The regeneration of monolithic wall-flow diesel particulate traps

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THE REGENERATION OF MONOLITHIC WALL-FLOW
DIESEL PARTICULATE TRAPS

by

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BTech, BEng, CEng, MIMechE

A Doctoral Thesis
Submitted in partial fulfilment of the
requirements for the award of
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of the
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1989

Supervisor: Professor J C Dent, PhD, CEng

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This thesis describes the behaviour of monolithic wall-flow diesel particulate traps during periodic cleaning or 'regeneration'. The concept and development of a new regeneration technique using low-power microwave energy is also presented.

Health and environmental concerns with diesel engine particulate emissions have resulted in standards which will become increasingly strict during the 1990's. To meet these standards it is argued that diesel engines will require some form of exhaust after-treatment.

Monolithic wall-flow traps which can filter 90% of particulates are shown to be a favourable form of exhaust after-treatment. Traps require regenerating if exhaust back pressures are to be minimised and power and fuel economy not greatly reduced. Regeneration techniques which promote oxidation of the trapped particulate are discussed and the key requirement of an ideal regeneration system is identified.

An understanding of the regeneration characteristics of wall-flow monoliths is derived from a new mathematical model and previous models are reviewed. The new model provides further insights and is shown to be in good agreement with published experimental results.

The concept of using low power microwave energy to promote trap regeneration is proposed and developed. Experiments leading to the design of the first prototype Microwave Assisted Regeneration (M.A.R.) system are described. The prototype consuming only 1 kW of electrical power during regeneration is shown to perform encouragingly well on bench and engine.

An improved prototype is developed and tested. It is also installed in a vehicle for road tests and results from these and further tests incorporating new ideas are described. A novel technique to assess the microwave heating field pattern is presented and used. A Third-Generation M.A.R. system is developed based on these findings and further bench tests are described which indicate the optimum conditions for trap regeneration.

Although the wall-flow monolith has good filtration efficiency and thermal strength, it is found to have some inherent features which can discourage complete regeneration. M.A.R. is shown to be a commercially attractive trap regeneration technique and has favourable size, cost and power consumption attributes. Finally, a short discussion on microwave assisted chemical reactions is given.
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"Trust in the Lord with all your heart and do not lean on your own understanding. In all your ways acknowledge Him and He will make your paths straight".

Proverbs 3 vv.5 and 6
PUBLICATIONS AND PATENT FROM THIS WORK

CHAPTER 3


CHAPTERS 4 AND 5


CHAPTERS 5 AND 6


PATENT

STATEMENT OF ORIGINALITY

This is to certify that the Author is responsible for the work submitted in this thesis, that the original work presented is his own except as specified in acknowledgements or with references, and that neither the thesis nor the original work contained therein has been submitted to this or any other institution for a higher degree.
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CHAPTER 1

1.1 INTRODUCTION

The 1980's have seen a rapid emergence of technologies which seek to control diesel engine particulate emissions. Research activity is now intense due to the strict vehicle emissions standards to be implemented in North America and elsewhere in the early 1990's.

In this thesis, the behaviour of a major contender for diesel particulate control: the monolithic wall-flow trap (which filters 90% of exhaust particulates) is described, and the concept and development of a new technique for its periodic in-situ cleaning or 'regeneration' using low power microwave energy is presented.

* * * * *

Diesel engines are becoming increasingly popular in a variety of applications primarily due to their good fuel economy. Despite their relatively low toxic emissions compared to petrol engines, diesel engines do emit appreciable amounts of particulate matter often seen as black, sooty particles exiting exhaust pipes of cars, trucks and buses. With increasing numbers of diesel engined vehicles there have been growing fears of the health risks associated with diesel particulates and also their effects on the environment.

Primary health risks are due to the particulates penetrating and remaining deep in the human lung tissue. Diesel particulate has a mean diameter of about 0.17 \( \mu \text{m} \), a size which is extremely penetrable [90].* Once inside the lung, particulates can remain for long periods of time [20].

* Numbers in square brackets designate references.
Diesel particulates consist of a carbon core surrounded by hundreds of hydrocarbon species, some of which (the Polycyclic Aromatic Hydrocarbons, PAH) have been shown to cause mutations and cancers in animal tissue [50][51]. Although it is unlikely that fully conclusive evidence will ever be found, the body of scientific opinion suggests that there is a significant carcinogenic risk related to diesel particulates especially among groups of people exposed to high levels of diesel exhaust emissions [87].

Other health risks which are perhaps less serious but certainly more widespread are associated with the aggravation of respiratory problems such as bronchitis and problems with eye, nose and throat irritation [21].

Environmental risks are numerous ranging from the external soiling of buildings (for example diesel particulates have been the biggest contributor in London [6]) to fears that diesel particulates may unfavourably contribute to global climatic changes [6]. Certainly poor visibility, especially in cities, is a problem due to a variety of engine emissions, and diesel particulate makes a significant contribution [87].

The increased awareness of the above risks compounded with the growing world diesel engine vehicle population [88] have led to tighter limits on acceptable engine emissions. On a world-wide scene the legislation is becoming increasingly strict for all classes of diesels, although there are large differences from country to country. Walsh, 1989 [88] provides a recent review of the world scene and highlights North America and Europe (both EEC and non-EEC countries) as being where tighter engine particulate emission standards are to be enforced. He
also mentions Hong Kong, South Korea, China, Taiwan, Brazil and Mexico in addition to the United States and European countries where retrofit controls on urban buses are being explored.

The United States has been among the first to introduce the most stringent standards, which will become increasingly strict in 1991 and 1994 (see Table 1.1) Buses are required to meet the 1994 limits in 1991. Strict limits were to have been introduced in 1985 but the technology required to meet them was not available and this led to a series of 'waivers', much debate and an intensifying search for a practical solution to the particulate emission problem. The US Environmental Protection Agency (EPA) has now decided that the standards shown in Table 1.1 will not be waived but must be met.

<table>
<thead>
<tr>
<th>Model Year</th>
<th>Hydrocarbons (HC)</th>
<th>Nitrous Oxides (NO\textsubscript{x})</th>
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</tr>
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<tr>
<td>1987</td>
<td>1.3</td>
<td>10.7</td>
<td>-</td>
</tr>
<tr>
<td>1988</td>
<td>1.3</td>
<td>10.7</td>
<td>0.6</td>
</tr>
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<td>10.7</td>
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<tr>
<td>1990</td>
<td>1.3</td>
<td>6.0</td>
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<tr>
<td>1991</td>
<td>1.3</td>
<td>5.0</td>
<td>0.25</td>
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<td>1993</td>
<td>1.3</td>
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<td>0.25</td>
</tr>
<tr>
<td>1994</td>
<td>1.3</td>
<td>5.0</td>
<td>0.10</td>
</tr>
</tbody>
</table>

**TABLE 1.1: US HEAVY-DUTY DIESEL EMISSION STANDARDS [54]**

3
To put these figures into perspective, Figure 1.1 shows the inherent trade-off between particulates and nitrous oxides (NO\textsubscript{x}) emitted from diesel engines. Generally engines can either be tuned to give low particulates and high NO\textsubscript{x} or vice versa. For any particular engine a single curve approximately parallel to the upper or lower bounds of the shaded region of Figure 1.1 is typical, but a range of engines (heavy duty in this case) lie within this shaded envelope.

![Diagram](image)

**FIGURE 1.1: PARTICULATE - NO\textsubscript{x} EMISSION CHARACTERISTICS FOR HEAVY-DUTY DIESEL ENGINES [54]**

The 1988 Heavy-Duty limits are already implemented in the US and most engines can conform to these requirements. The 1991 requirements, although well below the shaded region, can be met by some engines if careful modifications are made, but in 1994 it is almost certain that engines will require some form of exhaust after-treatment device to reduce engine-out particulates to below the required level. The case to support this view is presented later in this Chapter. Light-Duty Vehicles are under similar restrictions but the US market for this class of vehicle is small due to a variety of reasons including currently cheap US oil [88]. This has taken them from the US spotlight, but in Europe the situation is quite different where the light-duty diesel population is large, growing and under pressure from particulate legislation [31][38][88].
1.2 OVERVIEW OF THESIS STRUCTURE

Up to this point in Chapter 1, the health and environmental concerns with diesel particulate emissions have been briefly described together with some of the legislation to be implemented in the next five years. In subsequent sections, first the origin and nature of diesel particulate is discussed and then the case is put forward to support the view that some form of exhaust after-treatment is necessary if particulate emissions are to be reduced significantly. Various forms of particulate control are examined in Chapter 1, and the monolithic wall-flow trap is shown to be a strong contender for diesel engine exhaust after-treatment.

Chapter 2 discusses a variety of techniques which have been considered for trap regeneration (i.e. on-vehicle cleaning). The fundamental requirement of an 'ideal' regeneration system is identified and the concept of using low power microwave energy to promote trap regeneration is suggested.

Chapter 3 provides a more detailed understanding of the regeneration process itself by considering the modelling work of several investigators. A new model is developed which provides further insights into the regeneration process, and results from a parametric study show how engine variables and trap loading affect regeneration behaviour. The model is compared to some experimental results.

Chapter 4 elucidates the concept of using low power microwave energy to promote trap regeneration. The concept is justified by its size, cost, safety and power consumption attributes. Preliminary experiments leading to the design of the first prototype Microwave Assisted Regeneration (M.A.R.) system are described. The first prototype was
tested on both bench and engine, and its strengths and weaknesses are discussed.

Chapter 5 builds upon the experience and results of Chapter 4. A modified M.A.R. prototype is developed in an attempt to overcome some of the shortcomings of the original prototype. The modified prototype was bench and engine tested, and further, it was fitted to a vehicle. The vehicle installation design is described and its performance assessed. Key results of these and further bench tests point the way forward for system improvement.

Chapter 6 describes the development of a 'Third-Generation' M.A.R. system drawing upon all the results of the previous work. Bench tests which provide the working envelope for its optimum functioning are described. The Chapter ends by describing the durability test programme where repeated regenerations are currently being carried out on an engine operated on a varying speed-load cycle.

Chapter 7 discusses the commercialisation of M.A.R. with respect to cost, safety, performance and current industrial interest it has aroused. A discussion of the inherent limitations of the monolithic wall-flow trap is presented and the final section comments on some recent work with microwave assisted chemical reactions.

Chapter 8 provides the conclusions of this thesis and outlines areas of future work.
1.3 ORIGIN AND STRUCTURE OF DIESEL PARTICULATE

Before looking at controlling diesel particulate it is useful to know its origin and structure. Primary soot particles are formed in the fuel-rich parts of the diffusion flame in the engine cylinder by the pyrolysis of hydrocarbons. The particles are fairly spherical and are of diameters 10-30 nm. The pyrolysis involves many reactions; at high temperatures (2000 to 3500K) molecular 'splitting' or cracking is prevalent and at lower temperatures (1000-2000K) molecular addition becomes more significant as described by Broome and Khan, 1971 [16].

Many writers have provided information on the environmental conditions within the engine for soot formation and phenomenological studies have given some insights into the mechanisms themselves. Amann et al, 1980 [2] in their review of the rudiments of diesel particulate emissions highlighted work from both engine and 'non-engine' studies which have aided soot formation understanding. They suggest, in accordance with a host of other writers, that soot formation is an inherent feature of diesel engine combustion.

Once formed, the primary soot particles coalesce into larger agglomerates of irregular shape [52] and are polydisperse in size, having characteristic diameters mainly between 0.1 and 1 μm [65][83]. The chemical composition of these particulates has been the subject of much research and the actual composition has been shown to be dependent on the precise engine operating conditions [77]. A schematic of the chemical make-up of diesel particulate is shown in Figure 1.2.

As can be seen from Figure 1.2, diesel particulate does not just consist of carbon particles as many have assumed, but is a mixture of many organic and inorganic compounds. The US Environmental Protection
Agency has classified diesel particulate as being any matter, solid or liquid (except water) which can be filtered from the exhaust flow [2]. Since the legislation requires a reduction of the total particulate mass emitted, a total view of particulate formation and control is required. For example, particulate is not only derived from the combustion of fuel within the engine but is also derived from the engine's lubrication oil and the ingestion of particles through the engine's air inlet.
The various techniques to control diesel particulates are now discussed in the remainder of this Chapter.

1.4 DIESEL PARTICULATE CONTROL

The impending stringent emissions standards have forced manufacturers of engine equipment to take a long, hard look at all the factors affecting particulate/NO\textsubscript{x} emissions. Figure 1.3 schematically summarises the various aspects of diesel particulate control: engine consumables (air, fuel and lubrication oil), the engine itself (including combustion chamber, fuel injection equipment, and turbocharger etc) and exhaust after-treatment. The latter aspect is discussed in detail in the last part of this Chapter, but first the others are considered. These are grouped under the heading 'engine methods'.

1.4.1 Engine Methods

a) Fuel

One of the major influences on an engine's performance and emissions is the fuel itself. The amount of sulphur in the fuel has a significant effect on the total exhaust particulates since sulphates are formed in the engine. Richards and Sibley, 1988 [74] show that sulphates derived from the current US diesel fuel sulphur content (0.3% by weight) would make up 70% of the legal particulate limit in 1994. French, 1987 [25] also makes this point and suggests that desulphurised fuel would make it easier for manufacturers to achieve 1994 limits. Richards and Sibley enumerate this by providing experimental evidence on a range of engines showing a 13-22% particulate reduction if the fuel sulphur is reduced from the current 0.3% to 0.03%. However, the oil companies are reluctant to reduce sulphur content since it is costly. Ingham and Warden, 1987 [42] of
ENGINE DESIGN.
Fuel (quality, type, additives, etc.)

