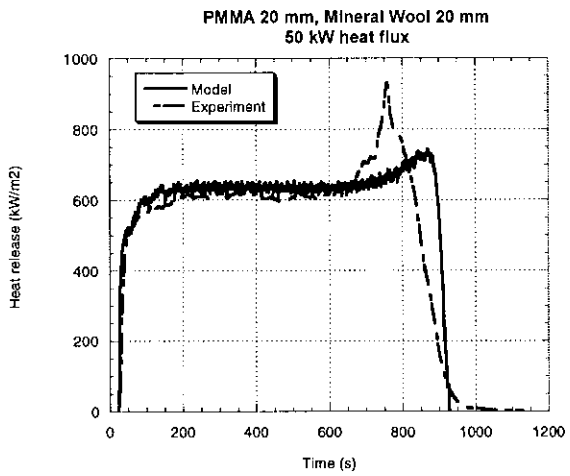

Figure 7-1 Simulation of a PMMA cone calorimeter test at 50 kW/m^2

7.1.2 Tests with particle board

Similarly a simulation of a 12 mm thick particle board with ceramic wool was performed. Figure 7-2 gives the results for a cone calorimeter test at 50 kW/m^2.

Also here the difference between simulation and test results is acceptable considering the complex behaviour of burning particle board. The second peak is not included in the simulation. In order to predict this second peak it is clearly necessary to have the possibility to include a temperature dependent thermal conductivity of the char. Even here simulations are slightly better compared to Yan's examples mainly due to the introduction of a composite particle board - ceramic wool.

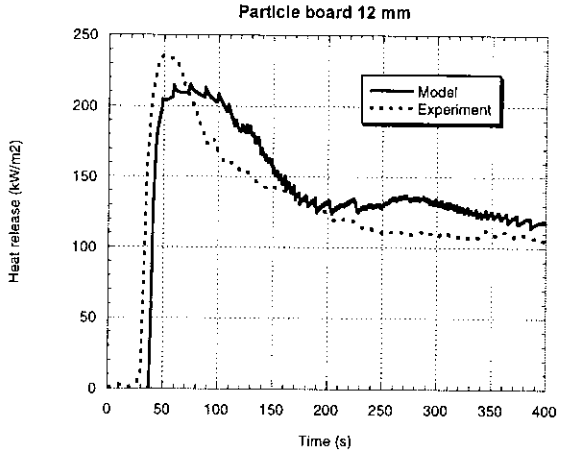

Figure 7-2 Simulation of a particle board test at 50 kW/m²

7.1.3 Tests with a PVC plaque

In the FIPEC project the procedure given in paragraph 6.9 was used to determine the input parameters for the pyrolysis model. In Figure 7-3 the result of the optimisation for a PVC material at 75 kW/m² is given. As can be seen the material simulation is quite good. Only the decay period is different. This can most likely be explained by the fact that the thermal conductivity of the char is identical to the thermal conductivity of the virgin materials. In future versions it is necessary to include a better representation of the thermal conductivity of the char in order to better predict the behaviour of materials with a highly active char during the combustion process.

Ignition times for different heat fluxes and peak heat release for other heat flux levels are within 10% of the measured values.

With the pyrolysis model a procedure for obtaining the composite behaviour was developed which allows a first prediction of acable behaviour by means of material tests results of the different cable components. Further information can be found in the final report of the FIPEC project [16].

From these results and the one obtained in the previous chapter it could be concluded that the code used was corresponding with the earlier developed code by Yan.

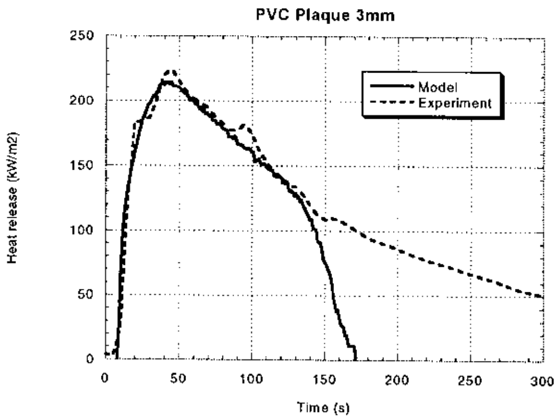

Figure 7-3 Prediction of a 3mm PVC plaque and comparison with the cone calorimeter test results at 75 kW/m².

