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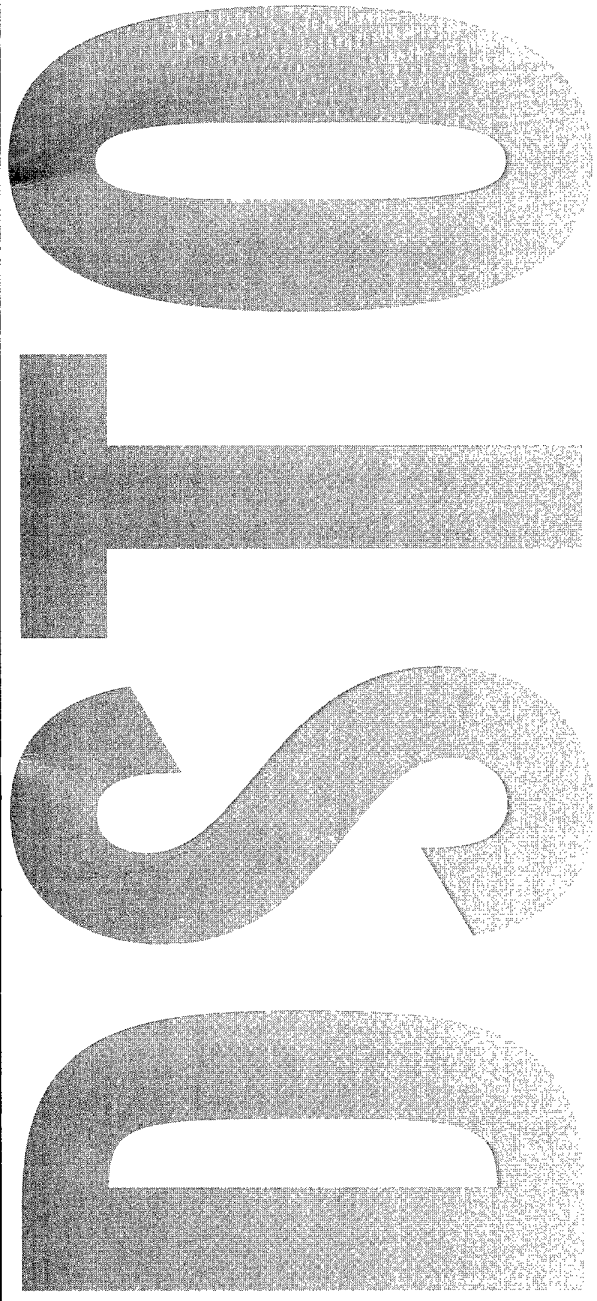

Thermochemistry and Kinetics Models for Magnesium/Teflon/Viton Pyrotechnic Compositions

Farid C. Christo

DSTO-TR-0938

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Farid C. Christo

Weapons Systems Division
Aeronautical and Maritime Research Laboratory

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ABSTRACT

This study examines in detail the equilibrium chemistry of Magnesium/Teflon (MT), Magnesium/Teflon/Viton (MTV), and MTV-air compositions. Gas-phase as well as solid-phase chemistry has been included. Equilibrium calculations accounting for over 47 species and various initial conditions have been performed. A comparison between MT and MTV combustion has been carried out with emphasis on investigating the effect of Viton on the combustion characteristics. The effect of air on MTV combustion has also been investigated for two possible MTV-air combustion models. A chemical kinetic mechanism with 18 reactions and 17 species, has been used to study the time evolution of reacting MT mixtures, accounting for finite-rate elementary reactions as well as performing sensitivity analysis with respect to reaction rates. Three different variations of the kinetic scheme have been studied and their effects on combustion products and flame temperature have been examined. Kinetic analysis has been repeated for three pyrotechnic compositions that are commonly used in flare and rocket motor igniter formulations.

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Executive Summary

A recent analysis of operational data over a period of 25 years (1973-1997) showed that over 51% of a total of 1434 military aircraft fatalities had fallen victim to infrared (IR)-guided air-to-air or surface-to-air missiles. The development of second (discriminatory)- and third (imagery)-generation missile seekers put more pressure on the IR countermeasure (CM) community for developing effective decoys to keep up with the advances in seekers technologies. Whilst the major thrust of the development in seekers is based on advances in electro-optic technologies, on-board IRCM technologies have not been progressing at comparable rate and still lag behind. However, passive off-board countermeasures remain the main effective in-service technology against IR guided missiles. Among the recent development in such IRCM's are the "kinematic flares", "special materials", "hot-bricks" and the "thrusted expendables" decoys.

The purpose of AIR 97/250 task "Modelling IR Countermeasures for Aircraft" is to develop computational capabilities to predict the aerothermochemical and radiative properties of generic pyrotechnic compositions. The process has been divided into three main stages; the first focuses on the development of thermochemical and chemical kinetic mechanisms, and is the main theme of this study. The second stage is the integration of chemical schemes into a flow field solver. This will provide a tool for simulating the effect of atmospheric turbulence on the combustion of the pyrotechnic mixtures under various operational conditions. The outcome of the first two stages will then be used to construct three-dimensional, time-dependent models to predict the thermal radiation characteristics and the overall performance of generic pyrotechnic compositions.

This study focuses on investigating the thermochemical properties and chemical kinetics of a number of Magnesium-Teflon-Viton (MTV) compositions, similar to those used in Defence applications. This comprehensive analysis focuses on calculating the chemical and combustion characteristics of MTV and MTV-air mixtures for a wide range of operational conditions. It includess chemical equilibrium calculations, sensitivity analysis of chemical kinetics, premixed combustion and perfectly stirred reactor modelling. Much of the discussion relates to understanding the effect of Viton and atmospheric air on the combustion of MTV mixtures. The analysis of the chemical kinetics scheme provides useful information on the dominant species and reactions that influence the combustion of MTV mixtures. This knowledge will be used to implement a realistic chemical model into a flow field solver, which is the focus of the next stage of this task.

Authors

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Farid Christo completed his B. Sc.(1986) and M.Sc. (1989) in Aeronautical Engineering at the TEHNION-Israel Institute of Technology, follwed by one year working as a research engineer at the Technion-R&D Institute. In his undergraduate studies he majored in thermo-fluids and propulsion systems. Farid's M.Sc. research was on experimental investigation of multiphase flows at low Reynolds numbers.

Between 1990 and 1993 he worked at the University of Sydney on a joint project with Pacific Power Corporation. His work focused on the development and validation of computer models to predict the flow field and erosion rate of heat recovery tubes inside the boilers of coal-fired power stations.

Between 1993-1996, he undertook a Ph.D. research at the University of Sydney, Department of Mechanical and Mechatronic Engineering. His research topic was the development of artificial neural networks for applications in turbulent combustion simulations. Upon completion of his doctorate Farid joined the Sydney-based company Biomass Energy Services and Technology, where he worked on modelling industrial aerodynamics and combustion processes. In April 1998 he joined the DSTO as a Research Scientist with Weapons Systems Division, Salisbury.

Farid's current research objective is to develop advanced computational capabilities for modelling the aerothermochemical and radiative fields of generic pyrotechnic compositions. This work will provide DSTO with the capability to evaluate the performance of new and existing pyrotechnic formulations with minimal dependence on complex and expensive experimental procedures.

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1. Introduction

Pyrotechnic devices, whilst having some civilian applications such as recreational fireworks and safety airbags in motor vehicles, are mainly used for military and Defence purposes such as illumination flares, masking smoke producers, incendiaries, ignition devices, tracers, and decoy flares to name just a few [1,2]. Infrared (IR) decoy flares have been in service since the 1960s, and they remain one of the most effective off-board countermeasures (CM) against heat-seeking guided missiles. Data collected over a period of 25 years (1973-1997) showed that over 51% of a total of 1434 military aircraft fatalities had fallen victim to IR-guided air-to-air or surface-to-air missiles [3]. The development of second (discriminatory)- and third (imagery)-generation missile seekers put more pressure on the IRCM community to develop effective decoys to keep up with the advances in seekers technology. Among the recent development in IRCM that worth mentioning are the "kinematic flares", "special materials", "hot-bricks" and the "thrusted expendables" decoys [4,5].

Magnesium/Teflon[1] (MT)-based compositions are widely used in IR decoy flares formulation because of their large energy output compared to other pyrotechnic mixtures, low hygroscopicity, low dependence of burning rate on pressure and temperatures, and relatively high degree of safety in preparation [6]. Viton[1] (a binder) is commonly added to MT mixtures to ease processing by improving homogeneity of the mixture, and also to protect the magnesium against oxidation by moisture during storage. In addition to its exceptional energy output Magnesium/Teflon[1]/Viton (MTV) composition has excellent environment and thermal stability characteristics and good compatibility with most materials used in pyrotechnic ordnance [7]. While a large number of studies [8-12] has been conducted on the dynamic performance of pyrotechnic compositions in general and MTV in particular (e.g. burning rate, processing technology, ballistic studies, spectral emission, thermal decomposition and so forth), only limited thermochemical and kinetics works have been carried out [7,13-15].

This study reports the results of a comprehensive numerical analysis of the thermochemistry of MT and MTV compositions. It also addresses the effect of atmospheric nitrogen on the combustion of MTV compositions and focuses on chemical kinetics and sensitivity analysis of different MT mixtures.

[1] Teflon (polytetrafluoroethylene) and Viton (copolymer of vinylidene fluoride and hexafluoropropylene) are trademarks of Du Pont.

2. Modelling Methodology

The modelling approach adopted here is based on numerically solving the governing equations that describe the thermochemistry and chemical kinetics of MT and MTV pyrotechnic compositions. It includes chemical equilibrium, perfectly stirred reactor (PSR), and premixed combustion models. Kinetics sensitivity analysis with respect to reaction rates has also been conducted. All calculations have been performed using commercial software packages Chemkin-III [16] and Surface Chemkin-III [17], and their EQUIL, SENKIN, PSR and PREMIX modules. A brief description of these modules is given in the following sections. Details on the mathematical and numerical schemes can be found in References [16, 17].

2.1 Chemical Equilibrium Model

Chemical equilibrium calculations, using EQUIL [16] code, have been used to determine the adiabatic flame temperature and concentration of combustion products of MT and MTV compositions. The approach used for evaluating chemical equilibrium is the element-potential method, which is based on the minimisation of Gibbs free energy. The equilibrium solution for given reactants and products is determined by establishing the distribution of the number of moles of each pure species in the system that minimises the system's Gibbs free energy, subject to atomic population constraints, namely atomic balance for each atom in the system. While chemical equilibrium calculations do not account for chemical kinetics they provide valuable information on the direction of chemical reactions and the effect of reactants and their initial state on the reaction products.

2.2 Kinetics Sensitivity Analysis

To examine the kinetics sensitivity with respect to reaction rates, SENKIN [16] module has been used to predict the time evolution of homogeneous reacting pyrotechnic mixtures, accounting for finite-rate elementary chemical reactions as well as performing sensitivity analysis. In general, sensitivity analysis determines quantitatively the relationship between the solution to a given chemical kinetic mechanism and various parameters, e.g. reaction rates.

2.3 Perfectly Stirred Reactor (PSR) Model

Perfectly stirred reactor (PSR) models are commonly used for testing and developing chemical reaction mechanisms. The PSR concept assumes that the contents of a well-mixed reactor to be nearly uniform due to high diffusion rate or intense turbulent mixing. That is the rate of reactants conversion to products is controlled by chemical reaction and not by mixing processes. PSR models solve the steady-state conservation equations of mass, species, and energy.

