SOLID FUEL COMBUSTION CHAMBER
PROGRESS REPORT XV

January-June 1989

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P.A.O.G. Korting
B.T.C. Zandbergen (ed.)
T. Wijchers
P. J.M. Elands
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F. Dijkstra

Delft, Rijswijk, The Netherlands

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ACKNOWLEDGEMENTS

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1. INTRODUCTION

In this Report, an overview of the activities carried out by the theoretical and experimental working group in the January-June 1989 period of the solid Fuel Combustion Chamber (SFCC) project [1] is given.
2. ACTIVITIES OF THE THEORETICAL WORKING GROUP (TWG)

2.1. Study of physical processes (combustion)

2.1.1. Flow dynamics

- Vortex generated acoustics (B.T.C. Zandbergen)

The final report on the direct simulation of vortex flow [2] has been published.

Work continued on the development of a physical and mathematical model to predict the 'eigen' frequencies and the amplitude of the pressure oscillations in the SPCC. This work is carried out by R. Poland (student General Fluid Dynamics section, FAEDUT) under the guidance of ir. G. Schouten (FAEDUT).

2.1.2. Combustion chemistry

- Background (B.T.C. Zandbergen)

Initially, combustion in COPPEF was modelled using chemical kinetics (finite reaction rates). However, it was soon realised that, at least for the present, the use of chemical kinetics is limited due to the fact that: 1) for most of the different species involved, data on reaction rates and reaction mechanisms are lacking, and 2) computing times were found to be very large.

ad 1) The use of chemical kinetics is presently limited to very simple fuels like e.g. hydrogen, methane and ethene.

ad 2) Computing times are of the order of hours on the FAEDUT IBM mainframe or on the FAEDUT Convex mini-supercomputer.

These considerations led to the incorporation in COPPEF of a model based on the diffusion flame concept (mixed is burned), thereby using the assumption that the combustion chemistry is determined by a simple one-step, irreversible and infinitely fast reaction.

Disadvantages of this simple reaction model, compared to the chemical kinetics model, were found to be, apart from neglecting the influence of finite reaction rates, its inability to predict the formation of pollutants and dissociation being neglected. Therefore, it was decided at the beginning of this period, to further extend the combustion chemistry modelling in COPPEF with a chemistry model based on the assumption of chemical equilibrium, see also below.

- Chemical equilibrium (P.J.M. Elands)

An existing code for chemical equilibrium calculations (STANJAN) has been implemented in the COPPEF computer code. A description of the method used and some results are presented in Appendix A.
2.1.3. Heat transfer

No work done

2.1.4. Fuel regression

- Fuel pyrolysis (J.P. de Wilde)

Background of the study: This study was initiated in 1987, due to the fact that evidence was found that during the pyrolysis of PMMA, not only MMA is formed, but e.g. also methane. The extent of this effect was such that this also significantly could influence the heat of combustion and the heat of gasification, i.e. the calculated regression rate. Furthermore, it was realized that the temperature of the gaseous fuel, which is closely related to the pyrolysis process, was not exactly known.

During this period, work concentrated mainly on four topics, 1) pyrolysis modelling, 2) heat of gasification, 3) heat transfer and 4) combustion. Note: At the 14th meeting of the User's Committee, pyrolysis modelling and heat of gasification have been presented as one topic.

ad 1) Pyrolysis modelling

Based on the assumption that the pyrolysis is essentially time-independent, an empirical pyrolysis model has been developed for polymethylmethacrylate (PMMA), which predicts the amounts of the different pyrolysis products formed (as a function of temperature). The different pyrolysis products are MMA, methane, acetylene, ethylene, ethane, carbon monoxide and carbon dioxide. The data for this model have been taken from the literature. It is found that the earlier assumption, that only monomer is formed, is at least valid until 700 K. Above this value, however, other pyrolysis products start being formed.