7.2 Verification with a stand-alone flame spread model

7.2.1 Description of the stand-alone flame spread model

The stand-alone flame spread model was developed to investigate if there was a possibility to simulate upward vertical flame spread in a simple way using the physical flame spread model alone without combining it with a CFD code.

The first step is to obtain all relevant physical parameters for the physical flame spread model according to chapter 6. The strategy is then to divide a panel of a certain material or composite into discrete, uniform cells or faces along an upward x-axis. Each face and material is subdivided in depth into a number of strips. A gas burner is then simulated by exposing a number of faces at the lower end of the panel to an external heat flux. The above faces are also exposed to a flux according to an exponential profile

$$\dot{q} = q_0 e^{-5.0(x - x_{f0})} \tag{18}$$

where q_0 is the burner flame flux and x_{f0} is the section of the panel directly exposed by the burner flames.

For each face the physical flame spread model is then called with each respective external heat flux and the material physical parameters. It returns heat release and temperature of each face, which is used to determine ignition and the position of the pyrolysis front. The flame length, x_f, is coupled to the total heat release from all faces and to the pyrolysis length by

$$x_f = \frac{x_p}{2} + k_f \dot{Q}^n \tag{19}$$

where x_p is the position of he pyrolysis front, k_f the flame height constant and $\dot{Q}$ the sum of heat release from all faces. The exponent n is taken as 2/3 for wall flames [14] and k_f as 0.054 $kW^{-2/3}$. All faces exposed by the flames are assigned a constant external flux while the faces above the flame are assigned an external flux according to the profile given in (18).

7.2.2 Results

The stand-alone flame spread model has been tested for two cases, a 12 mm particle board and a 3 mm PVC wire. Both cases have also been tested experimentally in the FIPEC project according to a test method developed for the project and using a standardised IEC method (IEC 60332-3).

7.2.2.1 Particle Board

The particleboard was experimentally tested in the IEC 60332-3 chamber as a 4 m high and 0.3 m wide panel vertically mounted on a ladder. A premixed-flame propane burner with a 20 kW output was applied to the lower part of the panel and flame spread was recorded visually and on video. As the cone calorimeter experiments used are not exactly from this type of particle board some uncertainty of the physical parameters should be considered. A cone experiment would make it possible to optimise the physical parameters in order to achieve a better simulation. The most important observation is that the model predicts correctly the fact that pyrolysis front stops and does not continue to the top of the 4 m rig, see Figure 7-5, which was also observed in the test. During the flame spread experiments the back of the boards ignited at a later phase. This cannot be predicted by the model for the moment and is thus ignored here.

7.2.2.2 PVC Wire

In the experiment the PVC wire was mounted on a vertical ladder in 4-m lengths. As for the particle board a 20 kW premixed-flame was applied to the lower part of the wires. The heat release was measured and flame spread recorded visually.

In the simulation the wire was represented by a 1.8 mm PVC panel, the thickness corresponding to the amount of combustible material mounted in the experiment. This is of course a very rough approximation of a wire but the result is certainly reasonable as can be seen in Figure 7-4. In the experiment the flame spread to the top in about 100 s and in the model the top was reached in 130 s, see Figure 7-5. The results prove that the pyrolysis model is capable of covering a lot of the physical phenomena occurring during the flame spread process. It should be noted that for cables an additional dimension in the numerical heat transfer model might be necessary to simulate the longitudinal heat transfer in the copper conductor.