In addition to testing chemical kinetics schemes, PSR calculations (using AURORA code [16]) are used to investigate the time it takes to reach a pseudo-equilibrium state. This is an important parameter as it indicates whether or not diffusion effects (e.g. diffusion of atmospheric air) would influence the reactions.

2.4 Premixed Combustion Model

Combustion of pyrotechnic mixtures can be classified as a premixed flame. That is the fuel and oxidant are completely mixed before the mixture is ignited. Calculations have been performed using PREMIX code [16], which accounts for chemical kinetics and molecular transport processes. The code is used to predict the flame temperature and species profiles in a burner-stabilised laminar flame configuration. The results are also used to determine ignition-delay time and understand the combustion process.

3. Compositions and Kinetic Mechanism Investigated

3.1 MT and MTV Equilibrium Models

This section lists the species and the initial conditions used in the various thermochemical and kinetics models investigated in this study. Since tetrafluoroethylene (TFE) is the main decomposition product from polytetrafluoroethylene (PTFE), it is assumed that PTFE and TFE systems are similar, and therefore calculations are made based on TFE properties. Due to lack of sufficient information on the thermodynamic properties of Viton, such as enthalpy-temperature dependence, the following simplifying assumption has been made in the calculations. Rather than treating the Viton as a unit molecule it has been assumed to consists of two separate molecules; a vinylidene fluoride (VDF) molecule and a hexafluoropropylene (HFP) molecule. It has been found (numerically) that the difference in the heat of formation of a unit molecule of Viton and that of a combined PVDF:HFP molecules, is negligible and has no significant effects on the flame temperature or on the concentration of the products.

3.1.1 Magnesium-Teflon Composition

Equilibrium calculations of MT compositions included the following species: $Mg(g)$, $Mg(l)$, $Mg(s)$, $C_2F_4(g)$, $MgF(g)$, $MgF_2(g)$, $MgF_2(l)$, $MgF_2(s)$, $MgF_4(g)$, $C(s)$, $C(g)$, $C_2(g)$, $C_3(g)$, $C_4(g)$, $C_5(g)$, $F(g)$, $CF(g)$, $CF_2(g)$, $CF_3(g)$, $CF_4(g)$, $C_2F_2(g)$, $C_2F_3(g)$, and $C_2F_6(g)$. The g, l, s letters represent phase state of gas, liquid, and solid, respectively. Two sets of calculations have been performed. The first set assumes all species are in a gaseous state (all-gaseous model), i.e. no liquid or solid phase species are included in the calculations. The second set allows species in solid and liquid phases (multiphase

model). The effect of the initial temperature of MT mixture on the adiabatic flame temperature and the products has also been examined for both cases. Calculations have been carried out for various MT compositions ranging from 10% to 80% magnesium (by weight).

3.1.2 Magnesium-Teflon-Viton (MTV) Composition

For MTV mixtures more species were included in the calculations (in addition to the species listed above). These are: MgH, HF, CHF, CH_2F, CHF_2, CH_3F, CH_2F_2, CHF_3, CH, CH_2, CH_3, and CH_4. Initial calculations for MT mixtures have shown that the amounts of higher carbons (C_2, C_3, etc.) are small and therefore no C_xH_y (x & y >2) compounds have been included in subsequent models. Calculations have been performed for two (fixed) Viton concentrations of 5% and 16% (by weight). In each case the magnesium component has been varied between 10% and 80%. Three commonly used MTV mixtures as listed in Table 1, have been selected in this study.

Table 1: MTV formulations used in chemical equilibrium calcualtions.

Composition Identifier	MTV ratio (% weight)	Typical application
MTV-1	54:30:16	US flare composition
MTV-2	55:40:5	UK flare composition
MTV-3	61:34:5	US igniter composition

3.1.3 MTV-Air Combustion

To examine the effect of atmospheric air on the equilibrium chemistry and combustion characteristics of MTV mixtures, calculations have been carried out for various MTV-air compositions. The inclusion of air in the chemistry equation means more species and radicals are involved due to possible reactions between O_2 and N_2 molecules from the air and C, F and H atoms from the MTV. The additional species included in the MTV-air combustion are: CO, CO_2, MgO(*g*), MgO(*l*), MgO(*s*), H_2O, MgC_2(*s*), Mg_2C_3(*s*), Mg_3N_2, MgN, NH_3, NO, NO_2, N_2O, and N_2O_5. The amount of air in the MTV-air formulations has been varied between 10% and 80% air (by weight).

Two models for MTV-air combustion have been considered. The first model, which has also been used in previous works [7,13], treats the air as a reactant in the MTV-air mixture. However, a more plausible scenario is to assume that the air is reacting with the combustion products of MTV, rather than as a reactant in the MTV-air mixture. This assumption is based on envisaging that burning flares in an airstream comprise of two distinct reaction zones. The first is an anerobic reaction zone where MTV thermally reacts, followed by a second reaction zone, that engulfs the anerobic zone, where mixing and afterburning of the combustion products with atmospheric air occurs [18]. Accordingly, the second MTV-air combustion model used consists of two stages: 1) MTV reaction and 2) MTV combustion products reacting with air. In this model the

adiabatic flame temperature and products of MTV formulations (listed in Table 1) are calculated first, then the major species from the products are used as reactants burning in air. The initial mixture temperature has been assumed to be equal to the flame temperature of the MTV. The major species included in the model are: Mg(*g*), MgF(*g*), MgF_2(*g*), C(*s*), MgF_2(*s*), MgF_2(*l*), and HF radicals. The initial temperature and species mole fractions of the three MTV mixtures are listed in Table 2.

Table 2: Initial state of combustion products used in MTV-Air reaction.

Flame Temperature T(K)	MTV-1	MTV-2	MTV-3
	2707	2847	2476
Species mole fraction			
Mg(*g*)	0.3463	0.3436	0.4598
MgF(*g*)	0.1354	0.1731	0.1143
MgF_2(*g*)	0.1147	0.1520	9.276×10^{-2}
MgF_2(*l*)	2.358×10^{-3}	1.625×10^{-2}	5.551×10^{-2}
MgF_2(*s*)	2.343×10^{-2}	1.252×10^{-3}	8.081×10^{-3}
C(*s*)	0.2910	0.2839	0.2389
HF	2.036×10^{-2}	2.748×10^{-2}	2.344×10^{-2}

3.2 Chemical Kinetic Scheme

The kinetics scheme used by Deyong and Griffiths [13] has been adopted in this study for the sensitivity analysis, the PSR and the premixed-flame calculations. The mechanism consists of 18 elementary reactions and contains 15 species as listed in Appendix A. It should be noted here that the Arrhenius factors for the higher carbons reactions are estimates as no accurate data is available.

4. Results and Discussion

4.1 Effect of Initial Temperature on Equilibrium Chemistry

The effect of the initial temperature of MT mixtures and their phase state (gaseous, liquid, solid) on the equilibrium chemistry has been examined for initial temperatures of 300K and 1366K. The latter is the boiling temperature of magnesium at atmospheric pressure, while the former represents a typical ambient temperature.

The results of the all-gaseous and the multiphase models are shown in Figs. 1 and 2, respectively. These figures show that the effect of initial temperature on the flame temperature is more pronounced in the all-gaseous model. Also, the flame temperature is strongly affected by the phase state of the species, irrespective of the initial temperature. In the fuel-lean region (Mg <33%) it is clear that the flame temperature is

noticeably higher for the multiphase model than the all-gaseous model, irrespective of the initial temperature of the mixture (for the same magnesium content).

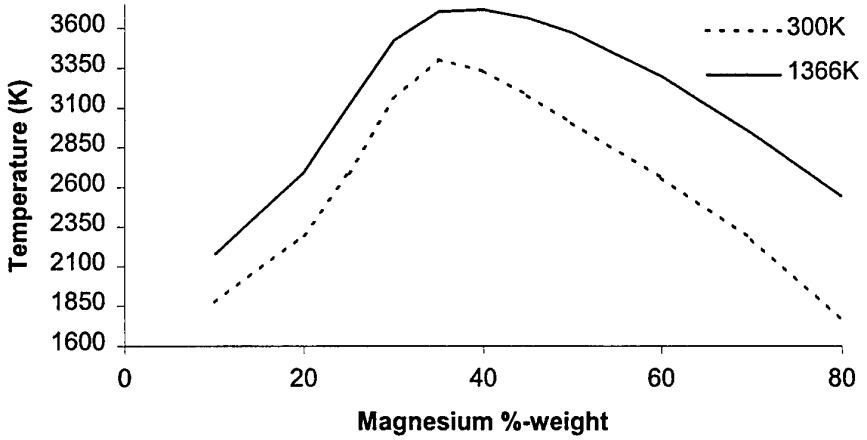

Figure 1: Effect of inlet temperature and phase state on the adiabatic flame temperature of MT composition (all species are in gaseous phase).

However, the reverse is true in the fuel-rich region. Nevertheless a similar stoichiometric flame temperature (~3700K) has been computed by both models (for an initial temperature of 1366K). The temperature gradient in the multiphase model is steeper than in the gaseous phase, especially on the fuel-rich side. These differences are probably due to the effect of solid and liquid properties in the energy equation such as heat of formation, sensible energy etc.

Figures 3 and 4, show equilibrium mole fraction profiles of major species for different MT compositions. The effect of the phase state on species concentrations is less evident in the region between 20% and 70% magnesium. Outside this region, the all-gaseous model shows lower concentrations for Mg, CF_2 and CF_4, than the multiphase model. This is likely to be due to the relatively lower flame temperatures calculated by the all-gaseous model (see Figs.1 and 2).

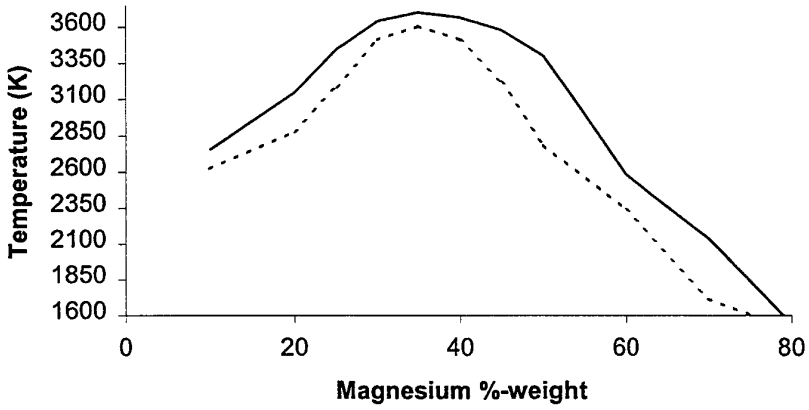

Figure 2: Effect of inlet temperature and phase state on the adiabatic flame temperature of MT composition (Species in liquid and solid phases are inlcuded). Legend as in Figure 1.

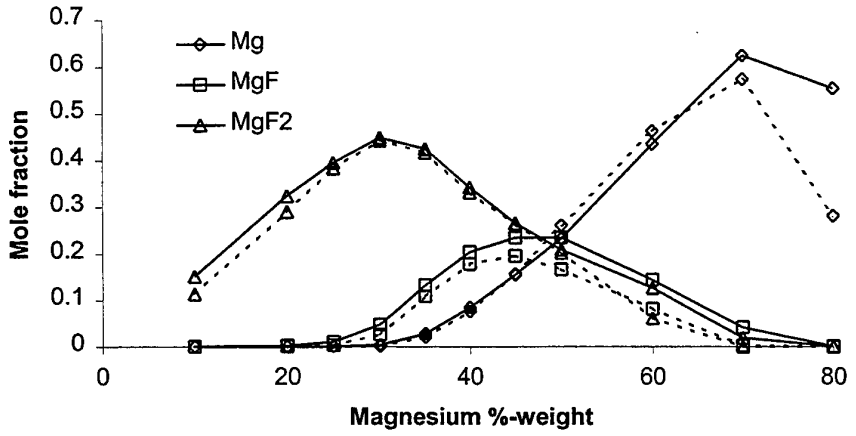

Figure 3: Equilibrium mole fraction profiles of major species of MT composition: inlet temperature 1366K: - - - gaseous species only, __ liquid and solid phases are also included.

