

BOUNDARY LAYER MODELLING OF THE HEAT TRANSFER PROCESSES FROM IGNITERS TO ENERGETIC MATERIALS

Clive Woodley, Mike Taylor, Henrietta Wheal

Building H7, QinetiQ, Fort Halstead, Sevenoaks, Kent TN14 7BP, UK

Current ignition models used in internal ballistics codes assume that heat transfer is primarily due to convection, and radiation in the case of electrothermal ignition. However, many other thermophysical and thermochemical effects in the boundary layer surrounding propellant grains play an important, if not a dominant, role in energy transfer leading to ignition. Modelling was conducted to estimate the heat transfer due to thermophysical and thermochemical effects within thermal boundary layers. Heat transfer by black powder combustion gases was compared with that due to condensing metal (copper) vapour. These heat transfer rates were then applied to propellant in order to predict ignition delay times, which were then compared to experimental ignition delay times. Convective heat transfer has also been estimated and direct comparisons made with heat transfer due to thermophysical and thermochemical effects.

INTRODUCTION

Thermal boundary layers exist between hot igniter material and the surface of cool energetic materials. It has been suggested that the behaviour of igniter material within these boundary layers dominates energy transport mechanisms for ignition (e.g. physical vapour deposition, thermochemical recombination reactions) [1]. To improve the current predictive modelling capability for the UK MOD, a move is being made towards explicitly modelling some of the important physics and chemistry occurring within the gas phase and at the interface with the solid phase. Initial work is being conducted with the ultimate objective of using the lessons learned to make intelligent modifications to existing internal ballistics codes. The benefits from this work will allow the design of optimal igniters for very insensitive gun propellant charges.

The approach taken in this study was to use the CHEMKINTM suite (CHEMKINTM is a registered trademark of Reaction Design) [2] to model the surface deposition rates and recombination chemistry within a thermal boundary layer at the interface of igniter gases and energetic material. The main aim of the work was to conduct preliminary modelling of an energy budget for both conventional black powder and plasma ignition and apply these to a gun propellant ignition scenario. The energy budget would compare heat transfer due to thermophysical/thermochemical effects with that due to convective heat transfer. Experimental ignition delay data were used to support the modelling.

Equilibrium modelling was conducted for black powder and copper vapour. Additionally, non-equilibrium modelling was conducted for black powder. The equilibrium modelling essentially ignored chemical reactions in the core flow and allowed only a limited set of reactions at the surface. The non-equilibrium modelling

allowed chemical reactions to take place everywhere, including condensation onto a surface.

CHEMKIN

The feature of CHEMKINTM that is particularly relevant to the ignition of energetic materials is the laminar boundary layer model. The boundary layer model is general in that it can be applied to any channel-flow system for which gas phase and surface kinetic mechanisms are known. The model predicts gas phase temperature and velocity fields, concentration fields for any number of chemical species, deposition or etching rates and surface-species coverage.

Flow conditions - pressure, temperature, velocity and species mass fractions - are input by the user at an inlet plane. Details on the gas phase and surface chemical reactions are also specified. The CHEMKINTM boundary layer code then predicts the steady state conditions for that set of input flow conditions and reactions.

Most charges used in large calibre guns comprise many grains that are in contact with each other. Between adjacent grains, there are many small channels through which igniter gas and plasma can propagate. Typical grain dimensions are 1-2 cm diameter and 1-100 cm long. These dimensions indicate that the interstitial gaps are less than 1 cm in 'width' and up to 100 cm long. Therefore the boundary layer model is very appropriate for modelling the flow along the interstices.

For the simulations, the flow along a cylindrical channel was modelled. This channel had a diameter of 1 cm (the order of interstitial gaps between propellant grains). The length was semi-infinite but only the first 100 cm was considered. Igniter gas enters the simulation with set initial conditions.

For the simulations reported in this paper, the following flow conditions were used:

- Black powder gas temperature 2000K (equilibrium and non-equilibrium);
- Copper vapour (plasma) temperature 4000K (equilibrium only);
- Velocity 200m/s, 300m/s and 400m/s;
- Pressure 0.1MPa and 5MPa.

