Ceramic-foam surface burners in high-temperature environments

Citation for published version (APA):

DOI:
10.6100/IR545299

Document status and date:
Published: 01/01/2001

Document Version:
Publisher’s PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

• A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher’s website.
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Ceramic-Foam Surface Burners in High-Temperature Environments

PROEFSCHRIFT

ter verkrijging van de graad van doctor aan de Technische Universiteit Eindhoven, op gezag van de Rector Magnificus, prof.dr. M. Rem, voor een commissie aangewezen door het College voor Promoties in het openbaar te verdedigen op woensdag 27 juni 2001 om 16.00 uur

door

Frederik Albert Lammers

geboren te Amsterdam
Dit proefschrift is goedgekeurd door de promotoren:

prof.dr. L.P.H. de Goey
en
prof.dr.ir. A.A. van Steenhoven

Dit proefschrift is mede tot stand gekomen door de financiële bijdrage van NOVEM te Utrecht.

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Printed by the Eindhoven University Press.

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Lammers, Frederik A.

Ceramic-foam surface burners in high-temperature environments / by
Proefschrift. - ISBN 90-386-2842-0
NUGI 837
Trefwoorden : keramische schuimbranders / oppervlaktebranders / laminaire verbranding / voorgemengde verbranding / warmtestraling / numerieke modellen
Subject headings: ceramic foam burners / surface burners / laminar combustion / premixed combustion / heat radiation / numerical modelling
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Chapter 1

Introduction

1.1 Ceramic-foam surface burners

A major disadvantage of using fossil fuels as an energy source is the emission of pollutants. Even though methane is in itself a very clean fuel, both air and natural gas contain nitrogen which can be oxidized to NOₓ. Because the emission of NOₓ affects the air quality, the government has, in the last decades, introduced legislation to minimize the emission of NOₓ. Furthermore, the allowed levels of NOₓ emissions are gradually being reduced. This has been an incentive for recent research into clean-burner technology.

The rate of formation of NOₓ strongly increases with temperature. The NOₓ emission can therefore be limited by keeping the temperature low and, furthermore, by reducing the residence time of the flue gases in the combustion chamber. The residence time can be minimized by reducing the size of the hot zone. However, a minimum size is required to guarantee the complete conversion of CO into CO₂. The flue gas temperature can be controlled by increasing the amount of air in the unburnt mixture and by directly cooling the flue gases. Lowering the flue gas temperature leads to a decrease of the efficiency of the convective heat transfer. However, in case of direct cooling the heat taken from the flue gases can be used as well. In this case the efficiency depends on the utilization of this heat.

Radiant surface burners convert the heat absorbed from the flame into radiation, which can be used directly in a heat exchanger or for heating up a product [58]. The conversion of convective heat into radiative heat takes place at the burner surface which is heated by the flame and cooled by radiative heat exchange with the environment. The burner surface can be constructed from several materials like metal fibers [20] or ceramic foams [8]. One type of ceramic-foam surface burner has been developed by ECN in Petten, the Netherlands [15]. During the last ten years these burners have been produced by ECO Ceramics in Velzen-Noord, the Netherlands. These burners have been developed primarily for domestic heating purposes but it has been acknowledged that they offer great opportunities in industrial applications as well. The burners can be used to heat the zinc bath in galvanizing equipment, to provide the heat for paper drying or for rapid heating of metal tubes to allow deformation and other applications. At Eindhoven University of Technology these burners have been studied since 1992. In this period of time the principles of
Figure 1.1: Stabilization principle of a ceramic-foam surface burner in the radiant mode. Gas and air flow through the porous burner and form a flame at the downstream side of the burner (a). Inside the burner the flame is cooled due to the difference between the gas temperature (solid line) and the burner temperature (dashed line) (b). The top layer of the burner is hot and radiates to the environment, the flame itself cannot be observed (c).

...
1.2 Ceramic foams and combustion

Ceramic-foam surface burners have been developed as low-NO\textsubscript{x} burners. The reduction of the NO\textsubscript{x} formation is realized by lowering the flue gas temperature through cooling of the flame. The principle of the flame stabilization is shown in Fig. 1.1. The gas and air are mixed upstream of the burner and flow with a velocity lower than the adiabatic burning velocity through the burner material. The foam itself is highly porous and allows the mixture to flow uniformly through the material. When the mixture is ignited at the downstream side of the burner, the flame moves faster upstream than the flow velocity of the mixture and the flame will eventually attach to the downstream face of the burner where it is cooled. The amount of heat transferred from the flame to the burner depends on the position of the flame and increases as the flame moves further upstream, into to the burner. The flame burning velocity decreases with increasing cooling rate and, therefore, the flame propagation speed decreases as the flame moves into the burner. A stabilization point will be found at which the burning velocity equals the unburnt-mixture velocity. The heat transferred from the flame to the burner heats up the burner which loses this energy to the environment by radiation. The burner surface is heated up to such a temperature that the radiative heat loss equals the cooling of the flame. This temperature can exceed 1000 K and in this condition the burner surface radiation is clearly visible. This can be seen in Fig. 1.1-c. The flame itself, which is very thin, is not visible as it radiates very weakly in the visible region. This operation mode of the burner is known as the radiant mode [7].

For unburnt-mixture velocities higher than the adiabatic burning velocity, flames can also stabilize on ceramic-foam surface burners. In this case the flame is not stabilized by cooling but as a collection of Bunsen flames on the surface. As the flame is not cooled, the final temperature of the flue gases approaches the adiabatic flame temperature and NO\textsubscript{x} formation is relatively high. This mode is known as the blue-flame mode [7].

Flames can also propagate and stabilize in the ceramic material itself. In this case the flame propagation is influenced by the ceramic material resulting in enhanced burning velocities. The flame can be stabilized at an interface between two different types of ceramic foam or by cooling part of the ceramic foam [37, 39, 46]. In Chapter 6 it will be shown that the flash-back process is related to the propagation of flames submerged in the ceramic material.

1.3 Aim of this work

The investigations in this thesis are focussed on the application of ceramic-foam surface burners in industrial processes. The central questions for these applications are the flame stability and the performance of the burners.

The stability of the flame is mainly affected by the occurrence of flash-back of the flame into the burner. During flash-back the flame travels through the burner and will ignite the fresh mixture in the plenum. It must be avoided at all circumstances to avoid dangerous situations. At normal conditions the stable operation range is limited by the
extinction limit and the blow-off limit which gives a wide operation range. Extinction occurs at velocities which are low enough not to pose any problem in practice. Blow off occurs at such high velocities that a large operation range of the burner is available. This allows the burner to be used in a modulating way. Flash-back, however, occurs in the radiant mode, as it is related to the stabilization process in the radiant mode, and does limit the application of the burners. The previously mentioned wide operation range is split in a lower and an upper stable part. Combustion is not stable in the region in between, which is the region where the maximum radiative efficiency occurs.

The flash-back phenomenon and the stability limits due to flash-back will be investigated in this thesis. Flash-back can be studied by only modeling the burner. The limits that are found, however, depend on the radiating temperature of the environment. This temperature in turn depends on the interaction between the burner and the application. Therefore, it is necessary to model the application in which the burner is placed completely. Such a model also allows the determination of the major aspects of the performance of the burner like the radiative efficiency, the overall efficiency of the heat transfer and the emission of pollutants.

The model derived to simulate a burner in an application will also be used to gain insight into the influence of the burner size on the heat transfer by gas radiation in the post-flame zone. The temperature profile in the post-flame zone has a major influence on the formation of pollutants like NOx. A correct description of the gas radiation is, therefore, required.

This study will be performed using numerical models and experiments. Methane will be used as a fuel in both the numerical models and the experiments as it is the main component of natural gas. The numerical models will be used to gain insight into the relevant processes and to predict the performance of new burners and combustion chambers. The experiments will be used to validate the assumptions and predictions of the numerical models and to investigate phenomena which are beyond the capabilities of the numerical models. Modeling applications of ceramic-foam surface burners requires a 2D or 3D description of the physical processes. The problems associated with such a description will be briefly dealt with in the following section. The experiment used in this thesis will be introduced in Section 1.5.

1.4 Numerical modeling

For a clear understanding of the performance and stability of ceramic-foam surface burners it is essential to model the interaction between the burner and the application. Therefore, the description of the burner and the description of the application in which the burner is mounted must be integrated. Both the combustion process on top of the burner and the heat transfer to the product or heat exchanger have to be modeled accurately. The main features to be modeled accurately are the flow in the combustion chamber, the chemical processes in the flame, the stabilization of the flame on the burner surface, the radiation inside the burner material and the radiation in the combustion chamber. All these fea-
1.4. Numerical modeling

![Diagram showing classification of combustion models]

*Figure 1.2: Classification of different combustion models available.*

tures have to be implemented in one model. Sophisticated models for 1D premixed laminar flames have been derived both in our group [55] as in other groups [59]. These models have been used for modeling combustion on ceramic foam burners by implementing the gas-solid heat transfer and the heat transfer in the solid [6, 7, 8]. Numerical simulation of weakly compressible flows and heat transfer has progressed significantly in the last decades. At this moment a number of commercial CFD packages is available in which most of this knowledge is implemented. These packages also have many possibilities regarding the geometry. The use of complex chemistry in multi-dimensional models is, however, still impossible. Special purpose 2D models have been developed for such reactive flows, but the application of these models is limited due to the enormous computing time needed [55]. The main problems associated with these simulations are the large number of strongly-coupled partial differential equations which have to be solved, the fine grid necessary due to the small length scales of the processes involving radical species and the slow convergence due to the stiffness arising from the large difference between the various time scales. Chemical reduction techniques have been developed which lower the number of equations and stiffness. These techniques reduce the complexity associated with the chemistry to such an extent that extension of these models to more-dimensional problems is possible within reasonable limits. The general idea is shown in Fig. 1.2, which classifies several combustion models according to the number of geometrical dimensions and the number of scalar equations. The computational time required for solving a problem with a certain model is a complicated function of these parameters. However, it increases drastically when any of the two is increased. For example, the computational time for a problem using a complex chemistry model is about two orders of magnitude higher than using the Flamelet-Generated Manifolds method (FGM) [44]. As the computational time is a constraint on the practical application of a model, the upper right corner of this graph has to be avoided. In this thesis two chemistry models will, therefore, be used: a 1D model with skeletal chemistry [54] (lower right corner) and a
2D model based on the Flamelet-Generated Manifolds method (FGM, upper left corner) [44]. Transient effects are included in the 1D model, whereas the 2D model is restricted to steady-state solutions.

Radiation modeling in a multi-dimensional geometry yields similar complications as the chemistry modeling. The emission and absorption of radiation by the gas in the combustion chamber is non-linear and a detailed description of the phenomena based on the inner spectral structure of the radiation is only available for line-of-sight models. These can be implemented relatively easily in 1D models but become very complicated for 2D and 3D models. Gray or gray-band models neglect a large amount of the spectral dependence of radiation. However, they give a much easier description which can be implemented in multi-dimensional models like the Discrete-Transfer [50], Discrete-Ordinates [18] and the Monte-Carlo method [24].

Two distinct models will be presented and used in this thesis. The first model considers a 1D geometry but includes complex chemistry and spectral radiation and will be used to study the interaction between the flame and the burner and the effect of gas radiation on the post-flame zone. The second model will be 2D and suitable for handling complex geometries. With this model applications of ceramic-foam surface burners will be simulated to investigate the flow, flame, heat transfer and radiation in such an application. To reduce the complexity of the model, FGM will be used for the chemistry and a gray-bands approximation for the radiation.

1.5 Experimental work

Two experimental setups have been used for this investigation. The first setup is a configuration in which several ceramic-foam surface burners can be placed. This setup allows accurate measurement of the burner surface temperature, gas temperature profiles and flue-gas analysis of the burner in an unconfined space.

For an investigation of the interaction between a ceramic foam surface burner and a hot environment a furnace has been built. This furnace is made of fire-resistant bricks with a Duraboard top plate with a ceramic-foam surface burner mounted in it. Opposite of the burner a heat exchanger is placed of which the position can be varied. By varying this position the hot gas volume and the surface of the surrounding hot walls can be varied, thus providing a way to change the average radiation temperature of the environment of the burner. Several thermocouples and a pyrometer allow measurement of gas, wall and burner temperatures.

1.6 Outline of this thesis

In the foregoing sections some of the modeling problems and proposed solutions have been presented. The next two chapters will give a more thorough description of the physics behind the models. In Chapter 2 the chemistry and physics which govern reactive flows
are described. Chapter 3 focuses on the radiation in the combustion chamber and the ceramic material. In these two chapters two models are presented. The first model is for 1D geometries with a detailed description of both the chemistry and the radiation. The second model is applicable for 2D flows in which the description of the chemistry and radiation is simplified.

The models and experiments are used in Chapter 4, Chapter 5 and Chapter 6 to investigate the performance and stability of ceramic-foam surface burners. In Chapter 4 the 2D model is validated using the results obtained for the hot furnace by comparing the results of simulations with experimental results. The model is also used to investigate the flame and the heat transfer in the furnace. In Chapter 5 the influence of gas radiation on the flue-gas temperature in the post-flame zone is studied. Most NO\textsubscript{x} formation occurs in this region and a simplified expression to describe the temperature field is, therefore, proposed. This expression is based on 2D simulations and experiments. In Chapter 6 the flash-back process is investigated in more detail. Based on steady-state and transient simulations a mechanism for flash-back is proposed. This mechanism is used to determine the stability limits for the ceramic-foam surface burner. The thesis is concluded by a discussion in Chapter 7.
Chapter 2

Laminar premixed combustion

The physical and chemical processes which play a role in the combustion and heat transfer on a ceramic-foam surface burner are presented in this chapter. Based on these processes two models are derived which will be used for the numerical analysis. The first model is a 1D transient complex-chemistry model which allows a detailed description of the burner-flame interaction. The second model is based on a reduced-chemistry model allowing numerical simulations of burner applications in 2D. Results of the two different models will be compared to determine the validity of the reduced chemistry assumptions. The radiation models used in both models are described in Chapter 3.

2.1 Physical modeling

A combustion process can be described using the conservation equations for a reacting flow. These equations are based on the conservation laws for mass, momentum and energy and on the balance between transport and conversion due to chemical reactions of the various species. These equations are presented in the following sections.

2.1.1 Governing equations

A flow can be described using the velocity \( \vec{u} \), the pressure \( p \) and the density \( \rho \) of the mixture. These are related by the continuity equation

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0
\]

(2.1)

and the momentum equation

\[
\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \nabla \cdot \tau + \rho \vec{g}
\]

(2.2)

with \( \vec{g} \) the acceleration due to gravity. An expression has to be inserted for the stress tensor \( \tau \). The stress tensor relates the viscous stresses to velocity gradients as well as the rate of
deformation of infinitesimal fluid elements and fluid properties. For a Newtonian fluid it is
given by
\[
\tau = -\mu \left[ \nabla \tilde{u} + \left( \nabla \tilde{u} \right)^T - \frac{2}{3} \nabla \cdot \left( \nabla \cdot \tilde{u} \right) \right].
\tag{2.3}
\]

For the gases considered in this thesis, it is assumed that the density \( \rho \), the temperature
\( T \) and pressure \( p \) are related by the ideal gas law
\[
\rho = \frac{p M}{RT},
\tag{2.4}
\]

with the universal gas constant \( R = 8.314 \text{ Jmol}^{-1}\text{K}^{-1} \). The average molecular mass of the
mixture \( M \) depends on the composition of the mixture. For \( N \) species it is defined in terms
of the mass fractions \( Y_i \) of the different species and their molecular weights \( M_i \) as
\[
\frac{1}{M} = \sum_{i=1}^{N} \frac{Y_i}{M_i}.
\tag{2.5}
\]

For low Mach number flows it generally holds that the difference between the actual
pressure and a reference pressure \( p_0 \) is very small [59]. So \( p \approx p_0 \) and
\[
\rho = \frac{p_0 M}{RT}.
\tag{2.6}
\]

As a result the pressure \( p \) is only present in the momentum equation Eq. (2.2), and for 1D
systems this equation can, therefore, be omitted from the model. For 2D systems it has to be included.

The temperature \( T \) can be deduced from the enthalpy \( h \) which depends on the specific
heat of each species, \( c_{pi} \), and the enthalpy \( h_{wi} \) of each species at the reference temperature
\( T_0 \), as
\[
h = \sum_{i=1}^{N} Y_i h_i = \sum_{i=1}^{N} Y_i \left( h_{wi} + \int_{T_0}^{T} c_{pi} (T') dT' \right).
\tag{2.7}
\]

For the mass fractions \( Y_i \) of the different species and the enthalpy \( h \), conservation
equations have to be solved as well. In a flame, the chemical conversion rate \( S_i \) of the
different species is balanced by transport due to convection and diffusion. This balance is
described by the conservation equation for each of the species:
\[
\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot \vec{F}_i = S_i.
\tag{2.8}
\]

The flux \( \vec{F}_i \) of species \( i \) is proportional to the velocity \( \tilde{u}_i \) of this species, which can be
split in the average fluid velocity \( \vec{u} \) and a diffusion velocity. For a mixture containing one
abundant species, the diffusion velocity \( \tilde{u}_i \) for the other species can be approximated by
Fick’s law [4], leading to
\[
\vec{F}_i = \rho \tilde{u} Y_i - \rho D_{uu} \nabla Y_i
\tag{2.9}
\]
and
\[ \frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho \bar{u} Y_i) = \nabla \cdot \left( \rho D_{im} \nabla Y_i \right) + S_i \quad \text{for} \quad i = 1, N - 1. \] (2.10)

The mass fraction \( Y_N \), of the abundant species, nitrogen, can be found from the algebraic relation
\[ \sum_{i=1}^{N} Y_i = 1. \] (2.11)

The chemical source term \( S_i \) depends on the reaction rates of the chemical system and will be treated in Section 2.1.2.

The enthalpy is carried by the chemical components and transported by heat conduction. The total flux of the enthalpy due to the species fluxes is given by
\[ \vec{F}_{hs} = \sum_i h_i \vec{F}_i. \] (2.12)

Combining this flux with the conductive flux, given by \( \vec{F}_{hc} = -\lambda \nabla T \), and the term due to the change in pressure, \( \frac{\partial p}{\partial t} \), gives finally [17]
\[ \frac{\partial p}{\partial t} + \nabla \cdot (\rho \bar{u} h) = \nabla \cdot \left( \lambda \nabla T \right) + \nabla \cdot \left( \sum_i \rho D_{im} h_i \nabla Y_i \right) + \frac{Dp}{Dt}. \] (2.13)

This equation can be rewritten using Eq. (2.7) to
\[ \frac{\partial p}{\partial t} + \nabla \cdot (\rho \bar{u} h) = \nabla \cdot \left( \frac{\lambda}{c_p} \nabla h \right) + \nabla \cdot \left( \frac{\lambda}{c_p} \sum_i \left( \frac{1}{Le_i} - 1 \right) h_i \nabla Y_i \right) + \frac{Dp}{Dt}, \] (2.14)

with \( Le_i = \frac{\lambda}{D_m \rho c_p} \) the Lewis number describing the ratio between the energy and mass diffusivities. The specific heat of the mixture, \( c_p \), is given by
\[ c_p = \sum_{i=1}^{N} Y_i c_{pi}. \] (2.15)

### 2.1.2 Chemistry

The basis of the chemical process considered in this thesis is the conversion of methane (CH\(_4\)) and oxygen (O\(_2\)) into the products, mainly carbon dioxide (CO\(_2\)) and water (H\(_2\)O). This conversion can be described using the following global reaction
\[ \text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}. \] (2.16)

This conversion leads to a large increase in the temperature of the mixture. Furthermore, traces of several other species are produced. Amongst these are the pollutants carbon-monoxide (CO) and the nitrogen oxides (NO\(_x\)).

The formation of the pollutants shows that the conversion of the reactions cannot simply be described using a single reaction as Eq. (2.16). Instead, it is found that a large
Figure 2.1: C-1 reaction chain for lean methane-air flames [54].
number of steps or elementary reactions are present in a methane/air flame. The main path for the oxidation of methane is shown in Fig. 2.1. It involves many radicals, like H, O and OH, which by themselves are not stable but they are crucial for the propagation of the flame. Each of these steps can be described by an elementary reaction. For example the first fuel consumption step is described by

\[ \text{CH}_4 + \text{H} \rightarrow \text{CH}_3 + \text{H}_2. \]  

(2.17)

The two arrows denote that the reaction can occur both in the forward and in the backward direction. The forward rate \( r_f \) of this reaction depends on a rate constant \( k_f \) and the mass fractions \( Y_i \) of the reactants:

\[ r_f = k_f Y_{\text{CH}_4} Y_h. \]  

(2.18)

The rate constants can be described using an Arrhenius law, which relates the rate constant \( k_f \) to the temperature using a pre-exponential factor \( A \), an exponent \( n \) and an activation energy \( E_a \):

\[ k_f = A T^n \exp \left(-\frac{E_a}{RT}\right). \]  

(2.19)

The description of the reactions can be generalized, using \( \nu'_{ki} \) and \( \nu''_{ki} \) to denote the coefficients of species \( A_i \) at the reactants and products sides of reaction \( k \), respectively. Each reaction is then written as

\[ \sum_{i=1}^{N} \nu'_{ki} A_i \rightarrow \sum_{i=1}^{N} \nu''_{ki} A_i. \]  

(2.20)

and the production and conversion of species \( i \), the source term \( S_i \) in Eq. (2.10), is given by the sum over all contributing reactions

\[ S_i = \sum_{k=1}^{M} (\nu''_{ki} - \nu'_{ki}) (r_{kf} - r_{kb}). \]  

(2.21)

with \( M \) the number of reactions and \( r_{kb} \) the rate of the backward reaction \( k \) for which similar relations as Eqs. (2.18) and (2.19) hold.

2.1.3 Flame modeling

The system of equations presented in the last two sections can be solved when the appropriate boundary conditions are specified and when the properties of the different species and the chemical data of the reactions are available. The boundary conditions depend on the flame type considered, but the species properties like the conductivities \( \lambda_i \), the specific heats \( c_{pi} \) and the diffusion coefficients \( D_{im} \) are tabulated functions of the temperature and the species concentrations [28]. For the chemical system several reaction mechanisms are available which define the necessary reactions and give tabulated expressions for \( A \), \( n \) and \( E_a \) for each of these reactions. The calculations in this thesis are based on a skeletal mechanism for lean methane/air combustion consisting of 25 reactions and 15 species that has been derived from the GRI mechanism [54].

The resulting system is, however, very stiff due to the large differences in the time scales of the reactions and the transport processes. Furthermore, the presence of several
short-living species requires a high spatial resolution in the flame front [55]. Solving this system in 3D and even in 2D is very time consuming. The 2D system will therefore be based on a reduced chemistry model which is described in Section 2.3. First, however, a 1D model for the ceramic-foam surface burner is presented which is based on the complete set of equations as presented above.

### 2.2 Flat flames on surface burners: 1D model

The equations presented in Section 2.1 form the basis for each combustion model. To model the combustion on ceramic-foam surface burners a description for the burner has to be added. For many applications a 1D description is sufficient. This description will be presented in this section. A more-dimensional description will be presented in Section 2.3.

#### 2.2.1 1D-model for premixed combustion on a ceramic-foam surface burner

The basis of the 1D model for the combustion on a ceramic-foam surface burner is the set of conservation equations and the chemistry presented in the preceding section. These can be used to model an adiabatic premixed flame by specifying the appropriate boundary conditions. At the inlet, Dirichlet conditions are specified for the species concentrations and the enthalpy (or the temperature of the mixture). At the outlet, Neumann conditions are specified for all these variables. Only for a single inlet velocity a solution is found and this inlet velocity can be found as the eigenvalue of the problem when the solution is fixed in space at a single point [55]. The solution of the equations, the flame, is a structure which moves upstream with a specific velocity. This burning velocity \( s_L \), or the adiabatic mass burning rate \( m_{b0} = \rho_u s_L \), is only a function of the inlet conditions. The influence of the temperature of the unburnt mixture on the mass burning rate \( m_{b0} \) is shown in Fig. 2.2.
Table 2.1: Properties of the 60 PPI ceramic-foam surface burners used in the experiments.

<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>burner thickness</td>
<td>$L$</td>
<td>1.0 cm</td>
<td></td>
</tr>
<tr>
<td>specific surface</td>
<td>$a$</td>
<td>40.0 cm$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>volumetric porosity</td>
<td>$\chi$</td>
<td>0.80</td>
<td></td>
</tr>
<tr>
<td>tortuosity gas</td>
<td>$\tau_g$</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>tortuosity ceramic-foam</td>
<td>$\tau_s$</td>
<td>0.4</td>
<td></td>
</tr>
<tr>
<td>conductivity</td>
<td>$\lambda_s$</td>
<td>$2.0 \cdot 10^{-2}$ W/cmK</td>
<td></td>
</tr>
<tr>
<td>heat capacity</td>
<td>$c_{ps}$</td>
<td>1.3 J/gK</td>
<td></td>
</tr>
<tr>
<td>density</td>
<td>$\rho_s$</td>
<td>3.0 g/cm$^3$</td>
<td></td>
</tr>
<tr>
<td>extinction coefficient</td>
<td>$K$</td>
<td>15.0 cm$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>emissivity</td>
<td>$\epsilon$</td>
<td>0.85</td>
<td></td>
</tr>
<tr>
<td>heat transfer coefficient</td>
<td>$h_v$</td>
<td>2.0 W/cm$^2$K</td>
<td></td>
</tr>
</tbody>
</table>

A higher inlet temperature gives a higher flame temperature and thus a higher conversion rate.

When a free flame is present above the burner and the unburnt gas velocity is lower than the adiabatic burning velocity, the flame will move towards the burner. As soon as it reaches the burner, the flame is, however, cooled by the burner surface. This cooling lowers the burning velocity in an analogous way as lowering the inlet temperature of the unburnt mixture. As the burning velocity depends on the cooling of the flame, which in turn depends on the position of the flame with respect to the burner, an equilibrium will be established at a position at which the burning velocity just equals the mixture velocity. The result is a stationary flame, stabilized at the downstream surface of the ceramic-foam surface burner.

To describe the combustion on a ceramic-foam surface burner, the burner properties must be included in the model. Even though the pore size $d_p$ of the burner (for a 60 PPI (pores per inch) foam $d_p = 25.4/60 = 0.42$ mm) is approximately equal to the thickness of the flame, the flame itself is flat. Due to the pressure drop over the flame front, flow irregularities damp out very fast when the mixture flows out of the burner [19]. A 1D description is, therefore, still valid and the burner can be modeled as a porous region where the interaction between the burner and the fluid is averaged over a representative volume.

The burner is modeled as a region in which two phases are present: a moving gas phase and a fixed solid phase. The conserved quantities of the gas phase, $\rho$, $\rho Y_i$ and $\rho h$, are multiplied by the volume fraction of the gas phase $\chi_g$ to account for the presence of the solid phase. The momentum equation is not solved because Eq. (2.6) is used for the density. The conservation equations for mass, species fractions and enthalpy are given by

$$\frac{\partial (\chi_g \rho)}{\partial t} + \frac{\partial}{\partial x} (\chi_g \rho u) = 0,$$

(2.22)
\[
\frac{\partial (\chi_g \rho Y_i)}{\partial t} + \frac{\partial}{\partial x} (\chi_g \rho u_i Y_i) = \frac{\partial}{\partial x} \left( \chi_g \tau_g \rho D_{mn} \frac{\partial}{\partial x} Y_i \right) + \chi_g S_i \quad \text{for} \quad i = 1, N - 1, \tag{2.23}
\]

\[
\frac{\partial (\chi_g \rho h)}{\partial t} + \frac{\partial}{\partial x} (\chi_g \rho u_i h) = \frac{\partial}{\partial x} \left( \chi_g \tau_g \frac{\lambda}{c_p} \frac{\partial}{\partial x} h \right) + \frac{\partial}{\partial x} \left( \chi_g \tau_g \frac{\lambda}{c_p} \sum_i \left( \frac{1}{Le_i} - 1 \right) h_i \frac{\partial}{\partial x} Y_i \right) - h_v (T - T_s) + S_{rg}. \tag{2.24}
\]

The mass fraction of nitrogen, \( Y_N \), follows from Eq. (2.11). Note that the convective fluxes and the source terms are also scaled by \( \chi_g \) and that the diffusive flux is scaled by the product of \( \chi_g \) and the tortuosity \( \tau_g \). The tortuosity accounts for the larger path lengths due to the presence of the foam. For the highly porous ceramic foam used in this study \( \tau_g \approx 1 \) and the influence of this factor is, therefore, neglected. The interaction between the solid and the fluid phase is modeled by the heat transfer term \( h_v (T - T_s) \) with \( h_v \) the volumetric heat transfer coefficient. When surface reactions take place at the internal or external surface of the burner, the species conservation equation Eq. (2.23) would also contain two-phase interaction terms. The burner material considered is, however, not known to behave catalytic in any way [7]. These interaction terms are therefore not implemented. A source term \( S_{rg} \) is added to the enthalpy equation (2.24) to account for heat loss due to gas radiation. This source term will be described in Chapter 3.

For the solid phase, no continuity, momentum and species equations have to be solved. Only an enthalpy equation without convective term is needed. This equation is completed with the term for the gas-solid heat transfer and a source term due to radiation \( S_{rs} \). This source term will also be described in Chapter 3. The resulting equation for the solid temperature \( T_s \) is given by

\[
\frac{\partial (\chi_s \rho c_p T_s)}{\partial t} = \frac{\partial}{\partial x} \left( \chi_s \tau_s \lambda_s \frac{\partial T_s}{\partial x} \right) + h_v (T - T_s) + S_{rs}. \tag{2.25}
\]

The sum of the two porosities must be equal to one: \( \chi_g + \chi_s = 1 \). For the solid phase the tortuosity cannot be neglected as it is approximately 0.4. The properties of the ceramic foam are shown in Table 2.1.