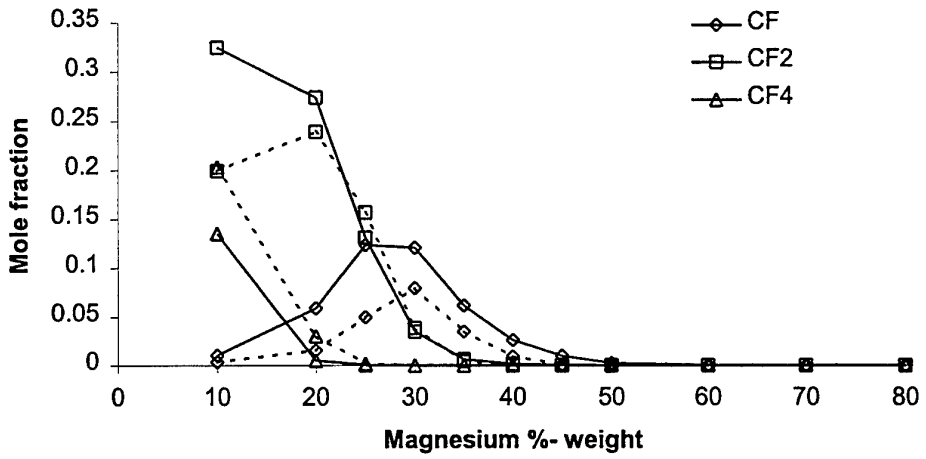

Figure 4: Equilibrium mole fraction profiles of C-F species of MT composition: inlet temperature 1366K: - - - gaseous species only, __ liquid and solid phases are also included.

Figure 5 shows the major liquid- and solid phase species in the combustion products of the various MT mixtures. The amount of liquid and solids species formed is minimal in the 20%-50% Mg region, probably due to the high flame temperature in this region. Since a multiphase model is more realistic than the all-gaseous model, it has been used in all subsequent calculations. Also, an initial temperature of 1366K (instead of a 300K) has been used. This simplifies the calculations because all reactants would be in a gaseous phase, hence alleviating the difficulties associated with the inclusion of surface reactions.

4.2 Effect of Viton on Equilibrium Chemistry

Equilibrium flame temperatures have been calculated for various MTV compositions with 5% and 16% Viton (by weight). Comparison of MTV temperature profiles with MT composition is shown in Figure 6. The figure clearly shows that Viton does not have a significant effect on the adiabatic flame temperature. Interestingly, Figure 6 shows that for the 16%-Viton mixture, the flame temperature is slightly lower than that of MT and the MTV with 5% Viton. This behaviour is more pronounced in the 40%-70% magnesium region, particularly around 50% Mg where a temperature difference of ~270K was calculated.

Comparison of species concentrations for various MT and MTV compositions are shown in Figs. 7-9. Figure 7 shows that Viton does not affect the concentrations of the liquid- and solid-phase species in magnitude or distribution, with the exception of MgF_2. The concentrations of MgH and HF, shown in Figure 8, however, indicate a significant difference between the 5% and 16%-Viton mixtures, especially in the concentration of HF. This is an expected result because increasing the amount of Viton

provides more hydrogen radicals that favourably reacts with fluorine. The figure also shows that Viton affects the distribution profiles of MgH and HF. However, the discrepancy in HF profiles is more pronounced in the region below 70%Mg, while for MgH species the effect of Viton is not evident for mixtures with 50% or less, magnesium.

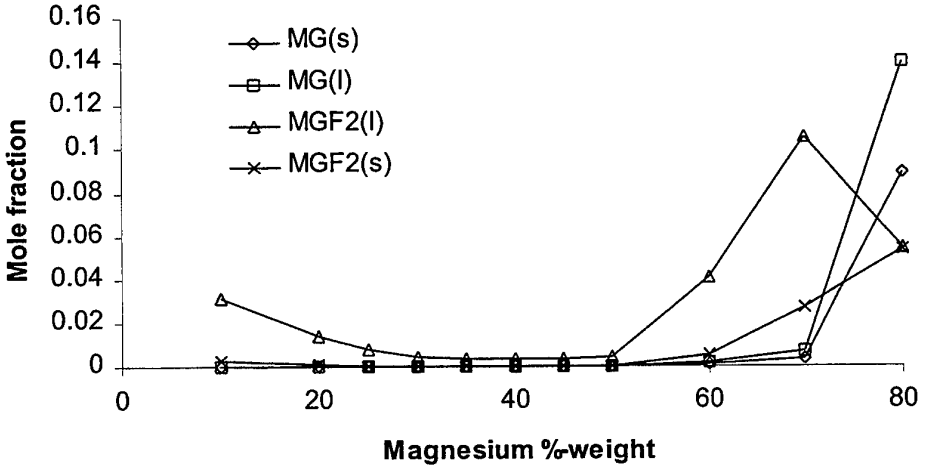

Figure 5: Equilibrium mole fraction profiles of major liquid and solid species (except carbon) of MT composition: inlet temperature 1366K.

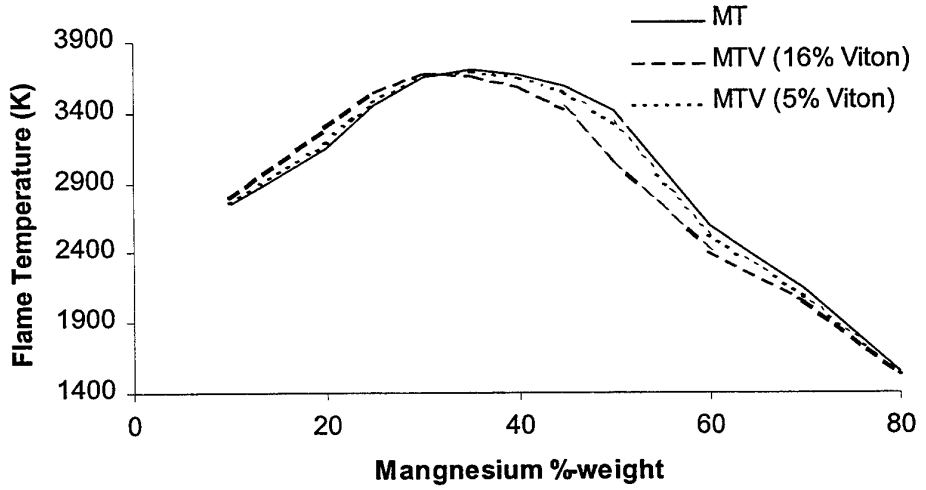

Figure 6: Flame temperature profiles of MT and MTV compositions with 5% and 16% Viton.

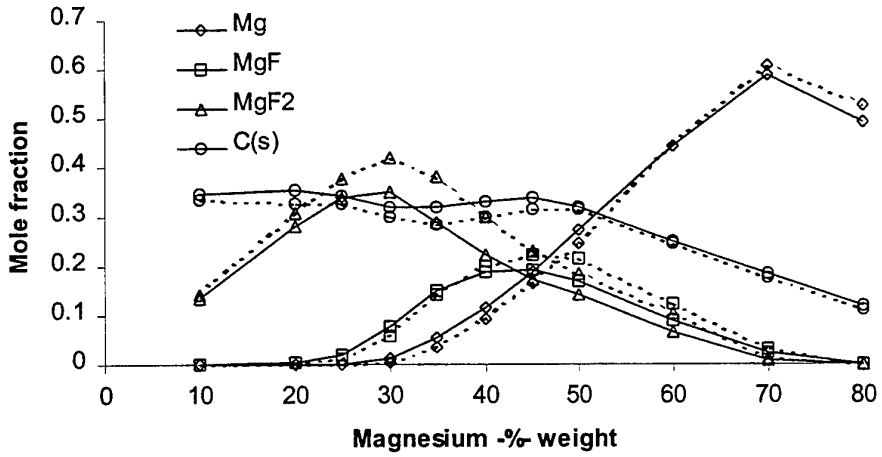

Figure 7: Products concentration of MTV mixtures: ___ 16% Viton, - - - 5% Viton. (inlet temperature 1366K).

Figure 9 shows a comparison between reaction products of MT and MTV (16%Viton) mixtures. The most noticeable difference in the concentrations is that of MgF and MgF_2 species. A possible explanation for the lower MgF and MgF_2 concentrations (for the MTV composition) is that hydrogen competes with the magnesium for free fluorine radicals to produce HF and MgH. Therefore less free F and Mg would be available to produce MgF and MgF_2. However, this scenario can not be verified without a kinetic mechanism for MTV reactions.

4.3 Effect of Air on Equilibrium Chemistry of MTV Mixtures

Equilibrium calculations have been performed for a MTV-air mixture (MTV-1 in Table 1) with air mass fraction in the range of 10% to 80%. The model accounts for the following compounds: NO_2, NO, N_2O, N_2O_5, Mg_3N_2, MgN, $MgC_2(s)$ and $Mg_2C_3(s)$. These species are in addition to those already mentioned in Sections 3.1.1 and 3.1.2. The results are shown in Figures 10-12. Figure 10 shows that magnesium oxidation by atmospheric oxygen commences only at air concentration of 40% and above, while magnesium oxidation by fluorine, Figure 11, occurs at any air content. This is probably because magnesium oxides begin to form only as excess oxygen (around 40% air content) becomes available as shown in Figure 12. Otherwise O_2 molecules are more likely to react with carbon to form CO, and magnesium reacts with fluorine to form magnesium fluorides. The results shown in Figure 12 indicate that nitrogen remains inert despite the inclusion of a large number of its compounds in the calculations. This is likely because N_2 molecules are unable to compete (with more reactive species, such as F and C atoms) for available O_2 and magnesium.

As mentioned in a previous section it is more plausible to envisage the burning of MTV in air as a two-stage process. Therefore calculations have been made using the initial composition shown in Table 2. The main assumption is that the initial air temperature is equal to that of the combustion products. This is a rough assumption dictated by a limitation in the computer model that does not allow different initial temperature for each species in the reactants.

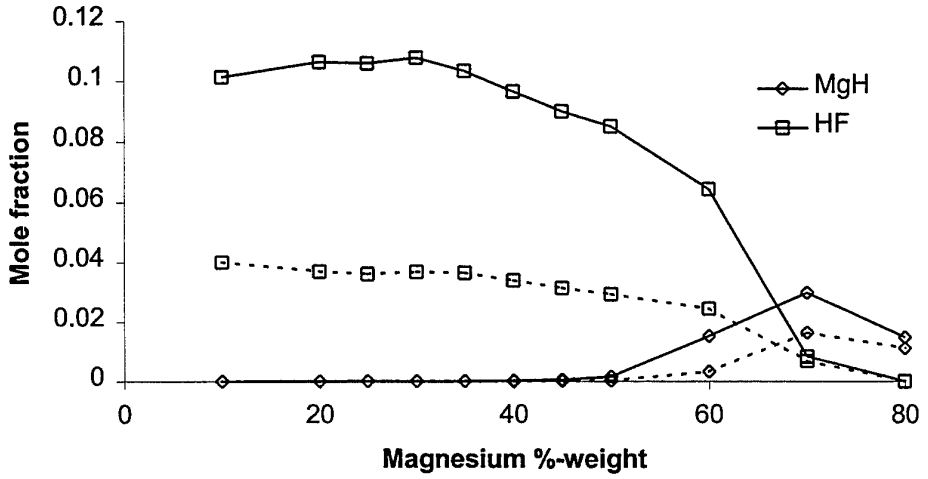

Figure 8: Concentration of MgH and HF for MTV mixtures: ___ 16% Viton, - - - 5% Viton. (inlet temperature 1366K).