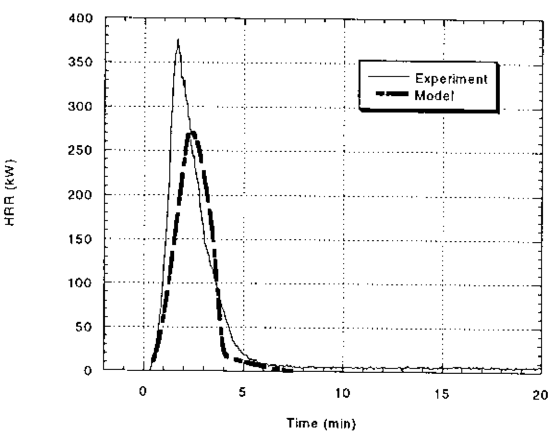

Figure 7-4 PVC Wire, model and experiment

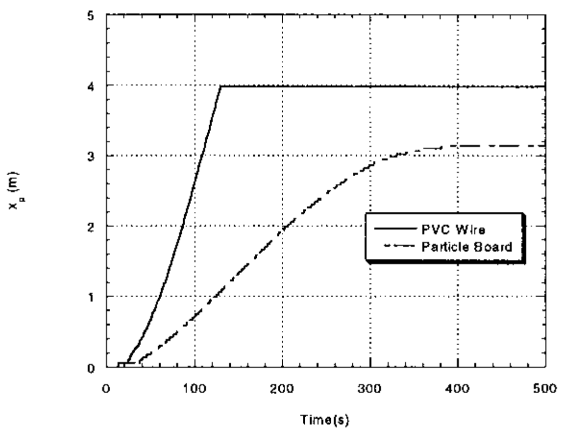

Figure 7-5 Simulated pyrolysed length in for the two cases

7.3 Verification inside the CFD code

A simple vertical panel was simulated by means of the flame spread code inside SOFIE. The simulation of this case revealed that temperature profiles were predicted satisfactory. It was only observed that once the material produced pyrolyses gases the risk of non convergence increased a lot. This revealed that more extensive code development was necessary which have the be implemented in the next SOFIE code. The SOFIE consortium have been taken this work has a high priority item.

8 Feasibility studies

The need to address flame spread and fire growth in geometries which are more complex than those considered in this project is large. Experimental data exist for several other scenarios of interest.

Part of this project was the investigation of the feasibility of both types of models for other applications. These feasibility studies are necessary in order to validate both the pyrolysis model itself and the correctness of its implementation inside the SOFIE code. It also allows further improvement of the thermal flame spread models.

Although effort has been spent to cover most scenarios it is possible that more scenarios than those listed can be considered.

8.1 Room and Room corridor tests

Data sets

- Within the Eurefic programme there is still a unique set of data available covering small scale testing such as cone calorimeter tests, room testing according to ISO9705 and large room tests.
- In Japan, both bench scale and full scale experiments (ISO 9705 room corner test and an intermediate scale test) are available.
- Within the SBI project (Single Burning Item) a large number of ISO9705 tests were conducted under the supervision of SP. Data is available from both room corner tests according to ISO 9705, cone calorimeter and SBI (single burning item) tests.
- Approximately 20 different floor coverings [17] have been tested in both room and room corridor scenarios at the University of Gent. Data is also available from cone calorimeter tests and a horizontal flame spread test (ISO9239 part 1).

Possible studies

Data from the Eurefic programme is highly valuable in order to test the flame spread models inside the CFD code. The main challenge is to predict the flame spread in both scales of room testing namely the small room tests and the large room test.

The studies in Japan can mainly be used for further fine-tuning of the thermal flame spread models.

The SBI project was already used in the thermal flame spread models for the room corner test results but can be further addressed for the link between cone and the SBI test method itself.

The floor covering study at Gent allows to address CFD flame spread modelling in a horizontal scenario both for room and room corridor scenarios. As it has been shown that ventilation is important in these scenarios the flame spread model inside the CFD code will be challenged with respect to its capabilities of predicting the change from wind opposed to co-current flame spread.

8.2 Cable scenarios

Data sets

- At SP a large number of different vertical and horizontal cable scenarios were tested within the FIPEC project (Fire Performance of Electrical Cables) in real scale. First a set of 25 tests with 4 cables were performed with different types of horizontal and vertical scenarios. Then one specific horizontal test set up was used to test 10 different market place cables.In addition one vertical test set up was chosen for testing of 40 different market place cables varying from medium voltage, low voltage, data cables, telephone cables, wires, coax to optical cables. Not only data from the cone calorimeter is available but also data of a vertical flame spread test similar to IEC 60332-3.
- At FRS a set of horizontal ventilated void tests on cables were performed. Data of full scale tests, a horizontal test method (Steiner tunnel) and cone calorimeter tests data have been generated.