The boundary conditions are equal to the boundary conditions for the adiabatic case except that the inlet velocity is specified. For the solid temperature, boundary conditions have to be specified at the upstream \( (x = -L) \) and at the downstream face \( (x = 0) \) to describe the surface heat-transfer. The boundary conditions are given by

\[
-\chi_s \lambda_s \frac{\partial T_s}{\partial x} \bigg|_{x=-L} = q_s L \tag{2.26}
\]

and

\[
-\chi_s \lambda_s \frac{\partial T_s}{\partial x} \bigg|_{x=0} = -q_s 0. \tag{2.27}
\]
2.2. Flat flames on surface burners: 1D model

At the upstream face of a thick burner the difference between the gas and solid temperatures is small and the heat transfer is, therefore, neglected giving

\[ q_{sL} = 0. \]  \hspace{1cm} (2.28)

At the downstream surface the temperature difference is considerable and the heat transfer is approximated by

\[ q_{sD} = h (T - T_s)_{x=0}. \]  \hspace{1cm} (2.29)

The heat transfer coefficient \( h \) is assumed to be related to the volumetric heat transfer coefficient \( h_v \). This latter has been measured and can be seen as the product of the heat transfer coefficient at the internal surface \( h_s \) and the specific internal surface area \( a \) as

\[ h_v = h_s a. \]  \hspace{1cm} (2.30)

The heat transfer coefficient at the downstream surface is assumed to be equal to this internal heat transfer coefficient, which gives

\[ h = \frac{h_v}{a}. \]  \hspace{1cm} (2.31)

2.2.2 Application and limitations of the 1D model

The model described in the previous section has been implemented in a 1D combustion code [7, 55]. This code uses an exponential finite-volume discretization in space and the
resulting system is solved using a fully implicit, damped-Newton technique. Adaptive re-gridding is implemented to increase the resolution around the flame front. Time integration is performed using an implicit scheme.

Solving the system of Eqs. (2.23), (2.24) and (2.25) gives a 1D description of a ceramic-foam stabilized flame as function of the inlet conditions including the inlet velocity \( v_a \). The result for an unburnt mixture velocity \( v_a = 15 \text{ cm/s} \) and an equivalence ratio \( \phi = 0.9 \) on a typical grid of 120 cells is shown as an example in Fig. 2.3. The equivalence ratio \( \phi \) is the methane to oxygen mole-fraction ratio divided by this ratio at stoichiometric conditions, i.e. as defined by the global reaction (2.16). The final flame temperature \( T_b \) of such a flame is lower than the adiabatic flame temperature because the flame is cooled by the burner material. The amount of cooling depends on the inlet velocity and this is shown in Fig. 2.4 which gives the final flame temperature as a function of the inlet velocity. The energy transferred from the flame to the burner is equal to the energy released as radiation to the environment \( q_r \). This amount depends both on the mass-flow rate and on the final flame temperature and has a maximum between 10 and 15 cm/s which is also shown in Fig. 2.4.

The model is 1D and, therefore, based on the assumptions that gradients in the other directions are small. The flame on the burner is flat to a good approximation and this 1D situation is in reality largely present. However, further away from the burner the flow and heat transfer is highly influenced by the geometry in which the burner is placed and the 1D assumption is no longer valid. Also the radiant heat transfer may influence the burner. In case of hot spots due to locally increased radiation impinging onto the burner surface, the stabilization position of the flame may locally be different. In these cases a 1D approach is no longer sufficiently accurate and a 2D or 3D model has to be used.

Figure 2.4: Flame temperature \( T_b \) (solid line) and radiant power \( q_r \) (dashed line) as a function of the inlet velocity \( v_a \) for an equivalence ratio \( \phi = 0.9 \).
2.3. More-dimensional flame modeling

For problems which focus on the burner, like for determination of the flame temperature and the radiant heat loss as a function of the inlet conditions (see Fig. 2.4) and for a first estimate of the NO\textsubscript{x} emission, the 1D approach is expected to be appropriate. For a detailed estimate of this emission, gas radiation should be included, but this is a 3D phenomenon. In Chapter 5, however, a relation for the radiative heat source, to be used in 1D models, will be obtained. The 1D model will also be used to investigate the flash-back process, in Chapter 6, as this requires detailed modeling of the interaction between the flame and the burner and transient simulations.

2.3 More-dimensional flame modeling

Numerical investigation of a ceramic-foam surface burner placed in an application requires 2D or 3D modeling. As a result of the stiffness of the system of equations presented in Section 2.1, solution of the complete set of equations is very time consuming. To deal with this stiffness a chemical reduction method is used which only requires one control variable for the chemical reaction system. The reduction technique by which this reduced system is derived will be introduced first. Then the resulting equations will be applied to the ceramic-foam burner system.

2.3.1 Reduction of the mechanism using Flamelet-Generated Manifolds

To reduce the time necessary for solving the problem, reduction of the chemical system is necessary. This reduction is aimed at removing the fastest processes from the system, thereby lowering the stiffness of the system.

The two most widely used reduction techniques are the partial-equilibrium and the steady-state assumptions. In the partial-equilibrium assumption the fastest reactions are assumed to be in chemical equilibrium. This gives relations for the ratios between the concentrations of the species involved in these reactions, which reduces the number of equations to be considered. The steady-state assumption on the other hand focuses on the short-living species. The source term \( S_i \) of the species conservation equation (Eq. (2.21)) can be split in production \( S_{i+} \) and consumption \( S_{i-} \) terms

\[
S_i = S_{i+} - S_{i-},
\]

(2.32)

giving the following expression for Eq. (2.10)

\[
\frac{\partial p Y_i}{\partial t} + \nabla \cdot (p \vec{u} Y_i) = \nabla \cdot (p D_{nm} \nabla Y_i) + S_{i+} - S_{i-}.
\]

(2.33)

When the separate production and consumption terms are much larger in magnitude than the other terms, this equation can be approximated by the following algebraic equation

\[
S_i = 0.
\]

(2.34)

The Intrinsic Low-Dimensional Manifold method (ILDM) is an extension of the steady-state approach [17, 36]. Instead of an a-priori determination of the steady-state
species, these species, or combinations of species, are derived from an eigenvalue analysis of the reactive system. The fastest processes are assumed to be infinitely fast and steady state is assumed for the combination of species associated with these processes. Each of these processes that can be assumed to be in steady state reduces the effective dimension of the chemical system. When the elimination process has lead to a sufficient reduction of the chemical system, the resulting manifold can be described with a small number of progress variables. As this manifold is determined before the actual flame calculation, the associated source terms and transport properties can be evaluated and stored in tables for future use. In the actual flame calculation these tables can then be used instead of calculating the values during run time.

The steady-state approximation, and thus also ILDM, is based solely on the chemical source terms. The structure of a laminar premixed flame is, however, determined by the balance between these chemical source terms and the convective and diffusive processes. Especially in the colder region of the flame, where the chemical terms are not so dominant, the transport equations cannot simply be replaced by Eq. (2.34). In the Flamelet-Generated Manifold method (FGM) the manifold is deduced from 1D flames or flamelets. Using these 1D flames the influence of the convective and diffusive terms in the transport equations is accounted for.

For the development of FGM [44] a control variable \( Y_{cn} \) is defined, which can be a species concentration or a linear combination of species concentrations. Using the iso-planes of this control variable in the flame a new coordinate system is defined. In this system \( \xi \) denotes the distance along a line perpendicular to the iso-planes of the control variable. All differential equations can be rewritten in this new coordinate system and these can be approximated as 1D-equations in the coordinate \( \xi \) as

\[
\frac{\partial}{\partial \xi} (\rho \omega Y_i) = \frac{\partial}{\partial \xi} \left( D_{im} \frac{\partial Y_i}{\partial \xi} \right) + S_i + P_i (\xi).
\]  

(2.35)

In this notation \( \omega \) represents the velocity in the \( \xi \)-direction and the perturbation term \( P_i \) contains the fluxes in the other directions and the contributions due to stretch, curvature and transient effects. Because the iso-contours of the species mass-fractions in laminar premixed flames are nearly parallel, the fluxes in the other directions can be considered to be small. In case of weak flame stretch the stretch terms are relatively small and \( P_i \) can be neglected as well. Furthermore, only steady-state situations are considered, so Eq. (2.10) can be replaced by

\[
\frac{\partial}{\partial \xi} (\rho \omega Y_i) = \frac{\partial}{\partial \xi} \left( D_{im} \frac{\partial Y_i}{\partial \xi} \right) + S_i,
\]  

(2.36)

which shows that Eq. (2.36) is a constraint for the solution. A similar reasoning can be introduced for the enthalpy giving another constraint:

\[
\frac{\partial}{\partial \xi} (\rho \omega h) = \frac{\partial}{\partial \xi} \left( \frac{\lambda}{c_p} \frac{\partial h}{\partial \xi} \right) + \frac{\partial}{\partial \xi} \left( \frac{\lambda}{c_p} \sum_i \left( \frac{1}{L e_i} - 1 \right) h_i \frac{\partial Y_i}{\partial \xi} \right)
\]  

(2.37)

The original system is constrained by the combination of Eq. (2.36) for each species and Eq. (2.37) for the enthalpy. When the mass flux \( \rho \omega \) is assumed to be constant, the solution
of this combination is the solution of a steady 1D flame. 1D flames can thus be used to determine the manifold.

In the original system, all species equations, except the equation for the control variable and the equation for the enthalpy, are now replaced by the extended steady-state relations given by Eq. (2.36) and Eq. (2.37), respectively. These quantities then follow from the solution of the 1D system on the coordinate $\xi$, with the control variable as the independent variable. As a result it is possible to solve the (steady-state) system by only solving the flow equations, a single equation for the control variable, given by

$$\nabla \cdot (\rho \bar{u} \nu_{cv}) = \nabla \cdot \left( D_{cv} \nabla \nu_{cv} \right) + S_{cv}$$

and an equation for the enthalpy

$$\nabla \cdot (\rho \bar{u} h) = \nabla \cdot \left( \frac{\lambda}{c_p} \nabla h \right) + \nabla \cdot (\alpha \nabla \nu_{cv}).$$

In which the various contributions of the diffusive species fluxes to the enthalpy flux are combined in

$$\alpha = \sum_i \left( \frac{1}{\text{Le}_i} - 1 \right) h_i \frac{\partial Y_i}{\partial Y_{cv}}.$$

In these equations all quantities which depend on the species concentrations ($\rho$, $D_{cv}$, $S_{cv}$, $\lambda$, $c_p$ and $T$) are taken from the manifold which is generated before the actual flame computation, as in case of ILDM. The manifold is determined from the solutions of adiabatic and burner-stabilized 1D-flames. The enthalpy of the adiabatic flames is varied by changing the temperature of the unburnt mixture. Burner-stabilized flames, in which the inlet velocity is varied, have been used to reach lower enthalpies [45].

2.3.2 Steady-state 2D-model for a ceramic-foam surface burner

The derivation of the steady-state more-dimensional model from the reduced chemistry equations is analogous to the derivation of the 1D model from the complex chemistry equations. The burner is implemented as a two-phase region with the solid-fluid interaction given by volume-averaged terms. The steady-state continuity equation is then given by

$$\nabla \cdot (\chi_g \rho \bar{u}) = 0.$$ 

In the more-dimensional system also the momentum equation has to be solved, which is given by

$$\nabla \cdot (\chi_g \rho \bar{u} \bar{u}) = \nabla \cdot \sigma + \chi_g \rho \bar{g} - R \bar{u}.$$ 

This equation contains a solid-fluid interaction term to account for the resistance to the flow of the porous medium. The porous medium is assumed to be isotropic with a resistance $R$ given by a Darcy-Forchheimer equation as

$$R = \frac{\mu}{k_1} + k_2 \rho |\bar{u}|$$
with the coefficients $k_1 = 3.0 \cdot 10^{-9} \text{ m}^2$ and $k_2 = 1.2 \cdot 10^3 \text{ m}^{-1}$ derived from experiments [7].

The chemistry is solved using FGM as described in the previous section. The equation for the control variable (Eq. (2.38)) for a two-phase system is given by

$$\nabla \cdot \left( \chi _g \tau _g \rho \bar{u} Y_{cv} \right) = \nabla \cdot \left( \chi _g \rho D_{cv} \nabla Y_{cv} \right) + \chi _g S_{cv},$$

(2.44)

and the equation for the enthalpy (Eq. (2.39)) by [44]

$$\nabla \cdot \left( \chi _g \rho \bar{u} h \right) = \nabla \cdot \left( \chi _g \tau _g \frac{\lambda}{c_p} \nabla h \right) + \nabla \cdot \left( \chi _g \tau _g \frac{\lambda}{c_p} \alpha \nabla Y_{cv} \right) - h_v (T - T_s) + S_{rg}.$$  

(2.45)

As in the 1D model the tortuosity of the gas phase $\tau _g$ is close to unity and is, therefore, neglected.

As in the 1D model a conduction equation with source terms for the solid-fluid interaction and the heat loss due to radiation is required to solve the heat transfer in the solid:

$$0 = \nabla \cdot \left( \chi _s \tau _s \lambda _s \nabla T_s \right) + h_v (T - T_s) + S_{rs}.$$  

(2.46)

For the gas phase boundary conditions have to be specified for the inlet, outlet and the walls. At the inlet the velocity and the composition of the unburnt mixture are prescribed. At the outlet the pressure is prescribed and the normal derivatives of all variables are assumed to be zero. At the walls all fluxes are zero except for the enthalpy equation. For the enthalpy equation, either a fixed temperature, a fixed heat-flux or a heat-transfer relation can be applied. The equation for the solid temperature (Eq. (2.46)) requires boundary conditions at the ceramic-foam surface and at the walls. For all these boundaries a zero heat-flux is prescribed. The surface heat-transfer at the downstream surface, which is present in the 1D model, is not implemented.

### 2.3.3 Application of the 2D model

The model described above is implemented into the commercial flow solver CFX-4.3 [10]. In this solver the equations are discretized using a finite-volume technique on a structured grid. The use of multiple blocks makes it possible to handle a variety of geometries. The solver is uncoupled, so the various variable fields are all solved independently. Overall convergence is realized using an outer iteration loop. The pressure-correction method in the solver is based on the SIMPLEC scheme. In the solver the standard definition of enthalpy is replaced by Eq. (2.7) by supplying appropriate specific heats and reference enthalpies. The coefficients stored in the manifold are supplied to the solver by several user-routines. Finally, in the burner region, the gas temperatures which are used as input to the radiation solver are replaced by the solid temperatures. The same is done for the source terms which are returned by the radiation solver.

The result is a very flexible system which profits both from the speed of the FGM implementation and from the features of the commercial packages. These latter features include complex geometries, Discrete-Transfer and Monte-Carlo radiation models (see Chapter 3), both 2D and 3D axisymmetric and Cartesian grids and conducting-solid grids. With this system it is possible to handle actual applications in a reasonable time.
2.4 Validation of the reduced-chemistry model

The manifold that is used in FGM is based on burner-stabilized laminar flat flames. These flames stabilize by heat transfer to an ideally cooled burner with an infinite heat transfer. The manifold is constructed from the results of simulations for various inlet velocities. If such flames, are subsequently modeled using FGM with this manifold, the results should be identical to the results using complex chemistry. However, for the ceramic-foam surface burner, the influence of the burner is different. The burner itself becomes hotter and the flames stabilize further upstream. As a result, the temperature profile of the gas inside the burner is highly influenced by the heat transfer inside the ceramic foam. Notably, it is less steep than the temperature profile for a burner-stabilized or adiabatic flame. In the FGM simulation of the ceramic-foam surface burner the temperature profile inside the burner is determined by the heat transfer in the solid phase as well. This can influence the results of the combustion model because FGM is based on the dependence of the profiles of both the mass fractions and the temperature on the profile of the control variable. In this section this influence is investigated by comparing the results of simulations using FGM to results of simulations using the complex chemistry model. The simulations using FGM are obtained from the 2D model in a 1D configuration.

The heat transfer from the gas to the ceramic foam increases the burning velocity when the effective conductivity of the ceramic material is higher than the conductivity of the gas. The effective conductivity of the ceramic material also includes radiation, which can be approximated using the Rosseland-diffusion approximation [52], and is given by

\[
\lambda_{\text{eff}} = \chi_{\text{r}} \tau_s \lambda_s + \frac{16 \sigma T_s^3}{3K}. \tag{2.47}
\]
Figure 2.6: Final flame temperature $T_b$, using the complex chemistry model (dashed line) and using the complex (solid line) and reduced chemistry (crosses) models for $\lambda_{ef}$ reduced with a factor 100, as a function of the unburnt mixture velocity $v_u$ with an equivalence ratio $\phi = 0.9$.

Figure 2.7: Gas- and solid-temperature and O and O$_2$ species mass-fraction profiles using the complex (solid line) and reduced chemistry (dashed line) models for an unburnt mixture velocity $v_u = 15$ cm/s, an equivalence ratio $\phi = 0.9$ and $\lambda_{ef}$ reduced with a factor 10.
For $\lambda_{eff} \approx \lambda$ the influence of the ceramic foam is small and, therefore, the results for a burner with a conductivity comparable to that of the gas are presented first. These results, the gas- and solid-temperature profiles and the O$_2$ and atomic-oxygen mass-fraction profiles, which gives an indication for the location of the flame front, are shown in Fig. 2.5 for $\phi = 0.9$ and $v_u = 15$ cm/s. In these simulations the effective conductivity of the foam has been reduced by a factor 100 by scaling the absorption coefficient $K$ and conductivity $\lambda$, The difference between the profiles for the two models is very small. The differences between the results of the two models are small for other inlet velocities as well. This can be concluded from the final flame temperatures plotted in Fig. 2.6.

To validate the application of the reduced chemistry model using the actual foam properties the comparison has also been performed with the effective conductivity reduced by a factor 10. These results, which show minor differences between results for the two models, are plotted in Fig. 2.7. The O$_2$ profile is less steep and the flame temperature is slightly too low. As a result, also the O-profile, which is determined from the O$_2$ and enthalpy profiles, is too low. For higher conductivities this effect becomes more prominent, and for the actual foam properties no solution can be obtained using the FGM model. The flame does not stabilize on the burner surface but moves into the burner, while this is not the case for the complex-chemistry model.

Using a reduced effective conductivity, implies that the foam which is simulated does not have the properties of the actual foam. Flames which stabilize outside the ceramic foam are, however, not sensitive to changes in the foam properties [7]. This can also be confirmed from a comparison of the final flame temperatures, using complex chemistry, for the actual foam properties and the scaled foam properties in Fig. 2.6. The maximum difference between these two profiles is less than 7 K. The physics of the flames that are stabilized on the ceramic-foam surface burner are included, but when the flame moves further upstream, into the ceramic foam, the flame becomes sensitive to the foam properties, as will be shown in Chapter 6. When this effect is important, simulations should not be made using the reduced chemistry model, because the reduced chemistry model cannot be used with the actual foam properties. However, for investigating applications of ceramic-foam surface burners for which the flame is located outside the burner, the actual properties will have no significant influence on the flame temperatures and the efficiency. For these simulations the reduced chemistry model can be an adequate model, as long as the effective conductivity of the ceramic foam is reduced, preferably by a factor 100. This value is used in this thesis.

### 2.5 Conclusions

In this chapter the physical and chemical processes that occur in a flat flame have been presented. Based on these processes two models have been developed. The first model is a transient 1D model based on complex chemistry which is to be used for fundamental investigations. The second model is a 2D model based on reduced chemistry which can be used to simulate the burner inside an application. Both these models have to be completed
with models for radiation inside the ceramic material and gas radiation, which will be presented in the next chapter.

Results from the reduced chemistry model have been compared with results from the complex chemistry model. From this comparison it follows that investigations which rely on the foam properties, like flame-stability analysis, cannot be performed using the reduced chemistry model. However, for applications of the ceramic-foam surface burner where the flame is located outside the burner, the reduced chemistry model can provide adequate results.
Chapter 3

Radiation

Radiative heat transfer has a completely different physical behavior as heat transfer by conduction and convection. There is no need for a medium to facilitate the transfer, even though radiation can interact with a medium. Radiation travels at the speed of light and considering the size of heat transfer equipment and the time scales prevalent in combustion processes, it can be considered instantaneous. The range of radiative heat transfer can be very large. In absence of any blocking inside the combustion chamber, radiative heat exchange between all walls of a combustion chamber must be taken into account. Finally, as opposed to convection and conduction, the radiative heat flux is not proportional to the temperature difference but proportional to the difference of the temperature to the fourth power. This means that radiation becomes very important at higher temperatures.

Radiation is important in combustion problems and essential for radiant surface burners. Even though flames are dominated by convection and conduction, radiation can play an important role in the heat transfer to the product. Furthermore, the temperature drop in the post-flame zone is to a large extent influenced by radiation, so radiation indirectly influences the production of pollutants like NOx.

In this chapter the physical processes involved in radiative heat transfer will be introduced. Furthermore, appropriate models for radiation inside the burner and the combustion chamber will be presented.

3.1 Theory

Radiation can be considered as an electromagnetic wave or as a photon traveling with the speed of light c. The wave can be described by its frequency $f$, wavelength $\lambda = c/f$ or wavenumber $\nu = 1/\lambda = f/c$. Photons are created and destroyed by quantum-mechanical processes. More precisely, they are created or absorbed when energy states of gas molecules or solid material change their population density. Emission of a photon takes place when, for instance, a molecule, falls from a higher into a lower energy state. Absorption of a photon leads to the migration of a molecule from a lower to a higher energy state. The energy of the photon is equal to the difference between the energy levels of the energy states. Besides absorption and emission, radiation can also be influenced by matter without
energy transfer. In this case only the direction of the radiation is changed. For surfaces this is known as reflection, for participating media as scattering.

The discussion of radiation follows Siegel and Howell [52] and is split in four parts. Section 3.1.1 describes the interaction between radiation and surfaces, Section 3.1.2 the interaction between radiation and media, Section 3.1.3 the radiation from hot flue-gases and Section 3.1.4 the interaction between radiation and the flow.

3.1.1 Emission, absorption and reflection of radiation at surfaces

Radiative heat transfer is described in terms of the concept of a black radiator or black surface. A black surface is a surface which absorbs all radiation which falls onto it. Its emission is a function of the wavelength of the radiation and the temperature of the surface. Radiation can be quantified in terms of the radiative intensity \( i_\lambda \), which is the emitted energy per unit of wavelength \( \lambda \), projected surface area \( A_p \) normal to the direction of the radiation and solid angle \( \omega \) around the direction. The direction itself is defined by the vector \( \vec{\Omega} \) as shown in Fig. 3.1. The projected surface \( A_p \) is equal to the surface area \( A \) multiplied by the cosine of the angle \( \theta \) between the direction of the ray and the normal vector on the surface \( \vec{n} \). Because of the definition in terms of the projected area, the emitted intensity of a black body is not a function of the direction and it is given by Planck’s law which in terms of wavelength is given by

\[
i_{\lambda} = \frac{2c_1}{\lambda^5(\exp\left(\frac{c_1}{\lambda k}\right) - 1)}.
\] (3.1)
and in terms of wavenumber by

\[ i'_{\nu} = \frac{2c_1 \nu^3}{\exp \left( \frac{c_2 \nu}{T} \right) - 1}, \]  

(3.2)

with the radiation constants \( c_1 \) and \( c_2 \) given by \( 5.955 \cdot 10^{-15} \) Wm\(^2\) and 0.01439 mK, respectively. Integration of Planck’s law over the wavelength space yields

\[ i'_{\nu} = \int_{0}^{\infty} i'_{\nu \lambda} d\lambda = \int_{0}^{\infty} i'_{\nu \nu} d\nu = \frac{\sigma T^4}{\pi}. \]  

(3.3)

The heat loss of a surface element due to emission of radiation is found by integrating over a hemisphere (as denoted by \( \odot \)), while correcting for the projected surface. The heat loss of a black surface per unit area by emission is therefore given by Stefan-Boltzmann’s law

\[ q_b = \int_{\odot} i'_{b} \cos \theta d\omega = \sigma T^4. \]  

(3.4)

For a real surface the emission is always less than this black-body radiation. Real surfaces are, therefore, characterized by an emissivity \( \epsilon \lambda \) which is in general spectrally dependent. For most surfaces, this value is fairly constant in the infrared region and such surfaces can be considered gray with an emissivity \( \epsilon \) independent of the wavelength. For such a gray surface the emission is given by

\[ i'_{e} = \epsilon i'_{b} = \frac{\epsilon \sigma T^4}{\pi}. \]  

(3.5)

From thermo-dynamical reasoning it follows that the absorptivity, the fraction of incoming radiation \( i'_{a} \) that is absorbed by a surface, must be equal to the emissivity. Therefore, the absorption of radiation by a gray surface with the emissivity and absorptivity given by \( \epsilon \) equals

\[ i'_{a} = \epsilon \int_{0}^{\infty} i'_{\nu \lambda} d\lambda. \]  

(3.6)

Radiation which is not absorbed by the surface is reflected. This reflection can be in any direction and the distribution over all directions can be a complicated function of wavelength and the incoming direction. Generally, however, two idealized types of reflection are considered: diffuse and specular reflection. Diffuse reflection represents an equal reflection of radiation into all possible directions. Specular reflection represents the mirror-like reflection of radiation into a single direction.

In the often used case of a diffuse gray surface the radiation \( i'_{o} \) coming from a surface is related to the temperature of the surface and the radiation falling onto the surface as

\[ i'_{o} = \epsilon i'_{b} + (1 - \epsilon) \int_{0}^{\infty} \int_{\odot} i'_{\nu \lambda} d\omega d\lambda. \]  

(3.7)

For a specular gray surface this is

\[ i'_{o} = \epsilon i'_{b} + (1 - \epsilon) \int_{0}^{\infty} i'_{\nu \lambda \phi_i = \pi - \phi_o} d\lambda. \]  

(3.8)
The difference between the incoming radiation and the outgoing radiation is the net heat absorbed or emitted by the surface. So the boundary condition for the radiation at the wall is given by

$$q_w = \int_0^\infty \int_\Omega (i^\prime_{\omega \lambda} - i_{\omega \lambda}') \cos \theta d\omega d\lambda = \epsilon \left( \sigma T^4 - \int_0^\infty \int_\Omega i_{\omega \lambda}' \cos \theta d\omega d\lambda \right). \quad (3.9)$$

This equation also reflects that the net wall heat flux $q_w$ is given by the difference between emission and absorption.

3.1.2 Radiation in participating media

Absorption, emission and reflection of radiation can also occur in participating media. The latter is known as scattering of radiation. The medium can be a gas, a cloud of droplets or particles, a semi-transparent solid like glass or some porous structure like a ceramic foam.

Absorption and emission are described using an absorption coefficient $k_\lambda$ which is in general spectrally dependent. The absorption in a small path-segment is the product of the absorption coefficient, radiative intensity and the length of the path-segment $ds$. Like for a surface, the emitted and absorbed radiation must be equal at thermal equilibrium so the emission in a small path-segment $ds$ is given by the product of the absorption coefficient, the black body intensity and the length of the path-segment $ds$. Scattering only changes the direction of radiation and is no net source or sink. The amount of radiation that is scattered away in a small path-segment $ds$ is the product of the radiative intensity, the path length and a scattering coefficient $\sigma_{s\lambda}$. This amount of radiation is distributed over all directions and its distribution depends on the structure of the medium. It is described by a bidirectional phase function $\Phi^{1,2}$ which describes the increase of radiation in direction $\Omega_2$ as a result of scattering of radiation coming from direction $\Omega_1$. For isotropic scattering $\Phi^{1,2} = 1$ for all directions $\Omega_1$ and $\Omega_2$. For non-isotropic scattering $\Phi^{1,2} > 1$ for those directions in which the radiation is preferentially scattered. For other directions the phase function must be less than unity as scattering may be no net source or sink of radiation [52].

Combining the absorption, emission and scattering terms gives the total change of radiation in a small path-segment $ds$. This can be written as a differential equation for the radiative intensity which is known as the radiative transfer equation (RTE)

$$\frac{dI_\lambda}{ds} = -(k_\lambda + \sigma_{s\lambda}) I_\lambda + k_\lambda I_{b\lambda} + \frac{\sigma_{s\lambda}}{4\pi} \int_{4\pi} \Phi^{1,2} I_\lambda' d\omega'. \quad (3.10)$$

Equation (3.10) takes scattering into account and is spectrally dependent. As will be shown in the next chapter this combination is not necessary for the subject of this thesis. The radiation is either gray while scattering must be included, or spectrally dependent without scattering. In the gray case the RTE can be written using the extinction coefficient $K = k + \sigma_s$ and the scattering albedo $\Omega = \frac{\sigma_s}{K}$ as

$$\frac{dI^d}{ds} = -K I^d + (1 - \Omega) K I^b_d + \frac{\Omega K}{4\pi} \int_{4\pi} \Phi^{1,2} I^d d\omega'. \quad (3.11)$$
3.1. Theory

Figure 3.2: Energy levels of an idealized di-atomic molecule. (A) and (B) represent two electronic states of the molecule, from [21]. The electronic states are split in vibrational states which are again split into rotational states.

For the case without scattering the RTE simplifies to

$$\frac{dI_\lambda}{ds} = -k_\lambda (I_\lambda - I_{b\lambda}).$$  \hspace{1cm} (3.12)

Solving this equation for hot flue-gases is complicated due to the irregular shape of the spectral absorption coefficient $k_\lambda$ as a function of the wavelength $\lambda$. Solving these equations, therefore, requires special models which are treated in the next section.