EQUILIBRIUM MODELLING

The CEA2 thermochemical code [3] was used to predict the equilibrium products at various temperatures and pressures. For each set of conditions, the output from the CEA2 code included the species and the mass fraction of each species. These values were input to CHEMKINTM to obtain heating rates at the surface. For the equilibrium modelling, these compositions were essentially fixed throughout the simulation. The only changes to this composition would be those due to condensation of species on the surface (surface reactions) and species diffusion (different species have different transport properties).

Figures 1 and 2 show the main predicted equilibrium combustion products, as a function of temperature, for black powder at 0.1 MPa and 5 MPa respectively. The composition of black powder used for this work was 75.5% potassium nitrate, 14.5%

carbon and 10% sulphur. In practice, the carbon is actually charcoal, consisting of only 70-80% carbon [4]. For this study it was decided to ignore other components as they were generally small and added considerably to the complexity of the chemical system. However, it is realised that the presence of some neglected species might be important in the reaction mechanisms.

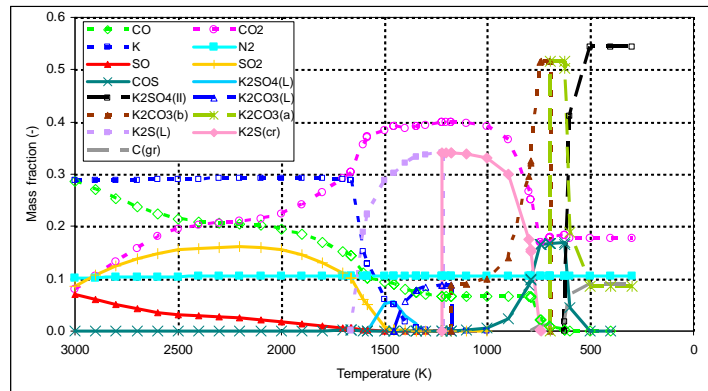


Figure 1. Predicted equilibrium conditions for black powder at 0.1MPa

Figure 1 shows that a key change in the concentrations of chemical species occurred at about 1700K. At this temperature, the mass fraction of potassium starts to decrease substantially as the temperature falls further. Commensurate with this, the potassium combines with sulphur dioxide to form condensed (liquid) potassium sulphide. The liberated oxygen combines with carbon monoxide to form carbon dioxide. Therefore it may be expected that there should be substantial differences in the predicted results for equilibrium and non-equilibrium conditions as gas species are condensed onto the surface, and cooling takes place near the surface.

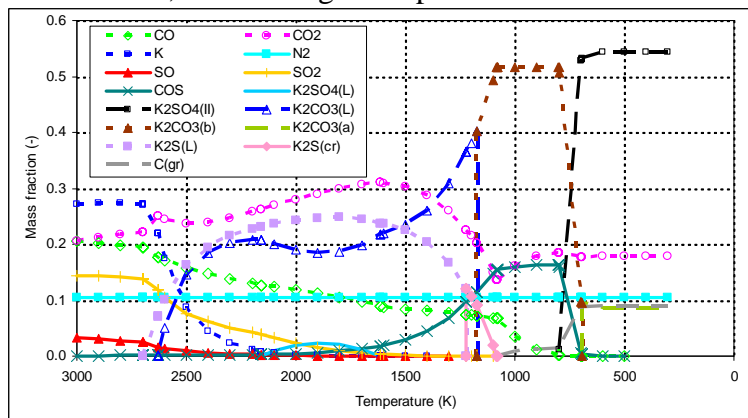


Figure 2. Predicted equilibrium conditions for black powder at 5MPa

Figure 2 shows substantial differences from Figure 1. The effect of the higher pressure results in a greater percentage mass fraction of condensed species at temperatures below 2700K.

CHEMKIN MODELLING RESULTS

Black powder - equilibrium

Figure 3 shows the predicted temperature and axial velocity distributions for inlet flow conditions of 2000K, 0.1MPa and 300m/s. Figure 4 shows the distributions for similar conditions but for an inlet pressure of 5MPa. In these figures, the wall is at a distance of 0.5cm for the cross-flow coordinate.