EXHAUST AFTER-TREATMENT
Trap etc.

Inlet Air
(quality, turbocharger etc)

Fuel Injection Equipment

Combustion Characteristics
Lubrication Oil

Exhaust Gas
To Atmosphere

FIGURE 1.3: FACTORS AFFECTING DIESEL PARTICULATE EMISSIONS
Chevron (Oil) Corporation estimate that sulphur reductions are at least an order of magnitude less cost effective than that of after-treatment and engine modifications. This may be a biased view, but it is interesting to note that the Californian Air Resources Board (CARB) in November 1988 adopted regulations limiting sulphur to 0.05% by weight together with aromatic hydrocarbon content of 10-20% by volume in an attempt to limit emissions [88]. However, changes of this kind are unlikely to be extended beyond California.

Other fuel factors are described by French, 1987 [25] and these include possible fuel quality deterioration in the future with increased aromatic content (which increases both hydrocarbons and particulates) and variable density fuel which can have a serious impact on power output and smoke.

Alternative fuels such as methanol which produce very low particulates are being actively studied especially in urban bus applications where the fuel can be made locally available [87]. Widespread use on trucks etc, however, is unlikely due to various problems including the lack of availability, low calorific value, corrosive properties and cost [89].

b) Charge Air

An engine's air supply is fundamental for combustion. Improved volumetric efficiencies and improved air motion resulting from better inlet port and combustion chamber design together with turbocharging can reduce particulates [2][52][74]. French, 1987 [25] states that the direct injection naturally aspirated engine has all but disappeared in the US due to the emissions legislation. He provides a useful graph showing how the particulate/NO\(_x\) trade-off curves are
affected by various engine modifications (see Figure 1.4). Clearly the addition of aftercooling (which further increases charge air density) to a turbocharged engine reduces emissions considerably.

![Graph showing particulate emissions vs NOx levels for different engine configurations](image)

**FIGURE 1.4: PARTICULATE/NO\textsubscript{x} TRADE-OFF FOR HEAVY TRUCK ON EPA TRANSIENT TEST CYCLE.** [25]

c) Fuel Injection Equipment

High pressure fuel injection equipment (FIE) also provides further dramatic changes. Richards and Sibley, 1988 [74] show how particulates are reduced by increased fuel injection pressure (see Figure 1.5) by improving fuel-air mixing.

![Graph showing performance vs injection pressure](image)

**FIGURE 1.5: EFFECT OF FUEL INJECTION PRESSURE ON PARTICULATE EMISSIONS [74]**
Unit injectors are becoming more popular due to the higher pressures they can achieve, and they also lend themselves to accurate electronic timing. Injector nozzle design is also important and Needham, 1987 [61] suggests that sac volumes be reduced to nearly zero to help reduce both hydrocarbons (HC) and particulates.

d) Exhaust Gas Recirculation and Injection Timing

Exhaust gas recirculation (EGR) is a further influence on diesel emissions. It is primarily a weapon against NO\textsubscript{x} and inherently causes particulate levels to rise, as shown in Figure 1.6, mainly due to lower temperature combustion and reduced oxygen availability.

![Figure 1.6: Effects of Exhaust Gas Recirculation (EGR) on Diesel Emissions of 5.7 Litre Oldsmobile Engine [53] (ordinate units in grammes per mile)](image)

Advancing the ignition timing, on the other hand, lowers particulate levels and Wade, 1980 [84] outlines how ignition timing and EGR can affect overall NO\textsubscript{x}, HC and particulate emissions and engine performance.
e) **Lubrication Oil**

Springer, 1988 [76] described lubrication oil as the "fourth dimension" of diesel particulate control. He estimates that half of the collected mass due to lubrication oil consumption consists of ash, metals and additive residual. To meet further legislation he suggests that many engines will require an 80% reduction in oil consumption along with other engine improvements.

Nearly all of the above quoted references in this section include exhaust after-treatment in their suggested particulate control strategies. Figure 1.4 (from French, 1987 [25]) shows particulate traps being required for engines to meet the 1994 regulations. Ingham and Warden, 1987 [42] suggest that after-treatment is a cheaper alternative to fuel desulphurisation. However, Richards and Sibley, 1988 [74] conclude that to meet 1994 regulations both low sulphur fuel and after-treatment will be required. Walsh, 1989 [88] states that to reduce particulates to meet the future stringent levels will probably necessitate the use of after-treatment devices. However, all of these writers (and there are many others) are also aware that diesel after-treatment technology is still relatively immature despite intensive effort throughout this decade, and many problems need to be overcome. Various diesel exhaust after-treatment techniques are now described.

**1.4.2 After-Treatment Techniques for Diesel Particulate Control**

a) **Cyclones**

To remove particulates from the exhaust gas flow, cyclones have been investigated. These cause the flow to rotate and the particles separate from the main flow by the centrifugal effect. Ludecke and Dimick, 1983 [53] describe these as having too short a residence time for the particles to be effectively separated and some means of
imposing a very high velocity to them would require extra energy. Recently Aldersey-Williams, 1989 [1] reported the development of a cyclone for diesel particulate control. He described it as "not being very efficient" at separating particles of less than 50 µm, in diameter and since Lipkea et al, 1978 [52] show more than 98% of diesel particulates on a mass basis are less than 6 µm in diameter, cyclones of this kind are unlikely to be practical and are generally receiving little current attention.

b) Electrostatic Precipitators
Since diesel particulates carry electrical charge*, they may be removed from the exhaust gas flow by using an electrostatic precipitator as described by Kittelson et al, 1986 [45]. These consist of a high voltage electrode inside a concentric pipe carrying the exhaust gas. Voltages of approximately 30 kV cause the particulates to be attracted to the pipe walls where they can be removed by a high voltage hollow grid. Problems occur when particulates adhere to each other and eventually bridge the electrode and pipe gap causing electrical breakdown. However, as Weaver et al, 1986 [89] indicate, the electrostatic precipitator does act as a reasonable particle agglomerator and hence might be used in conjunction with a cyclone (described above) as these can extract the larger particles more easily.

With both of the previous techniques and others, actual disposal of the particulate once collected presents a problem. Gibbs et al, 1986 [30] considered feeding the collected particles back into the engine's cylinder so as to reduce them by oxidation. Laboratory results showed that 40% of particulates (by mass) passed through an unfuelled,  

* Typically 1 to 5 electron charges [45].
motored engine without being oxidized. However the author is not aware of further developments of this technique.

c) Particulate Traps
By far the most popular method of exhaust particulate removal is the diesel particulate trap. These consist of a porous material placed in the exhaust flow to filter or 'trap' the majority of exhaust particulates.

Diesel particulate traps have been shown to filter 50-90% of engine exhaust particulates (by mass), but since the filtering medium retains the particulate it gets progressively blocked. This leads to high back pressures being imposed on the engine and hence reduced output power and fuel economy. The trap therefore needs periodic cleaning or 'regenerating' which can be accomplished by raising the essentially carbonaceous particulate to a sufficiently high temperature so that it rapidly oxidises with the free oxygen in the exhaust gases.

Two main problems with trap regeneration exist: firstly it is difficult to achieve the required particulate temperatures (approximately 450°C) to cause rapid oxidation, and secondly, because the reaction is exothermic, high trap temperatures (of over 1000°C) can occur and hence the oxidation process must be controlled to avoid trap damage by melting or cracking.

Howitt, 1987 [39] described the regeneration process as being 90% of the engineering problem with trapping being only 10%. Trap regeneration is discussed in more detail in Chapter 2, and is the main subject of this thesis. Here in Chapter 1 various trap types are now examined in terms of their trapping effectiveness and thermal strength.
Fibrous mesh traps are of the non-blockable type, the free flow area between the fibrous mesh elements being generally larger than the particles to be filtered. The filtering process is by a combination of interception of the larger particle sizes with the mesh elements and the deposited particulate matter, and diffusion to these surfaces by the smaller particles [63]. The particulate matter is therefore deposited throughout the length of the trap. Trapping efficiencies* of 50 to 60% are typical, however problems do occur when large agglomerates of trapped particulates are suddenly swept back into the exhaust gas during vehicle acceleration [85]. The uncertainties with this 'blow-off' phenomenon have discouraged fibrous trap development.

Fibre mesh materials were traditionally metallic wire of 50 to 200 μm in diameter. During regeneration excessive temperatures (over 1000°C) can cause melting [75] and therefore more recently ceramic fibres have been explored which can withstand higher temperatures; Nextel(R) (manufactured by 3M) for example can withstand 1200°C. Hardenberg et al, 1987 [35] used this type of material in a bus particulate trap system but experienced problems with the fibres breaking due to the mechanical action of the exhaust flow.

Porous ceramic foam materials have been considered as possible trapping media since they are relatively rigid and can withstand high temperatures of about 1200°C. Trapping efficiencies of around 50-60% are typical [58] but for a given trap volume their particulate capacity is limited since back pressure rises relatively quickly during trap loading [53].

---

* Trapping Efficiency = \[ \frac{\text{Total Trapped Particulate Mass}}{\text{Total Particulate Mass which has Entered Trap}} \]
The ceramic wall-flow monolith has received a tremendous amount of attention since it was first described by Howitt and Montierth, 1981 [40]. Figure 1.7 shows a ceramic monolith consisting of a honeycomb of square cross-section channels which are alternately blocked forcing the exhaust gases to pass through the porous walls before exiting the trap. This is shown schematically in Figure 1.8. The pores in the ceramic walls are small enough to cause most of the particulate to build up on the upstream side of the channel. Trapping efficiencies of 70-90% are typical. Figure 1.9 shows an enlarged section of a partially loaded wall-flow monolith with the inlet channels containing the particulate.

The Cordierite material used for wall-flow monoliths can withstand temperatures of 1200°C, the honeycomb structure imposes a relatively low exhaust back pressure (due to its high total filtration area) and can hold more particulate than similar sized ceramic foam traps [53]. These, together with its high trapping efficiency suggest it is a good medium for a diesel particulate trap.

Table 1.2 gives an overall comparison of different trapping media; clearly the wall-flow monolith exhibits the most favourable combination of trapping efficiency, working temperature and capacity.

<table>
<thead>
<tr>
<th>Trap Medium</th>
<th>Trapping Efficiency (%)</th>
<th>Maximum Working Temperature (°C)</th>
<th>Particulate Capacity</th>
<th>Refs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fibrous (wire)</td>
<td>50-60</td>
<td>900</td>
<td>Low. Blow-off a problem.</td>
<td>[53][85]</td>
</tr>
<tr>
<td>Fibrous (ceramic)</td>
<td>50-60</td>
<td>1200</td>
<td>Low. Rapid rise of back pressure.</td>
<td>[35][53]</td>
</tr>
<tr>
<td>Ceramic Foam</td>
<td>50-60</td>
<td>1200</td>
<td>Medium.</td>
<td>[53][58]</td>
</tr>
<tr>
<td>Ceramic Wall-Flow Monolith</td>
<td>70-90</td>
<td>1200</td>
<td>High.</td>
<td>[53][57]</td>
</tr>
</tbody>
</table>

**Table 1.2: Comparison of Different Trapping Media**

18
FIGURE 1.7: CERAMIC WALL-FLOW MONOLITH 5.66" DIA X 6" LONG

FIGURE 1.8: SCHEMATIC OF WALL-FLOW MONOLITH CHANNELS
FIGURE 1.9: A SECTIONED MONOLITHIC WALL-FLOW TRAP PARTIALLY LOADED WITH PARTICULATE (THE DARK AREAS). Magnification x 12 [85]
d) Through-Flow Oxidation Catalysts

Before concluding this section, the through-flow oxidation catalyst must be mentioned since it has received significant attention in the diesel industry [88]. The through-flow catalyst seeks to continually catalytically oxidise some of the Soluble Organic Fraction (SOF) part of the particulates (see Figure 1.2) thereby reducing the total emitted particulate mass. The exhaust gas flows straight through a medium e.g. wire mesh or ceramic substrate impregnated with a suitable catalyst (usually a precious metal such as platinum or rhodium) and some of the SOF is oxidised. The rationale behind using these oxidation catalysts is that trap regeneration technology generally has not yet reached the required reliability and cost targets. Therefore some engine manufacturers are considering adopting the oxidation catalyst in conjunction with the engine techniques described in Section 1.4.1 to just meet future emissions levels. Problems however, are associated with significant sulphate formation initiated by the catalyst [36]. Since these sulphates add to the particulate mass, fuel desulphurization would be a key requirement for adoption of these devices [88]. Another problem is that the soot portion of particulate can build up on the catalyst surface reducing the SOF conversion (oxidation) rate to zero after short periods [92].

1.5 CONCLUSIONS OF CHAPTER 1

This Chapter has introduced the need for reducing diesel engine exhaust particulates due to the health and environmental risks, and impending tighter emissions standards.

To reduce the particulate emissions significantly exhaust after-treatment is required. The monolithic wall-flow trap is favoured due to its high particulate filtration efficiency, good particulate
capacity and good thermal properties. However, like other traps, it requires periodic cleaning or 'regeneration'.

Regeneration techniques are the subject of Chapter 2.
2.1 INTRODUCTION

Trap regeneration is essential if exhaust back pressures are to be kept within acceptable limits. Regeneration is accomplished by oxidising the trapped particulate and this requires both heat and some available oxygen. Since the oxidation process is exothermic, trap temperatures may rise too high and cause cracking or melting of the filtering medium, and hence trapping effectiveness would be permanently lost. Therefore, the regeneration process must be carefully controlled.

Various regeneration techniques have been explored, none of which have yet been shown to be wholly satisfactory in terms of cost, reliability and energy efficiency. This Chapter discusses these techniques and highlights the fundamental requirement of a suitable regeneration system.

