COUPLED HEAT TRANSFER PROCESSES DURING FIRES – A NEW MODEL AND ITS APPLICATION TO NUCLEAR FACILITIES

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ABSTRACT

The application of numerical fire simulations to validate and to evaluate the propagation of fire and smoke is already a fundamental part of the preparation of fire protection or safety concepts, especially in the field of performance-based designs. Against this background, guidelines have been developed in the recent years, which describe and classify the available possibilities, approaches and models as well as provide suitable support for their application. Those programs and models respectively have to provide reliable results on the one hand and have to be efficient on the other hand. Thus, it is mandatory to continuously improve and extend the available possibilities of numerical fire simulations also in the future to satisfy the rising requirements as sufficiently as possible.

There is extensive need for improvement in numerical fire simulations especially in the field of heat transfer, both between the gas phase and the solid phase and within the solid phase itself. So far, the focus of further developments has mainly been on the modeling of the gas phase as well as pyrolysis and burning processes. In contrast to this, the physical processes of both convective heat transfer, in particular in the context of special configurations such as pipes or ducts (e. g. air ventilation ducts), and multidimensional heat conduction in solids have not been sufficiently accounted for so far.

Hence, a heat transfer model for coupled processes in fire simulations was developed, which is able to represent the process of convective heat transfer between the gas phase and the solid phase for both horizontal and vertical plane surfaces and in particular pipe and duct flows on the one hand and the process of heat conduction within multidimensional problems on the other hand physically correct. In addition to this the model is able to reproduce corresponding results using numerical simulation. The model was optimized both physically and numerically for the integrated usage within numerical fire simulations. It has a modular design, so it is suitable for integration into current and future fire simulation codes. Additionally, a basis was established with and within this model for a later expansion with appropriate pyrolysis models. A for the completion and demonstration concluding necessary integration of the developed heat transfer model for coupled processes into a state-of-the-art fire simulation code was exemplarily and successfully performed by means of the "Fire Dynamics Simulator" in its present and current version 5 [1]. Finally, the model was successfully applied amongst others to real scale fire tests in the context of nuclear facilities within the international OECD PRISME project.

In summary, the state-of-the-art was expanded with the heat transfer model developed and integrated into an internationally recognized CFD fire simulation code. Additionally, an important step was made on the way towards a fully coupled fire simulation imaginable in the future for instance for the purpose of the fire protection design of structures. Beyond that, the developed model can also make a valuable contribution in other fields, where extensions and improvements are still necessary in the future, in particular in upgrading pyrolysis models. Finally, the present possibilities in numerical fire simulations

were expanded with the developed model also in such fields, where calculations in fact are performed at this stage, whereas the applicability of the present and available models or the transferability of their constituents is however questionable or even incorrect.

PROBLEMS AND AIMS

The significant problems in the field of fire simulations can be summarized as follows. Currently, the consideration of the heat transfer to as well as within the solid phase is only possible with strong limitations. For example structural elements or installed equipment like ventilation ducts are meant by solid phase. However, the focus of further developments concerning the corresponding numerical codes was and still is on the specification of the gas phase as well as pyrolysis and combustion processes. Though, the precise determination of the temperatures on the surface and within the solid phase is a fundamental requirement especially for the latter question. The possibilities in the fields of convective heat transfer and heat conduction currently available are not sufficient for a lot of tasks. Especially a direct coupling of the gas phase and the solid phase with each other is an absolute necessary basis for both subsystems to safeguard an as appropriate as possible copy of the real fire scenario within the numerical simulation. Herefrom the main aims of this work arose which are to be discussed in the following. It was absolutely necessary to improve the modeling of convective heat transfer between the fluid/gas phase and the solid phase on the one hand. An aim of this work was to be able to consider appropriately amongst others also special situations in a fire scenario as they appear for example in the context of ventilation ducts. On the other hand work had to be done urgently to improve the modeling of heat conduction within the solid phase during numerical fire simulations. The multidimensional consideration of complex objects played an important role in this context as well as in particular the interaction of gas phase and solid phase in both directions, i. e. including the feedback of the aforementioned thermal processes on the fire event. This important coupling between gas phase and (detailed) solid phase is an important development in the field of numerical fire simulations.

Herefrom it results as a whole the developed heat transfer model for coupled processes in fire simulations which is published in [2] consisting of a model for convective heat transfer and a model for multidimensional heat conduction. The main attributes of the model are as follows. It is optimized both physically as well as numerically for the integrated usage within numerical fire simulations. Physically means in particular the consideration of the specific impacts caused by a fire and fire properties, e. g. temperature-dependent material data or the actual fluid in the fire room; numerically means in particular the choice of appropriate numerical methods. The development was performed with a view to the parallelization of the model. Moreover, the developed heat transfer model provides the basis for the later upgrading with appropriate pyrolysis models and was exemplarily integrated into the code "Fire Dynamics Simulator" (FDS) in its present and current version 5, a state-of-the-art fire simulation code. The items of the model are described in more detail later on. Before that, a short overview about the current statues of knowledge in the field of fire simulations is to be given in the following.