The application of a higher inlet pressure on the temperature and velocity distributions results in a significant narrowing of the boundary layer and produces nearly parallel velocity contours. The predicted temperature distributions did not vary significantly with inlet velocity over the range 200-400m/s.

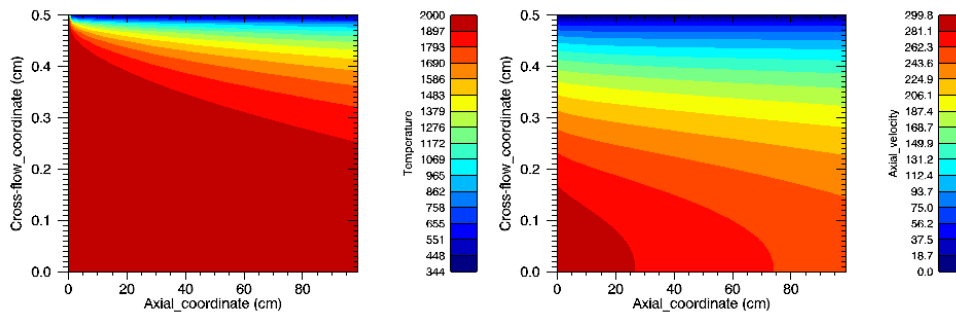


Figure 3. Predicted temperature (K) and axial velocity (m/s) distribution for inlet flow conditions of 2000K, 0.1MPa and 300m/s – black powder equilibrium conditions

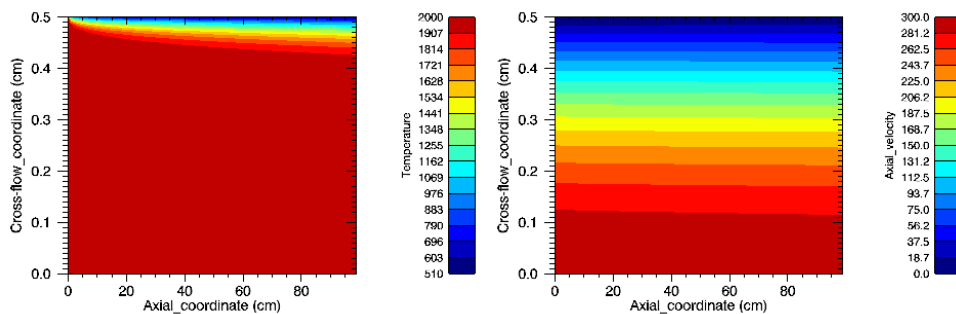


Figure 4. Predicted temperature (K) and axial velocity (m/s) distribution for inlet flow conditions of 2000K, 5MPa and 300m/s – black powder equilibrium conditions

Black powder – non-equilibrium

Figure 5 shows the predicted temperature and axial velocity distributions for inlet flow conditions of 2000K, 0.1MPa and 300m/s. Figure 6 shows the distributions for similar conditions but for an inlet pressure of 5MPa. The effects of a higher inlet pressure are similar to those for the equilibrium case, i.e. a narrowing of the boundary layer. Comparing the equilibrium and non-equilibrium cases, the only obvious

differences in the temperature and velocity distributions are that the temperatures are slightly greater for the non-equilibrium cases.

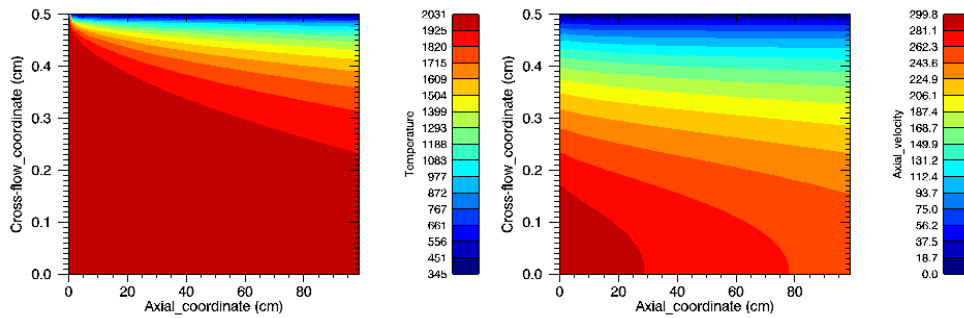


Figure 5. Predicted temperature (K) and axial velocity (m/s) distribution for inlet flow conditions of 2000K, 0.1MPa and 300m/s – black powder non-equilibrium conditions