2.2 REGENERATION TECHNIQUES

2.2.1 Use of Hot Exhaust Gas

The simplest regeneration technique is to operate the engine under a high speed, high load condition such that the exhaust gas is hot enough to cause rapid particulate oxidation. However, exhaust gas temperatures of between 450-550°C are required to initiate oxidation [40] and engines rarely provide these temperatures at the trap during normal drive-cycles. When they do, free oxygen levels in the exhaust gas are quite low.
As Murphy et al, 1981 [60] explain, heating the exhaust gas externally would require prohibitively high powers of the order of the engine's power, therefore throttling techniques have been developed [85]. By reducing the air flow through the engine, the overall air-fuel ratio is decreased from the normal unthrottled level and this causes higher average combustion gas temperatures and subsequently higher exhaust gas temperatures. Throttling also causes the engine to do more pumping work at the expense of useful shaft output power.

A range of throttling techniques have been explored, with the throttle placed either at the engine inlet, trap inlet or trap outlet [69]. With each technique the throttle is used to intermittently promote trap regeneration. The technique is relatively simple and has had some success especially in urban bus applications, described by Pattas et al, 1986a [69]. However, it is not without its problems. Engine power is much reduced and driveability is impaired, free exhaust oxygen is reduced and control of regeneration difficult. To overcome the latter problem Stiglic et al, 1988 [78] developed a sophisticated closed-loop system to help control the throttle and regeneration process. Noise due to the throttling process can also be a problem especially in applications where the regeneration is carried out with the vehicle stationary and the engine operated under free acceleration [67]. There are also concerns with increased thermal loading on the engine [70].

Despite the above problems, throttling systems are still being developed due to the relative simplicity of the concept.
2.2.2 Catalysts

The 'ignition' temperature of the particulate may be reduced to below 400°C by employing a suitable catalyst. This enables the trap to be regenerated in a wider range of engine speeds and loads.

Trap matrices impregnated with catalysts suffer deterioration with time and have a limited effect since the catalyst is not in contact with the major reaction sites of the particulate [62]. To introduce the catalyst to the particulate itself, fuel additives can be used [91].

Catalysts have several drawbacks. Firstly, they are expensive being usually a semi-precious metal, they either deteriorate with time (in the cases of filter matrix impregnation) or can lead to a build-up of incombustible material within the trap (when introduced via the fuel) which limits the trap's life. (Wade, 1983 [86] reported a typical monolithic wall-flow trap being blocked after 10,000 miles). Secondly, the trap cannot be regenerated at all speeds and loads. Finally, and perhaps most seriously, the catalyst promotes the oxidation of sulphur dioxide in the exhaust gas into sulphur trioxide which subsequently combines with water vapour to produce sulphuric acid aerosol in the atmosphere [48]. Fuel sulphur reductions would reduce this effect [17]. Both Wong et al, 1984 [93] and Hickman and Jaffray, 1986 [36] report a significant increase in emitted particulates when catalytic trap oxidisers of the wire mesh type were used. Enge et al, 1982 [23] similarly report a 40% particulate increase. There is much continuing research effort into developing a catalyst which will avoid these sulphate emissions problems. However, as Horrocks, 1987 [38] states, catalytic traps still cannot be regenerated at low exhaust gas temperatures without external
assistance. 'External energy' systems such as fuel burners or electrical heaters which do not necessarily require a catalyst are therefore now described.

2.2.3 Fuel Burner Systems

Diesel fuel burners located upstream of the trap have also received much attention. These burners provide a flame to heat up and promote oxidation of the trapped particulate, their main advantage being no additional load to the engine but they obviously require extra fuel. Wade et al, 1981 [85] described two fuel burner systems, one which used exhaust-fed gas and the other external air-feed. The latter types are much easier to control since both the oxygen concentration and air flow rate are constant but require the trap system to be by-passed for the period during regeneration. All fuel burner systems reported recently use external air for burner control, of which Macdonald and Simon, 1988 [54], Meinrad and Giorgio, 1989 [55], and Ha and Lawson, 1989 [34] are examples. Regeneration is carried out at low particulate loadings to reduce the risk of trap damage. Burner control is difficult and reliability problems have occurred especially with the fuel nozzle coking and ignition failure [86], but the biggest drawback is the cost. The fuel burners alone are of the order of £1000 each and truck and bus installations total 6% of the vehicle cost [3]. Macdonald and Simon demonstrated their system working well on a 100,000 mile simulated dynamometer test cycle and reported more than 6000 miles covered on a vehicle. They conclude that the system is feasible but prohibitively expensive for new vehicles. It appears that the present market for fuel burner regeneration systems lies with urban buses, especially in retrofit applications [34].
2.2.4 Electrical Heaters

Electrical resistance heaters to preheat the trap prior to regeneration have been explored. These are relatively simple and avoid the complexity and problems associated with the fuel burners described above. They do however require a significant amount of electrical power. Early examples [82] required several kilowatts, but by-passing the relatively cool exhaust gas around the trap during preheating can reduce powers significantly. Also to minimise power, most systems now preheat the front (inlet) face of the trap and externally fed air causes a hot oxidation zone to propagate through the trap consuming the trapped particulate. Barris and Rocklitz, 1989 [8] present a good example of this approach. Electrical resistance heating together with precious metal catalysts in the trap to reduce particulate ignition temperatures have been tried, and Arai et al, 1987 [4] describe their catalyst trap system as requiring 1.5 kW during preheating when an exhaust by-pass is used.

A brief mention of a type of electrical system not extensively reported is the porous element filter material developed by Fogarty Ltd. This filter medium could be heated dielectrically and thus the trapped particulate would in turn heat up and oxidise. However, Horrocks, 1987 [38] explained that filter sizes were too small even for a 2.5 litre engine and problems occurred with unreliable electrical connections to the filter elements. The author understands this system is not being currently developed.

2.3 FUNDAMENTAL REQUIREMENT FOR TRAP REGENERATION

The above regeneration techniques all have their strengths and weaknesses, and some are currently receiving much continued development effort, especially the 'external energy' systems such as
burners and electrical resistance heaters since these appear to be the most successful and have fewer problems. However it is important to look into trap regeneration more closely. It is clear that the prime requirement is not to heat the trap inlet gas or the trap itself, but it is the particulate that requires heating to promote rapid oxidation.

The author therefore proposed (in 1986) to use microwave energy to selectively and efficiently heat the trapped particulate to promote oxidation. Since the ceramic monolith itself was thought to be largely transparent to the microwave energy, only the particulate would be primarily heated. This approach appeared attractive and hence the idea was pursued further. This work is described in Chapters 4 to 7 of this thesis. Before this however, Chapter 3 provides a more detailed understanding of wall-flow trap regeneration with the development of a mathematical regeneration model.
CHAPTER 3

3.1 INTRODUCTION

In previous chapters it has been argued that both effective particulate filtration and trap regeneration are necessary to provide a practical means of significantly reducing diesel exhaust particulates. It was suggested that the monolithic wall-flow trap was the most suitable trap medium due to its good trapping efficiency and thermal strength. Various regeneration systems were described and finally a promising new concept proposed by the author of using microwave energy to promote trap regeneration was briefly mentioned. This will be further described in subsequent chapters.

Up to this point the details of the actual regeneration behaviour of monolithic wall-flow traps have not been described in any great detail, therefore the work in this chapter will attempt to provide this detail with the development and use of a mathematical trap regeneration model. This not only provides some insights to support further work presented in this thesis but also gives useful results for other developers of diesel particulate trap regeneration systems.

Models are useful for a variety of specific reasons. In their final form they hopefully provide useful results to aid system design; these detailed results may not be readily obtainable experimentally. However, perhaps more importantly, the process of developing the model encourages a systematic analysis of the problem and gives detailed insights into the important mechanisms involved. The model also exposes those areas where further research should be concentrated.
In the case of trap regeneration, direct measurements of the controlling parameters such as temperature, oxygen concentration and particulate oxidation rate (etc) within the filtering medium itself are very difficult, and intrusive measuring instruments may affect conditions and obscure the results obtained. Therefore despite the limitations and necessary simplifications, a mathematical model can be a useful design tool in assessing trap regeneration behaviour. This has led several investigators to develop trap regeneration models as part of their trap system development programmes.

The remainder of this chapter initially considers the physical structure of the monolithic trap with respect to modelling and then looks at how previous investigators have tackled the modelling problem. A new model developed during this present work is presented together with a full range of results of a parametric study and some experimental validation. Finally the usefulness of the model is discussed in the context of previous work, and subsequent trap modelling work that has been recently published is reviewed.

3.2 MODELLING THE MONOLITH'S PHYSICAL STRUCTURE

Referring to Figure 1.8 it can be seen that the physical structure of a loaded wall-flow monolith is not homogeneous but consists of discrete cellular channels which themselves are made up of a reactive porous layer of trapped particulate and an inert porous ceramic layer (the channel wall). This adds considerably to complexity of constructing an 'exact' model and constraints with computing power and a general lack of detailed physical data have encouraged significant simplifications and a range of modelling approaches to be made by different investigators.
The most significant simplification adopted by all investigators up to and including the present work was to consider a single composite section of particulate resting on the ceramic wall. Figure 3.1 shows this schematically.

![Schematic of Single Composite Section of Monolithic Wall-Flow Trap](image)

**FIGURE 3.1: SCHEMATIC OF SINGLE COMPOSITE SECTION OF MONOLITHIC WALL-FLOW TRAP**

Three general approaches to modelling this have been tried. These were to consider one-dimensional flow in the X direction, one-dimensional flow in the Z direction and finally two-dimensional flow in both the X and Z directions. Each approach makes the basic assumption that the composite section is typical of all the channels in the entire trap and that the channels are perfectly insulated. Both of these assumptions are reasonably true for channels a distance from the trap periphery. The interior channels in general experience the highest temperatures during regeneration and are hence of interest from the thermal melting/cracking point of view. The outer channels in practice often do not regenerate well but this depends on the degree of trap insulation.
Within the three general modelling approaches there are still a range of assumptions and simplifications which can be made. The following section considers how previous investigators have developed their models.

3.3 REVIEW OF PREVIOUS MODELLING WORK

3.3.1 Pauli et al, 1983 [71]

Pauli et al adopted the concept of discretizing the channel in the X (axial) direction (see Figure 3.1). Since the bulk flow is considered to flow in the X direction, and the end of the channel is blocked, some allowance must be made for 'leakage' flow through the porous particulate/ceramic layers and out of the adjacent outlet channel. Pauli et al assumed that the leakage flow continuously reduced with increasing X and became zero at the channel end, although they did assume some empirically chosen constants to allow for particulate/wall flow resistance depending on their respective thicknesses. The assumption that leakage flow at the channel entrance is the highest and flow at the channel end is zero is suspect. Experimentally the particulate layer presents the dominant resistance. For example the gas flow from a 2 litre engine at 1500 rpm, through a clean trap typically causes less than 1 cm Hg pressure drop across it, but in the loaded condition this rises to 10 cm Hg or more. Therefore if particulate at any position along the channel is preferentially consumed (by oxidation) then the major part of the gas flow through the wall would be at that point. So the basic assumption of continuously reducing flow with increasing X is not completely realistic.

Since Pauli et al chose a one-dimensional model, global convective flow of mass and heat were considered in the X direction, but in regard to the interaction with the particulate/ceramic layers gas was considered to diffuse through the porous layers in the Z direction exchanging heat and oxidising the particulate. The particulate and
ceramic layers were considered to be of the same physical structure and temperature, again due to the one-dimensionality of the equations.

The particulate oxidation rate was considered to be kinetically controlled and they supported this assumption through thermogravimetric analyses of diesel particulate samples. The oxidation rate was modelled using an Arrhenius relationship for carbon oxidation to carbon dioxide. They neglected source and sink mass balances for carbon dioxide and oxygen respectively.

Published results using the model were limited to particulate mass depletion (oxidation) along the channel during regeneration. The important result here was that the particulate mass depletion at the downstream end of the filter was greater due to the cumulative build-up of heat and the assumption of decreasing gas velocity at the downstream end. They also presented one temperature vs time profile for a single location in the trap which is reproduced here in Figure 3.2. Here the engine load and speed was increased to cause the
exhaust gas temperature $T_E$ to rise to 650°C. Since in this engine condition free oxygen in the exhaust is at a premium, additional oxygen was added to raise the oxygen concentration to 8.1% (by volume). Due to both the rise in inlet gas temperature and the heat release due to oxidation, the trap temperature $T_F$ rose to above the inlet temperature and peaked when the particulate upstream of the chosen point had been largely oxidised. If these temperature 'excursions' are too severe then trap damage can occur.

Overall, Pauli et al's model was reasonable but necessitated some simplifications which were restrictive such as ceramic and particulate layers being the same in all physical respects, and the leakage flow reducing with distance. Published results were disappointingly sparse and no temperature vs axial distance ($T_F$ vs $X$) profiles were presented which may or may not suggest problems with the model's temperature predictions at all axial points. However, Pauli et al did relate their model with some experimental findings and did contribute some very useful data on particulate oxidation rates which is to their credit.

3.3.2 Bissett, 1984 [13]

Bissett has made some impressive contributions to the understanding of diesel particulate trap regeneration behaviour, mainly through the development of mathematical models. In 1984 he presented work on a one-dimensional model not unlike Pauli et al, 1983 [71] discussed previously but developed it in a more thorough manner. The stimulus for such work was General Motors development of an upstream fuel-burner trap regeneration system. Bissett and Shadman, 1985 [15] also working concurrently on a one-dimensional model considering flow in the $Z$ direction (see later), indicated that for low gas flow rates encountered with fuel-burner systems (which isolate the trap by bypassing the exhaust gas around the trap during regeneration) require a
means of modelling non-uniform axial temperatures. Bissett therefore chose to model the trap channel in the axial, X direction (see Figure 3.1). Whilst citing Pauli et al, 1983 he stated that his work was more thorough and included a more detailed description of the temperature couplings between the heat and mass transfer and the oxidation effects.