For polyethylene (PE) work has begun on a stoichiometric model, which will also take into account the effect of time. So far, a reaction scheme has been worked out, thereby considering lumps (i.e. several groups of products) instead of the products themselves. Furthermore, the quantitative, time-dependent, datasets on product concentrations, obtained from the literature, have been regrouped into the different lumps considered in the model. From these data, reaction rate constants can be determined by means of a best fit procedure. This will result in the determination of the activation energies for each lump. With this parameter, the composition of the pyrolysis products can be predicted for any temperature and time. It is expected that this model will be ready in September of this year.

ad 2) The heat of gasification

Once the composition of the pyrolysis products of a certain polymer is known, the heat of gasification of the polymer can be determined as a function of temperature, provided that the heat of melting, the heat of vaporization, the heat of pyrolyzation and the specific heat at constant pressure of the different pyrolysis products are known [3].
In Fig. 1, the results are given for PMMA. The composition of the pyrolysis products has been determined using the empirical model mentioned above. For comparison also the values are given resulting from the assumption that during the pyrolysis of PMMA only MMA is formed. Note that at temperatures below 520 K the heat of gasification has no real physical meaning, since PMMA does not pyrolyze at these temperatures. From 520 K up to 700 K the two models show the same results, since in the empirical model also only monomer is formed. At higher temperatures, the results for the two models differ due to the different composition of the pyrolysis products. Assuming that pyrolysis of PMMA in an SFCC occurs at a temperature of 800 K, we find for the heat of gasification 2710 kJ/kg compared to 2360 kJ/kg when only MMA is formed. For comparison, in literature values between 2500 and 2700 kJ/kg are reported.

It is noted that for some of the pyrolysis products of PMMA, the necessary data (heat of pyrolyzation and the specific heat at constant pressure) were not known. These data have been determined by using the theory of group contributions, see e.g. [4].
ad 3) Heat transfer in the solid fuel

The temperature of the solid fuel determines to a large extent the fuel pyrolysis. This temperature is mainly determined by the heat transferred to the grain and the specific properties of the (solid) fuel itself. During this period, the use of TEMPROF, which is a computer code for heat transfer calculations in cylindrical geometries [5], has been evaluated. This was thought necessary, since TEMPROF does not take into account melting, pyrolysis and vaporization of the fuel.

The method used is based on a comparison between predicted and experimentally determined temperature profiles. The experimental profiles have been determined from experiments using hot air of up to 800 K to heat up the solid fuel. For these experiments, PE has been used as the solid fuel (see also section 3.1.1.). The results indicate good agreement for air temperatures below the melting point of the solid fuel. At higher air temperatures, the agreement was less. The latter is believed to be mainly due to the fact that, in TEMPROF, phase transitions are not accounted for and because TEMPROF only allows for temperature independent fuel properties. Therefore, it will be investigated whether it is possible to extend TEMPROF in order to include phase transitions and temperature dependent fuel properties (e.g. specific heat and conductivity).

ad 4) Combustion

In order to be able to perform chemical equilibrium calculations, the thermodynamic properties specific heat, enthalpy and entropy, as a function of temperature, have to be known for all the species involved. Therefore, during this period, as a first step, a literature search has been conducted to obtain these data. Secondly, for those species where literature does not give any values, the thermodynamic properties have been determined by using the earlier mentioned theory of group contributions. - At the moment, a Report on the use of this method is being prepared. - Thirdly, these thermodynamic data have been adapted for use in CET86 and STANJAN, which are dedicated computer programs for chemical equilibrium calculations. This has been illustrated by performing some test runs.

2.2. Validation/verification of COPPEP

No work done.

2.3. Programming and computing aspects

- The user's manual (H. Ablij).

A preliminary version of the User's manual is ready. A definite version is due when the program is finished.
3. ACTIVITIES OF THE EXPERIMENTAL WORKING GROUP (EWG)

3.1. Combustion experiments

3.1.1 Effect of operational conditions

- Testseries LPE (J.P. de Wilde and F. Dijkstra)

In order to be able to verify TEMPROF, see also section 2.1.4., a number of SFCC experiments have been carried out using vitiated air to heat up the solid fuel (no combustion). The purpose of these experiments was to determine temperature profiles as a function of time, at different locations along the grain. The vitiator temperatures were chosen with respect to the expected thermal behaviour of the PE fuel, i.e. melting at about 410 K and pyrolyzation at about 650 K, and were respectively 400, 550 and 800 K. Temperature histories have been determined through thermocouples (wire diameter 0.05 mm) which were embedded in the fuel grain (at different depths below the 'hot' surface). From the temperature histories, phase transitions could be detected, although this was not always the case. No further experiments are foreseen.