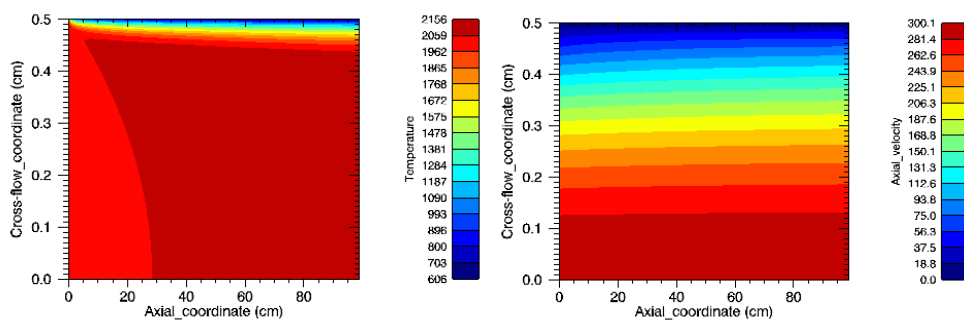


Figure 6. Predicted temperature (K) and axial velocity (m/s) distribution for inlet flow conditions of 2000K, 5MPa and 300m/s – black powder non-equilibrium conditions

Copper vapour

Figure 7 shows the predicted temperature distributions for inlet flow conditions of 4000K and 300m/s for pressures of 0.1MPa and 5MPa.

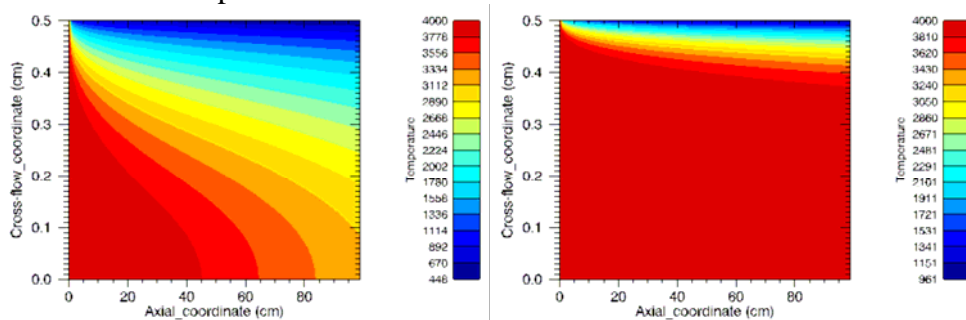


Figure 7. Predicted temperature (K) distribution for inlet flow conditions of 4000K, 0.1MPa (left), 5MPa (right) and 300m/s – copper vapour

At 0.1MPa and 5MPa, copper condenses from vapour to liquid at 2840K and at 4000K respectively. No account is taken of the variation in the boiling point of copper with pressure in the modelling. However, it can be seen from Figure 7 that the copper is able to condense a millimetre or two away from the wall in both cases. If the copper condenses, this will heat the cooler layers close to the wall and drive the boundary layer closer to the wall. One drawback of the version of CHEMKIN™ (4.0) used is that it does not allow the formation of condensed species within the core flow, only at the wall. The latest version (4.1) has a particle tracking module which should allow the formation of condensed species within the core flow.

Heating at wall

The predicted surface heat productions due to thermophysical and thermochemical effects for the equilibrium and non-equilibrium black powder simulations for inlet flow conditions of 2000K and 300m/s are compared in Figure 8 (left – 0.1MPa, right – 5MPa).

At 0.1MPa, the non-equilibrium simulation results in greater surface heat production rates by up to 10%. At 5MPa, the non-equilibrium simulation predicts lower surface heat production rates by about 50%. This reduction has occurred because most of the potassium and sulphur that could freely combine to form potassium sulphide have formed other products, such as carbonyl sulphide, or remained unreacted. However, it might be expected, based on the equilibrium predictions at 5MPa of CEA2, that condensed potassium sulphide would form in the free flow rather than at the wall, thus lowering the amount of vapour condensing at the wall and therefore reducing the heat production at that location.