STATUS OF KNOWLEDGE

Aside from algebraic models it can generally be differentiated between zone models and field or CFD models. As figure 1 [3] shows zone models (e. g. HARVARD VI, CFAST) permit a comparatively fast calculation of simple scenarios whereas CFD models (e. g. FDS, ISIS, Fluent, CFX) are used in particular for complex scenarios. With increasing development in all parts it is assumed that the up to now biggest disadvantage of CFD codes, their comparatively higher calculation time, can be reduced significantly in the future.

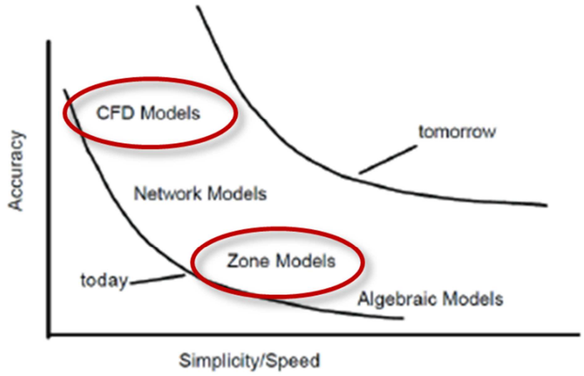

Figure 1: Hierarchy of fire simulation models [3]

In particular necessary are the specific for the numerical simulation of fire scenarios eminent important sub models like for example a pyrolysis model. However, general CFD codes like CFX or FLUENT do not contain those or only in a significantly limited range in contrast to CFD models which are especially concentrated on the simulation of fire scenarios like FDS. Due to this usually the prescription and knowledge of the temporal course of the heat release rate is necessary. This has to be abandoned and replaced by combustion/pyrolysis models in the future. That means, the temporal course of the heat release rate results directly from the fire scenario wherewith a real prediction of a fire and a modeling in line with reality respectively will primal be possible. As already mentioned the developed heat transfer model consequently provides the basis for the later upgrading with appropriate of such pyrolysis models.

A physical process that is also meaningful in the context of numerical fire simulations is the convective heat transfer between gas phase and solid phase. Zone models are limited per definition in this part, because amongst other things they do not solve the velocity field. CFD models do not have this limitation. Hence, the convective heat transfer there depends on how the gas phase related values are determined. An increased use of the Large Eddy Simulation (LES) method can be expected in the future. Currently, this method is already used very widely. However, simplifications are used during this way of gas phase modeling that now longer allow to determine the convective heat transfer straight from the values calculated in the gas phase as it is the case with the DNS method. Thus, sub models are necessary here which can be developed for example from empirical correlations (e. g. Nusselt relations). The current modeling of the convective heat transfer in fire simulations is insufficient and even wrong in several areas respectively. That is why a model or a modus operandi is necessary to be able to represent plane surfaces correctly on the one hand and specific items or configurations appropriately on the other hand.

An additional physical process that is also meaningful in the context of numerical fire simulations is the heat conduction within the solid phase. Up to now scant attention has been dedicated for example to the enclosure structural members, because they have only been regarded in their function as a boundary condition for the gas phase. Thus, only global energy considerations or one-dimensional heat conduction calculations through a homogeneous or in thickness direction layered ("multi-layer") solid phase have been performed so far. However, these approaches are problematical in particular in cases where multidimensional effects underlie. This is the case for example for frame corners or multilateral fire exposed structural members (e. g. columns). Thus, a model for multidimensional heat conduction ("multi-cuboid") is required. The currently propagandized way includes in this field the determination of transfer values for a downstream thermal analysis with separate programs or tools which however entails a plurality of disadvantages. Thus, an increased effort for modeling is caused by this and it lacks the already mentioned feedback which is however urgently required for example in the context of pyrolysis or heat transmission processes. According to this, it is absolutely necessary to develop a model that is integrated into the fire simulation code.

A NEW MODEL FOR COUPLED HEAT TRANSFER PROCESSES DURING FIRES

In the following the developed heat transfer model and its characteristics and specifics will be presented in more detail.

Model for convective heat transfer between gas phase and solid phase

The model for convective heat transfer between gas phase and solid phase forms the first part of the heat transfer model. This component sets the basis of the developed heat transfer model for coupled processes in fire simulations because it establishes the important coupling between gas phase and (detailed) solid phase. As already mentioned an alternative modus operandi, as it was used and further developed in this work, and the use of sub models are in this connection necessary for example for the LES (Large Eddy Simulation) method which will dominate the future at least for the short and medium term regarding the numerical simulation of fires with large volumes. The physical fundament is set by the basic equation for the determination of the convective heat flux [1].

$$\dot{q}_{conv} = h \cdot \left(\vartheta_{fluid} - \vartheta_{surface}\right) \qquad [1]$$

Due to the fact that ϑ_{fluid} can be taken from the CFD code and $\vartheta_{surface}$ from the heat conduction model that is presented later on, the problem can be reduced to the determination of the so called heat transfer coefficient h. In the course of this, this coefficient is in particular dependent from the type of convection, the type of flow as well as the geometry or configuration and additionally a function of for example temperature (difference), velocity, location and fluid. As already mentioned the determination of h can be carried out with empirical correlations, e. g. according to Nusselt and McAdams. A model based on these correlations has been developed, because those are already successfully verified in many cases. Moreover, an analogues procedure for other configurations is possible in the same way with this modus operandi.