3.1.3 Gas radiation

Gas radiation is caused by free molecules and is highly spectrally dependent. All emission and absorption is caused by state transitions. Each transition forms a line in the spectrum which is widened to a peak by several processes. In solids, radiation is also associated with transitions, but the peaks are much more widened and the result is rather smooth. For gases the widening processes are less rigorous and individual peaks can be identified. Therefore, the spectral dependence cannot be neglected for gas radiation but, on the other hand, scattering hardly exists in non-sooting conditions. The resulting RTE is given by Eq. (3.12).
Emission and absorption of radiation in gases is connected to the changes in electronic, vibrational and rotational states of individual molecules. The positions of these states are shown for an idealized molecule in Fig. 3.2 [21]. The wavelengths associated with electronic transitions are situated in the ultraviolet region and are not important for combustion modeling. The energy difference between vibrational states is smaller and the wavelengths associated with these transitions are situated in the visible and infrared regions. Rotational transitions have even less energy differences and have to be considered in conjunction with vibrational transitions. An exception is water which has a very high dipole moment and, as a result, relatively large energies associated with the rotational states.

Rotational transitions have to be taken into consideration as each vibrational transition must be accompanied by a rotational transition. As a result, the line at the wavelength associated with the vibrational transition is split into a large number of lines each belonging to a combination of that vibrational transition combined with a different rotational transition. This collection of lines is called an absorption band. Important bands in combustion are for water the pure rotational band (at higher wavelengths) and the 6.3, 2.7, 1.87 and 1.38 μm bands and for carbon dioxide the 15, 10.4, 9.4, 4.3 and 2.7 μm bands. These bands can be clearly identified in low resolution spectra as in Fig. 3.3. In these bands, each line is widened by broadening processes, most important are natural broadening, Doppler broadening and collisional broadening. The broadening depends on the temperature and composition [52].

The large number of peaks in each band makes the modeling of gas radiation very complex. In theory it is possible to divide the spectral range into such small intervals that for each interval a distinct, almost constant absorption coefficient can be identified. However, this would lead to millions of intervals. The averaging which is, therefore, necessary is complicated by the non-linearity of the resulting system. When the spectral RTE (Eq. (3.12)) is integrated over an isothermal path length s it gives the intensity at s as:

\[
i'_\lambda (s) = i'_0 \exp (-k_\lambda s) + i''_0 (1 - \exp (-k_\lambda s)).
\]  

This can be averaged over a wavelength interval but this averaged intensity is not equal to the intensity calculated using the averaged absorption coefficient. This holds especially when the shape of the absorption coefficient is very irregular as is the case for intervals which are much larger than the peak width. Consequently, when wavelength averaging is applied, as is the case for band models, the shape of the absorption coefficient distribution in the interval must be introduced and the path length must also be included. Two types of band models are widely used which differ on the width of the used interval. Wide-band models treat a complete absorption band whereas narrow-band models divide the bands in a large number of intervals [22, 56]. Each of these intervals still contains a large number of peaks, but the peaks can be assumed to be similar and regularly spaced. For a detailed study of gas radiation a wide-band model is used in this thesis and this is presented in Section 3.2.1.

In a wide-band model the absorption and emission are non-linear functions based on parameters which are averaged along a path. For 2D/3D systems, where more directions and
cells have to be considered, implementation of such a model is very costly. In the 2D model
the determination of gas radiation is, therefore, based on an effective absorption coefficient
for the complete spectrum or parts of the spectrum. This is a large simplification of the
underlying spectral structure but yields a simpler system of equations. The determination of
the effective absorption coefficients is based on the wide-band model and will be presented
in Section 3.3.2.

3.1.4 Coupling of radiation with the transport equations

The radiative transfer inside a medium is described by the RTE (Eq. (3.11) or Eq. (3.12))
which has to be solved in the complete domain. The boundary conditions for this equation
are given by the equations describing surface absorption, emission and reflection (Eq. (3.7)
or Eq. (3.8)).

For both the medium and the surfaces, absorption and emission are related to energy
transfer. The difference between the absorption $A$ and the emission $E$ must therefore
be included in the enthalpy equation of the medium and its boundary conditions. The
effect of emission and absorption at surfaces is given by Eq. (3.9) and this value must be
implemented into the boundary conditions. Emission and absorption in a medium leads to
an energy source or sink which can be found by integrating the absorption and emission
over all wavelengths and directions as

$$S_r = A - E = \int_0^\infty \int_{4\pi} k_{\lambda} I_{\lambda} d\omega d\lambda - \int_0^\infty \int_{4\pi} k_{h\lambda} I_{h\lambda} d\omega d\lambda.\quad (3.14)$$

In the combustion models presented in Chapter 2, $S_r$ is either passed to the enthalpy
equations (2.24) and (2.45) as $S_{r,\theta}$ or to the solid temperature equations (2.25) and (2.46)
as $S_{r,s}$. Alternatively, the heat source in the energy equation due to radiation can be seen
as the change in radiative intensity

$$S_r = -\vec{\nabla} \cdot \vec{q}_r\quad (3.15)$$

with the radiative flux being the net flux of energy due to radiation. The radiative flux $\vec{q}_r$
is found by integrating the radiative intensity weighted by the unit direction vector $\Omega$ over
all directions and wavelengths

$$\vec{q}_r = \int_0^\infty \int_{4\pi} I_{\lambda} \hat{\Omega} d\omega d\lambda.\quad (3.16)$$

Implementation of radiation in the combustion models presented in Chapter 2
requires modeling of the RTE inside the ceramic foam (Eq. (3.11)), and outside the ceramic
foam (Eq. (3.12)). Furthermore, the radiative heat sources have to be evaluated using
Eq. (3.15) or Eq. (3.16). The implementation for the 1D model is discussed in the next
section. For the 2D model the radiation is implemented using a Discrete-Transfer model in
a commercial code. This model will be presented in Section 3.3.
3.2 1D modeling of radiation

For the 1D model presented in Chapter 2, the radiation outside the ceramic foam and inside the ceramic foam is accounted for using two different approaches. The radiation of the hot-flue gases is based on the wide-band model and is treated in Section 3.2.1. The radiation inside the ceramic foam is modeled by solving Eq. (3.11) simultaneously with the combustion model. This is treated in Section 3.2.2.

Both models calculate the radiative intensity, which is to be used for evaluation of the radiative heat sources, for a discrete number of rays. The radiative heat sources are based on Eq. (3.15) as this equation provides a conservative formulation. In 1D the equation is given by

\[ S_r = -\frac{\partial q_r}{\partial x}. \]  \hspace{1cm} (3.17)

In a finite-volume discretization, Eq. (3.17) is implemented as the difference between the fluxes at the interfaces. The radiation grid is, therefore, defined at the interfaces of the volumes used for the enthalpy equation. On this radiative grid the radiative flux \( q_r \) has to be evaluated.

In 1D the direction of a ray can be described with a single coordinate \( \mu = \cos \theta \), with \( \theta \) the angle between the ray and the flow directions. Equation (3.16) can then be written as

\[ q_r = 2\pi \int_0^1 \int_{-1}^1 i_{\lambda \mu} d\mu d\lambda. \]

The angular integral in Eq. (3.18) can be approximated using a quadrature formula. Using Gaussian quadrature, the interval \([-1 : 1]\) is divided according to the zeros \( (\mu_m) \) of Legendre polynomials with the appropriate weights \( w_m \) \cite{13}. The discrete version of Eq. (3.18) is then given by

\[ q_r = 2\pi \sum_{m=1}^{M} \mu_m w_m \int_0^\infty i_{\lambda m} d\lambda. \]  \hspace{1cm} (3.19)

The evaluation of \( i_{\lambda m} \) depends on the nature of the radiation considered and is discussed in the next two sections. It will be treated in Section 3.2.1 for gas radiation and in Section 3.2.2 for radiation inside the ceramic foam.

3.2.1 Wide-band model for gas radiation

In a wide-band model each of the vibrational-rotational bands is assumed to be clearly distinguishable and is treated separately. As such the contribution of separate bands can be added to give the total heat transfer. This will be explained by focusing on the emission of an isothermal hot gas. When the wall intensity is neglected, the RTE (Eq. (3.12)) can be integrated from 0 to \( s \) to give the intensity at \( s \) as

\[ \dot{i}_\nu'(s) = \dot{i}_\nu (1 - \exp (-k_\nu s)). \]  \hspace{1cm} (3.20)
3.2. 1D modeling of radiation

The total emissivity is then obtained by integrating over all wavelengths and dividing by the total black-body intensity \( i'_{b} = \sigma T^4 \):

\[
\epsilon(s) = \frac{\pi \int_{0}^{\infty} i'_{w}(1 - \exp(-k_w s))\, dv}{\sigma T^4}. \tag{3.21}
\]

When the different bands are distinguishable and small enough to consider the black-body intensity constant in each band, Eq. (3.21) can be written as:

\[
\epsilon(s) = \frac{\pi \sum_j i'_{w,j}(1 - \exp(-k_{w,j}s))\, dv}{\sigma T^4}. \tag{3.22}
\]

This assumption is known as the band assumption [52], and the integral in Eq. (3.22) is replaced by the effective bandwidth \( A_j \), which is thus defined as

\[
A_j(s) = \int_{0}^{\infty} (1 - \exp(-k_{w,j}s))\, dv. \tag{3.23}
\]

Equation (3.22) is then written as:

\[
\epsilon(s) = \frac{\pi \sum_j i'_{w,j}A_j(s)}{\sigma T^4}. \tag{3.24}
\]

The same procedure can be followed for the absorption part of the RTE (Eq. (3.12)). This yields for the absorptivity due to radiation from a wall [52]

\[
\alpha(s) = \frac{\pi \sum_j i'_{w,j}A_j(s)}{\sigma T^4_w}. \tag{3.25}
\]

The integrated RTE can thus be written as

\[
i'(s) = i'_{w} - \sum_j A_j(s)i'_{w,j} + \sum_j A_j(s)i_{bj}. \tag{3.26}
\]

For a non-isothermal mixture with more than one absorbing species the integration of the RTE is slightly more complicated. This integration is treated in Appendix B.2, and results in the following expression for the intensity:

\[
i'(s) = i'_{w} - \sum_j i'_{w,j}A_j(0 \to s) - \sum_j \int_0^s i'_{bj}(s')\frac{\partial}{\partial s'}A(s' \to s)\, ds'. \tag{3.27}
\]

The bandwidth \( A_j \) can be calculated for a given path length \( s \), the concentrations of CO\(_2\) and H\(_2\)O and the temperature. The relations necessary for this calculation and the scaling which is necessary when the concentration and temperature profiles are not constant are treated in Appendix B. Equation (3.27) is an explicit relation which does not require any special solution methods. Only the integrals in Eq. (3.27) and the integrals necessary for evaluation of the scaled parameters (see Appendix B) have to be evaluated numerically.
3.2.2 1D modeling of radiation inside ceramic foam

Radiation is not only important for ceramic-foam surface burners because it provides the cooling mechanism of the burner, but also because it forms a major part of the solid-solid energy transfer inside the burner. In previous studies [7] the radiation inside the ceramic foam has been modeled using the optical-thick limit. Using the optical-thick limit approximation the contribution of radiation to the internal heat transfer can be treated as an effective conduction term [52]. This assumption is not valid near the ceramic-foam surfaces. For flames which stabilize very close to or inside the ceramic material the heat transfer inside the ceramic foam has a major influence on the burning velocity. Therefore, a more accurate treatment will be presented here for the 1D model.

As for the wide-band model for gas radiation, the source term in the enthalpy equation is based on Eq. (3.17) with the radiative flux discretized as in Eq. (3.19). The intensity in the latter equation is determined from the RTE (Eq. (3.11)) for an isotropic scattering medium ($\Phi^{1,2} = 1$)

$$\frac{\mu}{K} \frac{d\tau}{dx} = -I' + (1 - \Omega) \hat{i}' + \Omega \tau.$$  \hspace{1cm} (3.28)

where the average intensity $\tau$ is given by

$$\tau = \frac{1}{2} \int_{-1}^{1} I' d\mu.$$  \hspace{1cm} (3.29)

The angular integral in Eq. (3.29) can also be approximated using a quadrature formula, but $\tau$ will be determined in a different way as presented below. When Eq. (3.17) is implemented in a finite-volume method, the radiative flux $q_r$ has to be evaluated at the boundaries of the control volume. The intensities $i_m$ are therefore defined at these boundaries. The intensities are determined following the Discrete-Transfer Method [50] by integrating Eq. (3.28). For $\mu_m > 0$ this gives

$$i_{me} = i_{mw} f + S_i (1 - f)$$  \hspace{1cm} (3.30)

and for $\mu_m < 0$

$$i_{mw} = i_{me} f + S_i (1 - f)$$  \hspace{1cm} (3.31)

with

$$f = \exp \left(-\frac{K}{|\mu_m|} (x_e - x_w)\right).$$  \hspace{1cm} (3.32)

and

$$S_i = (1 - \Omega) \hat{i}' + \Omega \tau.$$  \hspace{1cm} (3.33)

The average intensity $\tau$ is found from the condition that scattering does not result in a net source or sink of radiation. The net effect of scattering along a path length $\Delta s$ is given by

$$\Delta i_m = \int_{0}^{\Delta s} \Omega K (\tau - i_m(s)) ds.$$  \hspace{1cm} (3.34)
3.3. 2D modeling of radiation

This integral is evaluated by integrating Eq. (3.28) giving

\[ \Delta s i_m = \Omega (\tau K \Delta s - i_{wu} (1 - f) - S_i (1 - f - \Delta s K)) \]  

(3.35)

with \( i_{wu} = i_{wu} \) for \( \mu_u > 0 \) and \( i_{wu} = i_{wu} \) for \( \mu_u < 0 \). The net effect of scattering must be zero, so the average intensity is found from the condition

\[ \sum_{m=1}^{M} \Delta s i_m = 0. \]  

(3.36)

3.2.3 Application of 1D radiation models

The radiation models for the gas radiation and the radiation inside the ceramic foam have been implemented into the 1D model based on complex chemistry presented in Section 2.2. For the radiation inside the ceramic foam, the equations are solved simultaneously and implicitly with the equations for the chemistry and heat transfer. The gas radiation is solved outside the implicit solver as the numerical integrations and the determination of the wide-band parameters require a large number of operations.

For the radiation equations boundary conditions have to be specified at the inlet and outlet. It is assumed that these boundaries are black surfaces. The inlet is assumed to radiate at the temperature of the unburnt mixture \( T_u \) and the outlet is assumed to radiate at the average temperature of the environment \( T_{env} \). The 1D combustion-model can be used using both radiation models, or by solving only the radiation inside the ceramic foam. When both models are used, the radiative intensities are coupled at the upstream surface of the ceramic foam. The 1D gas-radiation model is only used in Chapter 5. In all other simulations only the radiation inside the ceramic foam is accounted for.

3.3 2D modeling of radiation

For 2D/3D modeling of radiation several models are known. In the zone method [23] the radiative transfer is calculated by integrating the radiative transfer equation between pairs of volume or surface zones. For fine discretizations of the volume this results in a large matrix of view factors. The Monte-Carlo [24] and Discrete-Transfer [50] methods are ray-tracing methods which calculate the radiative transfer by integrating the RTE along rays in the volume. In the Monte-Carlo method these rays are chosen stochastically whereas the Discrete-Transfer method uses a predetermined set of rays. The Discrete-Ordinates method [18, 32, 34] solves the RTE as a differential equation on the same grid as the flow equations.

Narrow and wide-band models have been used to compute non-gray radiation using Discrete-Ordinates and Monte-Carlo models [38, 47]. However, these applications have mainly been limited to 1D. Due to the required computational effort the wide-band model is not suited for 2D. Therefore, instead of solving the complex spectral structure of the radiation, effective absorption coefficients are used which are based on the wide-band model.
The gas radiation and the radiation inside the ceramic foam are combined and calculated by the same model but with different absorption and scattering coefficients.

In this thesis the Discrete-Transfer method is used to compute the radiation in the 2D model because it is a flexible method which is more efficient than the zone and Monte Carlo methods. It does not suffer from false scattering as the Discrete-Ordinates method [11], but the ray effect can lead to unrealistic results [11, 33]. The Discrete-Transfer method will be introduced first and is followed by the determination of the effective absorption coefficients.

### 3.3.1 Discrete-Transfer method

In the Discrete-Transfer method [50] the computational domain is divided into cells which are assumed to have a constant temperature and absorption coefficient. The change in intensity along a ray passing through such a cell can easily be obtained by integrating the RTE over the path segment of the ray in the cell. The intensity on exit of the cell \( i'_n \) is related to the intensity on entry of the cell \( i'_{n-1} \) as (see Fig. 3.4)

\[
i'_n = i'_{b,n} (1 - \exp(-k_n (s_n - s_{n-1}))) + i'_{n-1} \exp(-k_n (s_n - s_{n-1})).
\]

(3.37)

The intensity at the cell faces along a ray can thus be related to the radiative flux leaving the wall at the origin of the ray and the composition of the cells through which the ray passes.

The division of the computational domain into volumes also divides the walls of the domain in surfaces. These surfaces have to be small enough to be considered constant.
in temperature. The net radiative heat transfer for the surface zone can be found from Eq. (3.9), provided that the intensity impinging on the wall is known. Therefore, the angular interval in Eq. (3.9) is discretized into a number of solid angles and for each solid angle a representative ray is traced back to its origin. Using the recurrent relation Eq. (3.37), the impinging intensity can be related to the radiative intensity leaving the origin walls and the temperatures and absorption coefficients of the volume through which the rays pass. In case of black walls with prescribed temperatures, the intensity of the radiation leaving the walls follows directly from the temperatures. In case of non-black walls or prescribed heat fluxes the incoming radiation has to be known and an iteration loop is, therefore, necessary.

The radiative heat source for each grid cell can be calculated in a similar way. This requires the determination of the radiating flux at all the cell faces by tracing rays in all directions. The radiative heat source then follows from the integral of the radiative flux over the cell boundaries. The number of rays which have to be traced, however, grows enormously when the grid size is reduced. Furthermore, many rays will (almost) coincide. Therefore, in practice, the radiative heat sources in the grid cells are approximated using the rays which have already been traced for the calculation of the wall heat transfer.

The rays which are traced, do not change throughout the computation, which makes the Discrete-Transfer method very efficient. The costly tracing work has only to be performed once. A disadvantage of this is, however, the vulnerability of the method to the ray effect (see Fig. 3.5). The ray effect is caused by interference between the angular and spatial discretizations and makes that small radiation sources are not ‘seen’ at places where this should be the case, whereas at other places the influence is overestimated. Another disadvantage of the method is the interpolation necessary to calculate the energy sources or sinks of the gas volumes. Another problem related to these sources is that the directions of the rays are based on the surface geometry which can be disadvantageous.
3.3.2 Determination of gray band absorption coefficients

The constant absorption coefficients in the 2D-model are determined by calculating the emission in a single direction at the mean beam length and a mean temperature. This determination is similar to the determination of the global absorption-emission coefficient in [5], except that in the present work the absorption coefficients are determined for gray bands. The mean beam length for an absorbing gas in a general geometry with volume \( V \) and area \( A \) is given by [52]

\[
L_e = 0.9 \frac{4V}{A}.
\]  

(3.38)

At the mean beam length the equivalent bandwidths \( A_j \) and the transmission \( \tau_j \) (see Appendix B.1) of all vibrational-rotational bands of all absorbing species are calculated. These values are calculated for an isothermal gas mixture at a temperature of 1700 K using the Edwards exponential wide-band model which is treated in Appendix B. The combination of the equivalent band width and the transmission defines the actual width of the band. As the band head location is fixed and given by either the lower limit \( \nu_{l,j} \), the upper limit \( \nu_{u,j} \) or the band center

\[
\nu_{c,j} = (\nu_{u,j} + \nu_{l,j})/2,
\]

the band limits follow from

\[
\nu_{u,j} - \nu_{l,j} = \frac{A_j}{1 - \tau_j}.
\]  

(3.39)

Neighboring bands might overlap, in which case the original bands are restricted to the non-overlapping regions. The overlapping region is considered to be a separate band with a transmission given by

\[
\tau_{jj'} = \tau_j \cdot \tau_{j'}.
\]  

(3.40)

For each interval a gray band absorption coefficient can be calculated by comparing the transmission to the transmission of a gray gas:

\[
k_j = -\frac{\ln \left( \frac{\tau_j}{\tau_j} \right)}{L_e}.
\]  

(3.41)

The mean-beam length \( L_e \) on which the absorption coefficients are based is determined from the geometry. For the gas temperature a reference value of 1700 K is used. For a mixture of hot flue-gases this leads typically to a combination of twelve absorbing bands and ten non-absorbing bands. An example of the absorption coefficients is shown in Fig. 4.13.

3.3.3 Application of the radiation model

The Discrete-Transfer method is a standard radiation model of the flow solver package CFX [10]. The application of the model is standard except for the radiation inside the ceramic material. In CFX the radiation is assumed to originate from the medium, and the radiation calculation is, therefore, based on the gas temperature and the resulting source terms are used in the enthalpy equation. In the present model this is not the case in the ceramic-foam region where the radiation originates from the solid phase. In this region
3.4 Comparing the exponential wide-band model and gray-bands model

The Edwards exponential wide-band model cannot be used in the 2D model. Therefore the gray-bands model is tested by comparing it to the results of the Edwards exponential wide-band model for a 1D isothermal gas. In the gray-bands model only the emissivity at the mean beam length is guaranteed to be equal to the spectral emissivity. To analyze the possible error which is made by using this approach, the emissivity along a path for the gray-bands model is compared with the emissivity for an Edwards exponential wide-band model. The band absorption coefficients are determined using two parameters, the mean beam length \( L_e \) and the temperature of the gas. In Fig. 3.6 the mean beam length is varied and in Fig. 3.7 the gas temperature is varied. In Fig. 3.6 the line from the Edwards exponential wide-band model is compared with results from the gray-bands model with the absorption coefficient based on mean beam lengths of 5, 10 and 20 cm. The result for 10 cm is accurate in the complete domain. The 5 cm line starts to deviate significantly after 20 cm, whereas the 20 cm line deviates slightly in the first 5 cm. From these results it is

Figure 3.6: Emissivity as a function of path length for flue gases at \( T = 1700 \) K and \( \phi = 0.9 \), calculated using the Edwards exponential wide-band model (solid line) and using the gray bands approximation with the absorption coefficients calculated with \( T = 1700 \) K and \( L_e = 5 \) (dashed line), 10 (dotted line) and 20 cm (dash-dotted line).
3.5 Conclusions

In this chapter a number of radiation models have been presented. These models are used in combination with the combustion models treated in the previous chapter. The Edwards exponential wide-band model is implemented in the 1D model to simulate gas radiation in the post-flame zone. Radiation inside the ceramic foam is also treated in the 1D combustion model.

In the 2D combustion model both the radiation inside the ceramic foam and the gas radiation are modeled using the Discrete-Transfer model with gray-bands.

concluded that the gray-bands approach gives a good approximation for $0.5L_c < s < 2L_c$. However, for larger path lengths the discrepancy is larger than for smaller path lengths.

In Fig. 3.7 results from the Edwards exponential wide-band model are compared with results from the gray-bands approximation based on three different temperatures. From this graph it follows that basing the absorption coefficient on a temperature which is higher or lower than the actual gas temperature, will underestimate or overestimate the emission by the gas, respectively. This will restrict the accuracy of the gray-bands model for applications in which there is no uniform temperature, or in which the temperature deviates significantly from 1700 K.

Figure 3.7: Emissivity as a function of path length for flue gases at $T = 1700$ K and $\phi = 0.9$, calculated using the Edwards exponential wide-band model (solid line) and using the gray bands approximation with the absorption coefficients calculated with $L_e = 10$ cm at $T = 1600$ (dashed line), 1700 (dotted line) and 1800 K (dash-dotted line).
Chapter 4

Ceramic-foam burner in a high-temperature furnace

Ceramic-foam surface burners have been developed for domestic heating equipment, but they can be very useful in industrial applications as well. If the radiative heat transfer can be used effectively, the energy consumption can be lowered. Also, the pollutant formation can be reduced due to the lower flame temperature. However, the risk of flash-back limits the application of the burner and the system must be well designed to make it as efficient as possible. A detailed investigation of the circumstances at which flash-back occurs will be presented in Chapter 6. From an analysis of the stabilization mechanism, which is based on radiative heat transfer with the environment, however, it follows that the radiating temperature of the environment is a key parameter for this process. Determination of this temperature requires detailed knowledge of the temperature distribution in the application. This can only be obtained by careful measurements or sophisticated modeling.

In this chapter an experimental set-up is described which is representative for a small-scale industrial-application with a hot environment. In this set-up temperature measurements are possible at both the walls and inside the combustion chamber. Using these measurements the 2D numerical model, as described in Chapter 2 and Chapter 3, is validated. The validation shows that the predictions of the model are generally in agreement with the experimental results, but that the heat loss of the flue gases appears to be underpredicted. The reason for this underprediction is investigated from an analysis of the heat transfer in the application and a limited sensitivity analysis of the numerical results. The heat-transfer analysis is also used to identify the importance of the main heat-transfer modes in such an application.

The experimental set-up is described in Section 4.1 and the numerical simulation in Section 4.2. The numerical results and the global validation of the reduced-chemistry model are presented in Section 4.3. The analysis of the heat transfer is presented in Section 4.4, and the chapter is concluded with a discussion in Section 4.5.

4.1 Experimental set-up

The experimental set-up is intended to investigate flash-back and to provide a reference system for the validation of the numerical models. The following requirements have been formulated prior to the design of the set-up:
4.1.1 Description of experimental set-up

Based on the requirements formulated above a set-up has been designed which is shown in Figs. 4.1, 4.2 and 4.3. In this set-up a hot environment is created by using the heat from the burner. The furnace consists of a cylinder of refractory bricks, referred to as wall or walls, and a duraboard plate which is referred to as the top disk. In the top disk the cylindrical burner is mounted. The burner radiates into the furnace with the flame located at the lower surface of the burner. This configuration has been selected instead of having the burner at the bottom of the furnace, radiating upwards, to prevent condensing water to fall onto the burner surface because this can cause fracture of the burner. The walls consist of two layers of twelve vertical bricks (size 114 mm × 63 mm × 230 mm). The inside of the bricks is polished to a cylinder with a radius of 155 mm as shown in Fig. 4.3, see also Fig. 4.2. The relevant properties of the walls and the top disk are listed in Table 4.1.

To achieve a steady-state situation with hot walls, part of the heat of the burner...
Figure 4.3: Cross-section of the furnace, including the positions of the thermocouples \( g_1 \), \( g_2 \), \( g_3 \) and \( w_1i \) to \( w_4o \). The thermocouple positions are listed in Tables 4.2 and 4.3. All dimensions are in cm.
Figure 4.4: Detail of the heat exchanger.

Figure 4.5: Thin-wire S-type couple.

Table 4.1: Selected properties of solid materials used in furnace.

<table>
<thead>
<tr>
<th>Material type</th>
<th>( T_{ref} ) [K]</th>
<th>( \rho ) [kg/m³]</th>
<th>( c_p ) [J/kg]</th>
<th>( \lambda ) [W/mK]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Refractory bricks</td>
<td>673</td>
<td>480</td>
<td>0.14</td>
<td></td>
</tr>
<tr>
<td></td>
<td>873</td>
<td></td>
<td>0.16</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1073</td>
<td></td>
<td>0.18</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1273</td>
<td>1050</td>
<td>0.20</td>
<td></td>
</tr>
<tr>
<td>Duraboard</td>
<td>478</td>
<td>240-280</td>
<td>0.075</td>
<td></td>
</tr>
<tr>
<td></td>
<td>700</td>
<td></td>
<td>0.105</td>
<td></td>
</tr>
<tr>
<td></td>
<td>922</td>
<td></td>
<td>0.144</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1144</td>
<td></td>
<td>0.192</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1255</td>
<td></td>
<td>0.222</td>
<td></td>
</tr>
</tbody>
</table>
must be removed by other means than by conduction through the walls. Possible solutions that have been considered are a large open outflow which allows the radiation and hot flue gases to escape from the furnace, a glass window which allows only the radiation to escape and a heat exchanger which absorbs convective and radiative heat. A water-cooled heat exchanger has been selected as it provides a good boundary condition for both the flow and the heat transfer. It is placed opposite to the burner which makes it possible to control the environment of the burner by changing the vertical position of the heat exchanger. This position is indicated by the distance \( H \) between the downstream surface of the burner and the heat exchanger. Lowering the heat exchanger lowers the view factor of the burner to the heat exchanger and thus increases the average radiating temperature of the environment of the burner. The heat exchanger is made of two steel disks through which water flows as shown in Fig. 4.4. It can be modeled as a wall with a constant, low temperature. Because it blocks the view from the lower part of the furnace to the burner, it forms the boundary between the upper hot part of the furnace and the, relatively cold, lower part. The distance between the heat exchanger and the wall should be small enough to isolate the upper part of the furnace from the lower part. It is, therefore, only necessary to model the upper part of the furnace. This assumption is further investigated in Section 4.2.2. Below the heat exchanger, the flue gases leave the furnace through a torus which is connected to the chimney (Fig. 4.3). The complete furnace is mounted on a steel rack to make it accessible from all sides.

The composition and flow of the unburnt mixture is controlled using two mass-flow controllers, one for the methane and one for the air. The uncertainty in the flow through the mass flow controller is 0.75% of the full range. In the furnace both gas and wall temperatures are measured. These measurements are discussed in the next two sections.
4.1.2 Wall temperatures

The temperature of the vertical brick walls is measured with K-type thermocouples. The couples are located at both the inside and the outside of the wall at four vertical positions (at \( h = 5, 15, 25 \) and \( 35 \) cm, \( h \) is measured from the downstream surface of the burner, see Fig. 4.3). At the first and third position, temperatures are measured at two sides of the furnace, giving a total of \((4+2)^2 = 12 \) thermocouples. At the inside the thermocouples are placed in vertical grooves in the wall. At the outside they are attached to the bricks. The thermocouple positions and nomenclature are summarized in Table 4.2. The thermocouples are read with a frequency of approximately 2 Hz and recorded with a frequency of approximately 0.2 Hz. The tolerance of the thermocouples is the maximum of 1.5 K or \( 0.4\% \) [43]. This corresponds to \( 1.5 - 2 \) K for the outer-wall thermocouples and \( 3.5 - 5 \) K for the inner-wall thermocouples.