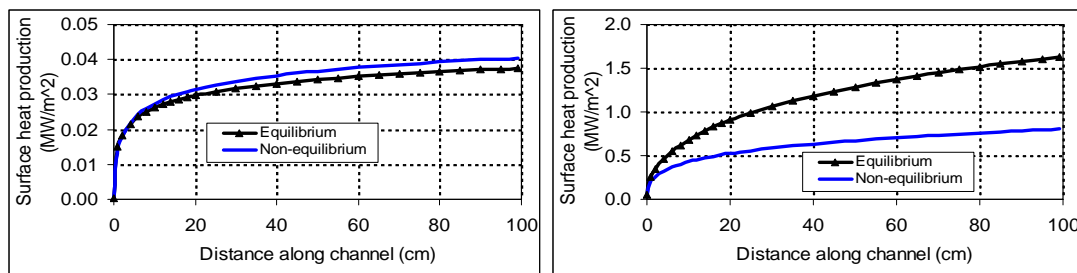


Figure 8. Predicted surface heating rates for inlet flow conditions of 2000K, 0.1MPa (left), 5MPa (right)

For copper vapour, the predicted wall heating rates for 0.1MPa and 5MPa are compared in Figure 9. These show a different profile from those shown in Figure 8. The reason for this difference is shown in Figure 10, which shows the predicted copper vapour distribution for inlet flow conditions of 5MPa, 4000K and 300m/s. Initially the deposition rate of copper is relatively high, and decreases with distance along the channel due to copper depletion close to the wall. This indicates that the deposition process is transport limited; the copper vapour can not easily reach the wall.

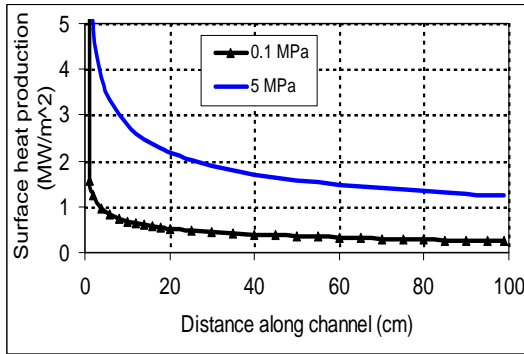


Figure 9. Predicted surface heating rates for copper vapour inlet flow conditions of 4000K and 300m/s

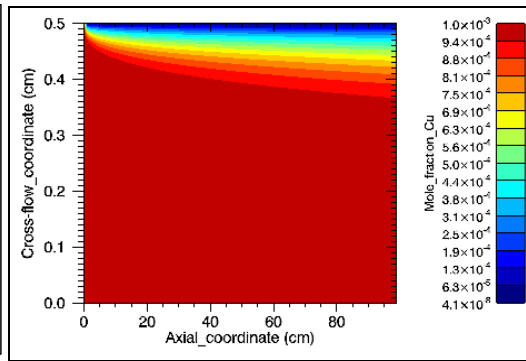


Figure 10. Predicted copper vapour distribution for inlet flow, conditions of 5MPa, 4000K and 300 m/s

The heating rates, at 50cm, shown in Figures 8 and 9 were used to estimate the time to ignition of JA2 propellant, which at 293K has a thermal diffusivity of $0.1334\text{mm}^2/\text{s}$ and a thermal conductivity of $0.290\text{W}/\text{m}/\text{K}$. Table 1 compares the estimated ignition delays assuming a constant surface heat flux to a semi-infinite solid. Also shown are estimated ignition times for convective heating using standard convective heating correlations applicable for internal ballistics [5].