As important properties of the model it can be said that for the present task the fluid within the fire room can be assumed to be equivalent to “ordinary” air. This was successfully proven in the work. Thus, “ordinary” air can be used as the considered fluid and the corresponding temperature dependent property values respectively within the framework of the model. Furthermore, turbulent flow conditions prevail as it is also the case in the majority of the technical applications. The worked out “concept of relocalization” sets a central component. Is was developed on the basis of appropriate criteria, because the both existing modus operandi – local and averaged – are not suitable for the present task. Figure 2 shows the basic idea of this concept. Through the usage of local values, like the property values of the fluid, a partially return of the course averaged for technical questions to the local curve, which is leaned against the really existing course of the curve, is possible. This applies in equal measure both for the heat transfer coefficient as well as the convective heat flux.

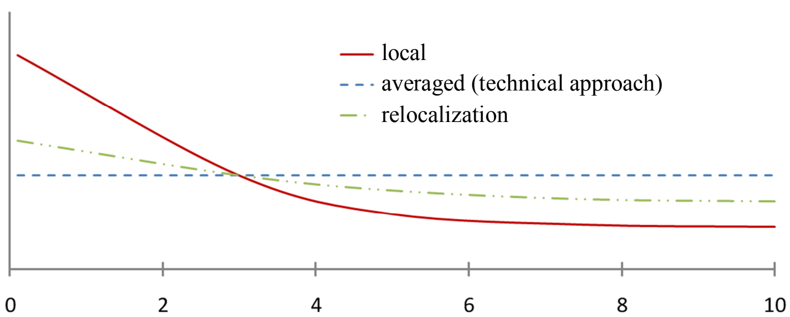

Figure 2: „Concept of relocalization“ – basic idea

The model covers horizontal and vertical plane surfaces as well as tube or duct flows as a special form. Concerning the plane surfaces the free convective heat transfer has to be considered, within the model according to the correlations from McAdams, as well as the forced convective heat transfer according to Petukhov/Popov and Nusselt. The simultaneous appearance of free and forced convective heat transfer is called mixed convection and is covered appropriately by the model. Concerning the tube or duct flows, i. e. in particular ventilation ducts, velocities of the flow between 6 and 12 m/s can usually be assumed. Thus, free convection does not appear alone and due to the flow it is not allowed to neglect the forced convection. The forced convective heat transfer is considered according to Gnielinski within the model. Mixed convection in horizontal ducts can usually be neglected [4]. The ability to neglect mixed convection in vertical ducts was proven in [2] using appropriate demarcation criteria according to Jackson/Hall in [2]. In addition to the conditions in the context of the prevailing turbulent flows approaches were developed for laminar flows and the transition region lying in between.

Model for multidimensional heat conduction

The heat transfer equation as it is shown in its general form in [2] – due to the consideration of the solid phase already without convective terms – sets the physical basis for the multidimensional heat conduction model. It is a PDE parabolic in time and elliptic in space which describes an initial boundary value problem.

$$\rho c \frac{\partial \vartheta}{\partial t} - \nabla \cdot \left(k \nabla \vartheta \right) = \dot{s} \qquad [2]$$

As a result of the parabolic type in time one initial condition for the time t = 0 and due to the elliptic type in space two boundary conditions in each coordinate direction, i. e. six for the Cartesian system in this problem, have to be formulated. The latter are formed by boundary conditions at the boundary surfaces of the whole volume of the solid phase – amongst others the convective heat transfer between gas phase and solid phase is considered here – and by matching conditions at contact surfaces of different solid phase objects.

An approximation of these analytical equations is required both temporal and spatial for the numerical calculation. An explicit Euler method is used for the temporal discretization in the model. It was successfully proven in the work that the time step of a CFD calculation Δt_{CFD} is in general already that small that the stability criterion does not play a meaningful role and the efficiency of the chosen method prevails. Because of that this method was preferred to the other reviewed methods. The Finite-Volume-Method (FVM) is used for the spatial discretization in the developed model. The special advantage of the FVM is that it is (flux) conservative and that is why it was preferred to the other reviewed numerical methods. With this method the domain that has to be calculated is divided into many so called control volumes and solved efficiently. The model equation to be solved then for the temperature in the point or node P and the control volume represented by this node respectively is given in [3] [5]. Here the term "b" contains the source term, i. e. heat sources/sinks.

$$\vartheta_P = \frac{1}{a_P^0} \left(b + \sum_{NB} a_{NB} \vartheta_{NB}^0 \right) \qquad [3]$$

The solution of the whole problem is finally carried out by a successive processing of universal units so called cells ("cell-by-cell-concept"). In FDS such a cell is for example a single-cell obstruction.