4.1.3 Gas temperatures

Gas temperatures are measured using thin-wire S-type thermocouples similar to those used in [7]. Such a couple itself consists of a combination of a pure platinum wire and a platinum wire with 10% rhodium. These wires are 200 \( \mu \)m in diameter and attached to support wires which are themselves supported by a ceramic tube. The construction is shown in Fig. 4.5 which also shows the way the ceramic tubes are inserted into the furnace through holes in the wall. The position of these holes and the nomenclature are shown in Table 4.3. Since the couples can be slid through the holes, the radial position of the thermocouple can be varied and radial profiles of the gas temperature can be obtained.

The temperature of theouples is measured at the junction between the Pt and the Pt10%Rh wires. The junction is heated up by the surrounding flue gas but loses heat through conduction in the wire and by radiative heat transfer with the surrounding walls and the hot gas volume. Combining these influences yields the following energy equation for the wire

\[ -\frac{d_c}{4} \lambda_c \frac{d^2 T_c}{dx^2} = h \left( T - T_c \right) - \epsilon_c \sigma \left( T_e^4 - T_{env}^4 \right). \] (4.1)

For long thin wires the conduction term on the left-hand side vanishes. For the thermocouples used in the furnace \((L/D = 125)\) the heat loss by conduction is expected to be less than 8% of the total heat loss \([14]\) and is, therefore, neglected. The gas temperature \( T \) then follows from the measured temperature \( T_e \) as

\[ T = T_e + \frac{\epsilon_c \sigma}{h} \left( T_e^4 - T_{env}^4 \right). \] (4.2)

The emissivity \( \epsilon_c \) of the couple can be found from the average of the emissivity of Pt \( (\epsilon_{Pt}) \) and Pt10%Rh \( (\epsilon_{Pt10%Rh}) \) with \([57]\)

\[ \epsilon_{Pt} = 8.67 \times 10^{-5} T_e + 0.0483, \] (4.3)

\[ \epsilon_{Pt10%Rh} = 8.44 \times 10^{-5} T_e + 0.0789. \] (4.4)
4.2. Numerical simulations

The heat-transfer coefficient $h$, can be found from a Nusselt relation for forced convection around a cylinder. Morgan [41] gives a detailed review of such correlations. Of the presented relations, four are applicable to the conditions found in the furnace ($0 < \text{Re} = \frac{\rho v d}{\mu} < 0.4$). From these four the following relation of Ref. 79 from [41] is used

$$\text{Nu} = \frac{h d_e}{\lambda} = 0.40 + 0.48\text{Re}^{0.5}. \quad (4.5)$$

For $0.05 < \text{Re} < 0.4$ the difference between this relation and the others is less than 25%. For the range $0.1 < \text{Re} < 0.4$ the difference between this relation and two of the others is less than 10%. Based on these results the inaccuracy of this relation is expected to be within 10%.

When Eqs. (4.3-4.5) are inserted in Eq. (4.2) the temperature of the surrounding gas can be deduced from the thermocouple reading, the flue gas properties, the thermocouple characteristics, the local velocity $v$ and the radiating temperature of the environment $T_{env}$. The latter two are not available from the experiment and have to be approximated or derived from the simulations. The corrected gas temperature profiles are shown in Fig. 4.17 and discussed in Section 4.3. The uncertainties shown in these graphs are based on

$$\Delta T = \Delta T_c + \left( \frac{\Delta e}{c} + \frac{\Delta h}{h} \right) + \frac{4T_c^3 \Delta T_c}{T_c^4 - T_{env}^4} (T - T_c). \quad (4.6)$$

The correction term in Eq. (4.2) $\left( \frac{c e}{h} (T^4_c - T_{env}^4) \right)$, ranges between 0 for a position close to the heat exchanger and 160 K close to the burner. The relative uncertainties in the emissivity is estimated to be about 10% and, as discussed above, the relative uncertainty in the heat-transfer coefficient is roughly 10%. The tolerance of the S-type thermocouples is the maximum of 1.0 K or 0.25% [43]. This corresponds to 4 K for positions near the burner and 2 K for positions near the wall. Using these values gives a final uncertainty in the gas temperatures of 2 K near the heat exchanger which increases to 40 K near the burner and varies from 6 to 12 K near the wall.

4.2 Numerical simulations

The experimental set-up, as described in the previous section provides a good opportunity for a global validation of the 2D numerical model. Furthermore, the model can be used to analyze the heat transfer in the furnace. This analysis can be used for the design of industrial applications of ceramic-foam surface burners. In this section the modeling assumptions, the computational domain and the boundary conditions, which are used to simulate the flow and heat transfer in the experimental set-up, are described.

4.2.1 Modeling assumptions

The 2D model, as described in Chapter 2, is used to simulate the flow and heat transfer in the experimental setup. Following the results from Section 2.4, the effective conductivity
in the burner is scaled with a factor 100. The experimental setup is designed as a 2D system and is described using an axi-symmetric coordinate system. The computational domain, shown in Fig. 4.6 and Fig. 4.7, is based on the cross-section of the setup as shown in Fig. 4.3. It includes wall regions for the side wall and the top disk. In these regions a conduction equation is solved:

$$ \nabla \cdot (\lambda \nabla T) = 0. $$

The model is restricted to the upper, hot part of the furnace. The lower part of the furnace, below the heat exchanger, is assumed not to influence the heat transfer in the upper part. This assumption is checked in Section 4.2.2.

A few simplifications have been made to represent the geometry of the experimental setup. Although the actual inflow into the plenum is not axi-symmetric these details have not been included in the computational domain. The plenum is restricted to the height of the top disk and the inlet boundary for the flow is positioned at its top. The thickness of the burner has been reduced from 1 cm to 0.1 cm to minimize the number of small cells which is necessary for a good radiation calculation with a high extinction-coefficient. In the experimental setup the top disk is covered with a steel plate. The conductivity of the steel is much higher than the conductivity of the duraboard of which the top disk is made. Therefore, the steel plate has not been included in the computational domain. The side wall is modeled as a solid wall with the properties of the bricks and an emissivity of 0.5 (see Section 4.2.3). The influences of the joints and thermocouple holes have been neglected. Besides these minor modifications it has been found necessary to include an insulating
4.2. Numerical simulations

layer around the plenum and the burner, i.e., a small insulating ring in the top disk (see Figs. 4.6 and 4.7). This insulation ($\lambda = 0.01$ W/mK) is necessary to prevent ignition of the fresh mixture. This insulation can be partly justified from the construction of the burner. In the set-up the burner is removable and there is a layer of duraboard and a thin air layer between the top disk and the plenum. So the burner and the plenum are not connected to the top disk and there will be a large thermal resistance for the heat transfer.

The inflow is prescribed at the inlet boundary with Dirichlet conditions for the velocity and the temperature and species concentrations, all assumed constant. At the outlet boundary only the pressure is prescribed. For the other variables Neumann, boundary conditions are implemented.

The heat exchanger is made of steel and cooled by water. The highest resistance against heat transfer from the flue gases to the cooling water is the convective one at the outside of the heat exchanger. The heat resistance at the inside of the heat exchanger and through the steel is, therefore, neglected and the heat exchanger is modeled as a wall with a temperature of 300 K and an emissivity of 0.4.

The heat transfer at the outer walls is more complicated as the heat resistance at the outside of the walls cannot be neglected. The heat transfer at the outer walls is, therefore, included by the heat-transfer relation

$$q = h \left( T - T_{env} \right).$$  \hspace{1cm} (4.8)

The heat-transfer coefficient $h$, which depends on the temperature, must account for both radiation and natural convection. The radiative part of the heat transfer is given by

$$q_r = -\epsilon \sigma \left( T^4 - T_{env}^4 \right)$$  \hspace{1cm} (4.9)

and the convective part is given by

$$q_c = -h_c \left( T - T_{env} \right).$$  \hspace{1cm} (4.10)

The heat-transfer coefficient for natural convection $h_c$ is found from a Nusselt-relation based on the Rayleigh number $Ra$ [3]

$$Ra = \frac{g \beta (T - T_{env}) L^3}{\alpha \nu}$$  \hspace{1cm} (4.11)

with the thermal diffusivity $\alpha$ given by $\alpha = \frac{\lambda}{\rho c_p}$ and the thermal volumetric expansion coefficient by $\beta = 1/T$ [25]. The length $L$ is the height of the hot wall, which is taken to be the distance between the burner and the heat exchanger, so $L = H$. For the walls, $Ra$ is of the order of $10^7$ and the applied Nusselt-relation is given by [3]

$$Nu = \frac{hL}{\lambda} = \left( 0.825 + 0.325 Ra^{1/6} \right)^2 \text{ for } 10^{-1} < Ra < 10^{12}. \hspace{1cm} (4.12)$$

For the top disk, $Ra$ is of the order of $10^6$ and the applied Nusselt-relation is given by [3]

$$Nu = \frac{hL}{\lambda} = 0.54 \text{ Ra}^{1/4} \text{ for } 10^4 < Ra < 10^7. \hspace{1cm} (4.13)$$
Figure 4.8: Response of the inner wall thermocouples \( w1i \) (solid line), \( w2i \) (dashed line) and \( w3i \) (dotted line), for two experiments at \( u_a = 15.0 \text{ cm/s} \) and \( \phi = 0.9 \): (a) \( H = 10 \text{ cm} \) and (b) \( H = 20 \text{ cm} \); see Table 4.2, Fig. 4.6 and Fig. 4.7 for the positions of the thermocouples. The curves for the left plot show a small twist because the experiment was conducted at \( u_a = 7.2 \text{cm/s} \) for the first 15 minutes.

with the length \( L \) defined as

\[
L = \frac{D}{4}.
\]  
\[ (4.14) \]

The heat-transfer coefficient then follows from

\[
h = \frac{q_c + q_r}{T - T_{cw}}.
\]  
\[ (4.15) \]

This relation is approximated by a linear function of the temperature \( T \), given by

\[
h(T) = h_0 + h_1 T.
\]  
\[ (4.16) \]

The Nusselt relations for natural convection are only approximations and do not take into account the temperature profile at the outside wall. Also the emissivity of the bricks is not known accurately. Therefore, the actual values for the heat-transfer coefficient \( h \) which are used in the model, are determined from experiments in Section 4.2.3. In this determination the value for the emissivity of the walls, \( \epsilon \) in Eq. (4.9), is varied.

4.2.2 Restriction of the computational domain

Some experiments have been analyzed to asses the interaction between the burner and the walls. The heat transfer at the inside of the furnace is analyzed by comparing the responses of the inner wall temperatures in different experiments during the start-up of the furnace.
4.2. Numerical simulations

Based on these processes the computational domain, necessary for an accurate modeling, is determined.

The typical response of the thermocouples at the inside of the furnace wall is shown in Fig. 4.8 for two experiments. The distance between the burner and the heat exchanger is $H = 10$ and $20$ cm in the two experiments. For both experiments one sees that the wall temperatures rise sharply after starting the burner. This indicates that the walls are heated up rapidly by radiative heat exchange with the burner. A further indication for this can be found from the difference between the two experiments. Note the difference in the response of thermocouple w2i. In the first experiment, with $H = 10$ cm, it is located in the lower part of the furnace, whereas in the second experiment, with $H = 20$ cm, it is located in the upper part. The result is that for the first experiment there is a time delay in the response which is also present for w3i in both experiments. In the second experiment thermocouple w2i reacts immediately, as w1i in both experiments. From the results of the inner wall temperatures it can be concluded that the top part of the walls, above the heat exchanger, are directly and mainly heated by the radiative heat exchange with the burner. The lower part of the walls is heated by the hot flue gases, by radiation from the walls and by conduction through the side wall. From the difference in the response between the upper and lower wall segments, it is concluded that the heat exchanger splits the furnace into two separate areas, with almost no radiative heat-exchange between them. The heat exchange between these two zones occurs only by the flow of the flue gases which must pass through the, relatively narrow, gap between the heat exchanger and the wall. Based on this observation it is assumed that the influence of the lower part of the furnace on the

Figure 4.9: Difference between the steady-state and the actual temperature of the thermocouples w1i (upper curve) and w2i (lower curve) for $v_n = 15.0$ cm/s, $\phi = 0.9$ and $H = 10$ cm. At $t = 3.7$ h the equilibrium was momentarily disturbed when a thermocouple was entered into the furnace to measure the gas temperature.
upper part of the furnace is small. Therefore, the computational domain is restricted to the upper part of the furnace, above the heat exchanger, and the gap between the heat exchanger and the wall. The lower part of the furnace will not be included in the numerical simulation.

From the experiments it also follows that the inner-wall temperatures increase very fast in the first half hour. This rate of increase is tempered in the remaining time of the experiment. This is shown in Fig. 4.9. After half an hour the difference with the steady-state temperature is within 25 K for the first two thermocouples. After 2.5 h the difference is within the scatter of about ±2 K.

4.2.3 Determination of boundary conditions at the outside wall

Some experiments have been performed to analyze the interaction of the furnace with the environment. From this interaction the boundary conditions for the numerical simulations \( (h_0 \text{ and } h_1 \text{ in Eq. (4.16))} \) are determined. This determination is based on a comparison of the response of the thermocouples to the results of a simple 1D model for the transient conduction through the walls. In the 1D conduction-model the emissivity \( \varepsilon \) of the outside walls is varied to reproduce the experimental results. The time scales of the heat-transfer processes are used to quantify the approximation of the steady-state situation.

The responses of the thermocouples \( w_{10}, w_{20} \) and \( w_{30} \) are shown in Fig. 4.10 for \( H = 10 \text{ cm, } v_u = 15.0 \text{ cm/s and } \phi = 0.9 \). The response of all thermocouples shows a delay, which is not present in the results for the inner wall thermocouples, followed by a rise in the temperature which is less steep than the rise for the inner-wall thermocouples. The time delay is the time necessary for the heat profile to 'travel' through the wall. The
difference between the steepness of the profiles for the inner wall (Fig. 4.8) and the outer wall (Fig. 4.10) can be explained from the difference in heat transfer. At the inner wall there is an equilibrium between absorption, emission, convection and conduction. The first two contributions are rather large and mainly determine the final inner wall temperature. At the outside there is an equilibrium between the heat transfer through conduction from the inside and through the free convection and radiation to the environment. The magnitude of these terms is, however, smaller than the magnitude of the radiation terms at the inside.

The heat conduction through the wall is simulated using a 1D-conduction model to analyze the radiation and natural convection at the outside. The 1D-conduction model is given by the differential equation for the temperature

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \lambda \frac{\partial T}{\partial r} \right)$$

(4.17)
on the domain $r_1 \leq r \leq r_2$ and by an initial condition and two boundary conditions,

$$T = T_0 \text{ for } r_1 \leq r \leq r_2 \text{ at } t = 0,$$

(4.18)

$$T = T_1 \text{ for } t > 0 \text{ at } r = r_1,$$

(4.19)

and

$$-\lambda \frac{\partial T}{\partial r} = h(T) (T - T_{env}) \text{ for } t > 0 \text{ at } r = r_2.$$

(4.20)

The temperature at the inner wall $T_1$ is assumed to be constant and equal to the steady-state value from the thermocouple readings because the heat transfer in the furnace is too complex to take into account. This approximation is justified by the fast response of the inner-wall temperatures. The heat transfer at the outside is calculated using the heat transfer relations from the previous section (Eqs. (4.8)-(4.16)). In these relations the emissivity is used as a free parameter. This parameter is fixed to a value of 0.5 from a qualitative comparison of the solutions of Eqs. (4.17)-(4.20) to the experimental results.

The experimental results and the solutions for $\epsilon = 0.5$ are shown in Fig. 4.10. The results for thermocouple who is underpredicted, whereas the results for the lower thermocouples are overpredicted. This is in agreement with the general view on natural convection, which predicts that a boundary layer will form, increasing in thickness from the bottom to the top, due to the natural convection flow along the outside [4]. At the lower parts of the wall the actual heat transfer is higher than the average value. As a consequence the real outside-temperature at the lower parts is lower than when based on the average heat-transfer coefficient. For the upper parts of the wall this situation is reversed. Inclusion of the boundary layer effect in the boundary condition for the outside is feasible, but would suggest an accuracy which cannot be validated. In further numerical simulations the heat-transfer relation for the outside walls will be based on the average value for the heat transfer coefficient with an emissivity of 0.5.

From the comparison of the experimental and predicted profiles in Fig. 4.10 it follows that the 1D conduction results give a good approximation for the actual situation. As such the results can be used to quantify the difference between the thermocouple readings and
the steady-state situation. From the results of the 1D conduction model, it follows that the
difference between the actual and the steady-state value is less than 1 K after two hours. The scatter in the experimental values is then ±2 K. At that time the system can thus be assumed to be in steady state.

4.3 Results of the furnace simulations

The 2D-model is used to model the experimental set-up. The model assumptions, the computational domain and the boundary conditions have been presented in the previous section. In Section 4.3.1, the results from a typical simulation are described. In Section 4.3.2, the numerical model is globally validated by comparing numerical and experimental results.

4.3.1 Simulation for $H = 20$ cm, $v_u = 15$ cm/s and $\phi = 0.9$

The results of a typical simulation are presented by describing the results for the case with $H = 20$ cm, $v_u = 15$ cm/s and $\phi = 0.9$. This simulation has been performed on the radiation and flow grids shown in Figs. 4.11 and 4.12. The flow grid is a rectangular mesh of 212 by 59 cells, with refinements at the flame front and at the walls. The radiation grid is constructed from the flow grid by combining multiple flow cells to a single radiation cell. The absorption coefficients used in the gray-bands radiation-model are shown in Fig. 4.13.

The calculated temperature distribution and flow pattern are shown in Fig. 4.14. The fresh mixture enters at the inlet and flows downwards towards the burner. The wall of the plenum is hot which causes a small recirculation zone in the plenum. The fresh mixture flows through the burner and is burned in the flame just below the burner. The flame front itself is too thin be visible on the scale of Fig. 4.14 and only shows as a jump in the temperature. The flue gases form a slow jet which flows towards the heat exchanger. Due to gas radiation the flue gases loose heat to the walls and the cooler gases. The center of the heat exchanger forms a stagnation point for the flue gases which are pushed towards the side. As they pass the heat exchanger, they are cooled by convection. The flue gases leave the combustion chamber as they pass the heat exchanger. In the top corner of the combustion chamber a recirculation zone is present. The expected single vortex is, however, not found, but under the influence of gravity a complicated flow pattern is found. This pattern cannot be very stable and transient effects should be included to model the stability of this flow pattern. The velocities in this region, are, however, small and the influence of these transient effects on the heat transfer is probably negligible. The isotherms in the side wall are nearly vertical, indicating that the conduction through the walls is almost completely 1D.

Even though the flame cannot be observed in Fig. 4.14, it is captured on a fine grid near the burner surface. The flame structure itself is shown in Fig. 4.15, by temperature and atomic-oxygen profiles at two radial positions on the burner. These profiles show that, at the rim of the burner, the flame stabilizes slightly further upstream than in the center. Possible causes of this difference in stabilization are differences in the radiation incident to the burner and preheating of the unburnt mixture. Of these two possible causes, differences
4.3. Results of the furnace simulations

**Figure 4.11:** Grid on which the radiation is solved for the simulations with \( H = 20 \text{ cm} \).

**Figure 4.12:** Grid on which the flow and combustion equations are solved for the simulations with \( H = 20 \text{ cm} \).

**Figure 4.13:** Gray bands and absorption coefficients used for the \( H = 20 \text{ cm} \) and \( \phi = 0.9 \) calculations.

**Figure 4.14:** Calculated temperature distribution and streamlines, for \( H = 20 \text{ cm}, v_u = 15 \text{ cm/s} \) and \( \phi = 0.9 \).
in incident radiation is unlikely as it would require a radiation profile which is higher at the rim of the burner. This is not in agreement with the presence of the core of hot flue gases at the center. As mentioned above, preheating of the unburnt mixture by conduction through the top disc is observed in the results, even though it is reduced by the presence of the insulating layer around the plenum (see Section 4.2). The isotherms in the top disc next to the plenum are nearly vertical and the flow in the plenum is influenced by the hot wall. Preheating of the unburnt mixture is known to have a large influence on the stability of the combustion and will make the flame stabilize further upstream [7]. As the flame stabilizes further upstream, the conduction inside the ceramic foam can influence the mass burning velocity of the flame. This influence is overestimated by FGM (see Section 2.4) and care must be taken while interpreting these results.

The effect of local preheating of the unburnt mixture can be very important for the stability of the combustion process when local flash-back causes ignition in the plenum. For a description of this effect, it is, however, essential to have a 2D model in which it is possible to simulate flames inside the ceramic foam with the actual properties of the ceramic material. This is not possible with the present model.

4.3.2 Model validation

The numerical model is validated by comparing the results from the experiments with the results from the simulations. The results considered are the wall temperatures at the inside and the outside of the furnace, and gas temperature profiles at three different heights \( h \) inside the furnace. Results have been obtained for four different experiments which are a combination of two inlet velocities \( v_u \) and two heat-exchanger positions \( H \).

The thermocouple positions are listed in Table 4.2, and the results of the wall-
4.3. Results of the furnace simulations

$T$ [K]

$H = 10$ cm, $v_u = 7.2$ cm/s

$H = 20$ cm, $v_u = 7.2$ cm/s

$H = 10$ cm, $v_u = 15$ cm/s

$H = 20$ cm, $v_u = 15$ cm/s

Figure 4.16: Inner and outer wall temperatures for $\phi = 0.9$ from the simulations (solid line and dashed line) and experiments (crosses and circles), see Fig. 4.6 and Fig. 4.7 for the positions of the thermocouples.
Figure 4.17: Gas-temperature profiles for $\phi = 0.9$ from experiments (crosses and circles) and simulations (solid line), see Fig. 4.6 and Fig. 4.7 for the positions of the thermocouples.
temperature measurements are shown in Fig. 4.16, together with the profiles from the simulations. In each of these graphs the results of the thermocouples located inside the hot part of the combustion chamber are plotted.

The numerical results for the inner-wall temperature for the cases \( v_u = 7.2 \text{ cm/s} \) are about 70 K too high for w1i and w1ic at \( H = 10 \text{ cm} \) and for w2i at \( H = 20 \text{ cm} \). The results w1i and w1ic for \( H = 20 \text{ cm} \) agree well with the numerical profiles. The results for \( v_u = 15.0 \text{ cm/s} \) show good agreement for all the inside positions. The outside wall temperatures in the simulations are highly influenced by the boundary conditions which are imposed. As these boundary conditions are based on the experimental results, the resulting profiles should agree well with the experimental results, and this is indeed the case. Only at the positions closer to the heat exchanger the numerical predictions are slightly too high. This was, however, already observed in Section 4.2.3.

The gas temperature profiles are compared in Fig. 4.17. Figure 4.17-a contains the profiles for \( v_u = 7.2 \text{ cm/s} \) with the heat exchanger located at \( H = 10 \text{ cm} \). The profiles for g1 and g1c, at \( h = 2.5 \text{ cm} \), are well predicted. Both the values and the profile show good agreement with the experimental results. This applies to the width of the inner core and also for the gradient close to the wall. For the profile of g2, at \( h = 8 \text{ cm} \), there is a difference between the numerical and experimental results of about 50 K near the center and of about 100 K closer to the wall. For the case with the higher inlet velocity \( v_u = 15.0 \text{ cm/s} \), presented in Fig. 4.17-b, the values of the numerical simulation are about 50 – 100 K lower than the experimental profiles for g1 and g1c. The shape of the profile shows a good resemblance. Both the width of the central core and the gradient towards the wall are, again, well predicted. For g2, the values are in good agreement. The experimental results do not show a large variation and this is also seen in the simulations. In the experiment for \( v_u = 7.2 \text{ cm/s} \), with the heat exchanger located at \( H = 20 \text{ cm} \), three gas temperature profiles have been obtained, which are shown in Fig. 4.17-c. For g1, the values are well predicted. The numerical profile, however, shows a core which is smaller than the experimental result. The gradient is well predicted. At g2 the profile is well predicted, but the values are about 60 – 100 K too high. Also the gradient is a somewhat larger in the experiments. Similar deviations are found for g3, located closest to the heat exchanger, with the exception that the largest difference is found near the center, instead of at the rim of the core. The profiles for \( H = 20 \text{ cm} \) and \( v_u = 15.0 \text{ cm/s} \) have not been measured.

From the comparison it is concluded that the model gives an adequate prediction of the wall temperatures and the gas temperature profiles in the upper part of the combustion chamber. Closer to the heat exchanger the prediction is reasonable, but the heat loss of the flue gases appears to be, slightly but systematically, underpredicted. Possible causes of this underprediction will be investigated in the next section. Overall, the model gives a good representation of the flow and heat transfer in the furnace.
4.4 Analysis of the heat transfer in the furnace

In this section, the numerical model is used to analyze the heat transfer in the furnace. Also, the sensitivity of the results to some radiative parameters and modeling assumptions is investigated and the most important heat-transfer modes are identified. Furthermore, it is tried to explain the lower heat loss of the flue gases found in the previous section. The analysis is split into influences of the gas-radiation model, the wall emissivities and the inlet velocity.

4.4.1 Influence of the gas-radiation model

Two aspects are further investigated in this section. First, the relative importance of gas radiation is studied as compared to other modes of heat transfer as convection and surface-to-surface radiation. Second, the accuracy of a gray-gas model with respect to gray-bands modeling is investigated.

For these two aspects the results of three simulations, one with a gray-bands model, one with a gray-gas model and one without gas radiation are compared. The importance of gas radiation is analyzed by comparing the results of the gray-bands model to the results without gas radiation. The importance of spectral modeling is determined by comparing the result of the two gas radiation models.

Gas radiation adds to the heat transfer. Differences in gas temperature will lead to heat transfer by radiation that reduces these differences. The temperature profiles will be less steep and the radiative heat transfer to the walls will be increased. The convective heat transfer depends on the steepness and will be reduced. The difference between the gray and spectral models is less clear.
4.4. Analysis of the heat transfer in the furnace

![Graph showing temperature profile](image)

*Figure 4.19: Temperature profile at the height of thermocouple 1 (h = 2.5 cm, see Fig. 4.6) for H = 10 cm, \( v_u = 15.0 \) cm/s and \( \phi = 0.9 \) without a gas-radiation model (dotted line) and with gray and gray-bands gas-radiation models (dashed line and solid line, respectively).*

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Radiation model</th>
<th>Convective Value</th>
<th>Convective Diff.</th>
<th>Radiative Value</th>
<th>Radiative Diff.</th>
<th>Total Value</th>
<th>Total Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat Exchanger</td>
<td>None</td>
<td>92.1</td>
<td>100.9</td>
<td>193.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Bands</td>
<td>74.7</td>
<td>-17.4</td>
<td>143.2</td>
<td>42.2</td>
<td>217.9</td>
<td>24.9</td>
</tr>
<tr>
<td></td>
<td>Gray</td>
<td>65.8</td>
<td>-8.9</td>
<td>169.5</td>
<td>26.4</td>
<td>235.4</td>
<td>17.5</td>
</tr>
<tr>
<td>Walls</td>
<td>None</td>
<td>56.3</td>
<td>-38.3</td>
<td>18.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Bands</td>
<td>35.4</td>
<td>-20.9</td>
<td>-14.8</td>
<td>23.5</td>
<td>20.6</td>
<td>2.6</td>
</tr>
<tr>
<td></td>
<td>Gray</td>
<td>23.4</td>
<td>-12.0</td>
<td>-1.6</td>
<td>13.3</td>
<td>21.9</td>
<td>1.3</td>
</tr>
</tbody>
</table>
The results will be analyzed on two points. First the heat flow-rates to the heat exchanger and the walls are compared. Then the temperature profiles in the combustion chamber are compared.

When comparing the heat flow-rates of the gray-bands calculation with the results of the simulation without gas radiation (see Table 4.4), one finds that by including gas radiation, the radiative heat transfer to the heat exchanger is increased by about 40%. On the other hand, the magnitude of the radiative heat exchange to the walls is reduced by 60%. The absolute difference is of the same order of magnitude as for the heat exchanger. The change in radiative heat transfer is partly compensated by the convective heat transfer. This effect is more dominant for the walls, where the differences in the total heat flow are very small.

The difference between the results for the heat exchanger and the walls is a result of the fixed, low temperature of the heat exchanger on one hand and the low heat transfer through the walls on the other hand. The heat exchanger absorbs all radiative and convective heat, but the walls are almost in radiative equilibrium: the absorption and emission are almost equal. The radiative heat transfer, which is the difference between the absorption and emission, is much lower than the absorption and emission terms. The walls are heated by the convective heat transfer but cooled by the radiative heat transfer. The heat transfer through the walls by conduction, given in Table 4.4 as the total heat flow, is the difference between the convective and radiative heat flows. Beside that the emission and absorption terms are much larger than the other terms, the dependence of the emission on the wall temperature is much larger than the dependence of the wall conduction and the convective heat transfer on the wall temperature. As a result the radiative heat transfer adapts to a change in convective heat transfer. For the heat exchanger there is no such balance. However, the radiative heat transfer from the gas to the heat exchanger leads to a temperature decrease of the flue gases. As a result the temperature of the flue gases in the vicinity of the heat exchanger is lower which results in a lower convective heat transfer.

A similar comparison can be made between the results for the simulations with the two gas radiation models. It is found that for the heat exchanger, the differences between the gray-gas radiation and gray-bands radiation are about 50% of the differences between the gray-bands radiation model and the model without gas radiation. When compared to the results with the gray-bands radiation-model, the gray-gas radiation-model overpredicts the influence of gas radiation by about 50%. The influence on the total heat flux is lower, about 8%, because of the influence of the convective heat transfer. This result is comparable to the result found by Boerstoel [5] when he compared the modeling of gas radiation in an experimental glass furnace using several radiation models. The differences between the results for a statistical narrow-band model and a model using an effective gray absorption coefficient was about 3% for the heat flux to the glass, but larger for the radiative source terms.