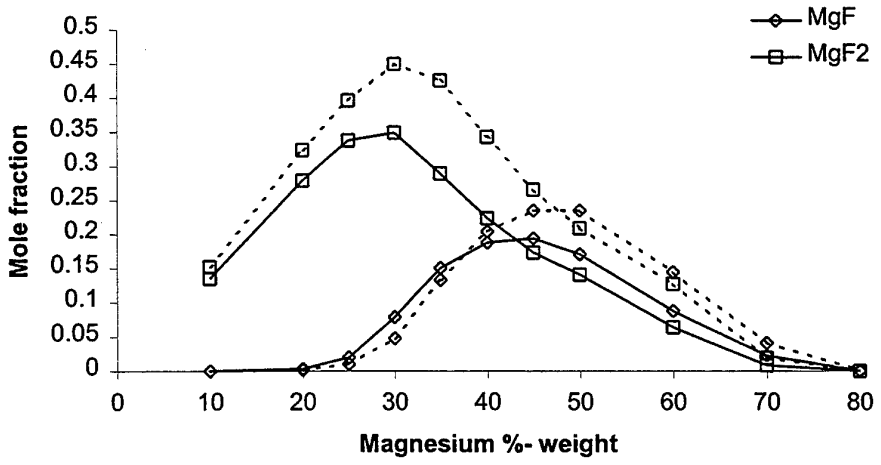

Figure 9: Comparison of MgF and MgF_2 profiles: - - - MT, ___ MTV (16% Viton).

Figure 13 displays the flame temperature for the reaction between the MTV combustion products (listed in Table 2) and air. The figure shows that for a mass fraction of 30% air and above, the flame temperature is similar for the three MTV-air formulations.

However, for an air content below 30% the temperature profiles vary noticeably, albeit the initial concentrations of the three MTV mixtures and inlet temperature are similar (see Table 2), with the exception of MTV-3 which has a higher magnesium content and a lower inlet temperature. The reasons for such discrepancies are not clear yet.

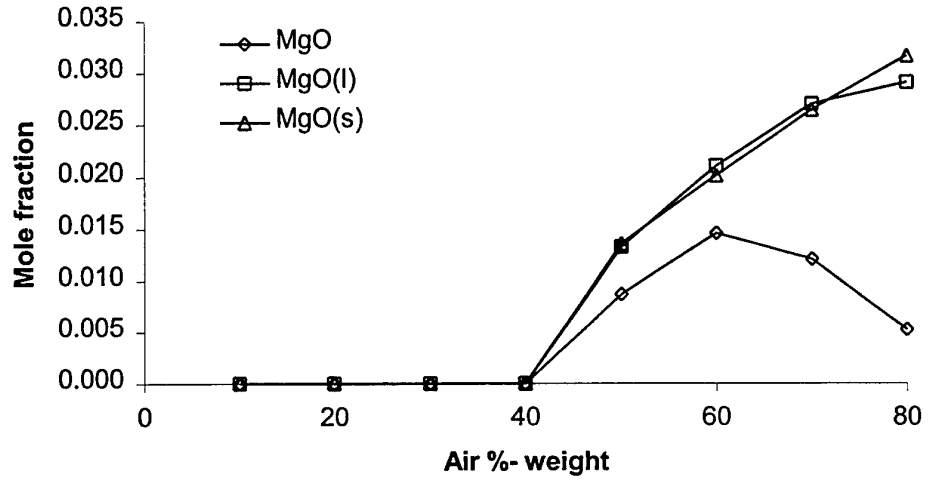

Figure 10: Effect of air on the concentration of magnesium oxides of MTV combustion.

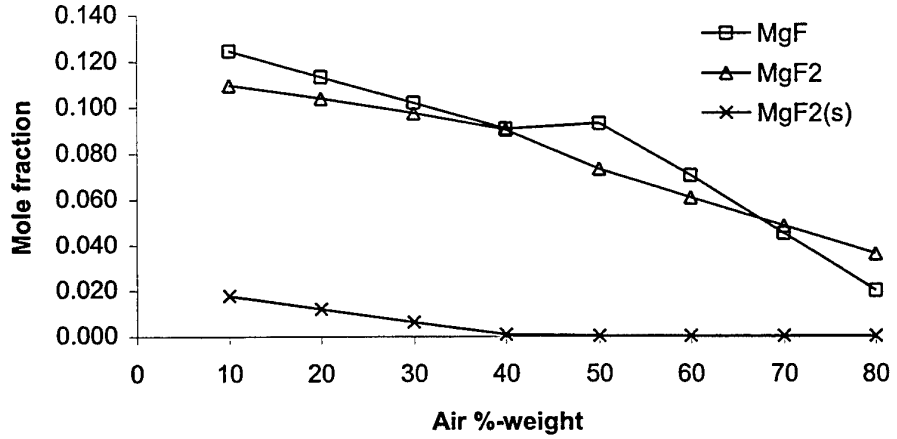

Figure 11: Magnesium fluorides concentration from combustion of MTV-air compositon (MTV-1 mixture in Table 1).

A comparison between the species profiles of the products from the three MTV formulations reacting in air is shown in Figure 14 (for simplicity only the results for MTV-1 formulation are presented). It shows no significant difference in the concentrations or the distribution of major species. The only exceptions are the profiles of HF, as shown in Figure 15.

It is worth noting that all three MTV formulations have similar inlet mole fraction of HF (0.020-0.028), as shown in Table 2. Explaining the discrepancies in HF based only on thermochemistry is not sufficient and a kinetic information for Viton (the only source of hydrogen) is needed.

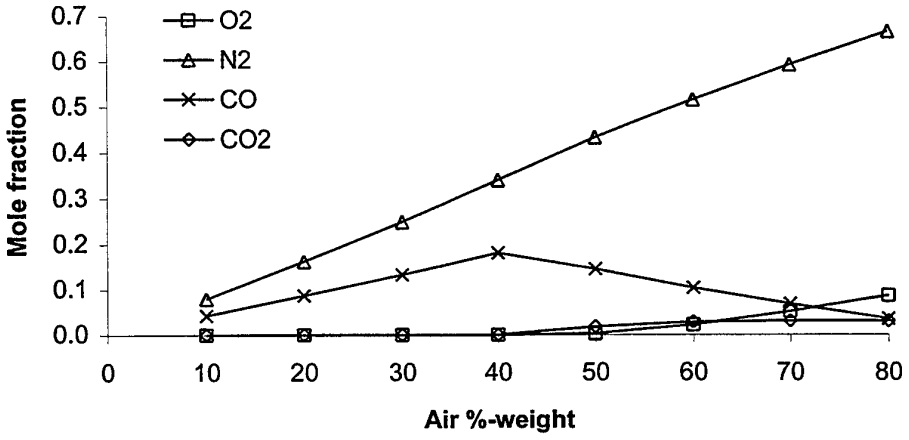

Figure 12: CO, O_2, CO_2 and N_2 profiles of MTV-air combustion.

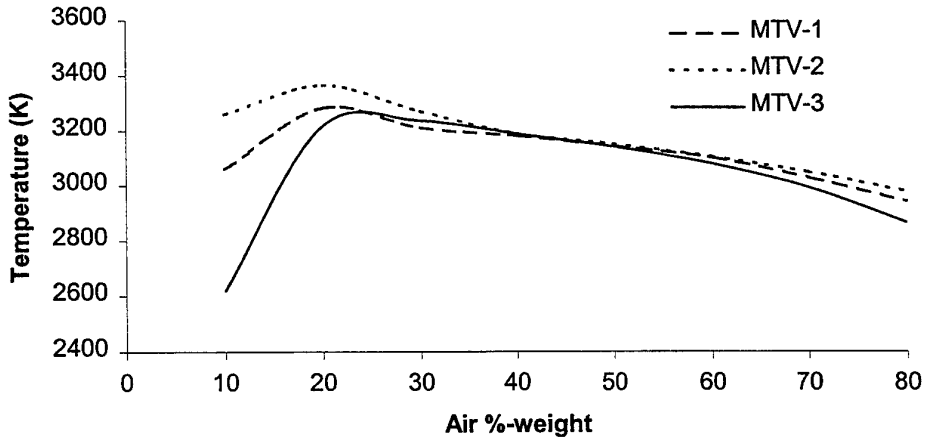

Figure 13: Temperature profiles for reaction between combustion products of various MTV compositions and air.

Another important result shown in Figure 16, is that the N_2 profile for MTV-1 formulation (N_2 profiles for all three MTV formulations are almost identical) indicates that nitrogen is no longer an inert species. For comparison, N_2 profile from the reaction of MTV and air is also plotted. It is clear that unlike the first model, in which the air is treated as a reactant, the nitrogen reacts and produces mainly NO (not shown). The results also show that no significant amounts of Mg_3N_2, MgN, Mg_2C_3 or MgC_2, are formed.

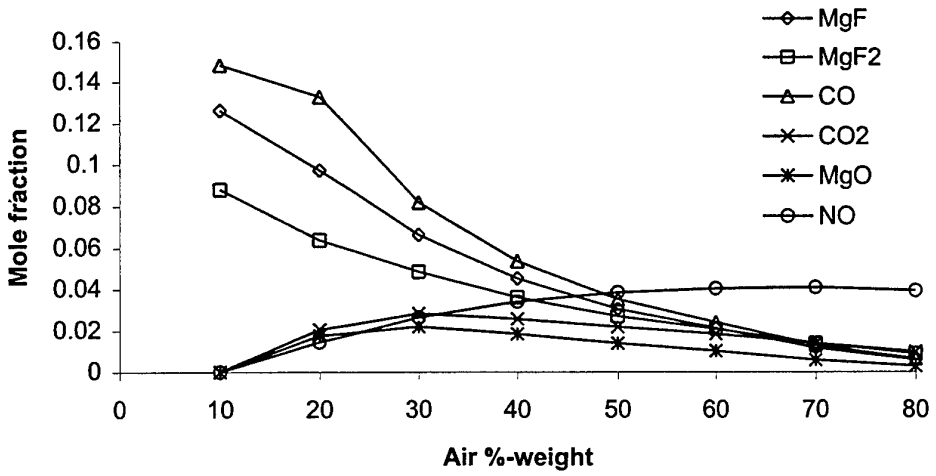

Figure 14: Concentration profiles of major species from MTV-1 products reacting with air.

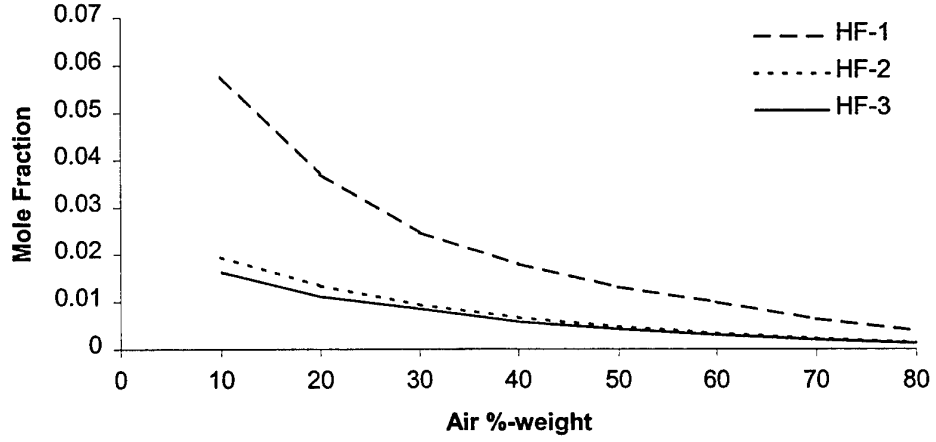

Figure 15: Concentration profiles of HF from various MTV-air reactions. (numerals HF-1 etc. refers to the MTV-1 formulation etc, respectively).