Table 1. Comparison of estimated ignition delays

Igniter material and conditions	Surface heat flux (MW/m^2)	Time to ignition (ms)	Convective heat flux (MW/m^2)	Time to ignition (ms)
Black powder at 0.1MPa (E)	0.0343	13200	0.509	59.9
Black powder at 5MPa (E)	1.29	9.32	2.74	2.07
Black powder at 0.1MPa (NE)	0.0367	11500	-	-
Black powder at 5MPa (NE)	0.670	34.6	-	-
Copper vapour at 0.1MPa	0.354	124	0.798	24.4
Copper vapour at 5MPa	1.58	6.21	5.63	0.489
E = equilibrium conditions		NE = non-equilibrium conditions		
Assumed ignition temperature is 470K				

The CEA2 code was used to calculate the thermodynamic data (density, molecular weight, ratio of specific heats, specific heat capacity at constant pressure, thermal conductivity, viscosity) for black powder. For copper, the REAL thermochemical code [6] was used.

There is relatively little difference between the estimated ignition delays using equilibrium and non-equilibrium chemistry for black powder. Comparing the ignition times obtained from the surface heat fluxes calculated by CHEMKIN™, the effect of increasing the density from 0.1MPa to 5MPa reduces the ignition times by factors of 1000 and 20 for black powder and copper vapour respectively. Comparing copper vapour and black powder, the estimated ignition delays are a factor of 100 shorter for copper vapour at 0.1MPa and comparable at 5MPa.

For convective heating, the ignition delay is a factor of 2-4 shorter for copper vapour than for black powder.

Experimental data to compare directly with these estimates are not readily available. However, crude comparisons may be made with results from experiments in which the ignition characteristics of 6g of black powder were compared with a 6kJ plasma discharge using a capillary plasma generator [7]. The geometrical configuration of the tests was such that the igniter material would have approached the propellant grains from a direction perpendicular to the grain surface; stagnation points may have developed and turbulent flow was very likely. Pressures developed were a few megapascal. However, the measured ignition delays were in the range 0.056-0.4ms for copper vapour and 4ms for black powder. These times are very comparable with those estimated in Table 1 for 5MPa.

CONCLUSIONS AND FURTHER WORK

Preliminary modelling of the boundary layer due to igniter material flowing over a propellant surface has been successfully conducted using the boundary layer model contained in the CHEMKINTM software. This modelling has allowed the estimation of surface heating effects due to thermophysical and thermochemical effects. The work confirms that the behaviour of igniter material within these boundary layers may be an important to energy transport mechanisms for ignition.

Comparisons of the heating effects due to black powder and copper vapour show that copper vapour gives rise to ignition delays 20-1000 times shorter, as a result of vapour deposition at the propellant surface. This reduction is in broad agreement with measurements from experiments.

The CHEMKINTM particle tracking module should be evaluated to determine the effect of allowing species to condense in the core gas flow on the heating at the propellant surface.

The CHEMKINTM boundary layer model assumes steady state laminar flow. Bespoke experiments are required to measure the heat flux under such conditions to validate the modelling work. Although conditions may occasionally be steady state for typical internal ballistics scenarios, the flow is more likely to be turbulent. Further work needs to be conducted to determine the effects of transient turbulent boundary layer flow on the heating rates at the propellant surface.

REFERENCES

1. M J Taylor, "Plasma Propellant Interactions in an Electrothermal-Chemical Gun", PhD Thesis, Cranfield University, September 2002, www.qinetiq.com/mjtaylor_thesis.
2. CHEMKINTM Theory Manual, June 2004.
3. S Gordon & B J McBride, "Computer program for calculation of complex chemical equilibrium compositions and applications", NASA Reference Publication 1311, October 1994.
4. E Freedman, "Thermodynamic Properties of Military Gun Propellants" in 'Gun Propulsion Technology', vol. 109 in the AIAA Progress in Astronautics and Aeronautics series, 1988.
5. C R Woodley, "Modelling the ignition of 40mm gun charges", 22nd International Symposium on Ballistics, Vancouver, November 2005.
6. G V Belov, "REAL - thermodynamic examination of combustion products under high pressure", Proceedings of the 28th ICT Conference, Karlsruhe, Germany, June, 1997.
7. M J Taylor, "Evidence for the Hypothesis of Ignition of Propellants by Metallic Vapour Deposition", Propellants, Explosives, Pyrotechnics, Vol. 27, pp 327-335, December 2002.

This work was carried out as part of the Weapons and Platform Effectors Domain of the UK MOD Acquisition Organisation.

© Copyright QinetiQ Ltd 2007