The one-dimensional model considered the particulate/ceramic layers to be of the same material and of the same temperature independent of the radial direction Z (see Figure 3.1). He too accounted for leakage flow through the wall in the conservation of mass expressions but did not place the restrictions on the leakage gas velocity profile as Pauli et al had done.

The oxygen concentration was assumed to be constant along the channel length since the oxygen in the bulk flow does not diffuse to the particulate by a concentration gradient but by convective flow. The actual amount of oxygen available, however is obviously dictated by the bulk gas mass flow rate.

The particulate oxidation was assumed to be kinetically controlled since very high specific surface areas in the particulate layer would enable mass transfer rates some two orders of magnitude higher than the kinetic reaction rates (this is discussed later). The reaction rate was described in an Arrhenius equation for carbon oxidation to carbon dioxide.

Bissett described in some detail his solution method of the coupled partial differential equations and essentially this was carried out by spatial discretization and solving them with proprietary software packages. Whilst no mention of computation time was given, a relatively "tame regeneration" (Bissett’s words) for which results were presented required some 2500 time steps for 212 modelled seconds.
The initial conditions of the trap were based on the fuel-burner data i.e. a temperature of 950°C and 15% free oxygen (by volume) and slow flow rate compared to normal engine exhaust flows (due to the trap bypassing technique). The initial mass loading of 10g of particulate is quite low (traps of the type modelled by Bissett could hold over 400g). Although this was in general accordance with the fuel-burner regeneration strategy of regenerating quite often to keep exhaust back pressures down and not allowing a large heat release during oxidation which might damage the trap, it is perhaps lower than would be likely in practice, 50g is more realistic. However, temperature excursions of over 1100°C were predicted with the model which seem very high considering the available oxidation enthalpy contained in the very small amount of particulate. Bissett presented temperature vs axial distance profiles which showed a form of 'travelling wave' starting at the heated upstream end and moving towards the downstream outlet end. These profiles are reproduced here in Figure 3.3. One very useful result was that the internal trap temperatures are very much hotter than the outlet gas temperatures up until the travelling wave reaches the downstream end and thus if a trap regeneration system uses outlet temperature to monitor and control the process large inaccuracies would be likely.

![Figure 3.3: Profiles of channel wall temperature during fuel-burner regeneration as a function of dimensionless axial distance at selected times [13]](image-url)
Bissett's approach was thorough and sound but he avoided analysing realistic particulate mass loadings. Relatively high temperature excursions predicted at the very low mass loadings imply significant errors at higher loadings. No experimental validation was provided but the work certainly provided useful understanding and insight into the regeneration process.

3.3.3 Bissett and Shadman, 1985 [15]

In conjunction with the model developed by Bissett, 1984 [13] discussed previously, Bissett and Shadman presented work on a one-dimensional model considering flow through the composite layers of particulate and ceramic wall in the Z direction (see Figure 3.1). When employing thermal regeneration techniques where the entire engine exhaust gas passes through the trap throughout the regeneration cycle the gas flow rates are high and therefore Bissett and Shadman argued that axial temperature variations are small and can be neglected.

The model geometry was considered to be a composite slab with an area equal to the total filtration area of the honeycomb channels. This is shown schematically in Figure 3.4. The slab consisted of a reactive layer of particulate deposit, followed by a non-reactive porous ceramic layer of a thickness equal to that of a single honeycomb channel wall.

![Figure 3.4: Monolithic trap model geometry used by Bissett and Shadman, 1985 [15]](image-url)
Bissett and Shadman presented a scanning electron micrograph of the fractured edge of a loaded wall-flow monolith which clearly showed the particulate deposit layer on the upstream surface of the channel walls. There was negligible penetration of the particulate into the internal pores of the ceramic wall and this gives some basis for the distinct 'reactive' and 'inert' layers in the model geometry.

The thickness of the particulate layer is always likely to be fairly uniform throughout the trap since if a particular channel fills up excessively it presents a higher gas flow resistance which then encourages flow to other channels. There is thus an equalising effect. The oxidation processes within the reactive particulate layer are complex and not fully understood. Bissett and Shadman simplified their model by considering only the top inlet face of the reactive layer oxidising and that after each time step the reactive layer's thickness was reduced to account for the particulate depletion. Thus the Z ordinate was assumed to move with time. This assumption can only be supported if all the oxygen flowing into the particulate is consumed by the top most layer. However, even during regeneration, some oxygen does pass through the entire layer without reacting with the particulate (since kinetic rates control the reaction) and it would therefore be more valid to assume that oxidation occurs throughout the layer and not solely at its upstream surface. This point is returned to later.

In accordance with previous work above, the oxidation of particulate was assumed to be the first order heterogeneous oxidation of carbon (i.e. \( \text{C} + \text{O}_2 \rightarrow \text{CO}_2 \)) and the reaction was assumed to be kinetically controlled and described with an Arrhenius expression. Bissett and Shadman neglected the reactant mass added to the gas phase from
deposit oxidation (i.e. they did not include 'source' and 'sink' terms in the mass continuity expressions) arguing that this added mass was small compared to the total convective flow. The solid and gas phase temperatures throughout the internal structure of the composite slab were assumed to be the same. The model slab was assumed to be effectively insulated from its surroundings at its edges.

Bissett and Shadman chose perturbation expansions [44] of temperature, oxygen concentration and reactive layer thickness expressions for the mathematical solution. A detailed mathematical description of the solution method was given by Bissett, 1985 [14], but this is not of prime interest here. However, Bissett claimed excellent precision in adopting this approach.

Thermal regeneration was initiated by increasing the inlet gas temperature from 600 to 800K in 240 seconds. Trap temperature and particulate mass vs time graphs were given. These identified three stages of regeneration: preheat, start of rapid oxidation and convective transport limited oxidation. Results also included a series of oxygen concentration profiles across the reactive layer which clearly demonstrated that even during rapid particulate oxidation, oxygen consumption was not complete and thus oxygen is generally available throughout the reactive layer and therefore oxidation is likely. This contradicts Bissett and Shadman's basic assumption of oxidation only at the particulate upstream surface.

An interesting parametric study was included of how the initial particulate mass loading affects regeneration time and peak temperatures (all other parameters being the same). These results are reproduced here in Figure 3.5. These show that high initial loading
led to faster oxidation with little effect on overall regeneration time but significantly increased the peak temperatures in the trap.

Bissett and Shadman explored altering the monolith's physical structure, namely the total filtration area and channel wall thickness. The filtration area is important since this directly relates to the overall size and hence cost of the monolith. The model showed that decreasing the filtration area promoted a faster regeneration but raised temperature excursions significantly. The decrease in filtration area effectively increases the particulate layers thickness (for a given particulate mass loading) and also increases the exhaust gas velocity. The effectively increased mass-loading follows the trend shown in Figure 3.5 but the effect of increased gas velocity is more complex. The increased gas velocity increases the convective cooling effect through the monolith and also simultaneously provides a high oxygen feed-rate to promote oxidation and hence heat release. Bissett and Shadman argued that for the range of interest in their study the latter effect dominated and hence higher temperatures were expected.
Bissett and Shadman also considered the effect of channel wall thickness. Decreasing it led to higher trap temperatures and faster regenerations since it would present less of a heat-sink to the oxidation heat release. The wall thickness does not affect the filtration efficiency significantly since wall-flow monoliths are surface filters, but reduced thickness does reduce pressure drop which is of basic importance. Bissett and Shadman concluded that a good strategy was to design monoliths with the thinnest wall thicknesses that mechanical strength and manufacturing limits would allow and to choose the largest filtration area possible in the vehicle installation.

Bissett and Shadman's work was a significant contribution to the understanding of monolithic wall-flow trap regeneration behaviour; they developed their model in a clear, unambiguous manner and provided useful basic trap data. They did not validate the model's results experimentally, but these were in general agreement with other investigators findings and were wholly reasonable.

3.3.4 Weidemann et al, 1984 [91]

Weidemann et al were investigating monolithic trap regeneration using catalytic fuel additives. In their previous work (Weidemann et al, 1983 [90]) they presented model equations to describe the oxidation process in the trapped particulate and the exhaust conditions, defining the ignition points. General results given in this work were only of a qualitative nature but significant experimental results were given. Later Weidemann et al, 1984 developed the model equations further to describe both the gas flow processes and the reaction kinetics for a particulate loaded channel section. Gas flow equations were empirically 'tuned' to give fairly accurate predictions of
pressure drop across a loaded trap. The reaction kinetics and energy expressions were applied to a model channel consisting of a particulate layer resting on the ceramic wall. The effect of the ceramic wall was ignored but the particulate layer itself was divided into a grid in the X and Z directions (as defined in Figure 3.1). Gas flow, however, was considered only in the Z direction. Gradients of relevant variables within each particulate layer were assumed to be zero and any build-up of particulate in the trap during the regeneration process was considered to be inert.

Weidemann et al, 1984 as stated above, were modelling catalytic regeneration and due to lack of kinetic data for the assumed Arrhenius expression they arbitrarily chose an activation energy and a frequency factor which gave reasonable results. A description of the numerical solution procedure was not given but they did point out that special care must be given in controlling the time-step size to give accurate solutions. They controlled this by limiting temperature changes to 1°C for each time-step.

Model results included gas mass flow rate, particulate thickness, temperature profiles in the X direction for various times during rapid oxidation. Results showed that the reaction began at the downstream end of the channel due to slightly reduced flow (and hence cooling effect) there. However, only a few seconds later the entire model channel length was shown to react uniformly. This uniformity gives some support to the slab model of Bissett and Shadman, 1985 [15]. Considering the particulate layers parallel to the ceramic wall, the model demonstrated that the interior layers began to react the earliest but once the top layer reacts significantly it consumes a substantial amount of the incoming free oxygen which significantly
reduces the reaction rate of the lower layers nearer the ceramic wall. Other results were temperature vs time profiles showing temperature excursions from 200°C to 1300°C, and temperature temporal gradients between 12°C/sec and -20°C/sec.

The work of Weidemann et al, 1984 gave further insight into catalytic regeneration of monolithic wall-flow traps. The model developed was not empirically validated but results appeared to be reasonable. The model itself was unusual since it was two-dimensional in nature, but they provided little detail of their basic assumptions, physical data for the model and solution procedure to allow a detailed critique.

3.3.5 Takama et al, 1984 [80]
Here a model describing the regeneration of ceramic foam traps was described and although it is not of prime interest here, it is worthy of brief mention for three reasons. Firstly, the basic equations and modelling approach are very similar to those developed for wall-flow traps and also some physical data is relevant. Secondly Takama et al described the model in a thorough manner unlike some other writers who perhaps tended to be fairly superficial in their model descriptions. Finally, they included some features in their model not previously incorporated by other writers.

Ceramic foam traps experience bulk gas flow entirely in the axial direction, although obviously at a microscopic scale radially-diffuse flow through the random foam structure does occur. Takama et al considered the usual first order heterogeneous oxidation of carbon to model particulate oxidation (i.e. \( \text{C} + \text{O}_2 \rightarrow \text{CO}_2 \)). They described this with an Arrhenius expression but also considered the mass diffusion step which at very high temperatures limits the overall reaction rate.
The model was axially one-dimensional and considered the coupling between the gas and solid phases with the respective temperatures distinct. Since the whole ceramic matrix was being considered (unlike the previous single-channel models) environmental heat loss terms were included in the energy equations.

Regeneration was initiated using an upstream heat-source and trap temperature variations with time during rapid oxidation showed that the modelled and experimental results were in good agreement. The model also showed an oxidation 'wave-front' (e.g. temperature peak) propagating axially downstream. Takama et al finally described regeneration limits for stable and unstable oxidation using their developed model.

3.4 THE PRESENT MODEL - Garner and Dent, 1988 [28]

The reasons for developing a regeneration model were given in the introduction to this Chapter. The detailed model equations here are developed in a generalised form which enables them to be applied to different trap types, e.g. fibrous, foam and wall-flow monolith, and for the latter, different model geometries, i.e. axial or radial dimensions. Only after the generalised model equations are developed are they applied to the chosen trap type and model geometry.

It is the intention here to use the model to describe the regeneration processes without being too dependent upon a particular regeneration technique or system. This is because most regeneration systems impose their own unique peculiarities on the trap's regeneration characteristics. Therefore, the simplest regeneration technique is chosen which uses high engine exhaust gas temperatures with a range of oxygen concentrations to promote thermal regeneration. This will give a good understanding of the regeneration process.
Since the whole exhaust gas flow is used throughout the regeneration cycle, axial gradients may be neglected in favour of analysing in detail the temperature and gas constituent gradients through the particulate and ceramic wall layers. This approach is supported by Bissett and Shadman, 1985 [15]. Thus a one-dimensional model is considered, with the spatial variable $Z$ being in the direction of flow through the porous deposit layer and ceramic wall. The model geometry is considered to be a composite slab with an area equal to the total filtration area of the honeycomb channels, see Figure 3.6.