A more detailed comparison can be made from the temperature profiles. Figure 4.18 contains the temperature profile along the axis and Fig. 4.19 the profile at h = 2.5 (the position of g1). In Fig. 4.18, the vertical profile along the axis, it is clear that for the simulation without gas radiation the flue gases do not lose any energy until they reach the
4.4. Analysis of the heat transfer in the furnace

4.4.2 Influence of wall emissivities

Radiative heat transfer is very important in the furnace. Besides gas radiation, which has been discussed in the previous section, the radiative properties of the walls are also of interest. In the model, all the surfaces are assumed to be diffuse and gray. This leaves the emissivities of the walls and the heat exchanger as parameters. In this section the influence of both these parameters is investigated. For computational speed this comparison is based on the gray-gas simulation which is used as a reference case.

Figure 4.20: Influence of the wall emissivity (solid line) and the heat exchanger emissivity (dashed line) on the heat transfer to the heat exchanger, for $H = 10$ cm, $v_u = 15.0$ cm/s and $\phi = 0.9$.
Chapter 4. High-temperature furnace

Figure 4.21: Inner-wall temperature profile for $H = 10$ cm, $v_u = 15.0$ cm/s and $\phi = 0.9$ for heat-exchanger emissivities of $\epsilon = 0.3$ (dashed line), 0.4 (ref. case, solid line), 0.7 (dotted line) and 1.0 (dash-dotted line).

Figure 4.22: Temperature profile along the axis for $H = 10$ cm, $v_u = 15.0$ cm/s and $\phi = 0.9$ for heat-exchanger emissivities of $\epsilon = 0.3$ (dashed line), 0.4 (ref. case, solid line), 0.7 (dotted line) and 1.0 (dash-dotted line).
4.5 Discussion

The influence of the emissivities on the heat transfer to the heat exchanger is shown in Fig. 4.20. In the previous section it was already found that the walls are almost in radiative equilibrium, but from this graph it can be seen that this means that the heat transfer to the heat exchanger is hardly influenced by the wall radiation. However, the wall emissivity has an influence on the wall temperature profile, as shown in Fig. 4.21, but this influence is only significant for very low emissivities.

The absorption of radiation by the heat exchanger is directly related to the emissivity. The influence of the emissivity of the heat exchanger on the heat it absorbs is therefore larger. It is, however, not linear as can be seen in Fig. 4.20. This is caused by multiple reflections of radiation. The emissivity of the heat exchanger has an influence on the gas temperature as can be seen in Fig. 4.22. Both the flame temperature and the gradient of the profile are influenced. The flame temperature is influenced as the radiation hitting the burner will increase for a lower heat exchanger emissivity. This can lead to a lower flame temperature as will be discussed in Chapter 6. The heat loss of the flue gases is influenced because the higher radiation level in the furnace increases the absorption.

4.4.3 Influence of inlet velocity

The uncertainties in the mass-flow controllers and the burner surface area, lead to an uncertainty in the velocity of ±0.6 cm/s. This makes the mass flow through the burner a possible error source in the experiments. The influence of the inlet velocity on the temperature profiles in the furnace is, therefore, investigated. Again this investigation is based on the reference case using the gray-gas radiation-model for the gas radiation. The resulting profiles are shown in Fig. 4.23. This graph shows that the influence of the inlet velocity is mainly limited to the flame temperature. The gradient of the temperature is hardly influenced. For this reason, an error in the inlet velocity is unlikely to be an explanation for the underprediction of the experimentally-found heat loss of the flue gases.

4.4.4 Conclusions

Radiative heat exchange is the most important heat-transfer mode in the furnace, which follows from a comparison of the heat-flow rates to the walls and the heat exchanger. Convective heat transfer, is however, also present and contributes to such an extent that it cannot be neglected. Gas radiation, is a very important heat-transfer mechanism and has to be taken into account.

The analysis shows as possible causes for the underprediction of the heat loss of the flue gases, the uncertainties in the band parameters of the gas-radiation model and the heat exchanger emissivity.

4.5 Discussion

An experimental set-up has been designed to provide a controllable hot-environment for a ceramic-foam surface- burner. The variation of the distance between the burner and the heat exchanger has shown to be a way to change the conditions of this environment.
Figure 4.23: Temperature profile along the axis for $H = 10$ cm, $v_u = 15.0$ cm/s and $\phi = 0.9$ for inlet velocities of $v_u = 14$ and $15$ cm/s (ref. case) (solid line and dashed line, respectively).

Originally, it was, however, the intention to use two sizes of burners in the experimental set-up. Experiments with the smaller burners showed that transient effects due to natural convection influenced the results significantly. These effects cannot be included in the present, steady-state, model and this reduces the applicability of the experimental set-up as a reference system for numerical simulations.

The boundary conditions of the system for the numerical simulations are well defined. The insulation of the brick walls is adequate to let the results be almost insensitive to the radiative properties of the walls. The results of the simulation are, however, sensitive to the value for the emissivity of the heat exchanger. For this reason, it would have been better to have a coating, with a well-defined emissivity, on the heat exchanger. Generally, the performed experiments provide a global validation of the model, and the results show that the model is applicable for heat-transfer analysis of this kind of systems. It must be noted that the accuracy of the gray-bands radiation model depends on the reference temperature used in the determination of the absorption coefficients. This could be a reason for the underprediction of the heat loss of the flue gases which is found in the validation.

It has been shown that the 2D model can be used to calculate the radiative environment of the burner in an application. This is the first step towards a quantitative prediction of flash-back in ceramic-foam surface burners. A second step is made in Chapter 6, where the influence of the radiating temperature environment on the flame stabilization is investigated. The numerical simulations have also shown that conduction through the top disc, which surrounds the burner and the plenum, can lead to preheating of the unburnt mixture. This can lead to a less-stable flame at the rim of the burner. The effect of conduction through the top disc is only included qualitatively as it has been necessary to reduce the effects of conduction close to the burner and inside the burner material to prevent (numer-
4.5. Discussion

cal) flash-back. The actual construction of the burner provides justification of this reduced conduction in the top disc. But the reduced conductivity in the burner has been necessary because flames calculated using FGM appear to be less stable than flames calculated using complex chemistry. On the other hand, modeling the effect of preheating in a quantitative manner would require more detail in the representation of the geometry and cannot be validated as such detailed measurements are not possible in the furnace.
Chapter 5

Gas radiation

Ceramic-foam surface burners have been developed as low-NO\textsubscript{x} burners. The reduction of the NO\textsubscript{x} formation is accomplished by lowering the flue-gas temperature by convective heat transfer from the flame to the burner. For a good estimate of the NO\textsubscript{x} emission it is, therefore, essential to model the burner-flame interaction accurately. NO\textsubscript{x} formation is, however, not restricted to the flame itself. Most of it is formed in the post-flame zone where the flue gases are still hot. In this zone the flue gases lose energy to the surroundings by convection at the boundaries and by gas radiation. In NO\textsubscript{x}-formation calculations an accurate description of the gas radiation must, therefore, be included in the computational method.

In most studies that incorporate gas radiation in the combustion model, this is accomplished using the optical-thin limit. This has been done, amongst others, in [26, 51] for premixed flames, by [1] for diffusion flames and in [12] for laminar flamelets. Bedir et al. [2] have compared a number of different radiation models, including the optical-thin limit, in case of a one-dimensional diffusion flame. They find that the optical-thin limit overpredicts the emission and underestimates the self-absorption by the gas substantially.

Liu and Rogg [35] used a Discrete Transfer Model with a modified wide-band model to study premixed and diffusion flames in 1D.

The difference between the results of the optical-thin limit and the other radiation models can be attributed to the influence of self-absorption. In the optical-thin limit this self-absorption is not included. On the other hand, 1D radiation models might overestimate the influence of self-absorption, because the optical thickness is related to the dimensions of the hot zone and this zone is infinitely large when a 1D model is used.

In this chapter the influence of gas radiation is investigated while taking into account the size of the hot gas volume in the post-flame zone. The post-flame zone is considered either as a 1D configuration, as shown in Fig. 5.1, or as an axi-symmetric configuration as shown in Fig. 5.2. In the latter configuration the post-flame zone is defined by two dimensions: the burner diameter \( d \) and the distance between the burner and the cold boundary \( H \). For large values of \( d \) the influence of the cold zone at the side becomes negligible and the configuration reduces to a 1D-configuration as shown in Fig. 5.1.

To explain the need for an accurate description of gas radiation, two limiting situations will be presented in the first section. These limiting situations correspond to the
optical-thin limit and the 1D radiation treatment of Fig. 5.1. Section 5.2 gives an estimate for the influence of the burner size. This influence is further investigated using the 2D numerical model with reduced chemistry, which was presented in Chapter 2. Based on several simulations, a simple model is proposed to incorporate the radiative heat loss as a function of the burner size in 1D simulations. This relation is based on the radiative heat loss in the optical-thin limit. The resulting source term for the radiative heat loss, is, however, scaled with a geometry factor to account for self-absorption. The results from the numerical simulations are compared with measurements of temperature profiles for four different burners in Section 5.4.

It will be shown that the optical-thin limit is only applicable for very small burners ($L_e < 1$ cm) whereas only for very large burners it is allowed to calculate the self-absorption by solving the radiation field using a 1D model. For most applications, detailed radiation computations should be applied, or instead the above mentioned simple model, to account for emission and self absorption, should be used.

### 5.1 Limiting situations

Gas radiation leads to a source term $S_{rg}$ in the energy equation of the gas. In Chapter 3 this source term has been given as the difference between a contribution due to absorption $A$ and one due to emission $E$ (Eq. (3.14)):

$$S_{rg} = A - E.$$  \hfill (5.1)
5.1. Limiting situations

The absorption $A$ depends on the local intensity field for which the radiation field has to be solved for the complete system. The emission $E$, however, depends only on local conditions, and can be evaluated using the tabulated Planck mean absorption-coefficient $k_P[52]$, the Stefan-Boltzmann constant $\sigma$ and the temperature $T$ as

$$E = \int_0^\infty \int_{4\pi} k_P' I_\nu d\omega d\nu = 4 k_P \sigma T^4. \quad (5.2)$$

Both $A$ and $E$ are positive, so the radiative heat loss is largest when $A \to 0$. This is the case in the optical-thin limit with low wall temperatures. In this case the intensity in the hot-gas region is very low compared to the black-body intensity of the medium ($A \ll E$) so:

$$S_{\nu g} \approx -E = -4 k_P \sigma T^4. \quad (5.3)$$

The optical-thin limit corresponds to a situation with a small path-length, i.e. a small gas volume and burner size. Therefore the temperature decrease, due to gas radiation, for burners with a diameter $d \to 0$ is given by Eq. (5.3).

Another limiting situation is obtained when the burner surface is very large, i.e. unbounded ($d \to \infty$). In this case the cold surrounding region is no longer present at the side and the hot region can also be viewed upon as unbounded. Therefore, the path lengths become infinitely large for directions parallel to the burner surface. No net radiative heat transfer is possible in isoplanes parallel to the burner. As a result it is possible to describe

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*Figure 5.3: Temperature profiles for a very large burner ($d \to \infty$, solid lines) with $H = 4$, $8$ and $20$ cm and a very small burner ($d \to 0$, dashed line) for $v_u = 15$ cm/s and $\phi = 0.9$. The temperature profiles are compared to the temperature profile of a flame without radiative heat loss (dotted line) and the adiabatic flame temperature (dash-dotted line). SR and GR denote the decrease in gas temperature due to surface radiation and gas radiation, respectively.*
Table 5.1: Average temperature gradient $\Theta$ for the optical-thin limit ($d \to 0$) and infinitely large burner ($d \to \infty$) and the geometry factor $C_r$ for the infinitely large burner for $v_u = 15 \text{ cm/s}$ and $\phi = 0.9$.

<table>
<thead>
<tr>
<th>$H$ [cm]</th>
<th>$\Theta$ [K/cm]</th>
<th>$C_r$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$d \to 0$</td>
<td>$d \to \infty$</td>
</tr>
<tr>
<td>4</td>
<td>69</td>
<td>33</td>
</tr>
<tr>
<td>5</td>
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<tr>
<td>20</td>
<td>49</td>
<td>17</td>
</tr>
</tbody>
</table>

the complete system, including radiation, using a 1D model. The height of the post-flame zone $H$ remains a parameter which can be varied. The post-flame zone length $H$ cannot be increased to infinity as this inhibits the radiative heat loss to the cold boundary. Without this heat loss the flame cannot stabilize on the burner. The height $H$ has been varied between 4 and 20 cm as this is a practical range for domestic combustion-chambers.

The results for the two mentioned limiting cases, at an inlet velocity of $v_u = 15 \text{ cm/s}$ and an equivalence ratio of $\phi = 0.9$, are shown in Fig. 5.3. The results are compared with the adiabatic flame temperature and with the temperature profile for the case without gas radiation. The difference between the latter two lines is an indication for the heat loss necessary for stabilization of the flame. This heat is converted into surface radiation. The difference between the lines for the two limiting cases and the burner-stabilized flame without gas-radiation is an indication for the amount of radiation produced by the hot flue gases. The graph shows that the amount of gas radiation is of the same order of magnitude as the surface radiation and should therefore be incorporated in calculations for the radiative heat transfer. This graph also shows the influence of $d$ and $H$ on the temperature decrease. There is a large difference in the heat loss due to gas radiation between $d = 0$ and $d = \infty$. This is further illustrated in Table 5.1 which lists the average temperature gradient $\Theta$ for the infinite burner and the optical-thin-limit calculations. The average temperature gradient $\Theta$ is calculated between the position $x_{\text{max}}$, at which the gas temperature has a maximum $T_{\text{max}}$, and $H$, where the temperature equals $T_H$, as

$$\Theta = \frac{T_{\text{max}} - T_H}{H - x_{\text{max}}} \quad (5.4)$$

For the infinite burner calculations there is a dependence on the length of the combustion chamber $H$. This dependence is, however, much smaller than the difference between the infinite burner calculations and the optical-thin limit.

The gas radiation also lowers the maximum value of the gas temperature near the flame. This influence ranges between 40 K for the infinite burner calculations and 60 K for the optical-thin-limit calculation. Numerical computations have shown that this effect has no significant influence on the mass burning rate and the internal structure of the flame which is only a few millimeters thick.
5.2. Estimate for the relation between radiative heat loss and burner size

From these preliminary results, it becomes clear that the importance of gas radiation is considerable, and should be taken into account for describing the transport and chemistry in the burnt gases. Besides the dependence of the gas radiation on the height of the combustion chamber $H$, there must be a significant dependence on the burner size $d$ because there is a large difference between the two limiting cases for $d \to 0$ and $d \to \infty$. The nature of these dependences will be investigated in the two following sections. First an estimate will be derived in the next section. This estimate is based on the weighted-sum-of-gray-gases model and is used to check whether the dependence on the geometry is also significant in the region of interest. In Section 5.3, the dependences are further investigated numerically for axi-symmetric situations.

5.2 Estimate for the relation between radiative heat loss and burner size

Although the influence of gas radiation depends on the burner size, it is not clear whether this dependence is also considerable in the region of practical interest: $2 < d < 50$ cm and $5 < H < 20$ cm. This will be investigated by using a simple description based on the Weighted-Sum-of-Gray-Gases model (WSGG-model) [53].

Integration of the RTE (Eq. (3.10)) over a path length $s$, while neglecting the intensity at $s^* = 0$, gives for the intensity at $s$:

$$\tilde{\iota}_\Lambda(s) = \tilde{\iota}_\Lambda^0 (1 - \exp (-k\Lambda s)).$$  \hfill (5.5)
When this relation is inserted in Eq. (3.14), the radiative heat source is given by

\[ S_{rg} = -\int_0^\infty \int_\pi^\pi k_\lambda' b_\lambda \exp (-k_\lambda s) \, d\omega \, d\lambda, \tag{5.6} \]

in which \( s \) depends on the direction associated with the solid angle \( \omega \). On the basis of Eq. (5.6) it is expected that the influence of gas radiation can be expressed in terms of the optical-thin limit scaled by a geometry factor \( C_r \)

\[ S_{rg} = -C_r A k P \sigma T^4. \tag{5.7} \]

The geometry factor \( C_r \) must account for the influence of self absorption. Consequently \( C_r \) should depend on the geometrical dimensions of the post-flame zone: the burner diameter \( d \) and the height of the combustion chamber \( H \). The WSGG-model gives the emission of an isothermal gas volume as a function of its volume and is, therefore, used to give a first approximation of the dependence of \( C_r \) on the geometrical dimensions \( d \) and \( H \).

In the WSGG-model the emission of an isothermal volume of gas is approximated by the emission of three gray gases and one transparent gas [53]. For this purpose absorption coefficients \( k_i \) and relations for weighing factors \( a_i \) for each of the gases are given. The emission can then be calculated using the mean-beam length \( L_e = C_r \frac{V}{A} \) with \( V \) the volume, \( A \) the bounding area and \( C_e \) a constant which is 1 for optical-thin media and 0.9 for absorbing media [52]. Using \( C_e = 1 \) gives for the effective emission \( E_{eff} = E - A \):

\[ E_{eff}(L_e) = \frac{A \sigma T^4}{V} \sum_{i=1}^3 a_i (1 - \exp (-k_i L_e)) = \frac{4 \sigma T^4}{L_e} \sum_{i=1}^3 a_i (1 - \exp (-k_i L_e)). \tag{5.8} \]

The Planck-mean absorption-coefficient can be found from Eq. (5.8), by taking the limit \( L_e \to 0 \) which corresponds to the optical-thin limit. This gives the optical-thin emission \( E_0 \) as

\[ E_0 = E_{eff}(L_e \to 0) = 4 \sigma T^4 \sum_{i=1}^3 a_i k_i \tag{5.9} \]

and the following expression for the Planck-mean absorption-coefficient

\[ k_P = \frac{E_0}{4 \sigma T^4} = \sum_{i=1}^3 a_i k_i. \tag{5.10} \]

The combination of Eqs. (5.7), (5.8) and (5.9) yields the following expression for the geometry factor \( C_r \)

\[ C_r(L_e) = \frac{E_{eff}}{E_0} = \frac{1}{L_e} \frac{\sum_{i=1}^3 a_i (1 - \exp (-k_i L_e))}{\sum_{i=1}^3 a_i k_i}. \tag{5.11} \]

For the axi-symmetric configuration shown in Fig. 5.2 the mean-beam length is given by

\[ L_e = \frac{2 d H}{d + 2 H}. \tag{5.12} \]
5.3. Numerical analysis

Table 5.2: Average temperature gradient $\Theta$ and geometry factor $C_r$ from the 2D simulations for $v_u = 15$ cm/s.

<table>
<thead>
<tr>
<th>$\phi$</th>
<th>$d$ [cm]</th>
<th>$H$ [cm]</th>
<th>$L_e$ [cm]</th>
<th>$\Theta$ [K/cm]</th>
<th>$C_r$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>20.0</td>
<td>10.0</td>
<td>10.0</td>
<td>27</td>
<td>0.38</td>
</tr>
<tr>
<td>0.9</td>
<td>20.0</td>
<td>15.0</td>
<td>12.0</td>
<td>25</td>
<td>0.36</td>
</tr>
<tr>
<td>0.9</td>
<td>10.0</td>
<td>5.0</td>
<td>5.0</td>
<td>40</td>
<td>0.57</td>
</tr>
<tr>
<td>0.9</td>
<td>5.0</td>
<td>5.0</td>
<td>3.3</td>
<td>52</td>
<td>0.74</td>
</tr>
<tr>
<td>0.9</td>
<td>5.0</td>
<td>15.0</td>
<td>4.3</td>
<td>43</td>
<td>0.70</td>
</tr>
<tr>
<td>0.8</td>
<td>20.0</td>
<td>10.0</td>
<td>10.0</td>
<td>25</td>
<td>0.44</td>
</tr>
<tr>
<td>0.8</td>
<td>10.0</td>
<td>5.0</td>
<td>5.0</td>
<td>39</td>
<td>0.64</td>
</tr>
</tbody>
</table>

The results for Eqs. (5.11) and (5.12), are shown in Fig. 5.4 as a function of $H$ for various $d$ and compared to the results from Table 5.1. The geometry factors in Table 5.1 have been determined by comparing the average temperature decrease of the 1D simulations to the corresponding values for 1D flames using the scaled optical-thin-limit (Eq. (5.7)). The results from the 1D calculations using the wide-band model from Table 5.1 lead to lower geometry factors than the WSGG-model. It must be noted that the WSGG model can only give an estimate and is not intended as a quantitative model. It does, however, reproduce the dependence of $C_r$ on $H$ as found for the 1D results. Besides that, from a comparison between the results for $d = 2$ and 20 cm, it follows that there is a significant dependence on the burner diameter $d$. This dependence cannot be modeled using the 1D model, because in the 1D geometry the burner surface is assumed to be unbounded. The dependence of the gas radiation on the burner diameter $d$ should be taken into account. As the estimate using the WSGG model is not accurate enough, this dependence is determined using 2D simulations in the next section.

5.3 Numerical analysis

In the two previous sections, it has been found that the radiative heat loss of the flue gases depends strongly on the burner diameter $d$ and the height of the combustion chamber $H$. In this section this dependence is investigated in more detail using the 2D numerical model presented in Chapter 2. For this investigation round burners, as in the configuration shown in Fig. 5.2, are simulated and the average temperature gradient $\Theta$ of the flue gases is compared to the average temperature gradient of 1D flames with the scaled optical-thin-limit (Eq. (5.7)). In these simulations the diameter $d$, the height of the combustion chamber $H$ and the equivalence ratio $\phi$ are varied. The values which are used are listed in Table 5.2.

The radiation and flow grids used in the simulation for $d = 20$ cm, $H = 10$ cm, $v_u = 15$ cm/s and $\phi = 0.9$ are shown in Figs. 5.5 and 5.6. The flow grid is a rectangular grid of 164 by 60 cells which is refined near the burner surface and at the side wall. The absorption coefficients which are used in this simulation are shown in Fig. 5.7.
Figure 5.5: Grid on which the radiation is solved for the simulation with \( d = 20 \text{ cm} \) and \( H = 10 \text{ cm} \).

Figure 5.6: Grid on which the flow and combustion equations are solved for the simulation with \( d = 20 \text{ cm} \) and \( H = 10 \text{ cm} \).

Figure 5.7: Gray bands and absorption coefficients used for the simulation with \( d = 20 \text{ cm} \) and \( H = 10 \text{ cm} \).

Figure 5.8: Temperature distribution for \( d = 20 \text{ cm} \), \( H = 10 \text{ cm} \), \( v_u = 15 \text{ cm/s} \) and \( \phi = 0.9 \).
Figure 5.9: Temperature distribution along the axis for $\nu_a = 15$ cm/s and $\phi = 0.9$ for $(d,H)$ in cm (solid lines). The temperature profiles are compared to the temperature profiles of 1D flames using the scaled optical-thin limit with $C_r = 0$, 0.38 and 1 (dashed lines).

The calculated temperature distribution above the burner is shown in Fig. 5.8. The burner is not shown in the graph but has been included in the simulation as shown in Fig. 5.6. The flame itself cannot be observed on the graph but is captured on the fine grid around the burner surface. In the flue gases two regions can be identified, a hot central core and a cold thermal boundary layer at the side wall. The gases in the boundary layer are rapidly cooled by convection, whereas the hot core is slowly cooled by radiation. In the central core the isotherms only show a small curvature, indicating that the central core is almost a 1D situation. The radiation grid is coarse, which is reflected in the isotherms.

The determination of the geometry factor $C_r$, for use in 1D flames with the scaled optical-thin-limit, is based on the temperature profile along the axis. These temperature profiles are shown for some geometries for $\phi = 0.9$ in Fig. 5.9. As in Fig. 5.3, the profiles are compared to the temperature profile for the flame without gas radiation ($C_r = 0$) and the optical-thin limit ($C_r = 1$). Comparing the results of the 2D model to the results of the 1D model, shows that the maximum flame temperatures are slightly underpredicted by the 2D model. This must be attributed to the FGM calculation (see Section 2.4).

From the profiles along the axis, the average temperature gradient $\Theta$ has been determined using Eq. (5.4). These values have been used to determine geometry factors $C_r$ as has been done for the 1D results in Table 5.1. The resulting $\Theta$ and $C_r$, are listed in Table 5.2 for all simulations. The profile for $d = 20$ cm and $H = 10$ cm has an average temperature gradient of $\Theta = 27$ K/cm, which is also found for a 1D simulation using $C_r = 0.38$. For visualizing the comparison, this latter profile is also plotted in Fig. 5.9.

From the results in Table 5.1, it follows that the geometry factor is a decreasing function of both $d$ and $H$. It has been found that the results correlate best using the mean-
beam length (Eq. (5.12)) which combines these two parameters. This is shown in Fig. 5.10, which combines the results from the 2D simulations (Table 5.2) and the 1D simulations (Table 5.1). This graph also shows the results from the WSGG estimate of the previous section (Fig. 5.4). The results of the 2D simulations have a similar shape as Eq. (5.11), and the results are, therefore, fitted to a similar function given by:

\[
C_r (L_e) = \frac{1}{L_e} \left( \frac{1 - \exp (-k_{r1} L_e) + a_r (1 - \exp (-k_{r2} L_e))}{k_{r1} + a_r k_{r2}} \right)
\] (5.13)

with \( k_{r1} = 0.287 \text{ cm}^{-1} \), \( k_{r2} = 0.00217 \text{ cm}^{-1} \), and \( a_r = 26.2 \). This fit is shown in Fig. 5.10 as well.

In Eq. (5.7) it is assumed that all the influences on the operating conditions are covered by the Planck-mean absorption-coefficient. The influence of the inlet velocity \( v_a \) on \( C_r \) is negligible as is shown in an earlier study [31]. The equivalence ratio has been varied in the simulations from 0.9 to 0.8. The results for \( C_r \) for \( \phi = 0.8 \) are slightly higher when compared to the results for \( \phi = 0.9 \) (see Table 5.2), but the difference is within the scatter of the results and is, therefore, neglected.

From the results in Fig. 5.10, it can be concluded that, for an accurate description of gas radiation, 2D effects should be taken into account. However, limiting the problem to 1D reduces the computational effort enormously. The magnitude of the geometry factor can be used to calculate the accuracy of the calculation. For this reason, Eq. (5.13) can be used to judge whether the approximation of the gas radiation using the optical-thin limit or using 1D radiation models is satisfactory. When the gas radiation is calculated
with the optical-thin limit, the difference between the actual temperature gradient and the calculated gradient is given by $1 - C_r(L_e)$. The relative error in the gradient following from a simulation using the optical-thin limit would then be equal to $1 - C_r(L_e)$ as well. It depends on the required accuracy whether this is acceptable or not, but when the required accuracy is, for example, 10%, this limits the applicability of the optical-thin limit to geometries with $L_e < 1$ cm.

The accuracy of a 1D model can be compared using Eq. (5.13) as well, i.e. by comparing the geometry factors calculated with the 2D mean-beam length (from Eq. (5.12)), to those using the 1D mean-beam length ($L_e = 2H$). The relative error for the temperature gradient $\Theta$ from the simulation using the 1D radiation-model is then given by

$$\frac{\Delta \Theta}{\Theta} = \frac{C_r(L_e) - C_r(2H)}{C_r(2H)}$$

(5.14)

For $H = 5$ cm the relative error is less than 10% for $d > 49$ cm. For larger $H$ this value is even higher, and it can be concluded, that by using a 1D radiation-model, the effect of self-absorption is significantly overestimated.

### 5.4 Experiments

In the previous section a relation for the geometry factor $C_r$ has been derived from the results of numerical simulations. In this section these results are compared with experimental results. For a direct comparison, experiments should be performed for the configuration...
shown in Fig. 5.2. This setup is, however, not available. Instead, experiments have been performed on burners operating in an open environment. For such a configuration the influence of gravity will lead to an increase of the velocity of the flue gases near the axis, due to the density differences between the hot and cold zones. This influence of gravity is investigated first using numerical simulations of burners in a configuration shown in Fig. 5.11. In this configuration the burner is surrounded by a co-flow of cold flue-gases. This co-flow is not present in the experiments but is added for numerical stability. It does not influence the temperature distribution in the core of the hot region.

A burner having a diameter of 10 cm operated at \( v_u = 14.6 \text{ cm/s} \) and \( \phi = 0.9 \) has been simulated with and without the effect of gravity. The temperature distributions of these simulations are shown in Fig. 5.12. The influence of gravity can be seen clearly from the differences in the shapes of the isotherms in the two results. In the case with gravity, the hot flue gas cone is contracted due to acceleration caused by density differences. Due to the higher velocities the temperature gradient is smaller for the case with gravity included.

Figure 5.12: Temperature distribution for a round burner with \( d = 10 \text{ cm} \)
for \( v_u = 14.6 \text{ cm/s} \) and \( \phi = 0.9 \) without (left plot) and with gravity (right plot).
5.4. Experiments

Figure 5.13: Measured temperature distribution along the axis (crosses) and from calculations with (dashed line) and without gravity (solid line) for \( v_\text{u} = 14.6 \text{ cm/s}, \phi = 0.9 \) and \( d = 10 \text{ cm} \).

Figure 5.14: Temperature distribution along the axis from measurements for \( v_\text{u} = 14.6 \text{ cm/s} \) and \( \phi = 0.9 \) for round burners of \( d = 20 \text{ (crosses)}, 10 \text{ (stars)} \) and \( d = 3 \text{ cm (squares)} \) and a square burner of size 11.4 cm (dots).
However, based on a residence time comparison of these two simulations, this effect should be more pronounced: the acceleration effect is partly compensated by extra radiative heat loss due to the smaller diameter of the hot cone. The temperature profiles at the axis are shown for the two cases in Fig. 5.13. From a comparison between the two curves, one finds that the difference between the slopes of the two profiles is less than 10% for $h < 3.5$ cm. The experimental results are only considered up to this height of $h = 3.5$ cm because the influence of the gravity becomes too large above this region.