4.4 Kinetics Sensitivity Analysis of MT Mixtures

To the best knowledge of the author no chemical kinetic mechanism is available yet for MTV, especially for Viton reactions. Therefore a MT kinetic mechanism [13] has been used in this study. The computer module SENKIN [16] has been used to predict the evolution of MT kinetics. The code calculates the time-evolution of homogenous reacting mixture for a given kinetic scheme that describes the chemistry of the mixture. It accounts for finite-rate elementary chemical reactions and performs kinetic sensitivity analysis with respect to reaction rates. Sensitivity analysis has been performed for three MT compositions with various M:T weight ratios. These are: a stoichiometric mixture 33:67, a typical UK flare composition 55:45, and a typical US igniter mixture 61:39. While a stoichiometric mixture is rarely used in applied systems it is commonly used as a baseline for research purposes.

Figure17 shows the time-evolution of the flame temperature for a stoichiometric MT composition. It shows a temperature rise from an initial temperature of 1366K to 1750K in approximately 13 μsec, followed by a rapid increase to 3570K in approximately 1μsec.

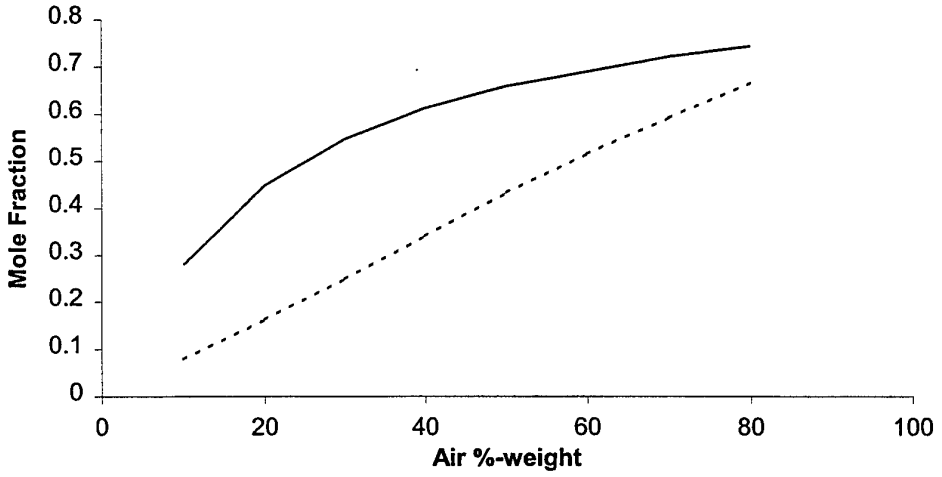

Figure 16: Concentration profile of N_2 for MTV-1 reacting with air : - - - MTV-air,___ MTV products-air.

Time-evolution profiles of major species, shown in Figure 18, are also consistent with the behaviour of the temperature profile. That is a slow change in the concentration in the first 13 μsec, followed by a rapid change reaching a steady state level in approximately 1μsec. Sensitivity analysis also provides information about the production/consumption rates of species with respect to the reactions in which they appear. For example, Figure 19 shows the time-dependent production rate of

magnesium. It identifies the dominant reaction that control the consumption (a negative production value represent destruction of species) of magnesium as $Mg+CF_2 \leftrightarrow MgF_2+C$. The figure clearly indicates that magnesium oxidation via the reaction $Mg+F \leftrightarrow MgF$, is negligible.

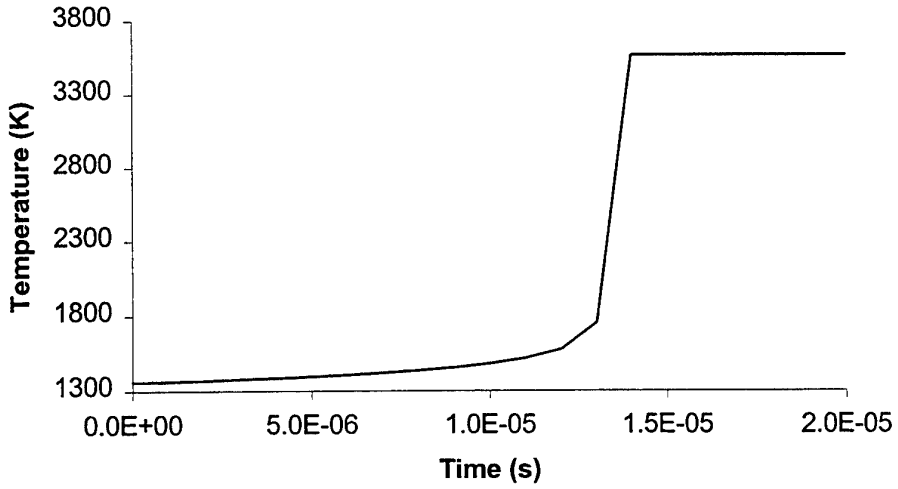

Figure 17 : Time evolution of flame temperature for a stoichiometric MT composition.

The normalised sensitivity for CF radicals, shown in Figure 20, explains why magnesium oxidation via F radicals is insignificant. It indicates that fluorine is primarily reacting with CF to produce CF_2, (which is a main agent for magnesium oxidation). That is fluorine plays an important but an indirect role in magnesium oxidation.

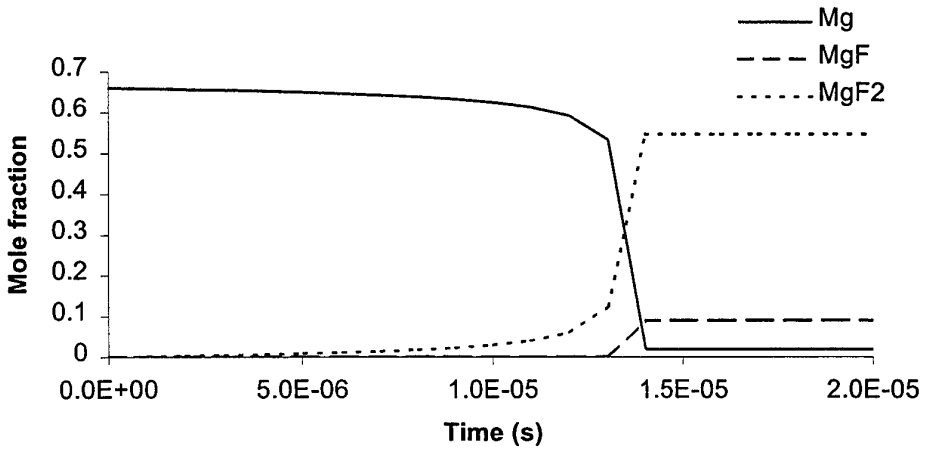

Figure 18: Time evolution of major species for a stoichiometric MT composition.

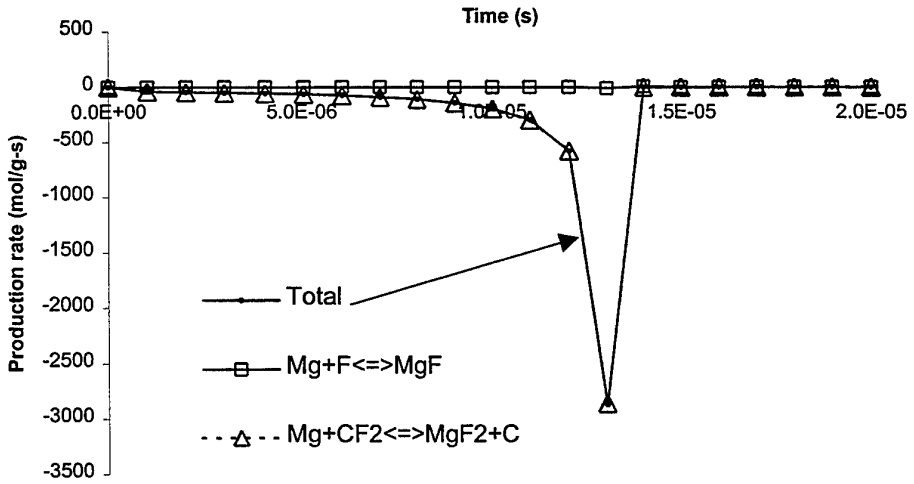

Figure 19: Production rate for Mg with respect to important reactions.

However, the main source of CF_2 is the dissociation of C_2F_4 (monomer of Teflon) reacting with a third-body species/radicals: $C_2F_4+M \Leftrightarrow 2CF_2+M$, as shown in Figure 21. The figure also shows that CF_2 is consumed by reacting with magnesium, $Mg+CF_2 \Leftrightarrow MgF_2+C$, producing magnesium di-fluoride and carbon. This reaction

represents the main bath for carbon production, while carbon consumption is carried out via the recombination reaction $2C \Leftrightarrow C_2$, as shown in Figure 22. The reactions of higher carbons however, do not contribute significantly to the overall carbon production or consumption.

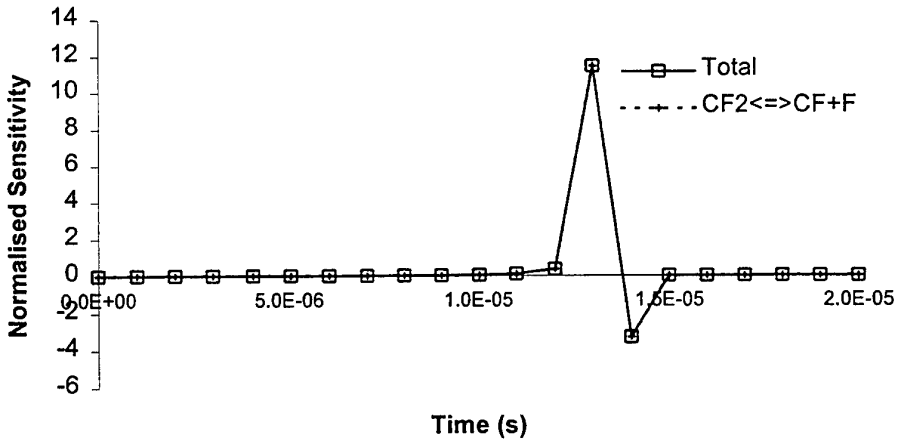

Figure 20: Normalised sensitivity for CF radicals for a stoichiometric MT mixture.

The sensitivity of the flame temperature with respect to reaction rates is shown in Figure 23. The results imply that the flame temperature is sensitive to two reactions: The first is the Teflon reduction: $C_2F_4+M \Leftrightarrow 2CF_2+M$, and the second is carbon recombination reaction: $2C \Leftrightarrow C_2$. The latter though is far less influential and practically negligible.