For the use in fire simulations it is additionally required to formulate the property values or material data dependent on the position as well as a function of temperature, because a lot of materials show significant changes in their thermal properties within the temperature band occurring in fire safety engineering. Within the model this is done at material changes favorably and in line with reality by a harmonic averaging of the heat conductivities. Besides the formulations for the domain also the boundaries have to formulated by appropriate boundary conditions within the numerical model. To do this three types of boundary conditions were foreseen. These are constant surface temperature and constant heat flux which are mainly intended for modeling (e. g. at the boundaries of the CFD domain) and diagnostics. The third boundary condition is the physically in the reality appearing heat flux consisting of convection and radiation due to a fire according to [4].

$$\dot{q}_{net}(t) = \dot{q}_{rad}(t) + \dot{q}_{conv}(t) \qquad [4]$$

In completion the developed model was provided with the corresponding algorithms for the consideration of heat sources/sinks. As already mentioned this provides a basis for the later integration of pyrolysis models. Moreover, the model is able to consider thermal contact resistances between discrete objects or materials.

VERIFICATION AND VALIDATION OF THE MODEL

In the following the verification and validation of the model is to be shown. The model and its properties as well as functions respectively were examined step by step beginning with simple and ending with complex questions. Furthermore, the max handling of the model was analyzed by varying the parameters. Now four meaningful examples are to be presented briefly as well as the results achieved.

The first example deals with the heat conduction including the convective heat transfer and is taken from the National Annex of Eurocode 1-1-2 [6]. As the figure shows the task is a three sided (five sided) adiabatically bounded cuboid with an initial temperature of 1000 °C that cools down by convective heat transfer with air (0 °C) over the remaining surface. The properties of the material (k = 1.0 W/mK; ρ = 1000 kg/m^3; c = 1.0 J/kgK) as well as the convective heat transfer coefficient (h = 1.0 W/m^{2}K) are stated by fictitious values. The aim is to calculate the temperature at point P (see figure 3).

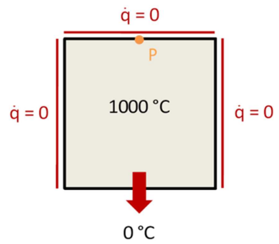

Figure 3: Mock-up for the example from the National Annex of EC 1-1-2 [6]

Table 1: Results of the comparative calculation regarding the NA-example

Time [s]	$\vartheta_{P,analytical}$ [°C]	$\vartheta_{P,numerical}$ [°C]	Difference [‰]
60	999.3	999.3	0.0
300	891.8	891.7	0.1
600	717.7	717.5	0.3
900	574.9	574.8	0.1
1200	460.4	460.3	0.3
1500	368.7	368.6	0.2
1800	295.3	295.2	0.2

The result is opposed to the analytical solution for different times in table 1. It appears a very good agreement of the respective values within the limits given by the National Annex. Thus, the model is appropriate for the use within the framework of the Eurocodes (thermal analysis).

The second example deals with the transient multidimensional heat conduction with convective and radiative heat transfer. A natural fire scenario of a room fire is assumed and it is to be studied a cube consisting of steel (very good heat conduction properties) and concrete (bad heat conduction properties but good thermal storage properties).

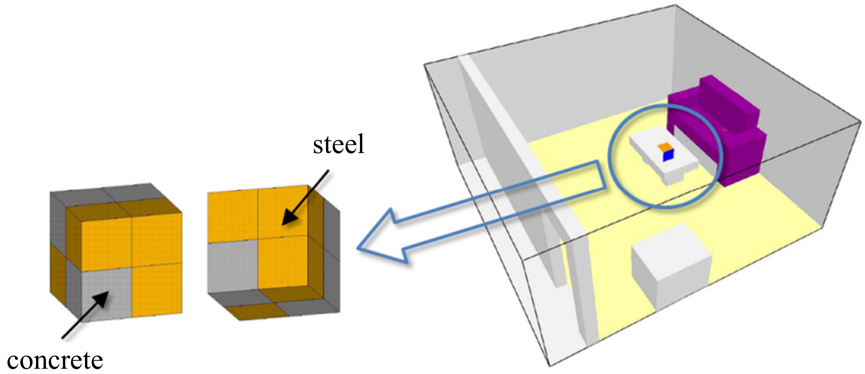

Figure 4: Realistic fire scenario of a room fire in FDS5

Figure 4 shows the scenario and the configuration. The material data were taken from the corresponding parts of the Eurocodes 2 [7] and 3 [8]. The really occurring heat flux caused by convection and radiation is used as boundary condition. The results are to be compared to the results of an ANSYS [9] calculation. The results of both calculations are shown in figure 5 for different times along two axes through the cube. It appears a very good agreement of the respective values. Furthermore, the boundary areas (left half of the figure) as well as material changes (right half of the figure) are reproduced correctly by the model.