Two round ceramic foam burners of $d = 10$ cm and 20 cm, one square ceramic foam burner of size 11.4 cm and a round water cooled-burner with $d = 3$ cm are used. The temperature profiles are measured using thermocouples as these provide a fast and reproducible means of temperature determination. The readings are corrected for radiative heat losses. The conductive heat losses are minimized by using thin couples with a large length diameter ratio. Based on the results in Chapter 4, the uncertainty in the temperatures is about 50 K, but the error in the temperature gradient is smaller.

Besides the uncertainty in the measured temperature, errors are caused by the mass-flow controllers, measurement of the burner surface and the position of the measurement. The combination of the uncertainties of the mass-flow controllers and the burner surface gives an absolute error for the inlet velocity of $\pm 0.6$ cm/s. For the equivalence ratio, which is determined by the two mass-flow controllers, the uncertainty is 4%. The absolute error in the position is about 1 mm. This is due to the difficulty in the determination of the position with respect to the burner surface, because the burner surface of the ceramic-foam burners is quite irregular. The uncertainty in the relative distance of the measuring points is much smaller, about 0.1 mm.

First the measured temperature profile of the burner with $d = 10$ cm operated at
5.4. Experiments

Table 5.3: Average temperature gradient $\Theta$ and the geometry factor $C_r$ from the experiments.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>$\phi$ [-]</th>
<th>$d$, $L$ [cm]</th>
<th>$H$ [cm]</th>
<th>$\Theta$ [K/cm]</th>
<th>$C_r$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Round</td>
<td>0.90</td>
<td>10</td>
<td>3.5</td>
<td>36.2</td>
<td>0.51</td>
</tr>
<tr>
<td>Round</td>
<td>0.90</td>
<td>20</td>
<td>3.5</td>
<td>35.8</td>
<td>0.51</td>
</tr>
<tr>
<td>Round</td>
<td>0.90</td>
<td>3</td>
<td>1.5</td>
<td>73.3</td>
<td>1.18</td>
</tr>
<tr>
<td>Square</td>
<td>0.90</td>
<td>11.4</td>
<td>3.5</td>
<td>29.0</td>
<td>0.41</td>
</tr>
<tr>
<td>Round</td>
<td>0.80</td>
<td>10</td>
<td>3.5</td>
<td>34.8</td>
<td>0.54</td>
</tr>
</tbody>
</table>

$v_u = 14.6 \text{ cm/s}$ and $\phi = 0.9$ is compared to the results of the simulations with and without gravity in Fig. 5.13. The temperature profile from the measurement agrees reasonably well with the calculated profile from the simulation including the gravity. It can be concluded that the model reproduces the measurements within the experimental uncertainty. The temperature decrease in the experimental results is, however, smaller than found in the numerical simulation. This might be caused by a higher self-absorption of radiation, but could as well be caused by a higher acceleration due to the density differences. This latter effect can be influenced by the differences between the configurations used for the experiments and the simulations.

The measured temperature profiles of the four different burners for $v_u = 14.6 \text{ cm/s}$ and $\phi = 0.9$ are shown in Fig. 5.14. Note that the temperature profile for the small burner is much steeper than for the other three burners. Also the slope of this profile increases with distance $h$, whereas for the other burners the slope of the profile decreases with distance. For this reason, care must be taken in the comparison to exclude the influence of the convective mixing. The other three burners show less difference. The temperature drop of the square burner is slightly less than that of the round burner of 10 cm. The slopes of the temperature profiles and the corresponding geometry factors, which are determined by comparing the average temperature gradient $\Theta$, are shown Table 5.3. The geometry factor for $d = 3 \text{ cm}$ is higher than unity, indicating that another cooling mechanism besides gas radiation is present. This is probably the influence of convection.

For a comparison of the experimental results to the results of the previous section, a mean-beam length has to be defined. The height of the hot gas volume is, however, unknown. From Fig. 5.12, it is concluded that the hot gas volume is a cone with a base diameter equal to the burner diameter and a height which is, roughly, two times the burner diameter. The mean-beam length for the round burners is then given by

$$L_e \approx \frac{8}{15} d.$$  \hspace{1cm} (5.15)

A similar, rectangular, equivalent is defined for the square burner, for which the mean-beam length is approximated as

$$L_e \approx \frac{8}{15} L.$$  \hspace{1cm} (5.16)

The geometry factors are plotted in Fig. 5.15 as a function of these mean-beam lengths.
and compared to the fit from the simulations (Eq. (5.13)). These mean-beam lengths are not well defined because they depend on $H$ which is unknown. For this reason the values are plotted using a relative error in the mean-beam length of 20%. This corresponds, for example, to using $H = d$ instead of $H = 2d$. The error in the geometry factor $C_r$ is estimated to be $\pm 0.1$. The clear dependence on the mean-beam length which is found in the numerical results is not found in the experimental values. It must, however, be noted that the variation in mean-beam length is not as large as in the numerical results. The magnitude of the geometry factors, except for $d = 3$ cm, is in agreement with the numerical results. The value for the square burner is much less than the result for the, comparable, round burner with $d = 10$ cm. Generally, the experimental results do not contradict the numerical results, but the dependence of the geometry factor $C_r$ on the mean-beam length $L_e$ cannot be confirmed, because of the poor definition of the mean-beam length.

By comparing the results from Table 5.3 to the results in Table 5.1, it follows that the optical-thin limit would not give accurate temperature profiles for these configurations. This affirms the conclusions of the previous section. Using a 1D model with $H = 4$ cm, see also Table 5.1, would give more accurate values. This 1D configuration shows, however, little resemblance with the experimental configuration and would, therefore, not be selected a priori.

5.5 Discussion

The temperature in the post-flame zone of a premixed flame is significantly influenced by gas radiation. From the numerical results it follows that for small combustion chambers, with $L_e > 1$ cm, the difference between the temperature gradient for the optical-thin limit and the 2D results is already more than 10%. This difference is caused by self absorption of radiation by the flue gases. Using 1D radiation models includes this self absorption, but overestimates its effects significantly.

For obtaining a higher accuracy in the temperature profile it is recommended to solve the complete 2D or 3D radiation problem. This is also recommended when gravity distorts the flow too much or when the flow is otherwise distorted by the application. If this is not possible or desired, it can be useful to model the gas radiation using the scaled optical-thin-limit (Eq. (5.7)) with the geometry factor given by the fit derived from the numerical results (Eq. (5.13)). Even though Eq. (5.13) is a fit, and Eq. (5.7) does not capture all the physics of the radiation problem, this scaled optical-thin-limit model is capable to describe the results for both the 1D simulations and the 2D simulations for different operating conditions. It provides a simple way to incorporate the effect of self-absorption while keeping a moderate accuracy, and can be used for other premixed burners and flamelet models as well. However, from the volume of the hot flue gases an appropriate mean-beam length has to be determined.
Chapter 6

Flash-back of laminar premixed flames in ceramic-foam surface burners

In the radiant mode, the flame stabilizes as a flat flame at the burner surface. The stabilization of this flame is based on heat transfer from the flame to the burner and from the burner to the environment. When part of this heat transfer cannot be realized stabilization of the flame is not possible and the flame propagates into the foam. As the flame reaches the upstream face of the foam, the unburnt mixture in the plenum is ignited. This is known as flash-back and limits the application of radiant surface burners.

Flash-back has already been studied by Bouma [7]. Bouma based his research on simple analytical models for the flame and did not consider the effect of enhanced flame propagation when the flame stabilizes deeper in the foam. In this chapter, detailed analysis, based on the detailed interaction of the flame and the foam using complex chemistry and radiation, is presented. It is shown that the enhanced propagation at deep stabilization plays a dominant role in the flame flash-back mechanism.

In this chapter the flash-back phenomenon is investigated using 1D numerical simulations, both steady-state and time-dependent. First, the stabilization of flames in a hot environment is compared to the stabilization of flames in a cold environment in Section 6.1. For some conditions it is not possible to obtain steady-state solutions and the behavior of the flame at these conditions is investigated using transient simulations in Section 6.2. These transient simulations show that flash-back occurs and indicate that flash-back can be related to the presence of the ceramic foam. Therefore, flames submerged in a ceramic foam are studied in Section 6.3. For a further understanding of the stabilization process, steady-state solutions are used to construct stabilization diagrams for both hot and cold environments in Section 6.4. The diagrams are similar to those presented in [48], but show more detail near the burner surface. Based on these stabilization diagrams, combustion regimes with and combustion regimes without steady-state solutions can be found in the parameter space. In Section 6.5, the stability diagrams are used to determine the stability limits of the burner. The chapter is concluded with a discussion in Section 6.6.
Figure 6.1: Flame stabilization on a ceramic-foam surface burner in a cold environment ($T_{\text{env}} = 293$ K, solid line) and in two hot environments ($T_{\text{env}} = 750$ K, dashed line, $T_{\text{env}} = 775$ K, dotted line) for $\phi = 0.9$. 
6.1 Stabilization at the downstream surface of the ceramic foam

In Chapter 2, a mechanism has been proposed to understand the stabilization of flat flames on ceramic-foam surface burners. The basis of this mechanism is that the burning velocity of the flame is determined by enthalpy loss of the flame to the burner. Consequently, there is a unique relation between the flame temperature and the burning velocity. This relation has already been observed in the past [7, 27] and more recently in [40]. In this section this enthalpy-loss mechanism will be compared with the results of ceramic-burner stabilized flames in both cold and hot environments. The results considered are the flame temperature $T_b$, the heat loss $q$ of the flame and the flame position $x_F$.

On the basis of the enthalpy-loss mechanism one would expect the flame temperature $T_b$ to be a rising function of the inlet velocity $v_u$, see [27], as

$$v_u = k \exp \left( -\frac{E_a}{2RT_b} \right).$$

The heat loss of the flame $q$ is the product of the mass flow and the enthalpy. The latter is only a function of the flame temperature which gives a direct relation between $q$ and $T_b$. The heat loss $q$, however, provides additional information as it is equal to the gas-solid convective heat transfer and the radiative heat transfer from the burner to the environment. The heat loss is given by [7]

$$q = \rho v \int_{T_b}^{T_{ad}} c_p dT = \int_{-L}^{0} h_v (T - T_s) dx = \varepsilon \sigma \left( T_{sr}^4 - T_{env}^4 \right).$$

Consequently, $q$ shows a maximum and is zero at $v_u = 0$ and at $v_u = s_L$.

The results for $T_b$, $q$ and $x_F$ are shown in Fig. 6.1 for a cold environment and two hot environments. For the cold environment the flame temperature rises and can be fitted to Eq. (6.1) with $E_a = 265 \text{ kJ/mol}$ and $k = 54.0 \cdot 10^3 \text{ cm/s}$ within an uncertainty of 1 cm/s. The curve for the heat loss $q$ can be derived from the flame temperature $T_b$. The results for the flame position $x_F$ show that there is no direct relation between the flame position and the heat loss of the flame; the maximum heat loss occurs around $v_u = 13 \text{ cm/s}$, whereas the stabilization point which is most upstream occurs at $v_u = 19 \text{ cm/s}$.

The enthalpy-loss mechanism can indeed explain the results for the cold environment. However, the mechanism cannot be used to predict the results for the hot environments. If this mechanism is valid, the temperature should only be a function of the inlet velocity, i.e. Eq. (6.1) should be valid independent of $T_{env}$. So there should be no difference in the flame temperature and the heat loss between the hot and cold environments. This is the case for the lower velocities ($v_u < 15 \text{ cm/s}$) but not for the intermediate range ($15 < v_u < 22 \text{ cm/s}$) and high velocities ($v_u > 22 \text{ cm/s}$) as shown in Fig. 6.1. At high velocities the results for the hot environment show higher flame temperatures. In the medium range, no steady-state solutions can be found for the hottest case and for the 750 K case the flame temperatures are significantly lower. The differences that are found for the flame temperature are more pronounced in the results for the heat loss. Especially in the intermediate region, the difference between the cold and hot cases is clear.
Figure 6.2: Flame temperature (solid line) and position (dashed line) as a function of the radiating temperature of the environment for \( v_u = 20 \text{ cm/s} \) and \( \phi = 0.9 \).

The influence of the radiating temperature of the environment on the flame temperature and the flame position is further illustrated in Fig. 6.2. This graph shows these quantities as a function of the radiating temperature of the environment for a single inlet velocity \( v_u = 20 \text{ cm/s} \). At low temperatures \( T_{env} < 500 \text{ K} \) there is hardly any influence on the flame temperature. The flame moves into the burner, but this can be expected from the higher burner surface temperature. For high temperatures \( T_{env} > 600 \text{ K} \) the flame temperature drops sharply and the rate of change of \( x_F \) increases. The results show that for a higher radiating temperature of the environment, the flame temperature drops. This indicates that the flame has to be cooled more to stabilize the flame. More cooling requires the flame to stabilize further upstream, which is indeed observed. More cooling also indicates that the difference between the inlet velocity and the adiabatic burning velocity grows with the radiating temperature of the environment. As the inlet velocity is constant, this requires the adiabatic burning velocity to rise.

The drop of the flame temperature, and thus the higher adiabatic burning velocity, as a result of the higher environment temperature cannot be explained by the enthalpy-loss mechanism. According to this mechanism only a single combination of inlet velocity and flame temperature should exist. So there must exist another influence which has not yet been accounted for. As the environment radiation does not act on the flame itself the influence must be expressed through the burner. The results that have been observed can be explained when the burner accelerates the flame movement and that this effect increases when the flame moves further upstream.

From the results of this section it follows that Eq. (6.1) is not sufficient to describe the stabilization of flat flames in a hot environment, but that the burner accelerates the flame for certain conditions. Furthermore, it is found that for some conditions steady-state
solutions cannot be obtained and that the differences between results for the hot and cold cases are most obvious close to these conditions. These results can be explained when the adiabatic burning velocity depends on the flame position. In the next sections these results will be investigated further. In Section 6.2, transient simulations, at a condition where no steady-state solution can be found, are presented. These simulations show that flash-back indeed occurs and that the ceramic foam greatly influences the adiabatic burning velocity. This latter effect is further investigated in Section 6.3, where flames submerged in a ceramic foam are studied. In Section 6.4, Fig. 6.1-c is extended to flames inside the ceramic foam. From these results the range of velocities for which steady-state solutions are possible, can be determined.

6.2 Transient simulations

In the previous section it has been observed that for certain operating conditions steady-state solutions cannot be obtained. In this section transient simulations are used to study what happens to flames when the burner is operated at these conditions.

The simulations are performed using an implicit time-integration scheme. The time step used should be lower than the typical time scale of the process. The time scale of the flame can be approximated by the ratio of the reaction-zone thickness $\delta$ and the adiabatic burning velocity $s_L$.

$$\tau_F = \frac{\delta}{s_L} = \frac{\lambda}{\rho s_L^2 c_p} \approx 10^{-3} \text{ s.}$$

(6.3)

This shows that the time step used should be no more than approximately $10^{-1}$ s. The
Figure 6.4: Gas (solid line) and solid (dashed line) temperatures upon changing the environment radiating temperature from 750.0 to 775.0 at $v_w = 20.0$ cm/s for $\phi = 0.9$. The ceramic foam is located between $x = -1$ and 0 cm.

Figure 6.5: Gas (solid line) and solid (dashed line) temperatures upon changing the inlet velocity from 16.0 to 20.0 cm/s at $T_{env} = 775.0$ K for $\phi = 0.9$. The ceramic foam is located between $x = -1$ and 0 cm.
6.2. Transient simulations

**Figure 6.6:** Flame response after changing the environment radiating temperature from 750.0 to 775.0 K at \( u_a = 20.0 \) cm/s (solid lines) and upon changing the inlet velocity from 16.0 to 20.0 cm/s at \( T_{env} = 775.0 \) K (dashed lines) for \( \phi = 0.9 \).
total simulation time, however, depends on the largest time scale which is the time scale for heating the ceramic material. This time scale is related to the length scale \( \delta_s \) of the flame in the ceramic foam, which is given by

\[
\delta_s = \frac{\tau_s \lambda_s}{\rho s_L c_p} \approx 10^{-2} \text{ m.} \tag{6.4}
\]

The time scale for heating the ceramic material is given by

\[
\tau_C = \frac{\delta_s^2 \rho_s c_{ps}}{\tau_s \lambda_s} \approx 10^2 \text{ s.} \tag{6.5}
\]

The total simulation time should be in the order of \( 10^2 \) s which would make a total of about \( 10^6 \) time steps necessary to simulate the flash-back process. For this reason we chose to use a quasi-steady-state approach instead. In this approach the response in the flame is assumed to be instantaneous so that the time derivatives of the flame equations can be omitted. Only the time derivative of the solid temperature is taken into account and the time step can be based on the time scale of this process.

First, the results of a transient simulation without flash-back are compared to experiments to validate the time integration of the 1D code and to check values which are used for the physical properties of the ceramic foam. Figure 6.3 shows the burner-surface temperature resulting from the transition from \( v_a = 7.2 \) to 9.0 cm/s. The surface temperature has been measured using a pyrometer and is corrected for the emissivity of the burner surface. When the velocity is increased, the burner-surface temperature rises sharply. In the numerical simulation the response is instantaneous, but in the experiment a time delay is present due to the reaction time of the mass flow controllers and the length of the tubes between the controllers and the burner. Furthermore, there is a significant difference between the experimental and the numerical final burner-surface temperature of about 45 K. This difference can be attributed to the influence of gas radiation. The hot flue gases radiate to the burner surface leading to a higher burner surface temperature, measured by the pyrometer. This effect has not been incorporated in the simulations. For a better comparison of the numerical and experimental results, the experimental curves are compensated for these two effects by shifting the curve 4.5 s to the left and 45 K down. After these compensations the results show good agreement. The sharp rise in burner surface temperature is followed by a gradual descent to the final value. As the gas velocity is increased the amount of heat transferred from the flame to the burner must increase (see Figs. 2.4 and 6.1-a). This extra heat transfer is concentrated in the top layer of the foam where the temperature difference between the gas and the solid is largest. Consequently the top layer is heated up rapidly and then the heat is redistributed over the foam.

From the comparison of the experimental and numerical results in Fig. 6.3, it follows that the 1D transient model, including the quasi-steady-state approach, gives a good representation of the transient interaction between the burner and the flame. It is, therefore, concluded that this model can be used for the transient simulations in this study.

In the previous section, no steady-state solutions could be found for a radiating temperature of the environment for inlet velocities between \( v_a = 18 \) and 23 cm/s. To check
whether there are indeed no steady-state solutions in this region, two transient simulations are presented with the burner operating conditions of \( v_u = 20 \text{ cm/s} \) for \( \phi = 0.9 \) at an environment radiation temperature of \( T_{env} = 775.0 \text{ K} \). The difference between these two simulations are the starting conditions. Both starting conditions are steady-state solutions presented in the previous section.

The first simulation starts at the steady-state solution with \( v_u = 20 \text{ cm/s} \) and \( T_{env} = 750 \text{ K} \). Flash-back is indeed observed in this simulation. This is clearly shown in Fig. 6.4 which shows the gas and ceramic temperature profiles during the simulation. Initially the ceramic material heats up and the flame moves slowly into the solid material. After approximately 80 s, an acceleration starts and then the flame propagates relatively fast through the burner. Finally a stationary solution is reached close to the downstream surface. In practice, the radiative heat transfer at the downstream surface will probably heat up the plenum and ignite the fresh mixture leading to fracture of the burner. This effect has not been included in the model as the inlet absorbs all radiation coming from the burner. It is also possible that the prevailing temperatures of 1500 K lead to fracture during the flash-back. The ceramic foam is designed for lower operating temperatures.

The second simulation starts at the steady-state solution for \( v_u = 16 \text{ cm/s} \) and \( T_{env} = 775 \text{ K} \) and the results are shown in Fig. 6.5. The results are similar to the results for the first simulation except that the acceleration starts at approximately 5 s, which is much earlier than in the first simulation. This large difference in response time is the time required to heat up the burner surface by the radiation from the environment in the first simulation. Eventually this leads to an upstream movement of the flame. In the second simulation the movement of the flame is a response to the changed inlet velocity of the flame itself. The flame response is much faster but eventually both simulations reach the same final situation. The flash-back process is further illustrated by Fig. 6.6 which shows the convective and radiative heat transfer at the burner and the flame position for both simulations. The results of the second simulation have been plotted with a time delay of 45.3 s. Using this time delay, the profiles give a perfect fit for \( t > 60 \text{ s} \). The two simulations only differ in the initial phase, which is, of course, determined by the initial condition.

Figures 6.6-b and c indicate that in the initial phase the convective heat transfer rises slowly, but it increases rapidly when the flame moves further into the burner. The radiative heat at the downstream surface rises as well, but cannot compensate the rise in the convective heat transfer. In the final part of the process the flame reaches the upstream surface which makes the radiative heat transfer rise significantly. Finally, the radiative heat transfer is large enough to compensate the convective heat transfer and the propagation of the flame is stopped.

The reason why flash-back occurs can be found from the results in Fig. 6.6. In the initial situation, which is a steady-state situation, there is a balance between the radiative and convective heat transfer. Due to the change in operating conditions, the convective heat transfer is larger than the radiative heat transfer and this will heat up the burner. As the burner heats up, the radiative heat transfer rises and the flame moves upstream. However, as the flame moves upstream, the convective heat transfer rises rapidly. It rises much more rapidly than the radiative heat transfer and this makes it impossible to find
a new equilibrium. Only when the flame reaches the upstream surface, the radiative heat transfer rises. However, this rise is only due to the heat transfer at the upstream surface (see Fig. 6.6-c) and then flash-back has already occurred. Central in the explanation is that the convective heat transfer rises when the flame moves into the burner. This has to be related to a raise in the adiabatic burning velocity inside the burner. This will be investigated in the next section.

### 6.3 Flames inside ceramic foam

The reason for the increase in the convective heat transfer when the flame moves into the burner must be related to the presence of the solid phase. Flames submerged in a ceramic foam are known to have a larger adiabatic burning velocity [48]. The studies in the literature have been performed using foams with different properties. Therefore, flames submerged inside the ceramic foam will be studied in this section. This investigation is performed using the 1D model described in Chapter 2 with the solid phase present in the complete computational domain. The system is made adiabatic by omitting the radiating surfaces and by changing the boundary conditions of the ceramic-foam temperature into the same boundary conditions as that are used for the gas-temperature.

The gas and ceramic-foam temperature profiles for an adiabatic premixed methane/air flame are shown in Fig. 6.7. When these profiles are compared with the temperature profile of an ordinary adiabatic flame one finds that the presence of the ceramic foam results in a much broader flame zone. The gas is heated up by the ceramic foam in the preheating zone and cooled in the post-flame zone. Conduction and radiation in the ceramic foam contributes to the upstream heat transfer. These effects result in a much higher burning
6.3. Flames inside ceramic foam

Figure 6.8: Adiabatic burning velocity for a flame submerged in a ceramic foam as a function of the ceramic-foam conductivity (dashed line) and extinction coefficient (solid line) for $\phi = 0.9$.

Figure 6.9: Adiabatic burning velocity for a flame submerged in a ceramic foam as a function of the ceramic-foam volumetric heat-transfer coefficient (solid line) and the porosity (dashed line) for $\phi = 0.9$. 
velocity of 81.2 cm/s as compared to 32.0 cm/s for an adiabatic flame without the ceramic foam present. The actual burning velocity depends strongly on the ceramic-foam properties: the conductivity $\lambda_s$, the extinction coefficient $K$, the volumetric heat transfer coefficient $h_v$, and the porosity $\chi$. The influence of these parameters is shown in Fig. 6.8 and Fig. 6.9. The influence of the conductivity and the reciprocal of the extinction coefficient is similar. The reason for this is that, in an optical thick medium, the influence of the radiation can be expressed as an effective conductivity, using the Rosseland diffusion model, given by [52]

$$\lambda_{rad} = \frac{16\sigma T^3}{3K}. \tag{6.6}$$

The volumetric heat transfer coefficient determines the difference between the gas and ceramic-foam temperatures. For $h_v = 0$ the ceramic foam has no influence except for the porosity. For $h_v \to \infty$ the gas and ceramic-foam temperature profiles become identical, leading to a maximum value for the burning velocity in Fig. 6.9. This graphs also shows that the porosity has a very small influence on the adiabatic burning velocity.

As for ordinary flames the burning velocity can be influenced by cooling of the flame by a burner. The burner is modeled as a perfectly cooled burner by applying the condition

$$T = T_s = T_{burner} \text{ at } x \leq 0. \tag{6.7}$$

The flame is then stabilized for a given inlet velocity $v_u$ by heat loss to the burner. The effect of heat loss on the burning velocity for flames submerged in a ceramic foam and for flames without the presence of a ceramic foam, is shown in Fig. 6.10. Both lines show a similar increase of the flame temperature with the inlet velocity, but the distance between the two lines is rather large. When a flame has to be stabilized at a certain inlet velocity,
the amount of cooling which has to be applied to stabilize the flame submerged in the ceramic foam is much higher than the cooling which has to be applied to stabilize a flame without the presence of the ceramic foam.

Figure 6.10 gives a preliminary explanation for the results found in the previous sections. The rise in the convective heat transfer as the flame enters the burner, can be explained from the larger difference between the adiabatic burning velocity for flames inside and outside the ceramic foam.

6.4 Stability diagrams

When a flame submerged in a ceramic foam is cooled, it can be stabilized at a certain position. In the absence of other cooling mechanisms, the cooling has to be established by radiative heat transfer at the surfaces of the foam with the environment. This implies that for each velocity two stabilization points can be found inside the burner, one with the radiative heat loss primarily at the upstream face and one with the radiative heat loss primarily at the downstream face. Furthermore, stabilization outside the foam surface is also possible. So for $u < s_L$ three stabilization points can be found.

These stabilization points are combined, for a cold environment, into a stabilization diagram as shown in Fig. 6.11. This graph shows that, besides the stabilization curve which was already shown in Fig. 6.1-c, there is another stabilization curve inside the ceramic material. This curve consists of submerged flames which are cooled by radiative heat transfer at the two faces of the burner. Flames can stabilize deep inside the burner at inlet velocities close to the adiabatic burning velocity of 81.2 cm/s of a submerged flame. Closer to the edges of the burner the cooling is larger enabling flames to stabilize on lower inlet velocities. At some positions two different flames with different mass burning rates can stabilize, one with a large enthalpy loss but low mass-flow rate and one with a lower enthalpy loss but a higher mass-flow rate. This is the case for both the curve inside the foam and the curve outside the foam. Solutions have not been found for $u < 10$ cm/s for flames deep in the ceramic foam. This can be caused by extinction, but this has not been investigated yet.

A similar diagram as Fig. 6.11 has been presented earlier by Sathe et al. [48]. They do not discriminate between the curve inside and outside the ceramic material and they do not mention the lower branches of the curves.

When the same stability diagram is constructed for a hot environment, both the curve inside the foam and the curve outside the foam are shifted towards each other near the downstream surface of the burner. This is shown in Fig. 6.12. For the hottest case, however, the curves inside and outside the foam are split and recombined into two separate curves for stabilization at low and high velocities. The connections between the curves at the inside and outside of the ceramic foam have been found by specifying the gas temperature at one point, while varying the inlet velocity until a converged solution is found. Solutions which are obtained in this way do not differ from the solutions found by fixing the inlet velocity.

From the stabilization diagram it can be concluded that the absence of steady-state
Figure 6.11: Stabilization diagram for flames stabilized in and on a ceramic-foam surface burner in a cold environment (environment radiating temperature $T_{env} = 293$ K).
6.4. Stability diagrams

![Stability Diagram](image)

**Figure 6.12:** Stabilization diagram for flames stabilized in and on a ceramic-foam surface burner in a cold environment \(T_{env} = 293 \, \text{K}, \) solid line) and in two hot environments \(T_{env} = 750 \, \text{K}, \) dashed line, \(T_{env} = 775 \, \text{K}, \) dotted line) for \(\phi = 0.9.\)

solutions in the intermediate velocity range for the hottest case has a physical significance. The stabilization diagram also provides the opportunity to find the window for which a steady-state solution cannot be found at \(T_{env} = 775 \, \text{K}.\) This window is also shown in Fig. 6.12.

The flame position curve in Fig. 6.1 can be explained from Fig. 6.11, as the latter is an extension of the former. The large upstream shift of the flame position is in fact related to the transition from the stabilization curve outside the foam to the stabilization curve inside the foam.

Based on the difference between the two stabilization diagrams the following mechanism is proposed. The flame must transfer heat to the burner to stabilize by means of enthalpy loss. When this heat transfer is insufficient the flame will move upstream. When during this movement the reaction zone of the flame enters the porous medium, the burning velocity of the flame is enhanced by the presence of the foam. To compensate for this higher burning velocity the flame must lose more enthalpy and will move more upstream. As such, the movement of the flame into the burner and the increase in the enthalpy loss necessary for stabilization amplify each other. This leads to a flame submerged in the ceramic foam which must be cooled to the flame temperature as shown in Fig. 6.10 by the solid line. This heat transfer to the burner must be compensated by a larger radiative heat transfer to the environment for which the solid temperature must rise. This will shift the flame even more upstream as the temperature difference between the gas and the solid must be
maintained. However, from Fig. 6.12 it follows that no steady-state solution is possible for the submerged flame stabilized at the downstream surface when the flame outside the foam cannot be stabilized. As gas-solid heat transfer, which heats up the burner, is higher than the radiative heat transfer, which cools the burner, the burner will slowly heat up, allowing the flame to propagate through the burner.