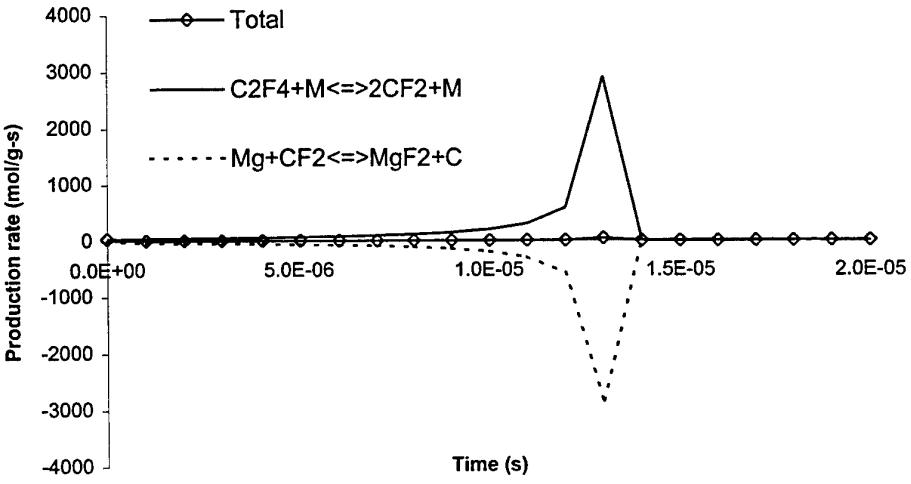

Figure 21 : Rate of production for CF2 via two major reactions (Mixture: stoichiometric MT compositon).

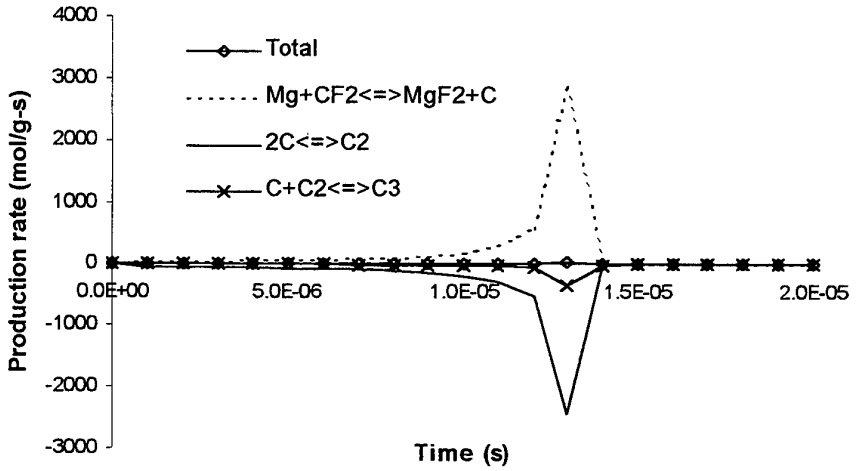

Figure 22: Production rate for Carbon via three main reaction (stoichiometric MT composition).

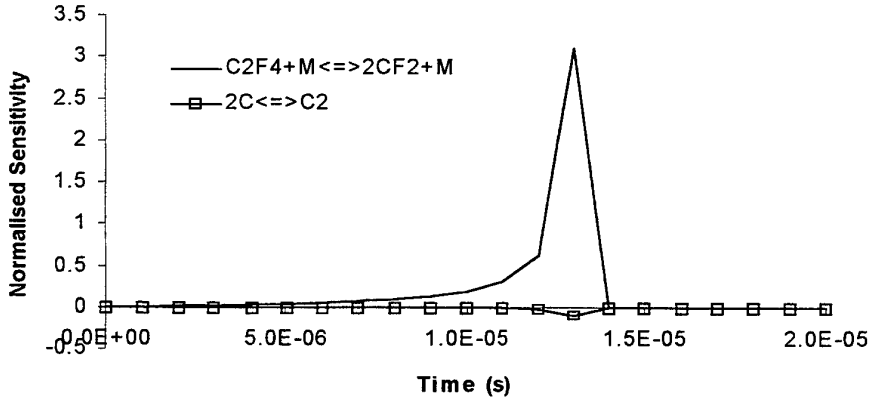

Figure 23: Normalised sensitivity for temperature with respect to important reaction rates (a stoichiometric MT composition).

Sensitivity analysis for the flare (55:45) and the igniter (61:39) compositions (not shown) revealed similar results to those of the stoichiometric mixture. As an example, Figure 24 shows a normalised sensitivity for temperature with respect to the reaction rates, for the three MT compositions. The main observation from Figure 24 is that the flame temperature is dominated by Teflon dissociation reaction i.e. $C_2F_4+M \Leftrightarrow 2CF_2+M$. The flare composition (55:45), however shows a higher sensitivity than the other mixtures. The figure also shows that there is a difference in the ignition-delay time between the compositions, the longest being that for the flare composition. The cause of this behaviour is not yet clear.

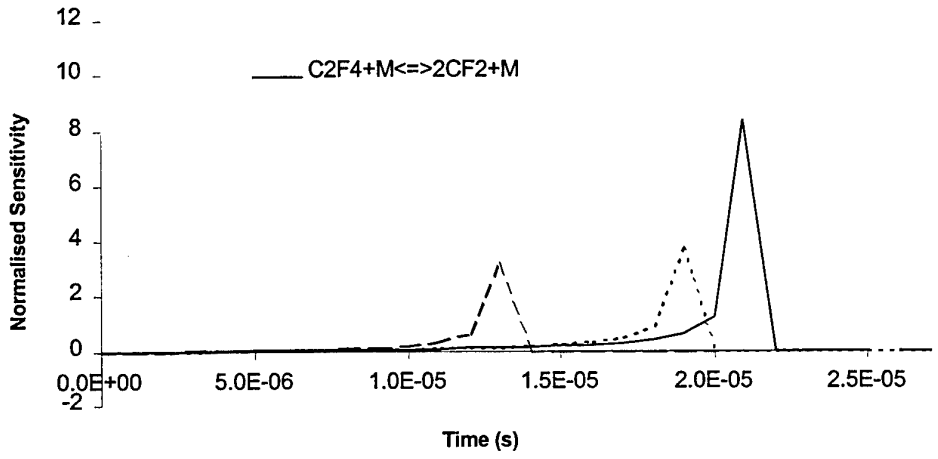

Figure 24: Normalised sensitivity for temperature with respect to a main reaction: ..... Stoichiometric mixture 33:67, ___ Flare composition 55:45, - - - Igniter composition 61:39.

Three variations for the Arrhenius coefficients (A, b and E) for the dominant reaction $C_2F_4 + M \Leftrightarrow 2CF_2 + M$, have been used to examine their effect on concentrations evolution, ignition-delay time and sensitivity characteristics. These are listed in Table 3. It has been found that the production rate, concentration and temperature profiles of major species are not significantly affected by variations in the Arrhenius factors. The most noticeable effect of the Arrhenius factors is on the ignition-delay time as shown in Fig 25. However, no systematic pattern has been established.

Table 3: Various Arrhenius coefficients for Teflon reduction.

	Arrhenius Equation: $k = A\,T^b\,e^{(-E/RT)}$		
Mechanism (identifier)	A	b	E (cal/mole)
Modica and Lagraph[19] (Mech-1)	7.82×10^{15}	0.5	55663
Keating and Matala[20] (Mech-2)	6.78×10^{16}	0	54700
Douglass et. al [21](Mech-3)	8.49×10^{17}	0	47085

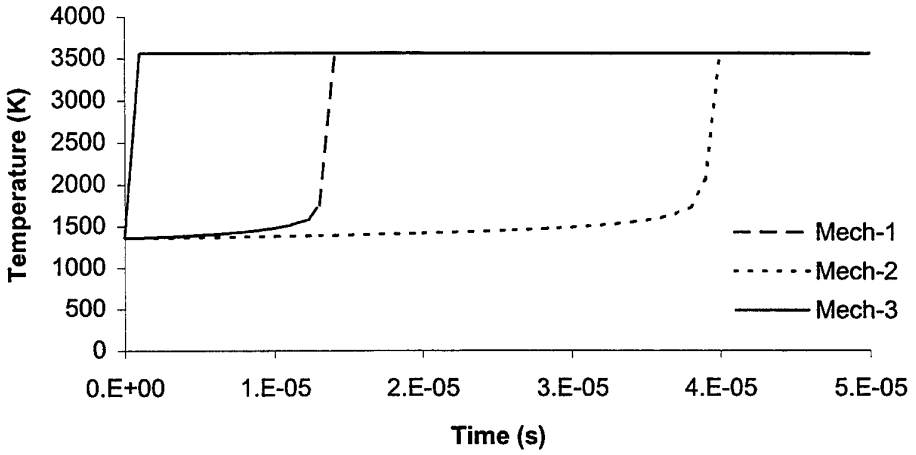

Figure 25: Temperature profiles against time for various kinetics mechanisms for a stoichiometric MT composiotion.References:Mech-1[19], Mech-2[20], Mech-3[21].

4.5 Perfectly Stirred Reactor Results

Perfectly stirred reactor (PSR) calculations have been performed using the AURORA module of Chemkin package [16,17]. The code predicts the steady state or time-averaged properties of a well-mixed reactor. The reactor is characterised by a reactor volume, residence time and incoming flow properties. The model accounts for finite-rate elementary chemistry reactions both in the gas phase and on the surface. In this study, however only gas phase reactions have been included due the lack of surface kinetics scheme for MT composition.

All calculations assumed a reactor volume of 130 cm^3, which represents a typical flare size (more specifically the PW118 flare). Calculations have been carried out for three different MT composition, namely a stoichiometric mixture 33:67, a typical UK flare 55:45, and a typical US igniter 61:39 formulation. For each mixture, calculations with various residence times have been performed. In general it has been found that a pseudo-equilibrium state has been reached in approximately 2-3 μsec, with no significance changes in the properties of the products over a residence time of 2 μsec.

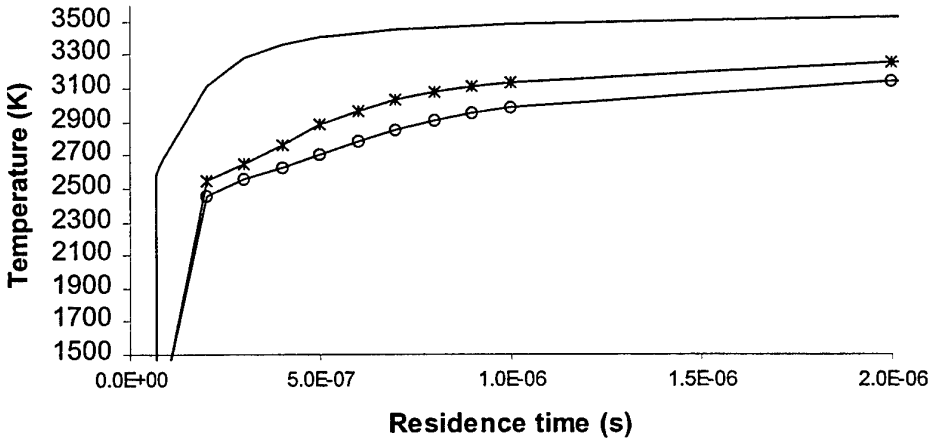

Figure 26: Flame temperature for different residence time of various MT compositions: ___stoichiometric, -- UK Flare, -o- US igniter.*

Figure 26 shows that the steady-state temperature decreases as magnesium content in the mixture increases. It also shows that as Mg concentration increases the residence time to achieve ignition is also increases. It is also clear that the temperature levels out for residence times over 2 μsec.