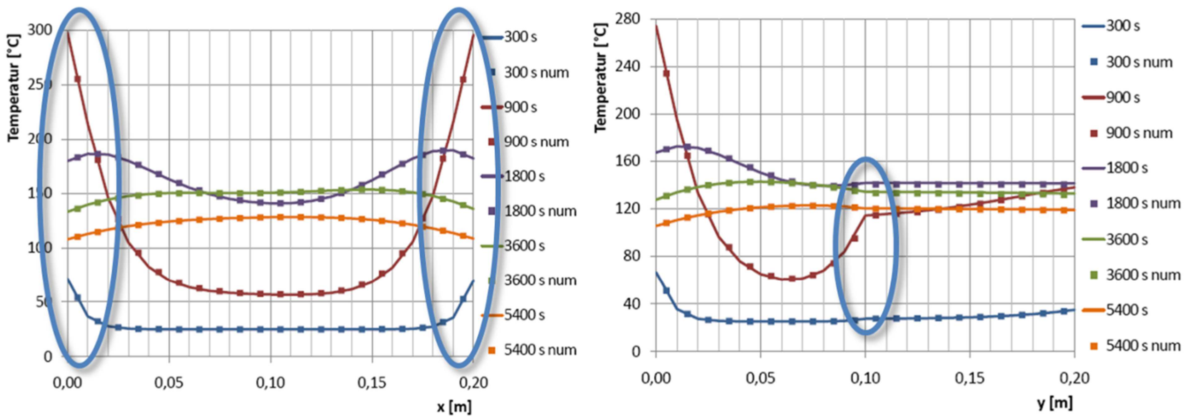

Figure 5: Results with convective and radiative heat transfer

Figures 6 and 7 show a cross section through the cube at 15 and 30 minutes respectively. In each case left the results of the developed model and right the results of the comparative calculation, the black frame marks the geometrically border of the object. It appears a very good agreement here again.

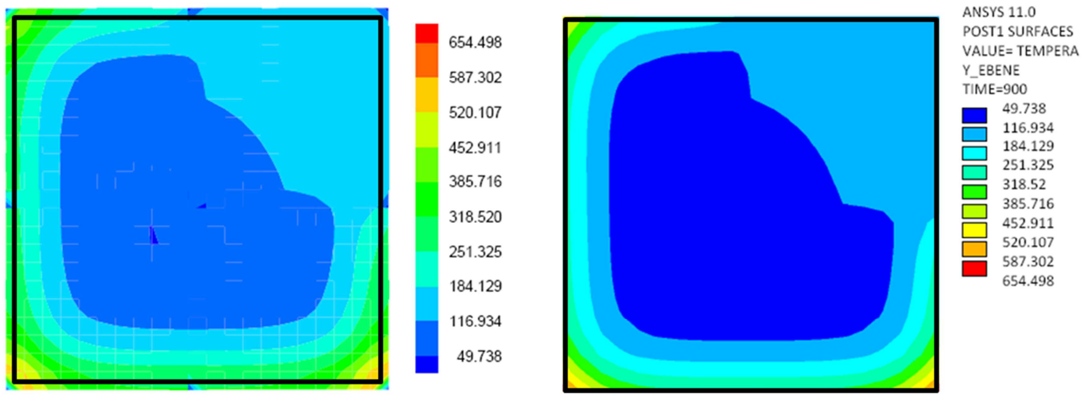

Figure 6: Results of the model and the control calculation (15 minutes)

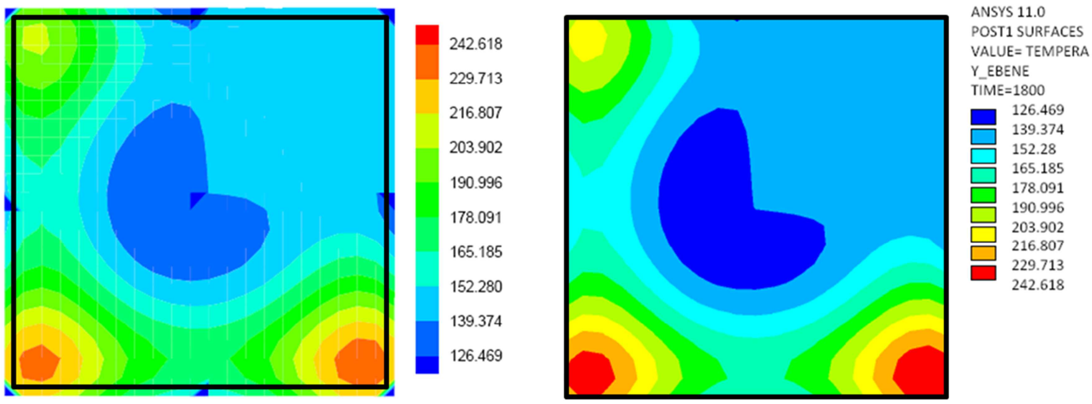

Figure 7: Results of the model and the control calculation (30 minutes)