### 6.5 Probing flash-back limits

In Section 6.4 stabilization diagrams have been presented for ceramic-foam surface burners in cold and hot environments. The stability diagram for a cold environment shows a situation for which all flames stabilize at the outside of the foam and no flash-back will occur. In the stability diagram for the hottest environment there is a range of velocities for which no steady-state solution can be found and it has been shown that for these cases flash-back occurs. The region for which a steady-state solution cannot be found can be considered as the flash-back window and the minimum and maximum velocities of this window follow from the local extrema for the lower and upper branches of the stability diagram, respectively. Using these flash-back windows a flash-back region can be drawn for a combination of a specific foam and a mixture composition. Such regions are shown in Fig. 6.13 for $\phi = 0.8 - 1.0$. These regions are determined by calculating the lower and upper stabilization curves, near the extrema, for a number of radiating temperatures of the environment $T_{\text{env}}$. The flash-back window for each temperature is then determined from the positions of the extrema. From Fig. 6.13 it follows that for $\phi = 0.9$ no flash-back will occur for any velocity as long as the radiating temperature of the environment is below $T_{\text{min}} = 753 \, \text{K}$. This temperature can be considered as the flash-back safety-limit.
Figure 6.14: Maximum radiating temperature at which no flash-back occurs at ceramic-foam surface burners for $\phi = 0.9$.

For $\phi = 0.8$ and 1.0 flash-back regions have been determined as well. The results are shown in Fig. 6.13. For mixtures with a lower equivalence ratio the flash-back region is shifted towards lower velocities and higher radiating temperatures of the environment. The risk of flash-back is decreased when the equivalence ratio is lowered. This is also shown in Fig. 6.14 by the critical radiating temperature of the environment as a function of the equivalence ratio.

6.6 Discussion

In this chapter flash-back of flames into ceramic-foam surface burners has been investigated by looking at steady-state solutions and by carrying out transient simulations for operating conditions for which steady-state solutions cannot be found. The transient simulations indicate that the absence of steady-state solutions can be attributed to the occurrence of flash-back at those conditions.

The transient simulations show, that flash-back occurs when the reaction zone of the flame enters the burner and is related to a large increase of the flame burning velocity by the presence of the porous medium. On the time scale of the flame, the flame is still stabilized by the burner, which is accomplished by a large convective heat-transfer from the flame to the burner. The burner heats up, but the large convective heat-transfer cannot be compensated by the increase of the radiative heat-transfer at the burner surface. As a result, the flame propagates slowly into the burner.

Flames submerged in ceramic foam have been studied to explain the larger flame burning velocity. Stabilization diagrams, in which both flames stabilized at the burner surface and flames submerged into the material are included, are constructed to find the conditions for which flash-back occurs. Based on the stabilization diagrams flash-back re-
gions are identified for $\phi = 0.8, 0.9$ and 1.0. Furthermore, maximum radiating temperatures of the environment are determined to completely exclude the risk of flash-back.

Bouma [7] has given an earlier analysis of flash-back on ceramic-foam surface-burners. In his analysis the flame is modeled using Eq. (6.1), which relates the flame temperature to the velocity, and activation-energy asymptotics, which gives a delta function for the chemical source terms, and the flame is assumed to be outside the foam. The foam surface temperature follows from the difference between the actual and the adiabatic flame temperatures and the differential equations in the ceramic foam, which do not contain source terms due to the flame anymore, are solved using an analytical method using constant coefficients. The flash-back condition is then constructed from the condition that the gas temperature at the burner surface must be less than the flame temperature. Note, that due to his definition and calculation of the stand-off distance, the value must be always positive, in fact negative values denote flash-back, whereas in the present work, the flame position $x_F$ can be negative for a stable flame.

Both his analysis and the present analysis emphasize that the convective heat-transfer must be equal to the radiative heat-transfer for stable combustion. Both methods give qualitatively equal results for the velocity region in which flash-back can occur. The stable operation range in the radiant mode is split into three parts. Two stable regions at high and low velocities and an unstable region in between.

The main difference between the analysis of Bouma and the present work is that Bouma uses an approximation of the flame equations, whereas the present work is based on the full equations. This allows the flame to move into the burner and lets the flame temperature follow from the equations. Bouma uses a fixed relation between the velocity and flame temperature whereas in the present work it is concluded that the flame temperature decreases when the flame moves into the burner (see Fig. 6.1). Also the approximation of the actual differential equations, which is used by Bouma, overestimates the gas temperature at the surface, his main parameter, by about 200 K [7]. The impact of these differences on the results can cancel themselves. The higher velocity of the burner will make the combustion less stable, which can also be said about the approximation used by Bouma.

The findings of this chapter should be compared to experiments. The limited experimental data which is available [7, 30], suggests that the trend is well predicted but that the actual limiting temperatures are higher. This can be caused by some of the limitations of the model which is used. The model does not include surface chemistry which could reduce the burning velocity due to recombination of radicals. Furthermore, the findings are sensitive to the value of the heat-transfer coefficient. The value used may be rather inaccurate, since it is hard to measure in the conditions of the top layer of the flame, where a strong temperature gradient is present. Also the volume-averaging method [7], which is applied to arrive at the set of 1D conservation equations, might not be justified, because the pore size is of the same order of magnitude as the flame thickness.

The analysis presented in this chapter is based on a 1D situation. In the absence of hot walls or mirrors in the vicinity of the burner, the radiation falling on to the burner will be evenly distributed. For the destabilizing effect of preheating, as found in Chapter 4,
this is not the case. Preheating will predominantly be present at the burner rim which is in contact with the surrounding material. Uniform preheating can be analyzed with the presented approach, but for the influence of non-uniform preheating the analysis should be extended to 2D, to include effects as flame stretch and the increased pressure drop over the burner. Flame-stretch effects could lower the burning velocity locally, adding to the stability of the flame. Local hot spots due to burner irregularities or local preheating, however, might induce a local increase of the pressure drop. This can lead to an unstable flame, because an increasing pressure leads to a decreasing gas velocity ahead of the hot spot. It is recommended for further study, to investigate how these effects influence the flame stability.
Chapter 7

Conclusions and future developments

In this chapter, it is reviewed to what extent this thesis facilitates the design of applications with ceramic-foam surface burners and what remains to be investigated. An example application is modeled and analyzed to show the actual use of the findings of this thesis. Finally, some remarks are presented regarding possible future investigations.

7.1 Conclusions of this thesis

The objective of this thesis is to develop methods to analyze and predict the application of ceramic-foam surface burners in high-temperature environments. In each application the performance and the stability of the system must be guaranteed and these are, therefore, the main objectives of the analysis. The performance can be split into two separate issues: the efficiency of the heat transfer and the formation of pollutants. The stability of the burner is mainly linked to the occurrence of flash-back.

Two numerical models have been developed. A 1D model that contains all the chemistry and the details of the heat transfer in the burner and the flue gases, and a 2D model, that has some limitations with respect to the heat transfer inside the burner, but allows the simulation of actual applications. The 2D model has been globally validated by comparing the results of simulations to results of experiments. Using the 2D model it is possible to predict the efficiency of an application.

The analysis of the heat transfer in the experimental furnace, has shown the importance of gas radiation as a heat-transfer mechanism in the combustion chamber. The modeling of gas radiation has been analyzed by comparing the results of 1D simulations, using the optical-thin limit and a 1D radiation model, with the results of 2D simulations. It is concluded that the above mentioned 1D models have limited applicability for actual burner systems. The difference between the optical thin limit, that neglects all the self absorption by the flue gases, and the 2D results are only less than 10%, when the mean-beam length of the combustion chambers is less than 1 cm. On the other hand, the 1D radiation model overestimates the influence of self-absorption significantly. For most applications the actual geometry should be taken into account, but for use in 1D models a simple model
is developed. This scaled optical-thin-limit model gives a fairly accurate approximation of the heat transfer by gas radiation.

The prediction of the formation of pollutants is not implemented in the 2D model and is, therefore, still restricted to the 1D model. The use of the scaled optical-thin-limit model for the heat transfer by gas radiation, however, gives an improved prediction of the temperature of the flue gases in the post-flame zone. This allows a better prediction of both NOₓ and CO levels using the 1D model. Nevertheless, extension of the 2D model with NOₓ and CO formation is preferable. Some remarks on this extension are made in Section 7.3.

With the use of the 2D model, it is possible to determine the radiative environment of the burner, which is a key parameter in the stability of the flame. Analysis has shown that, contrary to the results of earlier studies, the stabilization of a flame at the burner surface depends on the temperature of the environment. The reason for this dependence is found to be the acceleration of the flame by the burner, when the flame is forced to stabilize further upstream. This acceleration leads to a higher heat transfer between the flame and the burner that cannot be compensated by a rise in the radiative heat transfer. Analysis of the relation between the flame position and the flame velocity has shown that, for low radiating temperatures of the environment, two stability curves exist: one inside the burner and one at the outside. For a hot environment these two curves are split and recombined into two other curves. In the velocity range between these curves, flash-back occurs. This observation makes it possible to derive the flash-back limits.

### 7.2 Application to IR-heater

It is being investigated by ECO-Ceramics, whether ceramic-foam surface burners can be used as closed IR-heaters for domestic cooking-apparatus. Simulations of such a system have been performed to support this analysis. These simulations are presented here as an example of the application to practical design-problems of the models derived in this thesis.

The closed IR-heater is shown in Fig. 7.1. It consists of a ceramic-foam surface burner placed in a combustion chamber which is, at the top, closed by a glass plate. On top of the glass plate the pan is placed. In the simulations presented here, it is assumed that this pan is filled with boiling water. To improve the performance of the heater, a ring of ceramic foam is placed around the burner. Through this ring the hot flue gases are removed from the combustion chamber and led towards the outflow chamber. While the flue gases pass the ring of ceramic foam, they lose heat to the solid material that is converted into radiation. The ring is called the passive foam while the burner, on which the combustion takes place, is called the active foam.

The outflow chamber is located around the plenum which makes it possible to heat up the unburnt mixture with the remaining heat of the flue gases. This heat integration will lead to an improvement of the efficiency but can also cause dangerous situations by ignition of the unburnt mixture in the plenum.

The final design must have an efficiency of at least 50% but preferably in the order of 70%. It must be operated in a safe way, and the glass cover of the combustion cham-
7.2. Application to IR-heater

**Figure 7.1:** Computational domain, dimensions in cm.

**Figure 7.2:** Grid on which the flow and combustion equations are solved.

...ber may not become hotter than 1000 K. It is preferable that both the glass plate and the ceramic-foam surfaces have a homogeneous temperature distribution. To facilitate the design, simulations have been performed which focus on these issues.

### 7.2.1 Objectives of simulations

Based on the requirements defined for the final design, four questions are formulated which should be answered by the study:

1. What is the maximum temperature of the glass cover; is it below the maximum temperature of the glass and is the temperature of the lower glass surface uniform?
2. Is the temperature of the ceramic-foam surfaces uniform?
3. What is the efficiency of the system and how can it be improved?
4. How much is the preheating of the unburnt flue gases by the hot wall; is there a risk of ignition of the unburnt mixture?

### 7.2.2 Modeling assumptions

The simulations have been performed with the 2D-model presented in Chapter 2, with the effective conduction in the ceramic foam scaled with a factor 10 (see Section 2.4). The numerical domain is based on the configuration shown in Fig. 7.1 and consist, from top to bottom, of a steel plate that represents the pan, the glass plate, the combustion chamber, the active foam, the passive ceramic-foam, a conducting wall, the plenum and the outflow chamber. The plenum and active foam on one side are connected to the outflow chamber...
Table 7.1: Description of the simulations, the values for the variations are only shown when they differ from the ones for the base case.

<table>
<thead>
<tr>
<th>Simulation</th>
<th>( v_u ) [cm/s]</th>
<th>( d_{\text{active}} ) [cm]</th>
<th>( H ) [cm]</th>
<th>( A_{\text{passive}} / A_{\text{active}} ) [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base case</td>
<td>14.6</td>
<td>10</td>
<td>6</td>
<td>1</td>
</tr>
<tr>
<td>Half power</td>
<td>7.3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Small burner</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Low combustion-chamber</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Double passive active ratio</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 7.2: Results of the simulations, the temperature profiles for the variations are described with respect to the base case.

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Efficiency [-]</th>
<th>Temperature profiles</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Active</td>
</tr>
<tr>
<td>Base case</td>
<td>0.52</td>
<td>See Fig. 7.5</td>
</tr>
<tr>
<td>Half power</td>
<td>0.59</td>
<td>all ( \pm 100 ) K lower</td>
</tr>
<tr>
<td>Small burner</td>
<td>0.44</td>
<td>all ( \pm 25 ) K lower</td>
</tr>
<tr>
<td>Low combustion-chamber</td>
<td>0.47</td>
<td>( \pm 70 ) K lower</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \pm 25 ) K lower</td>
</tr>
<tr>
<td>Double passive active ratio</td>
<td>0.57</td>
<td>( \pm 50 ) K lower</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \pm 150 ) K lower</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \pm 50 ) K lower</td>
</tr>
</tbody>
</table>

and the passive foam on the other side, by the conducting wall. In this conducting steel wall a conduction equation is solved:

\[ \nabla \cdot \left( \lambda \nabla T \right) = 0. \quad (7.1) \]

In the glass plate radiation is possible, and this region has, therefore, been included in the radiation model. In this region, Eq. (7.1) has, therefore, been extended with a radiative heat source:

\[ \nabla \cdot \left( \lambda \nabla T \right) = S_{rg}. \quad (7.2) \]

The absorption coefficients used for the radiation inside the glass are shown in Fig. 7.3.

The inlet and outlet boundary conditions are similar to the ones in Chapter 4: Dirichlet conditions for the temperature, the species concentrations and the velocity at the inlet; prescribed pressure and Neumann boundary conditions for the other variables at the outlet. The side wall is implemented as an isolated wall and at the top of the pan, a fixed temperature of \( T = 373 \) K is prescribed to model the boiling water.

7.2.3 Results of the simulations

Based on the model and the computational domain described in the previous section, five cases have been simulated. These cases are summarized in Table 7.1. The dimensions for the configuration of the base case are a burner diameter of \( d = 10 \) cm, a distance between the burner and the glass plate of \( H = 6 \) cm, a conducting wall with a width of 0.5 cm and an outer diameter of \( d = 7.4 \) cm, that is chosen such that the total surface-areas of the passive and active foam are equal. In the base case, the burner is operated at 14.6 cm/s.
Figure 7.3: Glass absorption-coefficients used in the base-case simulation.

Figure 7.4: Temperature distribution for the base case.

Figure 7.5: Glass and ceramic-foam temperature-profiles for the base case.
with $\phi = 0.8$ giving a total power of 3.1 kW. The variations that have been investigated, are a reduction of the power by a factor two, a smaller burner at the same inlet velocity, a lower combustion chamber and a larger passive-foam area.

In the simulations it has been found that the use of the conductivity of steel (17 W/mK) for the conducting wall, causes ignition in the plenum. To prevent this, a lower conductivity of 0.1 W/mK is used. This value is comparable to the conductivity of a ceramic material.

The grid for the flow calculations is a rectangular grid of 126 by 45 cells and is shown in Fig. 7.2. It contains refinements near the burner surface, near the lower glass surface and near both sides of the conducting wall. The temperature distribution for the base case is shown in Fig. 7.4. The flame itself cannot be observed, but is captured on the fine grid near the burner surface. Note that the unburnt mixture near the conducting wall is strongly preheated, but the preheating is not fully captured because the grid is too coarse in the plenum and the lower burner region. The unburnt mixture does not ignite even though the temperature is about 900 K halfway into the burner. An improved preheating could lead to dangerous situations. The preheating leads to a radial variation in the flame temperature that is reduced as the flue gases come near to the glass plate. The lower temperature of the side wall, that is determined by an equilibrium of the radiation and the conduction, leads to a gradient in the radial direction.

The glass and burner surface temperatures are shown in Fig. 7.5. The temperature profile of the glass plate is fairly uniform and is not higher than the critical temperature of 1000 K. Also the variations do not show glass temperatures that are above the critical temperature. The surface temperature of the active and passive foam are in the same range of 1060 to 1220 K. There is a peak in the temperature of the active foam temperature which is caused by the preheating. This peak will show as a ring close to the rim of the burner. The most probable cause is the preheating of the unburnt mixture by conduction through the wall. A better distribution of this preheating can reduce the temperature of this ring.

The efficiencies of the five cases and the observations with respect to the temperature profiles have been summarized in Table 7.2. The difference between the temperature of the active and passive foam is smallest for the variation with the larger passive foam area. The efficiency is lowered for the small-burner and the lower combustion-chamber cases, whereas reducing the power and increasing the area of the passive foam increases the efficiency. Reducing the power increases the fraction of the heat release that is converted into radiation by the burner. In this light the increase of efficiency is less than expected. Apparently the rise in direct radiation is partially compensated by a reduction of the indirect radiation from the gas and the passive foam and a reduction of the convective heat transfer.

The decrease in efficiency for the lower combustion-chamber can be explained by a reduction of the gas radiation due to the lower gas volume. Increasing the passive foam area, increases both the radiation from the passive foam and the gas radiation because of the higher volume of the combustion chamber.

None of these variations has led to the objective efficiency of 70%, while two of the cases, the small-burner and the lower combustion-chamber cases, give an efficiency
that is lower than the minimal efficiency of 50%. An increase of the efficiency towards the objective of 70% may be realized by increasing the height of the combustion chamber and increasing the area of the passive foam. If the total area is to be kept constant, part of the gain, will, however, be lost due to the smaller burner area and the higher inlet velocity. A further increase of the efficiency can be realized by preheating the unburnt mixture. Local peaks in the temperature must, however, be avoided to prevent ignition. From the simulations it is clear that, even with the low conduction-coefficient in the conducting wall, the temperature is much higher near the wall than in the bulk of the mixture. Safely increasing the preheating can only be realized when the heat transfer between the unburnt mixture and the conducting wall is increased. Either by increasing the contacting surface by means of fins, or by increasing the velocity in the plenum by reducing the flow area.

7.2.4 Discussion

From the results of the simulations it follows that the efficiency of the system should be improved. Possible solutions that have been identified are a higher combustion-chamber, a larger passive foam area and an increased preheating. Preheating appears necessary when the objective of 70% efficiency has to be met but can be very dangerous in the present configuration. Especially when steel is used for the conducting wall. A new design should, therefore, give a better distribution of the heat conducted through the wall. This could also lead to a reduction of the peak which has been found in the temperature distribution over the ceramic-foam surfaces. The use of scaled ceramic-foam properties reduces the conduction in the foam and, therefore, the heat transfer between the passive and active foam. This does not interfere with the conclusion that the system can be dangerous and that the heat should be distributed more uniformly.

None of the simulations lead to a glass temperature that is above the critical temperature. Furthermore, the distribution of the heat over the glass plate is fairly uniform. From the simulations it follows that for the configuration considered, a pan with boiling water, there is no risk of fracture of the glass plate. Removing the pan from the plate will lower the heat transfer at the top of the plate and that could indeed be a problem but has not been investigated. Such an investigation could be made with the present model, but depends on the implementation of the heat transfer at the top of the glass plate.

7.3 Future developments

The example in the previous section shows that the 2D model can be effectively applied for design calculations. The numerical methods described in this thesis, can, however, be extended to cover a larger part of the design. At the moment, the prediction of the formation of pollutants is still limited to the 1D model. The 2D model should be extended to incorporate such calculations. Furthermore, the application of the 2D model for flames that are deeply stabilized in the ceramic-foam is inaccurate. 2D analysis of the stability of the combustion process requires a model that can handle such situations. Also the influence of preheating through a burner fitting, as observed in the experimental set-up in Chapter 4
and in the previous section, requires modeling of the conduction in the burner using the appropriate effective-conduction coefficients.

The formation of NO\textsubscript{x} can be implemented relatively easily in the 2D-model. As the NO\textsubscript{x} concentrations are very low and do not interfere with the chemistry of the methane conversion, they do not influence the flow and the combustion. The chemistry of the NO\textsubscript{x} formation can, therefore, be determined through post processing of the obtained results [17]. Such a post-processing step would require a manifold, based on a mechanism without NO\textsubscript{x} formation, that contains, besides the temperature and density which are already available, the concentrations of all the species in the mechanism. The post-processing step then consists of implementing an extended mechanism, that contains the NO\textsubscript{x} formation, by solving convection-diffusion equations for the extra species. This mechanism can be reduced by assuming steady-state relations for some species. This is presently under development.

The formation of CO and its conversion into CO\textsubscript{2} is now implemented as in a flamelet. In the cold part of the manifold it is assumed that the CO levels are given by the equilibrium. When this equilibrium is not reached, which is the case for rapid cooling of the flue gases, this assumption is not correct. In that case, CO should be traced as a separate species, and the combustion process should be split into two parts: the relatively fast initial conversion of the fuel and the slower conversion of the CO into CO\textsubscript{2}.

The limitations of the 2D model for flames inside the ceramic foam are related to the differences between the species and temperature profiles for burner-stabilized flames, on which the manifold is based, and those of flames on ceramic-foam surface burners. These differences are illustrated in Fig. 7.6, which shows the relation between the two progress variables, the enthalpy and the oxygen mass-fraction, for a number of inlet velocities for the two burners. This shows, that the reaction paths through the parameter space of the flames on the ceramic-foam surface burners are different from those of the burner-stabilized
flames. This is caused by the initial preheating of the gas which is more pronounced for higher burner temperatures. The 2D model can be improved by using a different manifold that is based on the flames on ceramic-foam surface burners. However, whereas the burner-stabilized profiles are nicely ordered, the profiles for the ceramic-foam surface burner intersect. This prevents the construction of a manifold based on enthalpy and the oxygen mass-fraction as the control variables. The enthalpy is only a good indicator for the different profiles in the gas outside the burner, but is less appropriate in the foam. Instead of the enthalpy a progress variable should be used which also gives a good indication of species and the gas and solid temperature profiles in the burner.
Bibliography


[42] C.A. Mors, Experimentele analyse van de warmteoverdracht tussen keramisch schuim


Principal symbols

Latin symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
<th>Unit</th>
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<tr>
<td>$A$</td>
<td>effective bandwidth</td>
<td>1/cm</td>
</tr>
<tr>
<td>$A$</td>
<td>absorption</td>
<td>W/m$^3$</td>
</tr>
<tr>
<td>$c_p$</td>
<td>specific heat</td>
<td>J/kgK</td>
</tr>
<tr>
<td>$d$</td>
<td>diameter</td>
<td>m or cm</td>
</tr>
<tr>
<td>$E$</td>
<td>emission</td>
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</tr>
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<td>enthalpy</td>
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<td>$h$</td>
<td>height</td>
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<td>height</td>
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<td>$i$</td>
<td>radiative intensity</td>
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<td>$k$</td>
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<td>W/m$^3$</td>
</tr>
<tr>
<td>$t$</td>
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<td>s</td>
</tr>
<tr>
<td>$T$</td>
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<td>K</td>
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<td>$Y$</td>
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Greek symbols

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<tr>
<td>$\lambda$</td>
<td>conductivity</td>
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### Principal symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Unit</th>
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<tr>
<td>λ</td>
<td>wavelength</td>
<td>m</td>
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<td>ν</td>
<td>wavenumber</td>
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<td>porosity</td>
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<tr>
<td>σ</td>
<td>Stefan-Boltzmann constant</td>
<td>W/m²K⁴</td>
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<tr>
<td>σₛ</td>
<td>scattering coefficient</td>
<td>–</td>
</tr>
<tr>
<td>τ</td>
<td>tortuosity</td>
<td>–</td>
</tr>
<tr>
<td>θ</td>
<td>angle</td>
<td>–</td>
</tr>
<tr>
<td>ω</td>
<td>solid angle</td>
<td>–</td>
</tr>
<tr>
<td>Ω</td>
<td>scattering albedo</td>
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### Subscripts

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<td>b</td>
<td>burnt</td>
</tr>
<tr>
<td>g</td>
<td>gas</td>
</tr>
<tr>
<td>P</td>
<td>Planck mean</td>
</tr>
<tr>
<td>s</td>
<td>solid</td>
</tr>
<tr>
<td>u</td>
<td>unburnt</td>
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</tbody>
</table>
Appendix A

Reaction mechanism

Table A.1: Reaction rate data for the Arrhenius relation: $k = BT^\gamma \exp (-E_a/RT)$. Units are mol, cm, s, K and cal [54].

<table>
<thead>
<tr>
<th>no</th>
<th>Reactions</th>
<th>$B$</th>
<th>$\gamma$</th>
<th>$E_a$</th>
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<td>r1</td>
<td>H + O$_2$ $\rightarrow$ OH + O</td>
<td>2.000E14</td>
<td>0.0</td>
<td>16800.0</td>
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<tr>
<td>r2</td>
<td>O + H$_2$ $\rightarrow$ OH + H</td>
<td>1.800E10</td>
<td>1.0</td>
<td>8826.0</td>
</tr>
<tr>
<td>r3</td>
<td>H$_2$ + OH $\rightarrow$ H$_2$O + H</td>
<td>1.170E09</td>
<td>1.3</td>
<td>3626.0</td>
</tr>
<tr>
<td>r4</td>
<td>OH + OH $\rightarrow$ O + H$_2$O</td>
<td>6.000E08</td>
<td>1.3</td>
<td>0.0</td>
</tr>
<tr>
<td>r5</td>
<td>H + O$_2$ + M$^a$ $\rightarrow$ HO$_2$ + M$^a$</td>
<td>2.300E18</td>
<td>-0.8</td>
<td>0.0</td>
</tr>
<tr>
<td>r6</td>
<td>H + HO$_2$ $\rightarrow$ OH + OH</td>
<td>1.500E14</td>
<td>0.0</td>
<td>1004.0</td>
</tr>
<tr>
<td>r7</td>
<td>H + HO$_2$ $\rightarrow$ H$_2$ + O$_2$</td>
<td>2.500E13</td>
<td>0.0</td>
<td>700.0</td>
</tr>
<tr>
<td>r8</td>
<td>OH + HO$_2$ $\rightarrow$ H$_2$O + O$_2$</td>
<td>2.000E13</td>
<td>0.0</td>
<td>1000.0</td>
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<tr>
<td>r9</td>
<td>CO + OH $\rightarrow$ CO$_2$ + H</td>
<td>1.510E07</td>
<td>1.3</td>
<td>-758.0</td>
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<tr>
<td>r10f</td>
<td>CH$_3$ + H $\rightarrow$ CH$_4$</td>
<td>1.9E36</td>
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<td>9050.0</td>
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<td>r10b</td>
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<td>r11</td>
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<td>3991.0</td>
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<td>0.0</td>
<td>0.0</td>
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<tr>
<td>r17</td>
<td>HCO + M$^a$ $\rightarrow$ CO + H + M$^a$</td>
<td>1.600E14</td>
<td>0.0</td>
<td>14700.0</td>
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<tr>
<td>r18</td>
<td>CH$_3$ + O$_2$ $\rightarrow$ CH$_3$O + O</td>
<td>7.000E12</td>
<td>0.0</td>
<td>25652.0</td>
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<td>r19</td>
<td>CH$_3$O + H $\rightarrow$ CH$_3$O + H$_2$</td>
<td>2.000E13</td>
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<td>r20</td>
<td>CH$_3$O + M$^a$ $\rightarrow$ CH$_3$O + H + M$^a$</td>
<td>2.400E13</td>
<td>0.0</td>
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<td>r21</td>
<td>HO$_2$ + HO$_2$ $\rightarrow$ H$_2$O$_2$ + O$_2$</td>
<td>2.000E12</td>
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<td>0.0</td>
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<td>r22</td>
<td>H$_2$O$_2$ + M$^a$ $\rightarrow$ OH + OH + M$^a$</td>
<td>1.300E17</td>
<td>0.0</td>
<td>45500.0</td>
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<td>r23</td>
<td>H$_2$O$_2$ + OH $\rightarrow$ H$_2$O + HO$_2$</td>
<td>1.000E13</td>
<td>0.0</td>
<td>1800.0</td>
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<td>r24</td>
<td>OH + H + M$^a$ $\rightarrow$ H$_2$O + M$^a$</td>
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<td>0.0</td>
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<tr>
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<td>H + H + M$^a$ $\rightarrow$ H$_2$ + M$^a$</td>
<td>1.800E18</td>
<td>-1.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

*) Third body efficiencies: CH$_4$ = 6.5, H$_2$O = 6.5, CO$_2$ = 1.5, H$_2$ = 1.0, CO = 0.75, N$_2$ = 0.4, O$_2$ = 0.4 and for all other species 0

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Appendix B

Exponential wide-band model

In Chapter 3 the Edwards exponential wide-band model is introduced. In this model the emission and absorption along a path length is determined from the effective bandwidth of a vibrational-rotational band. In this appendix the derivation of the effective band width from the optical properties of a gas and the application of the wide-band model in a 1D geometry is treated.

B.1 Effective band width

The derivation of an expression for the effective bandwidth \( A_j \) (following Edwards [16]) of a wide band is performed in two steps. The first step involves the determination of the average absorptivity \( \bar{\alpha} \) in a narrow band. The second step is the integration of this expression over the wide band.