3.1.2. Effect of geometry and configuration variables

- Testseries CHTPB and N2 (F. Dijkstra)

Following an earlier series of experiments, some additional experiments were performed to determine the effect of different inlet geometries on the (local) regression rate. In total, 7 different geometries have been investigated. It was found that some inlets, significantly, can enhance fuel regression. However, this effect is largely limited to the recirculation zone.

3.1.3. High energetic fuels.

- Testseries HTPB (F. Dijkstra)

Following earlier experiments, some additional experiments have been performed to investigate the combustion of HTPB and HTPB + additives. The additives used are aluminium, boron, magnesium, and ammonium perchlorate. Variables considered are regression rate and combustion efficiency. To evaluate the combustion efficiency, gas samples have been taken in the exhaust of the combustion chamber. First results indicate that HTPB + magnesium gives the highest regression rate. Further analysis is continuing.

3.2. Experimental instrumentation

3.2.1. Diagnostics and measurement techniques

- USPET (F. Dijkstra)
During this period, the new ultrasonic equipment, developed by AIMS, was tested. The test results clearly confirmed the proper working of this equipment. Based on this result, three additional systems were ordered from AIMS, which were delivered in June, this year. Integration of these systems is planned for the next period.

- LDV (T. Wijchers)

In 1988, a Laser Doppler system has been acquired with the help of STW, to allow for detailed gas flow measurements (Laser Doppler Velocimetry; LDV). The use of LDV is foreseen for the validation and evaluation of the COPPEF flow modeling.

During this period, a number of LDV experiments has been carried out to familiarize with the LDV system and, through comparison of experimental data with theoretical data, to gain further confidence with respect to LDV generated data. The experiments have been carried out using the perspex model of the 2-D burner, see section 3.2.2., and cold air as the gas medium. Measurements were made over a cross-section at the end of the inlet flow channel of the model (flow velocities of up to 30-35 m/s). The length of the channel was such that, under these conditions, a fully developed (2-D) turbulent pipe flow could be expected. Such a gas flow can be calculated analytically with Prandtl's universal velocity-distribution law:

\[ u(y) = 2.5 \cdot v^* \ln \left( \frac{y}{y_c} \right) + u_c \]

where \( u(y) \) is the velocity at a distance \( y \) from the wall, \( v^* \) is the friction velocity, \( y_c \) is the distance between the centerline and the wall, and \( u_c \) is the maximum velocity in the flow channel. Note: this formula is only valid in the region between 0.01 \( y_c \) and 0.2 \( y_c \).

![Figure 2: 2-D chamber inlet velocity profile (mass flow of cold air is 29-33 g/s)]
In Fig. 2, the experimental data have been plotted against the results of the universal velocity-distribution law for two sets of parameters. It is found that the experimental data agree best with the p-line; differences are comparable with fluctuations in the local mean velocity.

From these results, it is concluded that the LDV equipment gives reliable results at least for gas flow velocities of up to 20-25 m/s. However, since it is not expected that, for other gas flow velocities, the physics will change, it seems valid to assume that LDV will also give good results for these other gas flow velocities. At the moment, this will allow LDV to be used, without problems, for gas flow velocities up to 170 m/s. To measure higher velocities, the LDV optics should be modified slightly.

- Movable thermocouple

During this period, the following items have been addressed:

- The use of Pt/Pt-Rd thermocouples in the SFCC was found to be limited to gas temperatures of about 2200 - 2300 K. In order to extend this temperature limit, an experiment was conducted using a Tungsten-Rhenium type of thermocouple (useful up to about 2900 K). The experiment showed that especially the 26% Rhenium wire suffers from loss of material (up to 40% of the initial diameter). No influence on the measurements was detected. Therefore, it was concluded that this type of thermocouple was not applicable for regular use, but could be used incidentally when high temperatures must be measured.