With the third example the correctness of the model is examined in presence a heat source or sink. As figure 8 shows, a heat source is placed in the centre of an adiabatically bounded concrete cube – temperature dependent material properties according to Eurocode 2 [7]. The development of the temperature dependent rate of energy generation per unit volume follows an Arrhenius approach. This approach is often used in the practice for pyrolysis models. As before, the results are to be compared to those of an ANSYS [9] calculation

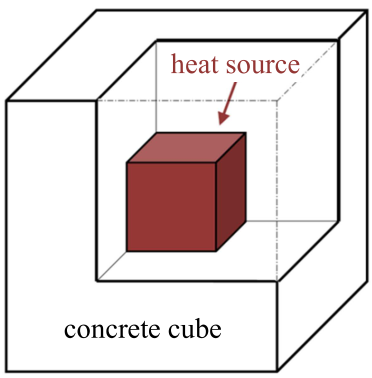

Figure 8: Structure for the example with heat source

The results of both calculations are shown in figure 9 for different times – due to the symmetry – to the midpoint of the cube. It appears a good agreement of the respective values with differences less than 3 %. Thus, the correct consideration of heat sources/sinks in particular with Arrhenius approach within the model is proven and consequently the developed model is suitable for the modeling of pyrolysis models, too.

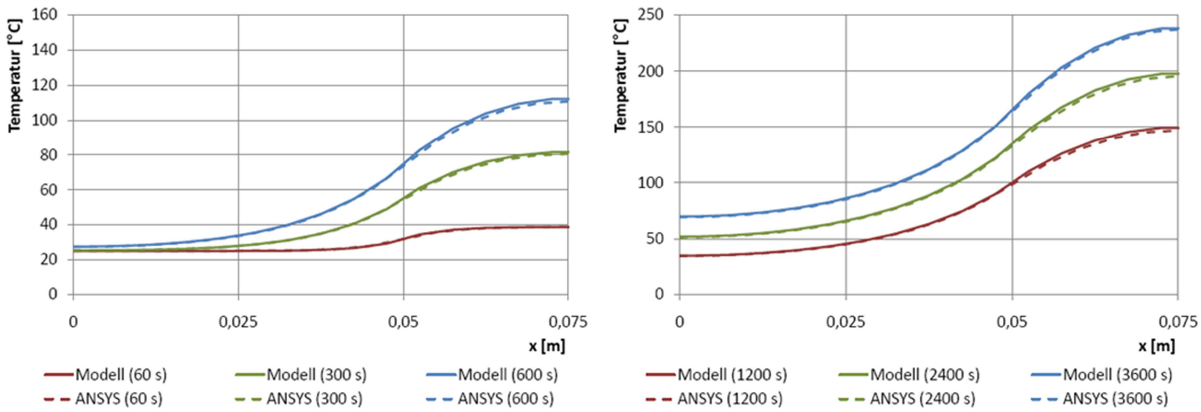

Figure 9: Results with a heat source in the style of a pyrolysis model

In the last example the convective heat transfer for a tube/duct flow is to be studied. The scenario consists of a ventilation duct (l x b x h = 10 m x 50 cm x 50 cm) which is turbulently flowed through by air (v_{air} = 6 m/s). The temperature of the incoming air is ϑ_{gas} = 150 °C and the (constant) surface temperature is ϑ_{gas} ± 50 °C. Thus, both cases "heating of the fluid" and "cooling of the fluid" can be analyzed. The achieved results are compared to the both existing verified empirical approaches. Those are the local and the averaged modus operandi. As already mentioned the latter is often used in practice (technical approach). The results are shown along the duct axis in figure 10 (heating) and 11 (cooling). It appears both for the heat transfer coefficient as well as the convective heat flux that the concept of relocalization functions properly. Furthermore, the balancing of the total heat flow transferred and the comparison of them also leads to a good agreement [2].