Possible studies

Thermal flame spread models have been addressed in the FIPEC project for a specific type of full-scale test based on IEC 60332-3. However the CFD modelling of flame spread was not included in FIPEC. A unique database is thus available addressing a wide variety of cable scenarios. In the FIPEC project it was also clearly shown that mounting and position of cables is the main driving parameter in the flame spread. Only by means of a well established pyrolysis model connected to a CFD model all different types of real scale cables scenarios can be addressed. The FRS data set could be used for investigating extensively the horizontal wind aided flame spread of cables.

8.3 Vehicle scenarios

Data sets

At NIST a number of complete train wagons were tested. Tests results are available from the full scale rig but also from cone calorimeter tests.

Possible studies

The flame spread inside a vehicle such as a train wagon can be studied and compared with the real test data.

8.4 Furniture fires

Data sets

- Between 1993 and 1995 a large European project (CBUF) was conducted to investigate the fire behaviour of upholstered furniture. Data from different furniture items in room tests (with different ventilation and size), furniture calorimeter tests and cone calorimeter tests are available.
- Similar data sets have been generated in the US by NIST. Data from cone calorimeter tests and furniture calorimeter test are available.

Possible studies

The data sets from furniture will allow testing of the pyrolysis model at a smaller "micro" scale to investigate whether it is possible to simulate the flame spread on the surface of a furniture item.

8.5 High storage stacks

Data sets

- At SP in Borås, Ingason [13] has measured the rate of heat release where industrial storage stacks burn both at full scale and at one third scale. Detailed measurements of temperature, gas velocity and heat release are available in all scales.
- At Factory Mutual Research Corporation experimental work on industrial storage scenarios have been carried out similar to the one at SP.

Possible studies

The simulation of high storage rack will investigate the possibility of the physical flame spread model to predict the flame spread inside small chimneys where thermal buoyancy effects are important.

8.6 Discussion

From the overview above it becomes clear that a large amount of feasibility studies are possible. All of them will investigate specific types of flame spread and will allow both for improvements and modifications in the models. The most logic strategy is to start with the more simple scenarios such as room and room corridor tests. Then flame spread where the "micro" scale plays an important role can be addressed. This scale concerns cable and furniture fires. At last the very large scale and complicated scenarios such as vehicles and storage racks can be addressed.

9 Conclusions

Before implementing the pyrolysis code inside a CFD code it was decided to perform a sensitivity analysis of the pyrolysis model by means of an input parameter analysis. For this purpose the programme was foreseen with an easy to us input module.

A sensitivity analysis of the pyrolysis model developed by Yan revealed the following:

- Parameters such as thermal conductivity, pyrolysis temperature and heat of pyrolysis seem to have most influence on the prediction results. Ignition temperature has only effect when using the non-charring mode.
- The onset of the HRR curve and the change in boundary conditions has been treated differently for charring and non-charring materials. The user should take caution when using the different modes.
- The numerical strips for the thermal heat transfer model have a considerable influence on the convergence of the model. More guidance has to be developed.

In order to apply the pyrolysis model a number of input parameters are required. A first simple procedure to determine the different input parameters by means of cone calorimeter test results has been outlined. More automatic determination is desirable in the future and also the use of other supplementary test methods or test procedure with the cone calorimeter, for example determination of pyrolysis temperature and heat of pyrolysis can be considered.

The pyrolysis model has been validated positively by means of:

- Cone calorimeter test results of PMMA, particle board and PVC.
- A stand-alone vertical flame spread model used for the vertical flame spread on a cable rig.
- A simple flame spread simulation inside the CFD code SOFIE.

The validation study learned that improvements of the model can be made by allowing a change of thermal conductivity of the char and possibly by introducing a two dimensional heat transfer model.

It has become clear that more research is needed to stabilise the pyrolysis model inside the CFD code SOFIE. Supplementary work is being done inside the SOFIE consortium to obtain these goals inside the next version of SOFIE. It would have been a waste of resources to address this problem already in the actual version of SOFIE. For this reason this part was limited.

By implementing a flame spread code inside a CFD code it can be shown that this type of flame spread model will give the fire researcher and engineers an unlimited resource for investigating different types of flame spread in different scenarios. Therefore an overview of future feasibility studies has been given in order to validate the flame spread code more extensively and to show the power of its applicability.

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