- Previously, it has been reported that conduction of heat through the thermocouple wires greatly can influence the measurements. To investigate this effect in more detail, an extra thermocouple was added to measure the temperature of the support of the thermocouple wires and to allow for a correction of the temperature measured. Experiments clearly justify this approach. Some further improvements, to reduce conduction losses, are planned.

- In addition to the experimental work, a theoretical study has been carried out to determine the influence of conductive heat transfer. Note: radiative heat transfer has already been treated independently. To determine the effect of conduction, a differential equation has been set up for the energy balance of an infinitesimal section of a wire heated through forced convection. As a result, the model gives a correction term for conduction losses of the thermocouple as a function of the effective diameter of the thermocouple, the thermal conductivity of the gas and of the wire material, the viscosity and the density of the gas. Initial calculations gave promising results.

- The pyrometer (T. Wijchers)

A method has been developed, which allows for the determination of the radiative heat transfer in the SFCC from the (soot) emissivity. The latter is determined from pyrometer measurements.
- Gas-sampling apparatus (J.P. de Wilde)

Construction of the gas-sampling apparatus is delayed for two months due to the high workload of the PML workshop. Testing, though, is still planned for August - September of this year.

3.2.2. The experimental facility (F. Dijkstra)

- The SPCC inlet section

The honeycomb structure, which is to reduce flow asymmetry in the inlet, is ready for testing. Testing is delayed due to problems with the new ignition system.

- The igniter

Several different igniter geometries have been tested to allow also ignition at high mass flows (1 kg/s and more). However, so far, test results have not been very succesfull. At the moment, further actions are under consideration.

- The aft mixing chamber/diffuser

The new aft mixing chamber has been tested. Testresults confirmed the validity of the design. No further work is foreseen.

- By-pass

Contrary to earlier reporting, the production of the variable area by-pass has not yet started. This is due to the fact that the design is delayed due to capacity problems at the FAEDUT construction bureau. No solution for this problem has yet been found.

- LDV particle generator

The LDV particle generator has been integrated in the automatic control system of the SFCC testfacility. No further work is planned.

- Production of HTPB fuel grains

The production facility of HTPB fuel grains is now fully operational. Only some small refinements are still planned.
- 2-D burner/2-D chamber

The 3-month preliminary design study of the 2-D burner, initiated in 1988, has been completed. This study was carried out by P. Oomen of the 'Hogeschool Haarlem' as part of his practical work. The work included internal ballistics, identifying the different components, some initial stress calculations and the construction of a perspex flow model. The results have been laid down in a Report [6]. No further work on the 2-D burner within the context of the SFCC-project is planned, except that, presently, the perspex flow model is evaluated for use with respect to validation/evaluation of the numerical flow model (COPPEF).
REFERENCES


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<th>ACRONYMS</th>
<th>DESCRIPTION</th>
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<tr>
<td>COPPEF</td>
<td>COmputer Program for calculation of (2D) Parabolic and Elliptic Flows</td>
</tr>
<tr>
<td>DUT</td>
<td>Delft University of Technology</td>
</tr>
<tr>
<td>EWG</td>
<td>Experimental Working Group</td>
</tr>
<tr>
<td>FAEDUT</td>
<td>Faculty of Aerospace Engineering, DUT</td>
</tr>
<tr>
<td>HDOTNO</td>
<td>Hoofdgroep Defensie Onderzoek, TNO (Defense Research Div., TNO)</td>
</tr>
<tr>
<td>HTPB</td>
<td>Hydroxyl Terminated Poly Butadiene</td>
</tr>
<tr>
<td>LDV</td>
<td>Laser Doppler Velocimetry</td>
</tr>
<tr>
<td>PE</td>
<td>PolyEth(y)lene</td>
</tr>
<tr>
<td>PMMA</td>
<td>PolyMethylMethAcrylate</td>
</tr>
<tr>
<td>PMLTNO</td>
<td>Prins Maurits Laboratory, TNO</td>
</tr>
<tr>
<td>SFCC</td>
<td>Solid Fuel Combustion Chamber</td>
</tr>
<tr>
<td>STW</td>
<td>Stichting voor de Technische Wetenschappen (Technology Foundation)</td>
</tr>
<tr>
<td>TNO</td>
<td>Organisatie voor Toegepast Natuurwetenschappelijk Onderzoek (Organization for Applied Scientific Research)</td>
</tr>
<tr>
<td>TWG</td>
<td>Theoretical Working Group</td>
</tr>
<tr>
<td>USPET</td>
<td>Ultra Sonic Pulse-Echo Technique</td>
</tr>
<tr>
<td>WGS</td>
<td>Werkgroep Gebruik Supercomputers (Working group for the use of supercomputers)</td>
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</table>
Implementation of a combustion model based on chemical equilibrium
in the COPPEF computer code