The narrow band is a spectral interval, defined using wavenumbers \( \nu \), which is large enough to contain a large number of lines, but small enough so that the lines in the interval can be assumed of to be of equal intensity \( S \). The lines in an interval are described by their intensity \( S \), half width \( \gamma \) and the average spacing \( d \). The actual spacing of the lines in the interval is assumed random and the average absorptivity \( \bar{\alpha} \) of the narrow band at mass-pathlength \( X = \rho s \) is then given by

\[
\bar{\alpha}(X) = \frac{1}{2\Delta \nu} \int_{\nu - \Delta \nu}^{\nu + \Delta \nu} 1 - \exp \left( -\frac{k_{\nu} X}{\rho} \right) d\nu = 1 - \exp \left( -\frac{\frac{S X}{d} \sqrt{1 + \frac{S X}{d \eta}}} \right). \tag{B.1}
\]

The ratio \( \eta \) between the line half-width \( \gamma \) and the line spacing \( d \) is correlated by

\[
\eta = \frac{\pi \gamma}{d} = \beta P_e. \tag{B.2}
\]

The effective pressure \( P_e \) incorporates the effect of self-broadening and is correlated using a coefficient \( b \) and an exponent \( n \) to the actual pressure \( P \), the reference pressure \( P_0 \) and the species pressure \( P_i \) as

\[
P_e = \left( \frac{P}{P_0} + (b - 1) \frac{P_i}{P_0} \right)^n. \tag{B.3}
\]
The expression for the average absorptivity $\bar{\alpha}$ (Eq. (B.1)), can be integrated over the wide band to give the effective bandwidth $A_j$ as

$$A_j(X) = \int_j \left(1 - \exp\left(-\frac{k_j X}{\rho}\right)\right) d\nu = \int_j \bar{\alpha}(X) d\nu = \int_j \left[1 - \exp\left(-\frac{\nu_0 - \nu}{\sqrt{1 + \frac{\require{cancel}\omega}{d \require{cancel}\omega} \frac{\nu_0 - \nu}{\require{cancel}\omega}}\right)\right] d\nu. \quad \text{(B.4)}$$

In the wide band the line intensity $S$ is not constant and the line intensity has to be specified as a function of wavenumber. In the exponential wide-band model an exponential variation is assumed, in which the line intensity is given as a function of the integrated bandwidth $\alpha$ and the exponential decay rate $\omega$:

$$\frac{S}{d} = \frac{\alpha}{\omega} \exp\left(\frac{-\nu_0 - \nu}{\omega}\right). \quad \text{(B.5)}$$

There is a theoretical basis for this variation, given in [16] and it gives a reasonable fit for isothermal and even non-isothermal data. The bandwidth is now given by inserting Eq. (B.5) in (B.4):

$$A(X) = \int_0^\infty 1 - \exp\left(\frac{-\frac{\omega}{\alpha} \exp\left(-\frac{\alpha \nu}{\omega}\right) X}{\sqrt{1 + \frac{\omega}{\require{cancel}\omega} \exp(-\frac{\alpha \nu}{\require{cancel}\omega}) \frac{X}{\omega}}}\right) d(\nu_0 - \nu). \quad \text{(B.6)}$$

This equation can be evaluated using numerical quadrature or approximated by a closed form relation. The most used relation, on which most correlations are based, is given by a four region relation depending on $\eta$ and the maximum optical depth at the band head $\tau_H = \frac{2X}{\omega}$:

- **linear region**: $\tau_H \leq 1, \tau_H \leq \eta$
  $$A_j = \omega \tau_H = \alpha X \quad \text{(B-7-a)}$$

- **square root region**: $\eta \leq \tau_H \leq \frac{1}{\eta}, \eta \leq 1$
  $$A_j = \omega \left(\sqrt{\frac{\alpha \eta \tau_H - \eta}{}\right) \quad \text{(B-7-b)}$$

- **log-root region**: $\frac{1}{\eta} \leq \tau_H, \eta \leq 1$
  $$A_j = \omega \left(\ln (\tau_H \eta) + 2 - \eta\right) \quad \text{(B-7-c)}$$

- **logarithmic region**: $\tau_H \geq 1, \eta \geq 1$
  $$A_j = \omega \left(\ln \tau_H + 1\right) \quad \text{(B-7-d)}$$

The formulation of the wide-band model based on Eq. (B.6) requires the determination of the parameters $\alpha$, $\omega$ and $\eta$.

The integrated bandwidth of the wide band $\alpha$ is the integral of $S/d$ over the band. It is based on the vibrational-rotational states of a harmonic oscillator and normalized to
its values at reference temperature $T_0 = 100$ K. Based on a molecule having vibrational quantum numbers $(\nu_1, \nu_2, ..., \nu_m)$ with a transition to $(\nu_1 \pm \delta_1, \nu_2 \pm \delta_2, ..., \nu_m \pm \delta_m)$ $\alpha$ is given by

$$\alpha(T) = \alpha_0 \frac{(1 - \exp (-\sum_{k=1}^{m} \pm u_k \delta_k)) \Psi(T)}{(1 - \exp (-\sum_{k=1}^{m} \pm u_0 \delta_k)) \Psi(T_0)}$$

(B-8)

with

$$u_k = \frac{h \nu_k}{kT}$$

(B-9)

and $\Psi(T)$ given by

$$\Psi(T) = \frac{\prod_{k=1}^{m} \sum_{x=0}^{\infty} \left( \frac{\nu_k + x + \delta_k - 1}{(g_k - 1)!} \right) \exp(-u_k \nu_k)}{\prod_{k=1}^{m} \sum_{x=0}^{\infty} \left( \frac{\nu_k + x + \delta_k - 1}{(g_k - 1)!} \right) \exp(-u_k \nu_k)}.$$  

(B-10)

In this formula $\nu_0$, $k$, denotes the lowest possible initial state, i.e. $\nu_0 = 0$ for $+\delta$ transitions and $\nu_0 = \delta$ for $-\delta$ transitions. To account for degenerated vibrations a set of weights $g_k$ is used.

The exponential decay rate $\omega$ is given by

$$\omega(T) = \omega_0 \sqrt{\frac{T}{T_0}}$$

(B-11)

and the line-width to spacing parameter $\beta$ from Eq. (B.2) is given by

$$\beta(T) = \beta_0 \sqrt{\frac{T_0 \Phi(T)}{T \Phi(T_0)}}$$

(B-12)

with

$$\Phi(T) = \left( \frac{\prod_{k=1}^{m} \sum_{x=0}^{\infty} \left( \frac{\nu_k + x + \delta_k - 1}{(g_k - 1)!} \right) \exp(-u_k \nu_k)}{\prod_{k=1}^{m} \sum_{x=0}^{\infty} \left( \frac{\nu_k + x + \delta_k - 1}{(g_k - 1)!} \right) \exp(-u_k \nu_k)} \right)^{2}.$$  

(B-13)

The coefficients used in these equations are given in Table B.1 for the different bands of H$_2$O, CO$_2$ and CO.

Based on the wide-band model the transmission $\tau_j$ of band $j$ can be expressed as

$$\tau_j = \text{Min} \left( \frac{\tau_{H_j}}{A_j} \frac{dA_j}{dT_{H_j}}, 0.9 \right).$$  

(B-14)

**B.2 Application of exponential wide-band model.**

The exponential wide-band model has been derived and correlated for isothermal and homogeneous gas mixtures with a single absorbing species. The integrated form of the RTE (Eq. (3.12)) for such a gas mixture is given by

$$i'_{\nu}(s) = i'_{0\nu} \exp (-k_{\nu} s) + i'_{b\nu} (1 - \exp (-k_{\nu} s)).$$  

(B-15)
Table B.1: Exponential wide-band model parameters.

<table>
<thead>
<tr>
<th>Gas</th>
<th>Vibrations</th>
<th>Weights</th>
<th>Band Energy</th>
<th>Pressure parameters</th>
<th>Spectral Location</th>
<th>Band Absorption parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>m = 3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H$_2$O</td>
<td>$v_1$ = 36.02</td>
<td>$v_2$ = 1595</td>
<td>$v_3$ = 37.96</td>
<td>$0.0,0.0$</td>
<td>$6.3 \mu m$</td>
<td>$0.14311$</td>
</tr>
<tr>
<td></td>
<td>$g_1 = 1$</td>
<td>$g_2 = 1$</td>
<td>$g_3 = 1$</td>
<td>$0.1,0.0$</td>
<td>$1000$</td>
<td>$5000$</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>$v_1$ = 1301</td>
<td>$v_2$ = 60.7</td>
<td>$v_3$ = 2306</td>
<td>$0.1,0.1$</td>
<td>$9.4 \mu m$</td>
<td>$0.14311$</td>
</tr>
<tr>
<td></td>
<td>$g_1 = 1$</td>
<td>$g_2 = 2$</td>
<td>$g_3 = 1$</td>
<td>$0.0,0.1$</td>
<td>$960$</td>
<td>$0.9017$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$1.0 \times 10^{-6}$</td>
<td>$1.0$</td>
<td>$0.24723$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$2.4 \times 10^{-6}$</td>
<td>$3.6$</td>
<td>$0.89888$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$3.4 \times 10^{-6}$</td>
<td>$1.0$</td>
<td>$0.83141$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$2.0 \times 10^{-6}$</td>
<td>$1.0$</td>
<td>$0.93005$</td>
</tr>
</tbody>
</table>

This equation is integrated over $\nu$ and rewritten using the band assumption by combining Eqs. (3.24) and (3.25) to

$$i'(s) = i'_{0} - \sum_{j} A_{j}(s) i'_{0j} + \sum_{j} A_{j}(s) i_{bj}, \quad (B-16)$$

and is as such sufficient to calculate the intensity at each point for a gas containing a single absorbing species. When a mixture is considered, bands from different species can overlap. Generally no relations are available which treat these overlapping bands as a single combined band. One method to account for the band overlap is to interpret the equivalent bandwidth as the width of the region with complete emission/absorption. Under this interpretation, which is known as the box model, the following approximations are made:

$$A_{j}(X) i'_{0j} = i'_{b} F_{j}(X, T_0) \quad (B-17-a)$$

$$A_{j}(X) i_{bj} = i'_{b} F_{j}(X, T) \quad (B-17-b)$$

with $F_{j}$ the fraction of black-body intensity in the band $j$

$$F_{j}(X, T) = \frac{1}{\sigma_{b}} \int_{\nu_{j}}^{\nu_{j}} i'_{b}, d\nu. \quad (B-18)$$
The lower and upper bandwidths \( \nu_{jL} \) and \( \nu_{jU} \) depend on the bandwidth and the location of the top of the band. If the upper or lower band-limit is prescribed, the remaining band limit is determined from

\[
\nu_{jU} - \nu_{jL} = A_j(X). \tag{B-19}
\]

If the center of the band is prescribed, the band limits are given by

\[
\nu_{jU} = \nu_{jc} + \frac{A_j(X)}{2} \tag{B-20-a}
\]
\[
\nu_{jL} = \nu_{jc} - \frac{A_j(X)}{2} \tag{B-20-b}
\]

Overlapping bands can now be treated by combining the overlapping bands and retaining the lowest lower band limit and the highest upper band limit. The intensity using the box-model is then given by

\[
i'(X) = i'_0 \left( 1 - \sum_j F_j(X, T_0) \right) + i'_b(T) \sum_j F_j(X, T) \tag{B-21}
\]

In this derivation the assumption has been made that the temperature and the composition of the gas are homogeneous. When this is not the case the integration of the RTE (Eq. (3.12)) is given by

\[
i'_\nu(s) = i'_{0\nu} \exp(-\kappa) + \int_0^s \exp(-(\kappa + \kappa^*)) i'_{bw}(s^*) k_\nu(s^*) ds^* \tag{B-22}
\]

with the optical thickness \( \kappa \) given by

\[
\kappa = \int_0^s k_\nu ds^*. \tag{B-23}
\]

Equation (B-22) can be rewritten to

\[
i'_\nu(s) = i'_{0\nu} \exp(-\kappa) + \int_0^s i'_{bw}(s^*) \frac{\partial}{\partial s^*} \exp(-(\kappa + \kappa^*)) ds^*. \tag{B-24}
\]

The equivalent bandwidth from Eq. (3.23) is defined between \( s_1 \) and \( s_2 \) using the optical thickness as

\[
A_j(s_1 \rightarrow s_2) = \int_0^\infty \left( 1 - \exp\left( -\int_{s_1}^{s_2} k_\nu ds \right) \right) dv = \int_0^\infty \left( 1 - \exp\left( -(\kappa_2 - \kappa_1) \right) \right) dv \tag{B-25}
\]

Therefore Eq. (B-24) is rewritten as

\[
i'_\nu(s) = i'_{0\nu} - i'_{0\nu} (1 - \exp(-\kappa)) - \int_0^s i'_{bw}(s^*) \frac{\partial}{\partial s^*} (1 - \exp(-(\kappa + \kappa^*))) ds^*. \tag{B-26}
\]
When Eq. (B-26) is integrated over $\nu$ and the band assumption is used the following equation is obtained

$$i'(s) = i'_0 - \sum_j i'_0 A_j(0 \to s) - \sum_j \int_0^s i'_b(s^*) \frac{\partial}{\partial s^*} A(s^* \to s) ds^*. \quad (B-27)$$

As the equations for the bandwidth have been deduced for isothermal and homogeneous conditions, a scaling of the different parameters is necessary. The recommended scaling is given by

$$X = \int_0^s \rho ds^{**} \quad (B-28-a)$$
$$\pi = \frac{1}{X} \int_0^X \omega dX^{**} = \frac{\xi_1}{X} \quad (B-28-b)$$
$$\varpi = \frac{1}{\xi_1} \int_0^\xi \omega d\xi^{**} = \frac{\xi_2}{\xi_1} \quad (B-28-c)$$
$$\eta = \frac{1}{\xi_2} \int_0^\xi \eta d\xi^{**} = \frac{\xi_3}{\xi_2} \quad (B-28-d)$$

**B.3 One-dimensional discretization of the exponential-wide-band-model equations**

The wide-band model is used in the 1D model to calculate the radiative flux $q_e$ in Eq. (3.18). This requires determination of the radiative intensity $i_m$ for $M$ rays on a staggered grid. Equation (B-27) is written for each direction and grid point using midpoint values for the numerical integration. For the positive directions this yields:

$$i_{mk} = i'_{mk0} - \sum_j i'_0 A_j \left(0 \to \frac{x_k}{\mu_m}\right) - \sum_{k^* = 0}^{k} i'_b(T_{k^* + \frac{1}{2}}) \left(A_j \left(\frac{x_{k^* + 1}}{\mu_m} \to \frac{x_k}{\mu_m}\right) - A_j \left(\frac{x_{k^*}}{\mu_m} \to \frac{x_k}{\mu_m}\right)\right) \quad (B-29)$$

Again the box model assumptions given in Eq. (17) are used, this yields

$$i_{mk} = i'_{mk0} \left(1 - \sum_j F_j \left(0 \to \frac{x_k}{\mu_m}, T_0\right)\right) - \sum_{k^* = 0}^{k} \sum_j i'_b(T_{k^* + \frac{1}{2}}) \left(F_j \left(\frac{x_{k^* + 1}}{\mu_m} \to \frac{x_k}{\mu_m}, T_{k^* + \frac{1}{2}}\right) - F_j \left(\frac{x_{k^*}}{\mu_m} \to \frac{x_k}{\mu_m}, T_{k^* + \frac{1}{2}}\right)\right) \quad (B-30)$$

The values needed for the the scaling of the parameters, $X$, $\xi_1$, $\xi_2$ and $\xi_3$, are also evaluated using numerical integration using midpoint values:

$$X_{i,m,k^* \to k} = \sum_{k^{**} = k^*}^{k-1} p_{k^{**} + \frac{1}{2}} \frac{1}{Y_{i,k^{**} + \frac{1}{2}}} \left(\frac{x_{k^{**} + 1} - x_{k^{**}}}{\mu_m}\right) \quad (B-31-a)$$
$$\xi_{i,j,1,m,k^* \to k} = \sum_{k^{**} = k^*}^{k-1} \alpha_{i,j} \left(T_{k^{**} + \frac{1}{2}}\right) \left(X_{i,m,k^{**} + 1} - X_{i,m,k^{**}}\right) \quad (B-31-b)$$
Table B.2: Calculated wall heat flux for benchmark problems.

<table>
<thead>
<tr>
<th>Case</th>
<th>Slab width</th>
<th>Gas temp.</th>
<th>H₂O press.</th>
<th>Wall temp.</th>
<th>Wall emiss.</th>
<th>Wall heat flux (kW/m²)</th>
<th>Calc.</th>
<th>Kim et al. [29]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.10</td>
<td>1000</td>
<td>1.0</td>
<td>0</td>
<td>1.0</td>
<td>-13.5</td>
<td>-14.4</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1.0</td>
<td>1000</td>
<td>1.0</td>
<td>0</td>
<td>1.0</td>
<td>-26.6</td>
<td>-27.7</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1.0</td>
<td>1000</td>
<td>Profile</td>
<td>0</td>
<td>1.0</td>
<td>-23.8</td>
<td>-25.1</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.40</td>
<td>Profile</td>
<td>1.0</td>
<td>400.0</td>
<td>0.99</td>
<td>-6.6</td>
<td>-8.0</td>
<td></td>
</tr>
</tbody>
</table>

\[
\xi_{i,j,2,m,k^* \rightarrow k} = \sum_{k^* = k^*}^{k-1} \omega_{i,j} (T_{k^*+1} + \frac{1}{2}) (\xi_{i,j,1,m,k^*+1} - \xi_{i,j,1,m,k^*}) \quad (B-31-c)
\]

\[
\xi_{i,j,3,m,k^* \rightarrow k} = \sum_{k^* = k^*}^{k-1} \eta_{i,j} (T_{k^*+1} + \frac{1}{2}) (\xi_{i,j,2,m,k^*+1} - \xi_{i,j,2,m,k^*}) \quad (B-31-d)
\]

### B.4 Benchmark problems

Kim et al. [29] have presented five benchmark problems of which four have been calculated. These cases are summarized in Table B.2 which also contains the wall heat fluxes. The profiles which are used for the H₂O concentration and temperature, are shown in Fig. B.1. The results of these calculations are presented and compared with the results of Kim et al. in Figs. B.2-B.5. Some small differences exist, but generally the results compare well. Therefore, it is concluded that the Edwards exponential wide-band model has been implemented correctly.
Appendix B. Exponential wide-band model

Figure B.1: Concentration and temperature profiles for case 3 and 4.

Figure B.2: Case 1, slab of water vapor at 1000 K with $L = 0.1\, \text{m}$.

Figure B.3: Case 2, slab of water vapor at 1000 K with $L = 1\, \text{m}$.
Figure B.4: Case 3, slab of water vapor and nitrogen at 1000 K with a parabolic H₂O-concentration profile and L = 1 m.

Figure B.5: Case 4, slab of water vapor with a parabolic temperature profile and L = 1 m.
Summary

Ceramic-foam surface burners have been developed as low NO\textsubscript{x} burners for domestic heating equipment. The lower NO\textsubscript{x} formation is a result of the cooling of the flame at the burner surface. This heat transfer causes the burner surface to heat up and radiate to the environment. The burners can be used in industrial applications as well, resulting in a low NO\textsubscript{x} formation and a possible reduction of energy use by efficient use of the radiation coming from the burner. The application of ceramic-foam surface burners in industrial applications is, however, limited because of the possibility of flash-back due to the high temperature of the environment of the burner.

In this thesis the application of ceramic-foam surface burners in a high-temperature environment is analyzed. The analysis is aimed at the prediction of the performance and the stability of the burner in an application, to facilitate its design. The key processes are the chemical reactions in the flame and the heat transfer by radiation in the burner material and the combustion chamber. For this analysis a 1D and a 2D model are developed. The 1D model, based on complex chemistry and a wide-band model for the gas radiation, is used for detailed investigations of the combustion process. The 2D model, based on reduced chemistry and a gray-bands approach for the radiation, is developed for determining the efficiency of the heat exchange in a burner application.

The 2D model is validated by comparing the results of simulations to experimental results. The experimental results are derived from a lab-scale furnace that is designed to provide a controllable hot environment for the burner. The setup is a furnace of heat-resistant bricks heated by the burner and cooled by a heat exchanger. It allows measurements of both the gas and wall temperatures. The comparison shows that the heat transfer in the furnace can be adequately modeled using the 2D model.

An important heat-transfer mechanism in the combustion chamber is gas radiation. The cooling by gas radiation depends on the size of the hot-gas volume and this dependence is investigated using numerical simulations. In most studies the gas radiation is implemented using the optical-thin limit or using 1D radiation models. For geometries with a mean-beam length larger than 1 cm, the optical-thin limit, in which the effect of self-absorption is neglected, is found to show more than 10% deviation in the temperature gradient. 1D radiation models include the effect of self-absorption, but overestimate its effect significantly for practical geometries. The simulation results are fitted for a more accurate implementation of gas radiation in 1D models.

The application of ceramic-foam surface burners in hot environments is limited due to the possibility of flash-back. Flash-back occurs when the flame cannot be stabilized at the
burner surface, but moves into the burner, leading to fracture of the burner or to ignition of the unburnt mixture upstream of the burner. The process of flash-back is analyzed using numerical simulations with the 1D model. The occurrence of flash-back is explained by the influence of the ceramic foam on the burning velocity of the flame. Flames submerged in the ceramic foam have a larger adiabatic burning velocity and therefore require more cooling from the burner in order to stabilize. This additional cooling becomes important for a high temperature environment when the higher burner surface temperature forces the flame to stabilize further upstream. When the presence of the ceramic foam requires additional cooling, the flame must stabilize even further upstream and for certain conditions this process does not lead to a stable situation, but to flash-back. These conditions have been determined from the stability diagram of the burner. Whether flash-back will occur in an actual application depends on the radiative temperature, with respect to the burner, of the application. This radiative temperature can be determined using the 2D model.

With the models described in this thesis, applications of ceramic-foam surface burners can be simulated. As an example, simulations of a closed IR-heater are presented for a base case and some variations. Based on the results of these simulations, some design improvements for the closed IR-heater are suggested.
Samenvatting

Keramische schuimbranders zijn ontwikkeld als lage NO$_x$ branders voor huishoudelijke toepassingen. Bij deze branders wordt de NO$_x$-emissie verminderd door het verlagen van de vlamtemperatuur door koeling van de vlam aan het branderoppervlak. Door deze warmteoverdracht wordt het branderoppervlak heet en straalt naar de omgeving. Zowel de lage NO$_x$-uitstoot als de stralingsoptbrengst maken dat het toepassen van deze branders in industriële processen voordelig kan zijn. Echter, de toepassing van de brander in industriële toepassingen is gelimiteerd doordat de kans op vlammerugslag wordt verhoogd indien de brander geplaatst is in een toepassing met een hoge stralingstemperatuur.

In dit proefschrift wordt de toepassing van keramische schuimbranders in een hete omgeving onderzocht. Dit onderzoek is gericht op zowel de prestatie als de stabiliteit van de brander in een toepassing, om het ontwerp van dit soort toepassingen te vereenvoudigen. De belangrijkste processen die hierbij een rol spelen zijn de chemische reacties in de vlam en de warmteoverdracht door straling in de brander en de verbrandingskamer. Voor het onderzoek zijn daarom twee modellen ontwikkeld. Een 1D model, gebaseerd op complexe chemie en een wide-band model voor de gasstraling, dat wordt gebruikt voor een gedetailleerde studie van de verbranding, en een 2D model, gebaseerd op gereduceerde chemie en een grijze banden stralingsmodel, dat is ontwikkeld voor het bepalen van de warmteoverdracht in een toepassing.

Het 2D model is gevalideerd door vergelijking van de resultaten van simulaties met experimentele resultaten. De experimenten zijn verricht aan een testopstelling die is ontwikkeld als een hoge temperatuur omgeving voor de brander. De opstelling is een oven van hittebestendige stenen die verwarmd wordt door de brander en gekoeld wordt door een warmtwisselaar. In de opstelling kunnen zowel de gas- als de wandtemperaturen gemeten worden. Het vergelijken van de resultaten laat zien dat de warmteoverdracht goed gemodelleerd kan worden met het 2D model.

In de verbrandingskamer is de warmteoverdacht door gasstraling erg belangrijk. De koeling door gasstraling is echter afhankelijk van de grootte van het volume aan hete gassen en deze afhankelijkheid is onderzocht met numerieke simulaties. In de meeste studies wordt gasstraling gemodelleerd met de optisch dunne limiet. Uit de resultaten volgt echter dat voor een geometrie met een gemiddelde straalsteven van meer dan 1 cm, de temperatuurgradiënt die berekend wordt met de optisch dunne limiet meer dan 10% afwijkt van de 2D resultaten. Dit verschil wordt veroorzaakt door zelfabsorptie van gasstraling. 1D stralings modellen nemen zelfabsorptie wel mee, maar overschatten die invloed aanzienlijk
voor praktische systemen. De resultaten van de simulaties kunnen gebruikt worden om in 1D modellen de gasstraling met een grotere nauwkeurigheid te implementeren.

De toepassing van keramische schuimbranders in een hete omgeving wordt beperkt door de mogelijkheid van vlamterugslag. Vlamterugslag treedt op als de vlam niet aan het oppervlak gestabiliseerd kan worden, maar steeds dieper de brander inloopt wat kan leiden tot breuk van de brander of tot ontsteking van het onverbrande mengsel in de mengkamer. Vlamterugslag is onderzocht met behulp van 1D numerieke simulaties en kan verklaard worden met de invloed van het brander materiaal op de vlamsnelheid. Vlammen die diep in een keramisch schuim zijn gestabiliseerd hebben een grotere adiabatische vlamsnelheid en vereisen daardoor een hogere koeling van de brander om te kunnen stabiliseren. Deze extra koeling wordt belangrijk in een hete omgeving omdat de hogere temperatuur van het branderdek ervoor zorgt dat de vlam dieper in het materiaal stabiliseert. De aanwezigheid van het brandermateriaal kan dan een hogere koeling vereisen waardoor de vlam nog dieper zal moeten stabiliseren. Voor bepaalde condities leidt dit proces niet tot een stabiele situatie, maar tot vlamterugslag. Aan de hand van stabiliteitsdiagrammen is bekeken voor welke condities dit het geval is. Of vlamterugslag optreedt in een toepassing hangt af van de stralingstemperatuur van de toepassing zoals die door de brander gevoeld wordt. Deze stralingstemperatuur kan bepaald worden met het 2D model.

Met de modellen zoals die in dit proefschrift zijn beschreven, is het mogelijk om toepassingen met keramische schuimbranders te simuleren. Als voorbeeld hiervan, is een gesloten IR-straler gesimuleerd voor een referentie case en een aantal variaties. Op basis van de resultaten van deze simulaties is een aantal ontwerpverbeteringen voorgesteld.
Nawoord

Vier jaar werk zit erop en is, gelukkig, ook opgeschreven. Ik had het nooit alleen kunnen doen en wil graag iedereen bedanken die een bijdrage heeft geleverd.

Ten eerste natuurlijk Philip, zijn kennis en enthousiasme hebben er in grote mate voor gezorgd dat het verhaal geworden is zoals het is. Ook de kritische kijk van Anton heeft daaraan bijgedragen. Voor beiden geldt ook dat ik heel blij ben met hun flexibele opstelling in de afgelopen tijd.

Wolter en Herman van ECO Ceramics wil ik bedanken voor hun inzet die tot een mooie oven heeft geleid. Zij hebben ervoor gezorgd dat ik het praktische nut van het onderzoek niet vergeten ben. De inbreng van Peter is heel erg belangrijk geweest voor dit onderzoek. Niet alleen omdat hij zoveel kennis heeft van keramische schuinbranders maar vooral ook omdat hij altijd bereid is deze te delen. Jeroen heeft mij FGM uitgelegd. Daarnaast had ik zonder hem en Roy, Chem1D niet kunnen laten doen wat ik wilde. Verder heb ik de hulp van vele anderen, zoals Karel, Koen, Corine, Frank en Frits, bij de experimenten enorm gewaardeerd. Mijn dank gaat verder uit naar de studenten die zich hebben ingezet voor dit project. Twan heeft de opstelling ontworpen en Robert heeft een aantal aspecten van de simulaties bekeken.

De afgelopen vier jaar zouden veel minder leuk zijn geweest zonder de relativerende opmerkingen van mijn kamergenoten Marco en Maurice. Zij weten een ongekend vermogen tot flauwe humor te koppelen aan een grote bereidheid tot hulp bij kleine en grote problemen. De goede sfeer, ook mede bepaald door de buren Marco, Misheck en René, heeft ervoor gezorgd dat ik het vier jaar naar mijn zin heb gehad.

De mensen bij mijn huidige werkgever, Twister, wil ik bedanken voor de ruimte en flexibiliteit die ik de afgelopen maanden heb gekregen om dit werk af te ronden.

Voor alles wil ik echter Claudia bedanken die mij altijd gesteund heeft maar er ook altijd voor zal zorgen dat ik andere belangrijke dingen niet uit het oog verlies.
Stellingen
behorende bij het proefschrift

Ceramic-Foam Surface Burners in High-Temperature Environments
van

Bart Lammers

1. Voor het berekenen van de temperatuurdaling door gasstraling van de rookgassen van een vlam op een oppervlaktebrander in een praktische toepassing, voldoen zowel de optisch dunne limiet als een 1D benadering niet. Daarom dient de straling ruimtelijk opgelost te worden. (Hoofdstuk 5 van dit proefschrift)

2. In vorige studies is gevonden dat de vlamtemperatuur van een vlam op een oppervlaktebrander niet afhankelijk is van de brandereigenschappen. Dit is echter niet het geval indien de brander op de rand van stabiliteit wordt bedreven. Dan zijn de eigenschappen van de brander en ook de temperatuur van de omgeving in hoge mate bepalend. (Hoofdstuk 6 van dit proefschrift)

3. Bij vlamterugslag is het niet primair de vlam die door de brander loopt, maar het temperatuurprofiel van de brander dat instationair is. De vlam past zich aan dit temperatuurprofiel aan en is op de korte termijn wel stabiel. (Hoofdstuk 6 van dit proefschrift)

4. In Nederland is de weg net zo slecht aangegeven als in het buitenland. Hier valt het echter minder op omdat je de weg kent.

5. Het in een file wisselen van baan kan worden gerekend tot vervelend gedrag van de automobilisten, maar het is wel nuttig omdat het snelheidsverschil tussen de rijstroken hierdoor verminderd waardoor de doorvoer eerlijker wordt.

6. Mensen die spreken over, bijvoorbeeld, de zestiger jaren van de vorige eeuw, zijn vijftig jaar te vroeg met het tweede deel van de tijdsaanduiding.

7. Máxima heeft laten zien dat een middagje schaatsen, een talencursus en een dagje keukenhof meer dan genoeg zijn als inburgeringscursus.

8. De meeste CFD plaatjes kun je ook met een tekenpakket maken.

9. De rondjes die je met een trein kunt maken omsluiten al snel een tiental kerken.

10. De verrijking van het grote aantal nieuwe tv-zenders bestaat voornamelijk uit het kunnen kiezen uit meerdere domme spelletjes.