![Figure 3.6: Geometry for Monolithic Wall-Flow Trap Model](image-url)
The slab consists of a reactive layer of particulate deposit, followed by a non-reactive porous ceramic surface of a thickness equal to that of a single honeycomb channel wall. This is similar to Bissett and Shadman's model geometry but important differences are included. Firstly, oxidation is allowed to take place anywhere in the particulate layer since as mentioned earlier (in Section 3.3.3) temperatures are sufficiently high and oxygen is available throughout the particulate layer. Secondly, the internal structure of the particulate layer changes before and during oxidation and these changes are complex in nature and not well understood. Therefore here the particulate layer is assumed to oxidise throughout (as localised conditions allow) leaving an inert material having the same physical structure as the original particulate. Thus the requirement of endeavouring to model the collapsing particulate structure and employing a moving coordinate system \( Z \) is avoided. Bissett and Shadman, 1985 [15] also avoided trying to describe the changing and collapsing particulate structure but they employed a moving coordinate system since only the topmost (upstream) layer was assumed to be oxidised at any one time and the total particulate thickness was assumed to shrink.

Here, as with all previously described trap regeneration models, the particulate is assumed to be carbonaceous and that a simple heterogeneous chemical reaction between the carbon and oxygen yields carbon dioxide.

The generalised model equations are now presented which describe the oxidation mechanism and mass and energy balances.
3.4.1 Oxidation Mechanism

Oxygen in the exhaust gas is transported to the particulate surface by convective mass transfer and this oxygen participates in the oxidation kinetics of the carbonaceous particulate matter.

The oxygen mass transfer rate per unit volume $\dot{G}_{G,O_2}$ (kg/m$^3$s) is given by

$$\dot{G}_{G,O_2} = g \cdot a \cdot [m_{G,O_2} - m_{S,O_2}] \left[ \frac{kg}{m^3s} \right] \quad (3.1)$$

where $g$ is the mass transfer conductance (kg/m$^2$s), $a$ is the specific area (l/m) (i.e. surface area of the porous media per unit volume) and $m_{G,O_2}$ and $m_{S,O_2}$ are the oxygen mass concentrations in the bulk exhaust gas flow and at the particulate surface respectively (kg O$_2$/kg exhaust gas).

The particulate kinetic oxidation rate per unit volume $\dot{R}_{S,O_2}$ (kg/m$^3$s) is given by

$$\dot{R}_{S,O_2} = K \cdot \rho_G \cdot m_{S,O_2} \left[ \frac{kg}{m^3s} \right] \quad (3.2)$$

where $K$ is an Arrhenius expression [49] (1/s) and $\rho_G$ is the bulk gas density (kg/m$^3$). Since in the steady state the rate of oxygen mass transfer equals the rate of particulate oxidation, i.e.

$$\dot{G}_{G,O_2} = \dot{R}_{S,O_2} \left[ \frac{kg}{m^3s} \right] \quad (3.3)$$
equations (3.1) and (3.2) may be equated to solve for the unknown oxygen mass fraction at the particulate surface $m_{s,o_2}$.

Hence,

$$m_{s,o_2} = \left[ \frac{g \cdot a}{K \cdot \rho_G + g \cdot a} \right] m_{G,o_2} \quad (3.4)$$

Defining the group $(g \cdot a/\rho_G)$ as the mass transfer rate $b \ (1/s)$ yields the overall reaction rate

$$\dot{R}_{s,o_2} = \frac{K \cdot b}{K + b} \rho_G \cdot m_{G,o_2} \quad \left[ \frac{kg}{m^2 \cdot s} \right] \quad (3.5)$$

The general significance of equation (3.5) is that the smaller of either the chemical reaction rate $K$ or mass transfer rate $b$ controls the overall reaction rate $\dot{R}_{s,o_2}$. At low surface temperatures $K$ is smaller than $b$ and hence the chemical kinetics limit or control the overall reaction rate. However, at high temperatures, since $K$ is strongly dependent on temperature (in an Arrhenius relationship) $K$ is larger than $b$ and hence the mass transfer rate $b$ controls the reaction. In both cases the mass fraction of oxygen in the exhaust gas flow $m_{G,o_2}$ influences the reaction rate at the particulate surface.

3.4.2 Mass Balances

a) Particulate - The mass of particulate is depleted as it is oxidised and is represented mathematically by
where $\beta_p$ is the concentration of particulate (kg/m$^3$), $t$ time (s) and $r$ the stoichiometric ratio for the oxidation of carbon to carbon dioxide.

b) Gas stream - Since oxygen is transferred from the exhaust gas stream to the particulate surface and carbon dioxide is transferred back to the gas stream, gradients of these two constituents will exist in the direction of the exhaust flow and with time. Reactions of other species can be accommodated in the model since the mass transfer and gradient expressions can be written in a general form. For a general constituent, $\eta$ in the gas flow the gradients of concentration in space and time are given by

$$-\phi \dot{G} \frac{\partial m G,\eta}{\partial z} - \phi \rho G \frac{\partial m G,\eta}{\partial t} = g \cdot a \cdot [m G,\eta - m S,\eta]$$

\[ \text{kg m}^{-3} \text{s}^{-1} \] \hspace{1cm} (3.7)

where $\phi$ is the medium porosity, $\dot{G}$ the gas flow rate per unit area (kg/m$^2$s), and $m_{G,\eta}$ and $m_{S,\eta}$ the concentration of gas constituent $\eta$ in the bulk gas and at the solid surfaces respectively. For oxygen transport to the particulate surface and consumption there, equation (3.7) may be rewritten as:

$$-\phi \dot{G} \frac{\partial m G,O_2}{\partial z} - \phi \rho G \frac{\partial m G,O_2}{\partial t} = \dot{R}_{S,O_2}$$

\[ \text{kg m}^{-3} \text{s}^{-1} \] \hspace{1cm} (3.8)
3.4.3 Energy Balances

a) Gas stream - Radiation effects in the gas stream can be neglected since they are very small. Therefore the loss of energy in the gas flow with time and in the flow direction is equal to the heat convected to the solid surface. This is expressed as

\[-\phi \dot{G} C_R G \frac{\partial T_G}{\partial z} - \phi \rho G C_R G \frac{\partial T_G}{\partial t} = h \cdot a \cdot [T_G - T_S] \quad \text{[kW/m}^3\text{]} \quad (3.9)\]

where \( h \) is the convective heat transfer coefficient. Note that distinct gas \( T_G \) and solid \( T_S \) temperatures are assumed here. Apart from Takama et al, 1984 [80] who modelled foam traps, all the previously reviewed investigators assumed these two phases to be the same temperature. Whilst this is a fair approximation, this would restrict the general nature of the model equations if assumed here.

b) Solid phase - Radiative heat transfer effects can be neglected since the channels are slender and each of the four surfaces of the inlet channel are assumed to exchange equal amounts of radiative heat with each other. The convective heat transfer to the solid from the gas stream increases the internal energy of the solid and hence its temperature setting up a thermal gradient due to conduction in the flow direction. If the temperature of the solid is high enough the particulate will oxidise liberating energy. This can be expressed mathematically as

\[(1 - \phi) \rho S C_R S \frac{\partial T_S}{\partial t} = \dot{R}_{\text{O}_2} \cdot (H + h \cdot a \cdot [T_G - T_S]) + k_s \frac{\partial^2 T_S}{\partial z^2} \quad \text{[kW/m}^3\text{]} \quad (3.10)\]
where $\rho_s$ is the solid density (kg/m$^3$) and $H$ the enthalpy of reaction for particulate oxidation (kJ/kg) and $k_s$ the bulk thermal conductivity of the porous solid (kW/mK).

3.4.4 Equation of State
This completes the set of equations that require solving. Since the change in gas pressure in the trap during regeneration is of the order of a few centimetres of mercury [37] the absolute gas pressure in the trap is assumed constant. The equation of state can therefore be expressed as

$$p_G T_G = \text{constant} \quad \left[ \frac{\text{kgK}}{\text{m}^3} \right] \quad (3.11)$$

3.4.5 Mathematical Solution
The above system of equations are coupled non-linear partial differential equations of mixed type which can be discretized and solved using a suitable finite difference scheme. In the course of this study it was found that the algorithm described by Lawson and Norbury, 1985 [47] modelled the same set of equations in an efficient manner. This algorithm coded in FORTRAN by Lawson and Norbury, was therefore used for the numerical solution.

The algorithm adopts a scheme using two levels of iteration: the outer iteration is essentially 'Gauss-Seidel' which uses the most up to date information in each subsystem to solve the linear equations and the inner iteration is from Newton's method and solves the subsystems containing the dominant non-linearities. These non-linearities occur in the gas and solid energy equations which are strongly coupled.
The boundary conditions at the trap inlet are known at each time increment and first approximations of the gas mass fractions $m_{o,g}$ and temperatures $T_{o}$ and $T_{s}$ are found. Using these approximations the energy equations are solved by the Newton Iteration to yield better estimates of $T_{o}$ and $T_{s}$. The remaining variables are then recalculated from the values of $T_{o}$ and $T_{s}$ obtained from the Newton Iteration, the gas density $\rho_{o}$ from the equation of state, the oxygen mass fraction from equation (3.8) and the particulate depletion rate from equation (3.6).

A better approximation to the values of the variables is achieved by setting up a second outer iteration (Gauss-Seidel) loop between the first approximation of values $m_{o,g}$, $T_{o}$ and $T_{s}$ and the computation of particulate depletion rate. All values are therefore evaluated for the first time step and the procedure is repeated for subsequent time steps. A full description of this algorithm is given by Lawson, 1984 [46].

The spatial and temporal increment sizes and computer processing time are discussed later.

3.4.6 Application of Model to Monolithic Wall-Flow Traps

So far the equations have been kept general enough to model gas flow through a matrix containing reactive particulate. These general equations are now applied to the specific geometry of the monolithic wall-flow trap. It is possible to model other types of trap, e.g. fibrous type (Garner and Dent, 1988 [28]), using the same foregoing equations in a similar manner.
a) **Model Geometry** - The model geometry described earlier and shown in Figure 3.6 considers oxidation in the porous particulate deposit layer. The thickness of this layer is given by

\[
Z_p = \frac{m_p}{\beta_{\text{Bulk}} \cdot A_{\text{fil}}} \quad (m)
\]

where \( m_p \) is the total trapped mass of particulate (kg), \( \beta_{\text{Bulk}} \) is the bulk density of the particulate (kg/m\(^3\)) and \( A_{\text{fil}} \) is the total filtration area of the monolith (m\(^2\)). The regeneration equations are solved along the total length \( Z \) of the model geometry, which includes the wall thickness \( Z_w \) (m). As explained before, to avoid using a moving coordinate system to define the reaction front of the oxidising particulate surface, and uncertainties regarding the 'collapsing' mechanisms occurring, it was assumed that the particulate is oxidised to an inert solid deposit having the same thermal and physical properties as the original particulate which remains in the layer and this can be accounted for by a simple mass balance from equation (3.6).

b) **Physical Characteristics of Particulate Layer** - The specific area of the solid is required for the heat and mass transfer rates. The particulate specific area depends on the size, density and shape of the particles. Although primary soot particles have diameters of the order of 10 to 30 nm these particles coalesce into larger agglomerates which have diameters of about 0.1 to 1 \( \mu \)m. The mean diameter based on the volume distribution was found to be 0.17 \( \mu \)m [83] and this value was chosen as the characteristic particle diameter.
There has been uncertainty concerning the bulk density of the particulate deposit, $\beta_{\text{Bulk}}$ (kg/m$^3$). Otto et al, 1980 [65] found that a sample shaken out of a monolithic trap had a bulk density of 56 kg/m$^3$. However, they found that particulate removed from an electrostatic precipitator had a bulk density of 20 kg/m$^3$ and some from an exhaust gas recirculation valve 400 kg/m$^3$. A literature survey [40,59,60,65,85] revealed that most investigators preferred to use a bulk density of 56 kg/m$^3$. The author has found experimentally that monolithic traps fully loaded up with diesel particulate suggest that the 56 kg/m$^3$ figure is very accurate and repeatable, consistently being within a tolerance of about five percent, and therefore this value was adopted for the purpose of the present work.

Depending on the particulate diameter its specific area $a_p$ varies. For an individual particle of density $\rho_p$ (kg/m$^3$) the specific area is given by

$$a_p = \frac{6\beta_{\text{Bulk}}}{d_p\rho_p} \quad \left[ \frac{1}{m} \right] \quad (3.13)$$

and assuming a particle density of 2000 kg/m$^3$ [65]

$$a_p = \frac{3 \times 10^{-3}}{d_p} \beta_{\text{Bulk}} \quad \left[ \frac{1}{m} \right] \quad (3.14)$$

In monolithic wall-flow traps the exhaust gas containing oxygen flows through the fine particulate deposit and the heat and mass transfer mechanisms are not well understood. A comprehensive study of heat and mass transfer rates between a non-reacting sphere in a
gas flow is given by Field et al, 1967 [24]. Pauli et al, 1983 [71] used the mass transfer equation, derived by Thoenes and Kramers, 1958 [81] for non-reacting spheres, in their mathematical analysis of the regeneration of particulate traps. A mass transfer coefficient for a non-reactive system was also used by Weidemann et al, 1983 [90] in the same application. For the work described here heat and mass transfer coefficients applicable to reacting beds of particles were used. Olson et al, 1968 [64] expressed the heat transfer coefficient as

\[ h_p = 3.787 \times 10^{-4} \left( \frac{\dot{G}_G T_G}{\phi_p d_p} \right)^{0.5} \text{[kW/m}^2\text{K]} \] (3.15)

and assuming constant \( \phi_p = 0.5 \) (a reasonable average) and \( d_p = 0.17 \text{ mm} \) this becomes

\[ h_p = \text{constant} \left( \frac{\dot{G}_G}{T_G} \right)^{0.5} \text{[kW/m}^2\text{K]} \] (3.16)

It should be mentioned here that the high heat transfer rates encountered in packed beds are not due to high heat transfer coefficients, but due to the large contact area (large specific area) between the gas and the porous deposit layer. Olson et al, 1968 [64] also recommended an expression for the mass transfer conductance

\[ g_p = 9.806 \times 10^{-4} \left( \frac{\dot{G}_G}{\phi_p d_p} \right)^{0.5} T_G^{0.33} \text{[kg/m}^2\text{s]} \] (3.17)
So, for constant $\phi_p$ and $d_p$ as before:

$$g_p = \text{constant} \left[ \dot{G}_G \right]^{0.5} T_G^{0.33} \left[ \frac{\text{kg}}{\text{m}^2 \text{s}} \right]$$  \hspace{1cm} (3.18)

The mass transfer conductance $g_p$ can also be found from the heat transfer coefficient using $g_p = \frac{h_p}{C_l}$ when the mass transfer rate is low which is so for low values of $[m_{G,G_2} - m_{G,L_2}]$ and a Lewis number of unity. Hence from equation (3.16) the mass transfer conductance can be written as

$$g_p = \text{constant} \left[ \dot{G}_G \right]^{0.5} T_G^{0.5} \left[ \frac{\text{kg}}{\text{m}^2 \text{s}} \right]$$  \hspace{1cm} (3.19)

Equations (3.18) and (3.19) derived for $g_p$ yield similar arithmetic results. For the present work equation (3.19) was employed.

c) Physical Characteristics of Ceramic Wall - The specific area used here is based on the assumption of cylindrical pores of uniform diameter $d_{pore}$ and is given by

$$a_c = \frac{4\phi_c}{d_{pore}} \left[ \frac{1}{\text{m}} \right]$$  \hspace{1cm} (3.20)

where $\phi_c$ is the porosity of the ceramic wall.