The purpose of the implementation of a chemical equilibrium combustion
model in the COPPEF computer code is easily explained. A chemical
equilibrium model allows all species to exist, provided their thermodynamic
data are given. Furthermore, since chemical equilibrium is achieved,
dissociation of species is accounted for. Also it is possible to include
the effect of turbulence on the combustion process by weighting the
elemental mass fractions with a probability density function. Last but not
least a chemical equilibrium calculation will require significantly less
computing time. A disadvantage is that it is based on infinitely fast
chemistry, hence it can be used only in regions where the reactions are
fast and where mixing is dominant.

The chemical equilibrium combustion model can be placed between the
diffusion flame combustion models and the finite rate chemical kinetics
combustion model. These models are discussed in Ref. 1 and 2.

The chemical equilibrium model is based on the STANJAN computer code
[3], which makes use of the element-potential method to obtain chemical
equilibrium.

A number of calculations will be presented to compare the results
obtained with the chemical equilibrium combustion model with the results
obtained with the other combustion models, for an H₂/O₂ flame. A combustion
model in the COPPEF computer code is used to solve for the source term in
the equation for the mass-fractions, Eq. 1.

\[ \frac{\partial}{\partial x} (\rho u_j Y_s) - \frac{\partial}{\partial x} (\Gamma_j \frac{\partial Y_s}{\partial x}) = S_{Y_s} \]  \hspace{1cm} (1)

convection diffusion source term

1

APPENDIX A

(No. of P.: 8)
COPPEF takes care of the convection and diffusion of species, but the combustion model must calculate the source term. It is convenient to keep all the other variables in a grid cell constant, while calculating the mass-fractions in this grid cell. Therefore the chemical equilibrium calculation is carried out at constant pressure and with a constant enthalpy. Of course the temperature will get a different value, but this will be calculated after the calculation of mass-fractions.

For the STANJAN program it is required that the mixture composition is given in mole fractions or mols of the elements present in the gas. These mole fractions can easily be calculated from the elemental mass-fractions. These elemental mass-fractions are conserved scalars, hence they can be calculated directly from the mixture fraction $f$. The elemental mass fraction $Z$ for nitrogen for example can be calculated from:

$$Z_N = f \cdot Z_{N,\text{fuel wall}} + (1 - f) \cdot Z_{N,\text{inlet}}$$  \hspace{1cm} (2)

In this manner the chemical equilibrium combustion model can be combined with the diffusion flame model. The convection and diffusion of mass-fraction of species is represented by convection and diffusion of mixture fraction, while the STANJAN program takes care of the source term.

In order to enhance convergence, first only the diffusion flame model is used during a number of iteration steps. Then the equilibrium model is 'switched on', i.e. the species mass-fractions are no longer calculated directly from the mixture fraction. The mixture fraction $f$ is used to provide the chemical equilibrium module with the elemental mass-fractions, together with the pressure $p$, the enthalpy $h$ and the temperature $T$ of the mixture. From the mass-fractions, the enthalpy and the temperature are

2
calculated as usual in COPPEF.

A schematic flowchart is given in Figure 1.