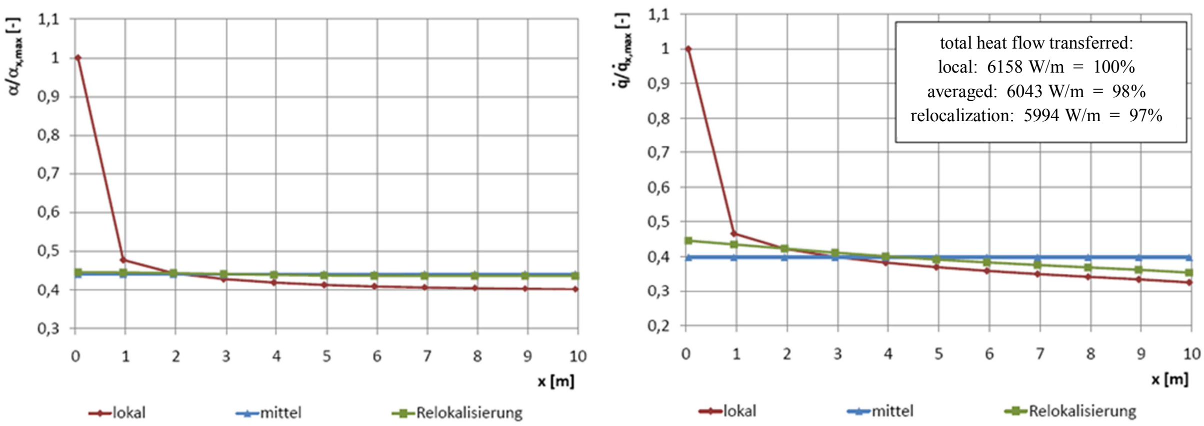

Figure 10: Distribution of the heat transfer coefficient and of the convective heat flux along the duct (normalised) – "heating of the fluid"

Thus, the model for convective heat transfer between gas phase and solid phase and the developed modus operandi respectively has to be declared as appropriate and correct. The same is also valid after the successfully performed verification and validation for the model for multidimensional heat conduction and consequentially at the end for the whole developed heat transfer model for coupled processes in fire simulations, too.

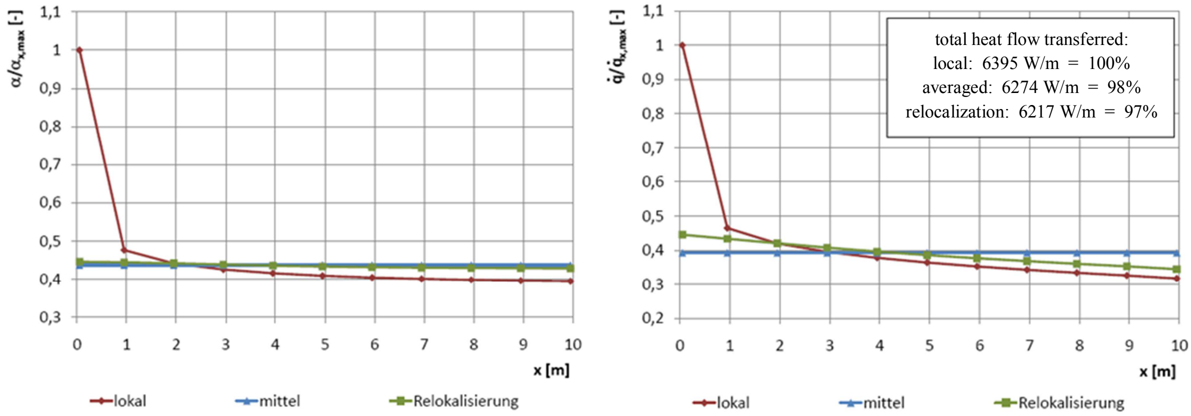

Figure 11: Distribution of the heat transfer coefficient and of the convective heat flux along the duct (normalised) – “cooling of the fluid“

APPLICATION OF THE MODEL

In the following the developed and reviewed model was applied to a practical fire scenario. In doing so a fire in a repository for insulation panels made of PS rigid foam was to be analyzed. The design fire could be determined with the help of [10] and has a maximum power of 4.22 MW with a whole dire duration of 1200 s [2]. Thereby it is looked at a duct which is made of reinforced concrete and converted to a ventilation duct. This duct crosses a fire compartment in horizontal direction and ventilates another following fire compartment. In addition a complex slab object is located in the fire room which has an unsymmetrical build-up with thermally widely varying materials (e. g. PVC) and which could for example represent an electrical cable. Amongst others due to the natural fire exposure as well as the constructions of the duct and the wall a performance based procedure with the use of engineering methods (numerical methods) is required here. The questioning of the performance based procedure is or could be: Is the wall thickness of the duct sufficient to provide for thermal impact within required limits in the neighboring room/fire compartment? This question can definitely be affirmed based on the numerical simulation. Furthermore, the possibility exists to reduce the wall thickness. In addition the results show that the super ordinate mechanisms are reproduced correctly. The model properly reproduces the temperature distribution and development within the slab object. It becomes apparent that only a three dimensional heat transfer model is able to reproduce the occurring effects correctly. Further results in particular concerning the model for convective heat transfer were also included and analyzed in [2].

In addition to this practical fire scenario the developed and reviewed model was very successfully applied to real scale fire tests in the context of nuclear facilities. These experiments were performed in the framework of the second test series PRISME-LEAK of the international OECD/PRISME project. Details to this project and respectively the experiments as well as the test facility and performance can be taken from the reports of the OECD/PRISME project. Due to the publication regulations within the international project it is currently not possible to show both the experimental data and the results achieved by the developed model. A distribution can possibly take place when a corresponding request is formulated to the project coordinator (Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, division project coordination (reactor safety research)); the corresponding information is included in [11].