A heat transfer coefficient correlation quoted by Bear and Corapcioglu, 1984 [10] for flow through porous media yields
\[ h_c = 3.588 \times 10^{-3} k_G \left[ \frac{G_G}{\mu_G} \right]^{1.375} \cdot d_{\text{pore}}^{0.375} \left[ \frac{\text{KW}}{\text{m}^2\text{K}} \right] \quad (3.21) \]

where \( k_G \) is the gas thermal conductivity (kW/mK) and \( \mu_G \) is the gas dynamic viscosity (kg/ms).

Bird et al, 1960 [12] gives these as

\[ k_G = 1.49 \times 10^{-6} T_G^{0.5} \left[ \frac{\text{KW}}{\text{mK}} \right] \quad (3.22) \]

and

\[ \mu_G = 1.28 \times 10^{-6} T_G^{0.5} \left[ \frac{\text{kg}}{\text{ms}} \right] \quad (3.23) \]

Therefore

\[ h_c = \text{constant} \left( \frac{G_G}{\mu_G} \right)^{1.375} T_G^{-0.1875} \left[ \frac{\text{KW}}{\text{m}^2\text{K}} \right] \quad (3.24) \]

for constant \( d_{\text{pore}} \).

d) Other Data - The chemical reaction rate \( K \) is given by the Arrhenius equation

\[ K = A \cdot \exp \left[ -\frac{E}{GT_S} \right] \left[ \frac{1}{\text{s}} \right] \quad (3.25) \]

where \( A \) is the frequency factor (1/s), \( E \) the activation energy (kJ/kg-mol) and \( G \) the universal gas constant (kJ/kg-mol.K).

The global kinetic rate equations of the Arrhenius type are an over-simplification of the chemical kinetic processes they represent and the variables \( A \) and \( E \) are strongly dependent on the precise experimental conditions under which data are obtained. A
survey of the frequency factors and activation energies adopted by several investigators modelling trap behaviour showed significant variations in their form and value as shown below in Table 3.1.

<table>
<thead>
<tr>
<th>Frequency Factor</th>
<th>Activation Energy (kJ/kg-mol)</th>
<th>Reference No</th>
</tr>
</thead>
<tbody>
<tr>
<td>87100 kg/m²s atm</td>
<td>149 476</td>
<td>[15, 24]</td>
</tr>
<tr>
<td>300 m³/sg</td>
<td>111 000</td>
<td>[71]</td>
</tr>
<tr>
<td>7700 (N) m³/sg</td>
<td>54 500</td>
<td>[66]</td>
</tr>
<tr>
<td>40.95 kg/m²s atm</td>
<td>142 000</td>
<td>[59]</td>
</tr>
<tr>
<td>3000 m/s</td>
<td>90 000</td>
<td>[91]</td>
</tr>
</tbody>
</table>

**Table 3.1: Variation in Frequency Factors and Activation Energies**

Otto et al [65] recommended activation energy values for carbon oxidation ranging from 70 000 to 420 000 kJ/kg-mol. Although values of frequency factor and activation energy depend on the mode of oxidation (thermal or catalytic) frequency factors for thermal oxidation used by Bissett and Shadman, 1985 [15] and Mogaka et al, 1982 [59] differ by a factor of 2000.

Some of these reaction rates yielded unrealistic results so it was decided to adopt the activation energy used by Pattas et al, 1985 [66] since their value was based on experimental results pertinent to monolithic wall-flow diesel particulate traps. Their frequency factor \( A \) was not defined in the form required in this study so a value of \( 1 \times 10^5 \) 1/s was adopted. These values give a reaction rate within the range of those obtained by the different investigators quoted above.
Table 3.2 gives the data used for the present study of the monolithic trap. The overall size and structure of the monolith gives a total filtration area $A_{fi}$ of $2 \text{ m}^2$ and the maximum amount of particulate it can contain is 45g.

Ceramic Monolith:

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter 5.66 inch</td>
<td></td>
</tr>
<tr>
<td>Length 6.00 inch</td>
<td></td>
</tr>
<tr>
<td>Cell structure:</td>
<td></td>
</tr>
<tr>
<td>Diameter, 0.012 inch</td>
<td></td>
</tr>
<tr>
<td>Cell density, 200 cells/inch$^2$</td>
<td></td>
</tr>
<tr>
<td>Wall thickness, 0.012 inch</td>
<td></td>
</tr>
<tr>
<td>Cell density, 200 cells/inch$^2$</td>
<td></td>
</tr>
<tr>
<td>Wall porosity, $\phi_w$</td>
<td>0.49</td>
</tr>
<tr>
<td>Mean pore diameter, $d_{pore}$</td>
<td>16.5 $\mu$m</td>
</tr>
</tbody>
</table>

Specific heat capacity $c_p = 1.11 \text{ kJ/kgK}$

Bulk density $\beta_c = 1400 \text{ kg/m}^3$

Bulk thermal conductivity $k_c = 0.0011 \text{ kW/mK}$

Particulate:

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Enthalpy of reaction $H$</td>
<td>32 800 $\text{ kJ/kg}$</td>
</tr>
<tr>
<td>Activation energy $E$</td>
<td>54 500 $\text{ kJ/kg-mol}$</td>
</tr>
<tr>
<td>Frequency factor $\Lambda$</td>
<td>$1 \times 10^5 \text{ l/s}$</td>
</tr>
<tr>
<td>Porosity $\phi_p$</td>
<td>0.50</td>
</tr>
<tr>
<td>Mean diameter $d_p$</td>
<td>0.17 $\mu$m</td>
</tr>
<tr>
<td>Specific heat capacity $c_p$</td>
<td>1.51 $\text{ kJ/kgK}$</td>
</tr>
<tr>
<td>Bulk density $\beta_{bulk}$</td>
<td>56 $\text{ kg/m}^3$</td>
</tr>
<tr>
<td>Particle density $\rho_p$</td>
<td>2000 $\text{ kg/m}^3$</td>
</tr>
<tr>
<td>Bulk thermal conductivity $k_p$</td>
<td>0.00084 $\text{ kW/mK}$</td>
</tr>
</tbody>
</table>

**TABLE 3.2: DATA USED FOR MONOLITHIC WALL-FLOW TRAP MODEL**

e) **Engine Data** - The engine operating conditions used in the model are given in Table 3.3. For modelling purposes a simple regeneration method is adopted where the engine is operated at high load to obtain high exhaust gas temperatures. The exhaust temperature map in Figure 3.7 shows the initial (A) and final (B) inlet gas temperatures the trap is exposed to during regeneration. At medium speed these represent operating the engine at light
(24%) load and increasing this at constant speed to a high (91%) load which in turn increases the exhaust gas temperature to promote trap regeneration. Although it is sometimes the practice to reduce the inlet gas temperature once rapid oxidation is underway, for the following results the temperature was maintained at a constant high level so that direct comparisons for different oxygen concentrations and trap loadings could be made.

Perkins Prima High Speed DI 1.992 litre N/A Diesel

Rated speed 4500 rpm
Exhaust gas temperatures at trap inlet (see 'Med', Figure 3.7)
473K prior to regeneration (at 2750 rpm, 24% load) rising to 773K (in 30 seconds) during regeneration (at 2750 rpm, 91% load)
Volumetric efficiency, 85% at 2750 rpm
Exhaust gas pressure, 1 x 10^5 N/m^2

TABLE 3.3: ENGINE DATA USED IN MODEL

FIGURE 3.7: ISO-EXHAUST TEMPERATURE MAP FOR PERKINS PRIMA ENGINE
(OPERATING LINES TO PROMOTE TRAP REGENERATION ARE SHOWN FOR LOW, MEDIUM AND HIGH SPEEDS)
3.5 RESULTS

Results obtained using the model with the input data given previously are now presented.

Figure 3.8a shows how the inlet exhaust gas and particulate-ceramic wall interface solid temperature vary with time. For the first 62 seconds the solid temperature is cooler than the inlet gas temperature which is heating up the trap matrix and causing some oxidation of the particulate. Between 62 and 143 seconds the oxidation reaction liberates sufficient heat to cause the solid temperature to rise 75K above the inlet gas temperature. At 143 seconds the reaction begins to cease since the particulate has been largely consumed and the trap matrix subsequently cools down to the inlet gas temperature. Figure 3.8b shows how the total particulate mass within the trap varies with time during regeneration. Fresh particulate being trapped during regeneration is neglected.

Temperature variations across the composite slab are shown in Figure 3.8c. Clearly the hottest part of the ceramic wall occurs, as one would expect, adjacent to the particulate layer but the particulate layer itself reaches higher temperatures. The way in which the particulate layer oxidises during regeneration is shown in Figure 3.8d. The interior of the particulate layer reaches the highest temperatures and hence oxidises at a faster rate.

3.5.1 Effect of Oxygen Concentration and Particulate Mass

Previous investigators [37,90] have shown that the temperatures within the trap vary considerably with oxygen concentration and trapped particulate mass. Using the same inlet gas conditions as before these were varied. Figure 3.9a shows how the particulate-ceramic wall
FIGURE 3.8: MONOLITHIC WALL-FLOW TRAP DURING REGENERATION (INITIAL PARTICULATE LOADING 15g, 9% INLET OXYGEN)
FIGURE 3.9: EFFECT OF OXYGEN CONCENTRATION

FIGURE 3.10: EFFECT OF INITIAL PARTICULATE MASS (5% OXYGEN)
interface temperature varies with time for different inlet gas oxygen concentrations (% by mass); the initial particulate mass was kept constant at 40g. Clearly the high oxygen concentrations lead to high temperatures and fast regeneration times (see Figure 3.9b) but regeneration can still occur at low oxygen concentrations of 3%. In Figure 3.10 the oxygen concentration is fixed at 5% and the initial particulate mass varied between 10g and 40g. Here it can be seen that although the high mass loadings lead to higher temperatures the total regeneration time stays relatively constant. This is because the higher temperatures promote a faster oxidation rate but more particulate requires oxidising.

The results for the full variation of oxygen concentrations and initial particulate masses of 3-10% and 10-40g respectively are summarised in Figure 3.11. These emphasise that the oxygen concentration has the most significant effect on overall regeneration time and that both high oxygen concentration and high initial particulate mass loadings lead to high and perhaps dangerous trap temperatures. To avoid melting, it is best to regenerate at low to mid-range particulate mass loading. The results also demonstrate that theoretically with a low mass loading (10g) and low oxygen concentration (3%) the trap can be regenerated at the chosen exhaust gas inlet temperature.

3.5.2 Effect of Exhaust Gas Flow Rate
The exhaust gas flow rate was varied while maintaining the trap inlet temperatures as before (see the speeds used in Figure 3.7 indicated by 'Low' and 'High').
FIGURE 3.11: SUMMARY OF RESULTS (VARYING MASS AND OXYGEN CONCENTRATION)

As Wade et al., 1981 [85] point out and is demonstrated here (Figure 3.12a) low flow rates with high oxygen concentrations lead to high trap temperatures which will cause melting or cracking of the ceramic substrate. The regeneration times however are not significantly affected by the exhaust gas flow rate; the oxygen concentration is the controlling factor, see Figure 3.12b.

3.5.3 Comparison with Experimental Results
Higuchi et al., 1983 [37] provided useful experimental results with a monolithic wall-flow trap connected to a combustion chamber. They varied the oxygen concentration and measured the gas temperatures at the outlet faces of the ceramic walls and showed that the temperature
profiles vary depending on the cell position in the trap. The results from their study are shown together with the prediction from the model presented here in Figure 3.13.

![Graphs showing](image-url)

**FIGURE 3.12: EFFECT OF EXHAUST GAS FLOW RATE (ENGINE SPEED) (40g Initial Particulate Mass)**

The conditions used are given in Table 3.4 and the thermocouple locations are as shown in Figure 3.13. The maximum temperature lies along the axis of trap and hence the model developed here can give some indication of maximum temperature variation with time for
channels near the trap axis. It can be seen that the trends are followed in a reasonable manner. The peak temperatures obtained using the model are about 100K higher than those found experimentally probably due to the basic assumption of an insulated composite slab and one dimensional heat flow.