![Flowchart of the chemical equilibrium combustion module.](image)

In subroutine SJTP the thermodynamic quantities of the mixture are calculated, while in SJEQLB the equilibrium composition is calculated. In order to compare the chemical equilibrium combustion model with the other three combustion models, already implemented in the COPPEF computer code, a test series of calculations has been carried out. The three different combustion models already implemented in this COPPEF computer code are: a combustion model based on finite rate chemical kinetics, a combustion model based on the mixed is burnt concept, called the diffusion flame combustion model, and a turbulent diffusion flame combustion model. For a comparison of these three models the reader is referred to References 1 and 2.
Figure 2. Dimensions of the combustion chamber.

Four different calculations have been carried out on the Convex C220 of the Delft University of Technology. In Fig. 2 the dimensions of the combustion chamber can be seen, while in Table 1 the geometry and conditions of the calculations are given.

The calculations with the diffusion flame combustion model and the turbulent diffusion flame combustion model use only the species H₂, O₂ and H₂O. The other species are only used by the finite rate chemical kinetics combustion model and the chemical equilibrium combustion model, since these two models take into account the dissociation of species. That this dissociation is important will become clear in the following. The calculation example has been chosen such, that high temperatures will occur in the recirculation region of the combustion chamber. Due to dissociation,
Table 1. geometry and conditions

<table>
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<tr>
<td>Diameter</td>
<td>0.200 m</td>
</tr>
<tr>
<td>Stepheight</td>
<td>0.050 m</td>
</tr>
<tr>
<td>Length</td>
<td>0.750 m</td>
</tr>
<tr>
<td>FACGRY</td>
<td>0.98</td>
</tr>
<tr>
<td>$u_{in}$</td>
<td>30 m/s</td>
</tr>
<tr>
<td>uniform inlet velocity profile</td>
<td></td>
</tr>
<tr>
<td>$p_{in}$</td>
<td>$1 \cdot 10^6$ N/m$^2$</td>
</tr>
<tr>
<td>$T_{in}$</td>
<td>1100 K</td>
</tr>
<tr>
<td>$T_{wall}$</td>
<td>1100 K</td>
</tr>
<tr>
<td>viscosity</td>
<td>$2.08 \cdot 10^{-3}$ m$^2$/s</td>
</tr>
<tr>
<td>$Re_{h}$</td>
<td>72,000</td>
</tr>
<tr>
<td>$v_{inj}$</td>
<td>0.100 m/s</td>
</tr>
<tr>
<td>species</td>
<td>$O_2, H_2, O, H, OH, H_2O, H_2O_2, HO_2$</td>
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Temperatures will be lower for the finite kinetics and for the equilibrium combustion models. The diffusion flame based models do not account for dissociation, and therefore they will predict much higher temperatures in the recirculation region.

In the next Figures, some results will be presented. From the temperature profiles in radial direction, Figs. 3.1 to 3.8, it can be seen clearly that the difference between the chemical equilibrium model and the diffusion flame models is obvious. Especially at locations, where the diffusion flame models predict the highest temperatures ($\approx 4500$ K), the equilibrium model predicts much lower temperatures ($\approx 3300$ K). This is due to the dissociation of species, just as is the case with the finite rate chemical kinetics model. At the end of the channel, where temperatures are lower, the differences become smaller. It can also be seen that the reactions are fast in this calculation, because there is no difference in results between the chemical equilibrium model and the finite rate chemical kinetics combustion model.

In the recirculation region, the difference between the diffusion
flame model and the turbulent diffusion flame model is apparent, in the
other part of the flow, there is no difference. Apparently, the
'unmixedness' is fairly large in the recirculation region, and small
outside.

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Fig. 3.1.

$\text{U/UA}\ 
\text{R: X/D = 0.12}$

Fig. 3.2.

$\text{U/UA}\ 
\text{B: X/D = 0.25}$

Fig. 3.3.

$\text{U/UA}\ 
\text{C: X/D = 0.50}$

Fig. 3.4.

$\text{U/UA}\ 
\text{D: X/D = 1.25}$