CONCLUSION

Within the conclusion first of all an analysis of additional value versus additional expense is to be done. In general it can be stated for procedures and methods in engineering that an additional expense is then justified if an additional value is combined. Concerning the model for convective heat transfer between gas phase and solid phase the essential additional values can be summarized as follows. It is now possible to consider plane surfaces correctly independent of their orientation. Furthermore, an in line with reality and physically correct consideration of special forms of convective heat transfer, i. e. here tube or duct flows, is possible for the first time. The developed modus operandi is also unrestrictedly able for the further special forms of convective heat transfer. A particular advantage of this model part is that there is no (meaningful) additional expense combined with. Concerning the model for multidimensional heat conduction the essential additional values can be summarized as follows. It is now possible to determine multidimensional temperature fields within the solid phase without an additional thermal analysis and for the first time also complex heterogeneous objects are possible in fire simulations. The feedback of the effects of the (multidimensional) temperature field calculation within the solid phase as well as at its surface on the fire scenario is existing now with the developed model for the first time. The model forms the basis for a further expansion by a mechanical analysis as well as by pyrolysis models. For both expansions a feedback of the aforementioned effects on the fire scenario is essential. Moreover, for pyrolysis models the correct determination of the temperatures within the solid phase, i. e. a multidimensional calculation, is an urgent basis and requirement respectively. Furthermore an additional value lies in the fact that a more efficient solution of fire protection questionings concerning the solid phase is possible, because only one model assembly will be necessary. Looking at the additional expense thus there is some existing due to the multidimensional calculation for sure, but with the use of parallelization techniques – thus the model was developed correspondingly and coordinated on it respectively – the additional time requirement can significantly be reduced again, i. e. the additional time requirement increases less than proportionally compared to the additional expense. The additional expense for model assembly (and calculation) of the thermal analysis in separate programs is however irreducible.

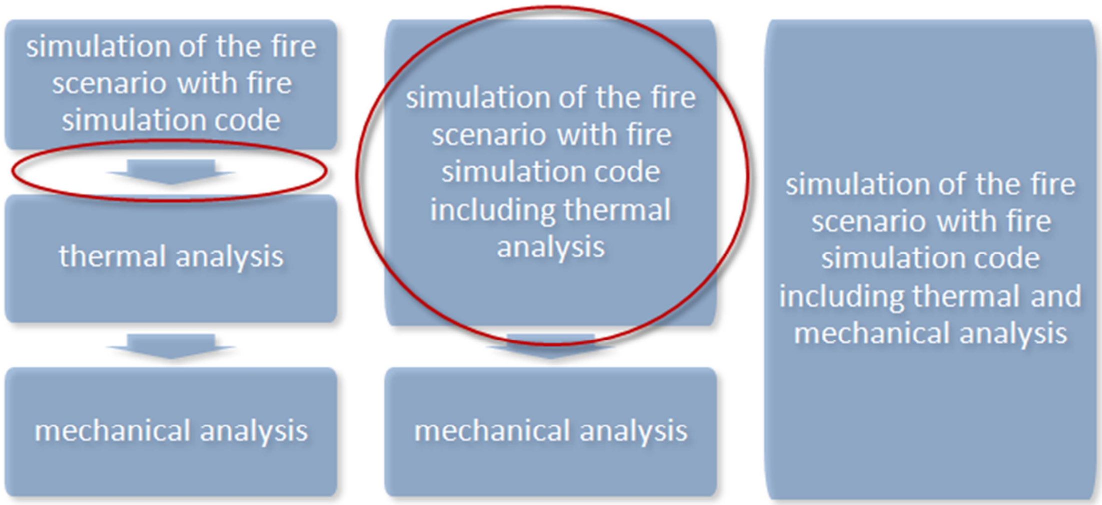

Figure 12: Modus operandi for the structural fire design in combination with natural fires

Within the work a heat transfer model for coupled processes in fire simulations was developed. By doing that the modeling of convective heat transfer between gas phase and solid phase for both horizontal and vertical plane surfaces as well as tube or duct flows (in particular ventilation ducts) was improved. Additionally the modeling of heat conduction within the solid phase was toughened up. Furthermore, it can provide a basis for pyrolysis models. The model was exemplarily and successfully integrated into a state-of-the-art CFD fire simulation code and extensively reviewed. Finally, the model was successfully applied amongst others to real scale fire tests in the context of nuclear facilities. The developed heat transfer model can be understood as a first step towards a fully coupled numerical fire simulation [2]. Using the example of the structural fire design in combination with natural fires the different ways are shown in figure 12. Left the current modus operandi and right the (possible) future. In the center the new and consistent way with the developed heat transfer model. Factual this means in the present context a mergence of fire simulation and thermal analysis with influence in both directions and the important coupling between gas phase and (detailed) solid phase which is a substantial further development in the field of numerical fire simulations.

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