---

Ceramic Monolith:

Diameter, 4.65 inch
Cell structure:

Length, 6 inch
wall thickness 0.012 inch
cell density, 200 cells/inch²
wall porosity, 0.40-0.50
mean pore diameter, 15-30 μm

Inlet Gas Condition

Figure 3.8a
Final temperature 863K
Flow rate (at STP) 0.6 m³/min
Oxygen concentration 10%
Particulate Loading 14.4g

Figure 3.8b
Final temperature 853K
Flow rate (at STP) 0.6 m³/min
Oxygen concentration 3%
Particulate Loading 14.9g

---

TABLE 3.4: CONDITIONS USED BY HIGUCHI ET AL, 1983 [37]

Inlet and Outlet Gas Temperatures vs Time
(Comparison with NGK Data)

Inlet Gas Condition

Flow rate (at STP) 0.6 m³/min
Oxygen concentration 10%
Particulate Loading 14.4g

Outlet Gas Temperature vs Time
(Comparison with NGK Data)

---

FIGURE 3.13: COMPARISON WITH EXPERIMENTAL RESULTS OF HIGUCHI ET AL, 1983 [37]
3.6 COMPUTER PROCESSING TIME
The monolithic trap model proved to be numerically stable for a range of step sizes and the time step can be greater than 1 second and the number of spatial increments less than 20. To obtain a reasonable resolution for the computer generated graphs given in this thesis a time step of 1 second and 40 spatial increments were chosen. Using these, 300 modelled seconds took 3 minutes CPU time on a Honeywell Multics computer and 18 minutes on a standard IBM PC/XT with mathematics co-processor.

3.7 DISCUSSION
Regardless of a model's complexity or simplicity its merit depends upon its usefulness. This section discusses some of the model's strengths and weaknesses, and judges its usefulness.

The generalised equations have the advantage that they can be applied to different trap types, but the one-dimensional form of the heat and mass flow equations impose some restrictions on attempting to model the entire physical structure of the wall-flow monolith. The options of either an axial or radial coordinate system were examined earlier. However, a three-dimensional model of each channel extended throughout the whole trap would impose its own restrictions requiring a high computing power and extending the model's complexity might have limited return since there are uncertainties with the basic physical data used.

A major uncertainty with the physical data highlighted during the model's development was in describing the particulate oxidation rate. It was shown earlier that a wide range of empirical constants for the Arrhenius relationship have been used by different investigators and
it appears that measured values vary with engine type and operating condition as well as trap type. Clearly more work is required in either describing the oxidation with a more detailed phenomenological equation compared to the relatively crude Arrhenius equation or by conducting specific experiments for each engine trap system.

The results from the model presented here were consistent with the observed behaviour of actual systems and the modelled results of other investigators. The one-dimensionality restricted reproducing the axial and radial variations of trap temperature observed by Higuchi et al 1983 (see Figure 3.13) but the trend was reasonable which gives some confidence in the findings of the parametric study of variations in exhaust gas flow rate, oxygen concentration and particulate loading. The model development and results have provided insights into regeneration behaviour which are useful in the general sense and also in later chapters where the development of a new trap regeneration system is described.

3.8 RECENTLY PUBLISHED TRAP REGENERATION MODELS
Since the development and publication of the model described here some further work has recently been reported.

Bella et al, 1988 [11] presented a model describing the one-dimensional gas flow in an engine exhaust manifold and incorporated a zero-dimensional wall-flow particulate trap model to describe soot oxidation. The exhaust manifold model was used to compute the gas pressures and temperatures entering the trap and it enabled different manifold configurations to be analysed. The particulate trap model discretized the channel wall into five axial control volumes and the rate of heat gained by each control volume was equated to the heat
release rate due to particulate oxidation less the heat removed due to convection. Particulate and ceramic temperatures were assumed to be equal and the heat capacity of the particulate neglected. Bella et al did not explain how the gas velocity was computed within the trap and since the convective heat transfer coefficient they used was velocity dependent, this would be important.

Bella et al presented results of analysing trap position in the exhaust system and the effect of catalytic fuel additives on regeneration rates and temperatures. Since the physical data used in the model equations were absent, especially the chemical reaction rate term (whose form was not even defined) and no experimental validation was provided, it is doubtful whether too much credence should be placed on their results. However, the general concept of considering the engine, exhaust manifold, trap and silencer together is considered a novel and useful approach since they are interrelated.

In their development of a trap regeneration system employing an electrical resistance face heater, Barris and Rocklitz, 1989 [8] used a two-dimensional computation fluid dynamics (CFD) software package to model the fluid flow and temperature profiles within a wall-flow trap. The trap matrix was considered globally in the radial and axial directions. Although input data and model assumptions were not given, comparisons of measured axial temperature during regeneration were provided and shown to be in very good agreement, as shown in Figure 3.14.

Two-dimensional plots of temperature showed how a 'skewed' (uneven) regeneration pattern can occur if the upstream heating effect is uneven. It is of prime importance to minimise this effect to reduce
thermally induced stresses and improve the amount of particulate oxidised during regeneration (the 'regeneration efficiency'). This latter point will be returned to in later chapters. The work of Barris and Rocklitz, in the author's opinion, represents the best global description of regeneration to date and marks the way forward in trap modelling.

Pattas and Samaras, 1989 [68] presented a sub-model describing the transient operation of wall-flow monoliths which is worthy of mention. Pattas and Samaras were considering regeneration by exhaust gas throttling and had developed an overall model which calculates the engine thermal loading and exhaust gas characteristics from the drive-cycle and vehicle data. These characteristics were input into the transient trap model. Pattas and Samaras adopted a particulate mass loading model which considered the particulate laden inlet channel to
deplete by oxidation in the direction as shown in Figure 3.15 ($U_o$ is the inlet gas velocity, $W$ is the wall flow velocity):

This is a novel approach and it does have some validity especially for the very high mass loadings. The inlet and outlet channels separated by the ceramic wall were discretized in the axial direction and modelled in a two-dimensional manner, as shown in Figure 3.16 ($\dot{m}$ signifying gas mass flow rate and $\dot{Q}$ signifying heat flow rate).

FIGURE 3.15: SCHEMATIC OF TRAP LOADING MODEL OF PATTAS AND SAMARAS, 1989 [68]

FIGURE 3.16: TRAP MODEL GEOMETRY OF PATTAS AND SAMARAS, 1989 [68]
For each of the three control volumes (inlet channel, ceramic wall and outlet channel) heat and mass balance expressions were described, and the particulate oxidation rate was calculated in the usual manner. Temperature vs time profiles were shown to be in good agreement with experimental results. Pattas and Samaras also included predicted temperature profiles along the channel length - these showed some signs of an axially moving oxidation zone being evident. An interesting feature of their work was an analysis of trap transient operation during different vehicle drive-cycle scenarios; the ECE 15 drive-cycle, sudden vehicle braking, and an uphill-downhill situation. Each of these are of particular practical importance. The ECE 15 drive-cycle simulates city driving and the model showed relatively low clean trap wall temperatures of 200-300°C which were fairly uniform along the channel length, though too low for regeneration. On vehicle acceleration or high load cruise condition trap regeneration can commence. If the vehicle is braked then the trap experiences a reduction in the convective gas cooling effect due to low flow together with a high oxygen content. Driving uphill and then downhill also produces a similar effect and both situations can lead to trap failure.

Using their model Pattas and Samaras showed that theoretically very high trap wall temperatures can be experienced (> 1500°C) which would lead to melting. Therefore a by-pass pipe on their throttling trap regeneration system was provided to protect the trap by diverting the oxygen rich exhaust gas. Also one important result was that the wall temperatures can be of the order of 400°C greater than outlet gas temperatures and therefore monitoring this latter temperature is a poor indicator and should not be incorporated in a regeneration control system unless wide error margins are allowable. Bissett, 1984 [13] found the same, as stated previously.
Pattas and Samaras also conducted a parametric study of the effect of initial mass loading which gave results similar to those in the model described in this thesis.

3.9 CONCLUDING REMARKS

In this chapter several trap regeneration models have been reviewed. The presented model provides further insights into the regeneration behaviour of a wall-flow monolith characterised as gas flow through a composite layer of reactive particulate resting upon a non-reactive ceramic wall. A key result is that particulate mass be kept below the mid-loading level if high temperatures leading to trap melting are to be avoided.
4.1 INTRODUCTION

In Chapter 2 various trap regeneration systems were explored and it was suggested that an ideal system would be one in which the trapped particulate itself is directly and efficiently heated to a sufficiently high temperature for rapid oxidation to occur. To achieve this it was proposed that low-power microwave energy might be used.

In this and subsequent chapters the design and development of a microwave diesel particulate trap regeneration system is discussed in detail. Specifically in this Chapter the basic concept and initial experiments are discussed which led to the design and testing of the first prototype. The microwave technique is henceforth referred to as Microwave Assisted Regeneration or M.A.R. for short.

4.2 MICROWAVE ASSISTED REGENERATION (M.A.R.)

4.2.1 Microwave Heating

Non-ionising electromagnetic waves at frequencies typically 1000 to 300 000 MHz are called microwaves. The electromagnetic waves excite certain media through which they pass, causing them to heat up as their molecules oscillate. This effect is used in domestic microwave ovens and in industrial applications such as rubber curing and paper drying.

As will be apparent to anyone using a domestic microwave oven, only certain materials heat up due to the microwave action. Water in a glass beaker can boil when exposed to microwaves but the beaker itself
remains relatively cool and only warms up as a secondary effect of heat conduction from the hot water. Thus the beaker can usually be removed from the oven by hand. The reason for the preferential heating of certain materials is because different materials exhibit different dielectric properties. Water for example has a high dielectric loss-factor and therefore microwave energy is lost to the water molecules which rapidly oscillate and heat up. Glass conversely exhibits a very low dielectric loss-factor and the microwave energy passes through with almost zero attenuation and the heating effect is negligible. This is equally true for loaded ceramic diesel particulate traps where the particulate is selectively heated by microwave energy but the ceramic is not.

Dielectric loss is a complex phenomenon and the dielectric properties themselves usually depend on empirical determination. The dielectric behaviour depends on the electromagnetic excitation frequency and to attain efficient heating both of these require matching.

It is perhaps useful to explain further the heating mechanism itself. An electric field polarises the electrons, atoms and molecules within a dielectric. The polarisation of the electrons and atoms are not of importance here but molecular polarisation is. Certain groups of molecules are natural polar entities and are known as dipole molecules or polar molecules where the centres of gravity of the positive and negative charges do not coincide but are separated by a small distance. Entities of this kind are found where atoms are linked together through electron pairs and in this way their electron shell is stabilised. A water molecule $H_2O$ is an example.
When a dipole is exposed to an electromagnetic field a dipole moment is induced and there is a finite time in which dipoles react to this field and orient themselves accordingly. The time-lag is due to various properties of the medium, e.g. viscosity etc. The time in which dipoles reorient is known as the relaxation time, $T$. The term dielectric loss involves the total energy dissipated due to the effect of all the elastic distortions, deformation and displacements which occur under stimulation from the field and the restoration forces. The energy change (loss) due to absorption accounts for the heating effect. Maximum absorption occurs when the angular frequency of the excitation wave $\omega$ (rad/s) equals the reciprocal of the relaxation time, $T(s)$ and this is the resonant frequency of the dipoles in the material. Puschner, 1966 [73], discusses the behaviour of a dielectric in more detail.

The next section considers using this heating effect to assist the regeneration of diesel particulate traps.

4.2.2 Application to Diesel Particulate Trap Regeneration

The general principal proposed here is to introduce microwave energy into the metal trap casing to heat the trapped particulate. Since the trap is of a ceramic material the microwave energy can readily pass through but on encountering the particulate is absorbed and only the particulate is primarily heated ready for oxidation. It is this direct and selective heating which makes the system inherently energy efficient and therefore attractive.

When the particulate is at a sufficiently high temperature rapid oxidation occurs and the trap regenerates. This process is greatly enhanced since the oxidation is exothermic and therefore energy is
liberated by the particulate which helps to promote rapid heating and sustain the oxidation. A trap loaded with 40g of particulate contains some 1.3 MJoules of energy which is released on oxidation and can be put to useful effect in sustaining the reaction.

A simple experiment was conducted to establish whether or not diesel particulate does in fact heat up and oxidise when exposed to microwave energy and air. Diesel particulate was obtained from a diesel engine exhaust system and was essentially powdery and dry in nature. A thin layer of particulate was used so that it just covered the bottom of a 75 ml Pyrex beaker. The beaker was placed in a standard 650W (output) domestic microwave oven and the particulate almost instantaneously glowed an orange colour and after a few minutes completely oxidised leaving only very slight traces of metallic particles (presumably pieces of rust from the exhaust system).

This experiment was repeated on a later occasion with diesel particulate removed from a trap. The microwave source (the magnetron) took 2.44 seconds to energise but as the photographs in Figure 4.1 (taken from video pictures) show oxidation is rapid. It is thought that the polar compounds (see Figure 1.2) contained in the particulate are greatly excited by the microwave energy causing rapid heating and hence oxidation. In Chapter 7 this phenomenon is addressed further.