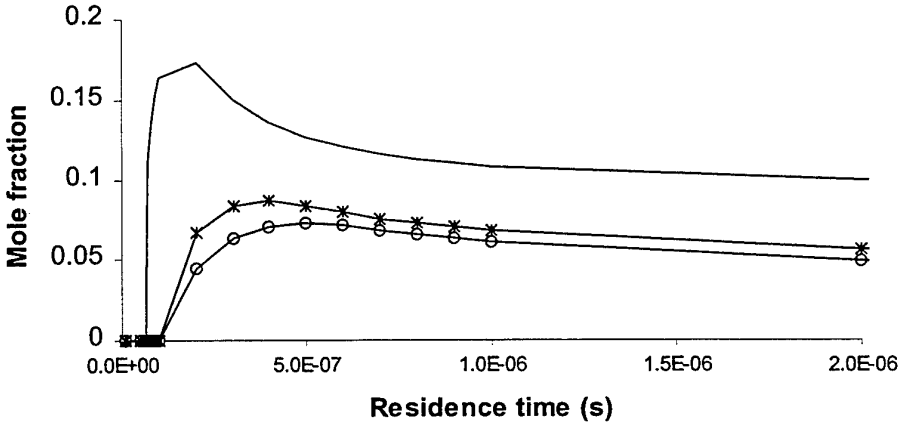

Figure 27: Profiles of Magnesium fluoride (MgF) for various residence times and MT composition:___stoichiometric, -- UK Flare, -o- US igniter.*

Concentration profiles of MgF, shown in Figure 27 are consistent with the temperature behaviour. That is, a magnesium-rich mixture tends to reduce MgF levels and causes a

time-delay in reaching its peak value. Similar trends and consistency are also visible for MgF_2 and CF profiles, shown in Figs. 28 and 29, respectively.

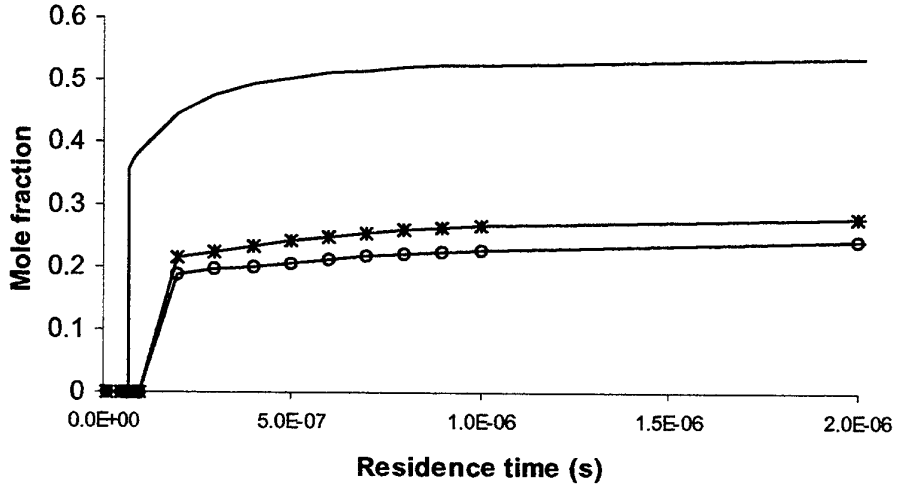

Figure 28: Distribution of MgF_2 against residence time. MT compositions:___stoichiometric, -- UK Flare, -o- US igniter.*

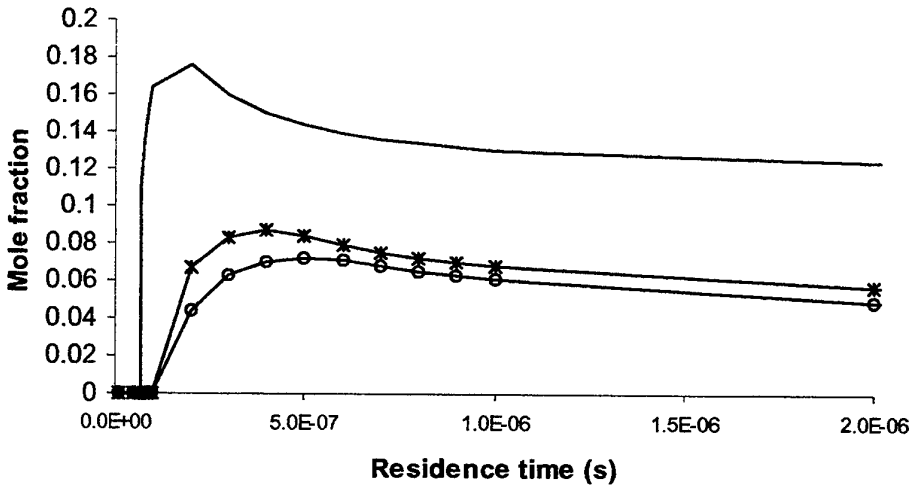

Figure 29: Profiles of CF against residence time. MT compositions:___stoichiometric, -- UK Flare, -o- US igniter.*

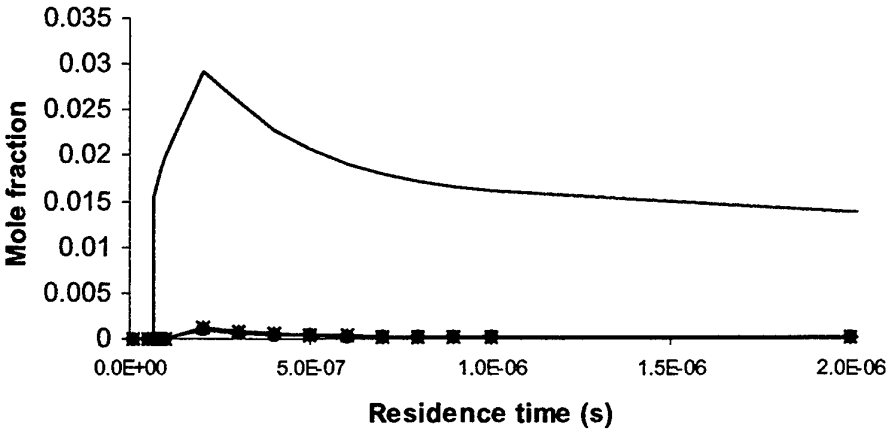

Figure 30: Profiles of CF_2 against residence time. MT compositions:___stoichiometric, -- UK Flare, -o- US igniter.*

However, for CF_2 profiles there is a significant difference between the stoichiometric and the magnesium-rich mixtures. It is likely that as the amount of Teflon (which is the main source of CF_2 as shown in Figure 21) in magnesium-rich mixtures decrease less CF_2 is produced as shown in Figure 30. However, the effect of lowering the Teflon content in the mixture is less pronounced for CF than it is for CF_2 concentration. This is likely to be influenced by the fact that magnesium-rich mixtures have lower flame temperature hence the $CF_2 \leftrightarrow CF+F$ conversion is not fully completed. It is worth also remembering that the flame temperature is strongly affected by CF_2 concentration as shown earlier in Figure 23.

The distribution of total carbon (C, C_2, C_3, etc.) for the three mixtures is shown in Figure 31. Since the main source of carbon production is the reaction: $Mg+CF_2 \leftrightarrow MgF_2+C$, as shown in Fig 21, reducing CF_2 means less carbon.

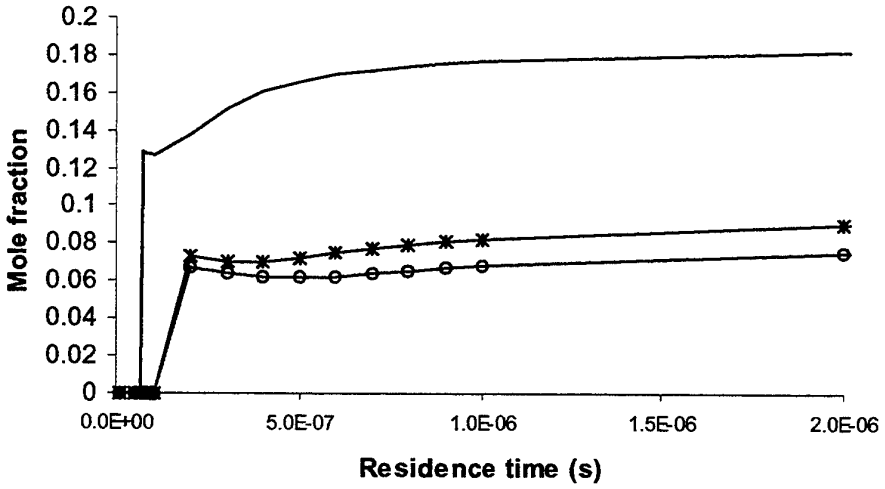

Figure 31: Total Carbon (C, C_2, C_3, etc.) against residence time. MT compositions:___stoichiometric, -- UK Flare, -o- US igniter.*

4.6 Premixed MT Combustion

Calculations using the PREMIX module [16] have been carried out for the three MT compositions (33:67, 55:45, and 61:39). Figure 32 shows temperature profiles in the axial direction for the various mixtures. The figure indicates that the temperature profiles have similar distribution and reach their pseudo-equilibrium state at a very short distance from the exit plane of the burner. The gradient of the temperature profiles though, varies slightly with composition, decreasing as the magnesium content in the mixture increases. Profiles of CF radicals, shown in Figure 33 (top), also point out to some effect of the magnesium content on the magnitude and location of peak concentration. Increasing magnesium content reduces the peak level of CF radicals and shifts the peak location further downstream. Nevertheless, the CF magnitude is comparable in all MT mixtures. For CF_2 profiles however, Figure 33 (bottom), the trend is different from that of CF profiles. CF_2 levels for the stoichiometric mixture are an order of magnitude larger than in the other compositions. This is because the main source of CF_2 is the dissociation of C_2F_4 (Teflon). Hence, lower C_2F_4 content as in the flare and igniter mixtures means lower CF_2 also. Figure 33 also shows that CF and CF_2 concentrations reach a super-equilibrium level before dropping to their equilibrium state. It is also noticeable that CF peaks slightly earlier than CF_2 for the stoichiometric mixture, but the reverse is true for the other mixtures. The reason for such discrepancy is not yet clear.

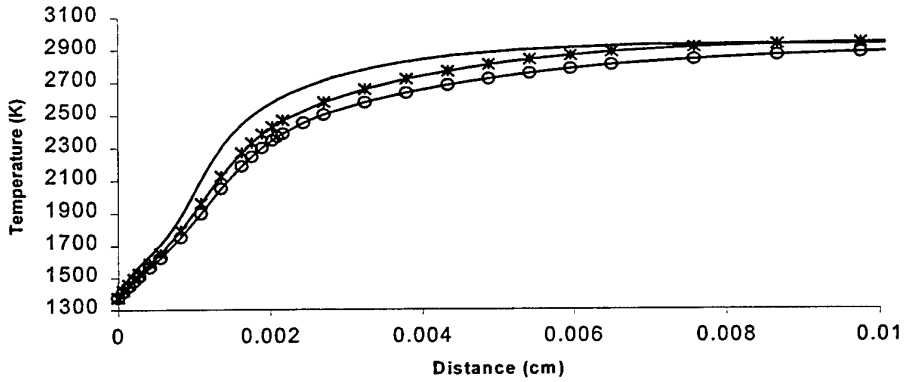

Figure 32: Temperature profile in the downstream direction of a burner-stabilised premixed MT mixtures:___stoichiometric, -- UK Flare, -o- US igniter.*

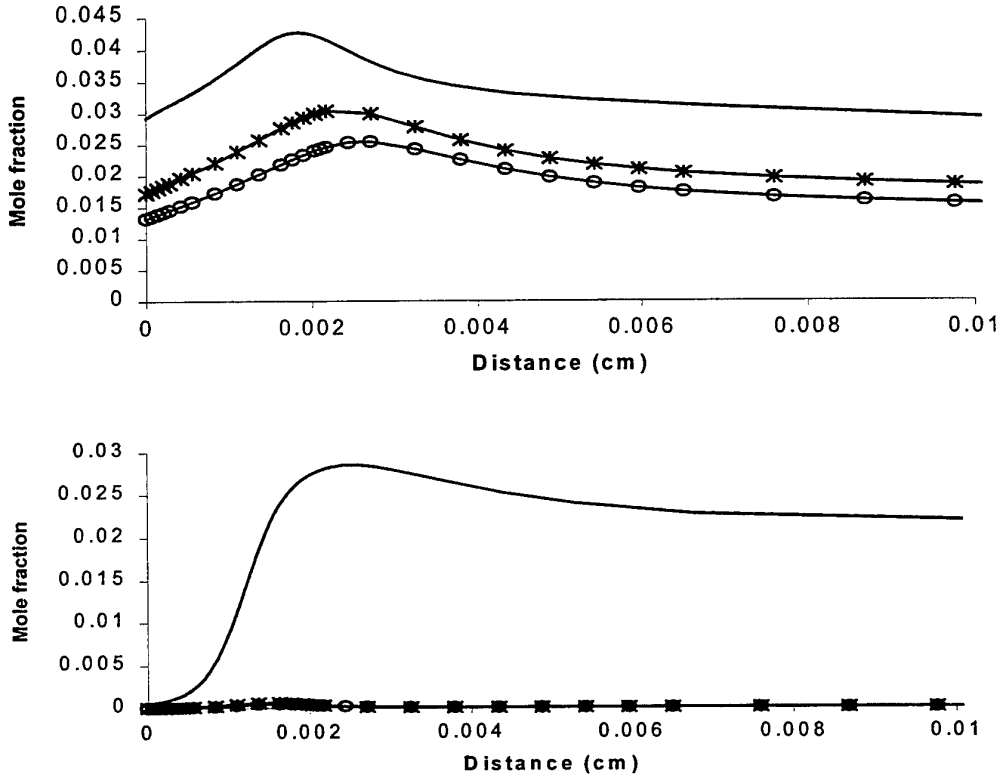

Figure 33: Profiles of CF (top) and CF2 (bottom) species against distance from burner's exit plane. Mixtures:___stoichiometric, -- UK Flare, -o- US igniter..*

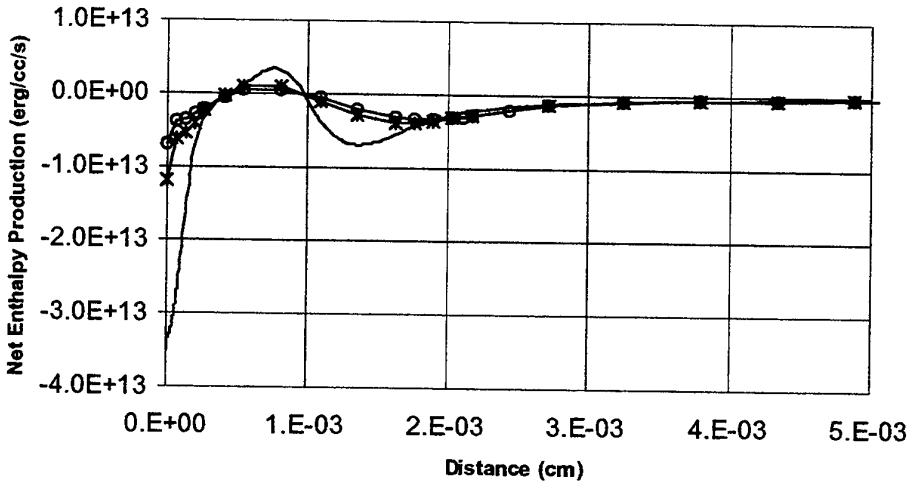

Figure 34: Net enthalpy production for different MT compositions: ___stoichiometric, -- UK Flare, -o- US igniter..*

Figure 34 shows the net enthalpy production for the three MT mixtures. The figure points out an initial stage in which combustion generates large amount of energy, the largest corresponds to a stoichiometric mixture, followed by a region between 0.005 and 0.02 mm from the surface where the enthalpy exhibits an oscillatory behaviour. The zone with the positive net enthalpy indicates an endothermic reactions. This range corresponds to the flame region where radicals and species are produced and consumed at high rates. At a pseudo-equilibrium state, where endothermic and exothermic rates are equilibrated, the temperature of the products stabilises. This is clearly shown in Figure 32, where the temperature profiles begin to level out after 0.05 mm downstream. The effect of this endothermic zone did not affect the flame temperature, though its existence slightly noticed in the gradient of the temperature profile shown in Figure 32, where a slight depression in temperature curve is noticeable at 0.001mm.

5. Conclusions

Equilibrium chemistry calculations have shown that the initial temperature of MT mixture and the phase state of the species do not affect the stoichiometric flame temperature, but do have a significant influence in other mixture ratios. The Viton content does not seem to have a significant effect on flame temperature or on concentrations of major species. Flame temperature and major species are similar for MT and MTV mixtures with similar M:T ratios. For MTV reacting with atmospheric air, it has been found that N_2 remains inert if the air is treated as a reactant in the MTV-air

mixture. However, if a two-stage combustion model is used the nitrogen reacts with oxygen to produce mainly NO species.

Sensitivity analysis of three typical MT formulations showed that the flame temperature is strongly influenced by the dissociation reaction of Teflon, that is $C_2F_4+M \Leftrightarrow 2CF_2+M$. This reaction is also the main source of CF_2 species, which in turn is the main path for magnesium oxidation via the reaction $Mg+CF_2 \Leftrightarrow MgF_2+C$. This reaction controls the source for C production, while C consumption is dominated by the recombination reaction $2C \Leftrightarrow C_2$. The results also showed that the content of magnesium in the mixture affects the ignition-delay time however, no systematic pattern has been established that correlates these parameters. Slight variations in the Arrhenius factors of the reaction $C_2F_4+M \Leftrightarrow 2CF_2+M$, do not have significant influence on flame temperature, production rates and concentration profiles of major species.

The results of premixed calculations indicated that the flame stabilises on the surface of the burner. From a practical viewpoint this is a desirable behaviour because a portion of the flame energy will be radiated backwards, towards the surface of the mixture, causing preheating of the reactants thus enhancing flame stability (temporally as well as spatially) and reducing the possibility of lift-off and subsequent complete blow-off of the flame.

6. Recommendations and Future Directions

The results of the sensitivity analysis, premixed flames and perfectly stirred reactor modelling for the various MT mixtures, showed that a typical chemical reaction time scale is in the order of ~10^{-6} Seconds. This time scale, when compared with a characteristic time scale of turbulence ~10^{-3} sec, gives a Damköhler number (defined as the ratio between a characteristic reaction and flow time scales) in the order of ~1000. Therefore, a fast-chemistry assumption would be reasonable for modelling turbulence-chemistry interaction in MT combustion. This is currently the focus of the next stage of AIR 97/250 task.

Whilst the kinetics scheme used in this study consists of a relatively small number of reactions, its implementation into a flow solver is likely to be complex because the flow solver needs to handle the additional 18 transport equations (18 reactions), which requires large memory allocation. Also, the stiffness of the chemical reactions causes numerical instability, making convergence more difficult and time consuming. It is therefore recommended to:

- Investigate the possibility of reducing the size of the kinetic scheme to a more manageable dimensions, while retaining a realistic representation of the chemistry.

For example, this study showed that reactions of higher carbons (C_2, C_3, ..) do not contribute significantly to the overall production rate of carbon. It might be possible then to eliminate these reactions from the mechanism without having much effect of the accuracy of the scheme.

- Implement a chemical mechanism into a flow solver starting with a simple scheme, such as a single global reaction.

- Validate the results of the flow-chemistry coupling by comparing them with a benchmark calculations such as a plug-flow reactor using Chemkin-III package.

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Appendix A: Chemical Kinetic Mechanism

Kinetics Scheme for Magnesium-Teflon Composition[13]
The Scheme used contain 18 reactions and 17 species, as shown below:

Table 4: Species used in Kinetics Mechanism for Magnesium-Teflon.

SPECIES	MOLECULAR	TEMPERATURE		ELEMENT COUNT		
CONSIDERED	WEIGHT	LOW	HIGH	C	F	MG
1. MG	24.31200	300	5000	0	0	1
2. MGF	43.31040	300	5000	0	1	1
3. MGF2	62.30880	300	5000	0	2	1
4. F	18.99840	300	4000	0	1	0
5. F2	37.99680	300	4000	0	2	0
6. C	12.01115	300	5000	1	0	0
7. CF	31.00955	300	3000	1	1	0
8. CF2	50.00795	300	3000	1	2	0
9. CF3	69.00635	300	3000	1	3	0
10. CF4	88.00475	300	3000	1	4	0
11. C2F4	100.01590	300	3000	2	4	0
12. C2F6	138.01270	300	5000	2	6	0
13. MG2F4	124.61760	300	5000	0	4	2
14. C2	24.02230	300	5000	2	0	0
15. C3	36.03345	300	5000	3	0	0
16. C4	48.04460	300	5000	4	0	0
17. C5	60.05575	300	5000	5	0	0

Table 5: Chemical kinetic mechanism for Magnesium-Teflon composition.(NOTE: A units mole-cm-sec-K, E units cal/mole).

		K = A T**b exp(-E/RT))		
	REACTIONS CONSIDERED	A	b	E
1.	C2F4+M=2CF2+M	7.82E+15	0.5	55663.4
2.	CF4+M=CF3+F+M	6.15E+34	-4.6	122362.4
3.	CF4=CF2+F+F	9.24E+14	0.5	95556.6
4.	CF4+F=CF3+F2	1.00E+12	0.5	85589.1
5.	2CF3+M=C2F6+M	7.14E+17	0.5	0.0
6.	CF2+F2=CF3+F	1.98E+11	0.5	2120.0
7.	CF3+M=CF2+F+M	1.57E+49	-9.0	92209.9
8.	CF2+M=CF+F+M	4.20E+26	-2.9	105949.0
9.	CF2=CF+F	2.07E+14	0.0	33707.6
10.	F2+M=M+F+F	2.12E+13	0.0	33707.6
11.	MG+F=MGF	4.00E+16	0.5	20000.0
12.	MG+F2=MGF2	4.00E+16	0.5	20000.0
13.	MG+CF2=MGF2+C	4.00E+14	0.5	20000.0
14.	MGF2+MGF2=MG2F4	4.00E+14	0.5	20000.0
15.	C+C=C2	1.80E+21	-1.6	0.0
16.	C+C2=C3	4.00E+14	0.5	20000.0
17.	C+C3=C4	4.00E+14	0.5	20000.0
18.	C+C4=C5	4.00E+14	0.5	20000.0

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19. ABSTRACT

This study examines in detail the equilibrium chemistry of Magnesium/Teflon (MT), Magnesium/Teflon/Viton (MTV), and MTV-air compositions. Gas-phase as well as solid-phase chemistry has been included. Equilibrium calculations accounting for over 47 species and various initial conditions have been performed. A comparison between MT and MTV combustion has been carried out with emphasis on investigating the effect of Viton on the combustion characteristics. The effect of air on MTV combustion has also been investigated for two possible MTV-air combustion models. A chemical kinetic mechanism with 18 reactions and 17 species, has been used to study the time evolution of reacting MT mixtures, accounting for finite-rate elementary reactions as well as performing sensitivity analysis with respect to reaction rates. Three different variations of the kinetic scheme have been studied and their effects on combustion products and flame temperature have been examined. Kinetic analysis has been repeated for three pyrotechnic compositions that are commonly used in flare and rocket motor igniter formulations.