To establish whether the Cordierite ceramic absorbs microwave energy a clean wall-flow monolith was placed in the microwave oven. After 3 minutes of microwave exposure, the ceramic was not noticeably warm to the touch and this suggested that microwave energy (at 2450 MHz) passed through with negligible attenuation.
FIGURE 4.1: DIESEL PARTICULATE IN DOMESTIC MICROWAVE OVEN
(Photographs from Video Pictures) (continued overleaf)
FIGURE 4.1: (continued from previous page)
4.2.3 Feasibility Study

The above experiments demonstrating that microwave energy could be used to help regenerate diesel particulate traps raised the question as to whether the research emphasis should be broadened to explore this technique further. A feasibility study was therefore carried out (Garner, 1987 [26]), and the main conclusions were that an M.A.R. system was considered practical and commercially attractive from the power, size, shape, safety and cost aspects, and that further work would be worthwhile. Potential advantages and disadvantages of M.A.R. contained in the feasibility study were as follows:

a) Advantages:
   • No engine throttling required during regeneration
   • Efficient heating of the particulate itself
   • Provides heating only when particulate is present
   • No catalyst is required
   • Electrically controllable
   • Trap need not be close to engine
   • Few moving parts; maybe a cooling fan for the microwave source (magnetron)
   • Relatively cheap and freely available microwave components; trap itself uses standard components.

b) Disadvantages:
   • Safety aspects
   • Electrical supply and control system required
   • Load to vehicle's electrical system.

There are of course others and many of these will become evident later.
4.3 PRELIMINARY EXPERIMENTS

The advantages of M.A.R. were clearly evident and therefore a prototype was developed. Firstly, some experiments were conducted to help with its design.

4.3.1 Initial Experiments

A ceramic wall-flow monolith of construction given in Table 4.1 was loaded with 45g of particulate from a 2 litre DI diesel engine. The trap casing was of split construction and bolted together enabling the monolith to be removed (see Figure 4.2).

<table>
<thead>
<tr>
<th>Uncatalysed</th>
<th>Length, 6.00 inch</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter, 5.6 inch</td>
<td>wall thickness 0.012 inch</td>
</tr>
<tr>
<td>Cell structure:</td>
<td>wall density 200 cells/in²</td>
</tr>
<tr>
<td></td>
<td>wall porosity 0.49</td>
</tr>
<tr>
<td></td>
<td>mean pore diameter 16.5 μm</td>
</tr>
</tbody>
</table>

The monolith loaded with 44.8g of particulate was placed inside a microwave oven of a nominal output power of 650W. Starting from 20°C the monolith periphery reached about 120°C in 10 minutes and at 25 minutes the central core of the monolith outlet channels could be seen to glow bright orange - the outer 16 mm peripheral region of the 143 mm diameter being below radiant temperature. (A photograph of a similarly loaded monolith exposed to microwave energy in an oven on another occasion is shown in Figure 4.3). At 66 minutes the microwave
FIGURE 4.2: EXPERIMENTAL TRAP CASING DESIGNED FOR EASY REMOVAL OF MONOLITH
oven was switched off and the monolith was allowed to cool in ambient air. Reweighing the monolith revealed that 86% of the particulate had been oxidised (thus the regeneration efficiency was 86%).

This experiment confirmed the idea of microwave energy penetrating the 'transparent' ceramic and preferentially heating the particulate causing it to oxidise. On an engine the initial temperature of the trap would be in the region of 200-300°C and although free oxygen in the exhaust would be typically reduced to less than 10%, the oxygen feed-rate would be higher since it is forced through the monolith by the exhaust pressure. Both of these factors would lead to much more rapid heating and oxidation than found in the above experiment.
4.3.2 Loaded Monolith Inside Metal Casing

It was important to establish whether microwaves could be successfully introduced into the relatively small cavity of the trap casing. This is because cavity dimensions of about one quarter the microwave wavelength are approximately the cut-off point where wave propagation is not possible. Here the wavelength is 12.2 cm which is of a similar order to the trap diameter of 15 cm (6 inch).

A special semi-circular shell top was made out of copper sheet and this was clamped onto one half of the steel separable trap casing (Figure 4.2) thereby securing the monolith, see Figure 4.4. An aperture in the copper top was made to be the same size as the output of the waveguide in the microwave oven. Thus microwave energy could be introduced into the side of the loaded monolith.

The whole unit was placed inside the domestic microwave oven. After 5 minutes the top region of the monolith below the aperture could be seen glowing orange even up to the edges of the monolith by looking axially along the outlet channels. This hot region travelled downwards as the particulate above it was consumed by oxidation as depicted in Figure 4.5. This was an extremely important result and the following conclusions could be drawn:

a) The microwave energy could be introduced into the relatively small trap cavity.

b) The particulate was effectively absorbing all the microwave energy and attenuating it so that little energy was passing through it.
FIGURE 4.4: SEMI-CIRCULAR COPPER SHELL WITH APERTURE TO INTRODUCE MICROWAVE ENERGY INTO METAL MONOLITH CASING

FIGURE 4.5: PROPAGATION OF OXIDATION ZONE THROUGH MONOLITH
c) Since the hot region migrated downwards as the top particulate was oxidised, the ceramic was causing little microwave attenuation i.e. it absorbed very little energy.

d) This migrating effect could be used more effectively if the microwaves were introduced in the upstream end of the monolith. The exhaust gas would then help the hot zone propagate downstream oxidising the rest of the particulate. This is more efficient and is also easier to design in real traps since the side aperture described above would cause mechanical sealing problems with the Interam(R) (3M Company) mat which secures the monolith in the metal casing.

4.3.3 Axial Heating of Monolith

Initially a stainless steel trap containing a loaded monolith was placed in a second domestic microwave oven with the 60 mm diameter inlet pipe aligned with the outlet of the waveguide. Power fluctuations (measured with a Watt meter) from the magnetron (i.e. the microwave producer) indicated that power was reflecting back to the magnetron and little energy was propagating into the pipe. This was not surprising since the pipe diameter approaches the cut-off wavelength below which wave propagation is not possible. This was a useful result since it demonstrated that an exhaust pipe diameter of 60 mm was sufficient to significantly attenuate stray microwaves trying to leave the trap casing along the exhaust pipe.

Without the end-cones (Figure 4.2), the loaded monolith was successfully heated at one end. To investigate the axial heating more thoroughly a brass rectangular cone was fabricated to fit axially onto the steel trap casing. The small inlet end was of the same dimensions
as the waveguide and the large end was a square of diagonal length equal to the trap diameter (see Figure 4.6). Again, heating and oxidation was successful and it was observed that more uniform and spread-out heating on the filter matrix occurred.

![FIGURE 4.6: RECTANGULAR END CONE FOR AXIAL HEATING](image)

4.3.4 Use of Forced Convection
Once the particulate is sufficiently hot it should be possible to pass air through the ceramic monolith and cause very rapid oxidation of the particulate. To demonstrate this, once the ceramic and particulate was glowing an orange colour, warm air of approximately 60°C was passed through the trap. The monolith glowed very bright orange indicating rapid oxidation. The oxidation was not extinguished by the forced convection but enhanced.
4.4 DESIGN OF M.A.R. PROTOTYPE

The previous preliminary experiments pointed the way forward towards a prototype M.A.R. system. Here the general principle of operation of the system is given followed by a description of the actual prototype design.

4.4.1 Principle of Operation

Figure 4.7 shows schematically the basic design concept and the method of operation is as follows. Exhaust gas laden with particulate passes through the ceramic monolith, and particulate is trapped and accumulates inside the inlet channels. When the trapped mass reaches a predetermined level measured by the effective pressure drop across the trap the regeneration process may begin.

![Schematic of M.A.R. System](image)

**FIGURE 4.7: SCHEMATIC OF M.A.R. SYSTEM**
The by-pass valve is opened allowing the majority of the exhaust gas to flow around the trap. The microwave system is switched on causing the trapped particulate to be energised resulting in a hot zone at the inlet end of the trap (see Figure 4.8). As the temperature rises the oxidation rate increases. Note that only one valve is used here. Other systems often use a second valve to stop any flow entering the trap during preheating. Here however, the availability of some exhaust gas containing free oxygen is a distinct advantage since oxygen is available to initiate oxidation and thereby the exothermic reaction liberates its own energy to help considerably with rapid heating. The particulate can draw in oxygen from the upstream exhaust gas as the oxidation process consumes it.

The microwave energy therefore initiates particulate heating and the exothermic reaction enhances this. Once the particulate is preheated sufficiently, the by-pass may be closed and at this stage the microwave source may be either switched off, continued or pulsed. The incoming exhaust gas now provides a much higher oxygen feed rate to promote rapid oxidation. A high temperature reaction zone then sweeps downstream as particulate is progressively consumed in the exhaust gas flow and the whole monolith is regenerated (see Figure 4.9).

The timing of this process depends on a number of factors including flow rate, oxygen concentration and particulate mass loading as was shown in Chapter 3. Thermal transients during rapid oxidation may be controlled either by regenerating at low to medium particulate mass loadings or by modulating the by-pass opening.
FIGURE 4.8: PREHEATING

FIGURE 4.9: REGENERATION
4.4.2 Actual Prototype Design

The above conceptual design was embodied in the prototype shown in Figure 4.10 and this section describes the design in more detail.

a) Monolith Casing:

The monolith casing consisted of separable stainless steel parts enabling the monolith to be removed for experimental purposes (see Figure 4.10). Under normal circumstances a standard lightweight stainless steel trap casing suitably seam-welded with the monolith inside could be used.
The type of stainless steel was chosen for its electrical and mechanical characteristics. Microwaves reflect better from non-magnetic metals than magnetic ones, and high electrical conductivity enables very low $I^2R$ heating losses in the walls [7]. Copper, brass, aluminium and stainless steel are suitable for this, but stainless steel has the highest temperature stability and was therefore chosen. The actual type of stainless steel chosen was virtually non-magnetic, had fairly high electrical conductivity and was readily available. (The electrical conductivity, however, was low enough to provide some no-load protection to the magnetron).

The two semi-circular casing halves hold the monolith with an Interam(R) sealing mat [33], which is standard practice. The inlet cone which is attached to the main body has a rectangular waveguide of suitable length inserted and welded into the side of the cone at 45°. This angle is fairly arbitrary but in this particular situation was the easiest to accommodate in the trap casing.

The two end cones and the two semi-circular casing halves are all bolted together to enable the monolith to be removed for experimental purposes, and sealed by a standard asbestos-based gasket material used for engine auxiliaries. This material is arbitrary but was shown to absorb microwave energy by placing it in a microwave oven and checking that it warmed up and therefore would absorb any slight microwave leakage from the joints. (Note again that the casing here is of bolted construction to enable the monolith to be removed for experimental purposes. A normal M.A.R. system would use a standard seam-welded trap casing allowing zero microwave leakage).
b) Waveguide Design:

The waveguide shape was chosen to be the classic rectangular cross-section with the magnetron anode protruding into the side through a suitable hole. The waveguide dimensions were chosen to be the optimum for the standard domestic/industrial frequency of 2450 MHz (see Appendix 1). This frequency is internationally recognised for microwave heating and the corresponding wavelength (12.2 cm) results in ideally sized waveguides and cavity dimensions for trap use (see Appendix 1). In addition its widespread use has meant magnetrons are very cheap and easily obtainable.

The waveguide material was the same type of stainless steel as used for the trap casing and end cones and chosen for the same reasons.

Since the waveguide is hollow and open ended, a seal must be provided somewhere along its length to allow microwaves to pass through with negligible attenuation but not allow exhaust gases and particulate to reach the magnetron anode. The seal material must have these characteristics up to the expected maximum operating temperature of 700°C.

For the prototype a proprietary glass material with a low microwave loss-factor and a high working temperature (950°C) was chosen. The glass was also fairly cheap and machineable. Some details of the glass are given in Appendix 3, together with some experimental results on its performance.

Mounted on the waveguide and onto the magnetron housing was a cooling fan. Since magnetrons are nominally 55% to 75% efficient [7], cooling is usually necessary to remove the heat generated at the anode.
c) Trap Inlet and Outlet Shields
For test purposes it was useful to see inside the trap and also allow
gas to pass through it. To achieve this without allowing any microwave
leakage, perforated metal discs mounted in aluminium rings were bolted
to the inlet and outlet flanges. Zero microwave leakage occurred. On
an engine, these are not necessary.

d) Power Supply
To accelerate the prototype build-time a standard domestic microwave
oven was 'cannibalized'. The high voltage supply and low voltage key-
pad and controller were separated for ease of construction (see Figure
4.10) and for test purposes a normal single phase mains supply was
used. Obviously on a vehicle a different 'front-end' to the power
supply is necessary and this is discussed later, however the total
input power requirement is within the capability of a normal vehicle's
electrical system (see Appendix 2) at 1 kW.

4.5 INITIAL PROTOTYPE EXPERIMENTS
4.5.1 First Test
For the first test of the system, instead of a particulate-laden
monolith inside the casing, a 465g potato with a thermocouple inserted
inside it was used as the 'dummy' load.

The potato heated up from 18.8°C to 60°C in 3 minutes. The input power
to the whole unit was stable at 1 kW (measured with a Watt meter).
Therefore, very approximately (assuming the potato had a specific heat
capacity similar to water) the system had an overall heating
efficiency of 45% which is very good considering the magnetron is
nominaly 55% to 75% efficient and the potato cannot be considered as
a well matched load in the microwave circuit.
Very little leakage from the trap joints was measured - the maximum value being 2 mW/cm$^2$. (Note again that a seam-welded unit would emit zero microwave energy). The limit for a domestic microwave oven is 5 mW/cm$^2$, and 10 mW/cm$^2$ is the usual accepted maximum where no injuries have ever been reported [18].

4.5.2 Test with Loaded Monolith

A test using a monolith, loaded with 45.6g of particulate, was carried out.

A thermocouple embedded 20 mm from the inlet face inside an inlet channel full of particulate indicated a rapid temperature rise to 900°C from 20.6°C in 1 minute. After the particulate surrounding the thermocouple tip was largely oxidised, temperatures of 700-810°C were maintained for 58.5 minutes. A thermocouple mounted at the outlet end of the monolith rose from 421 to 696°C during the last 30 minutes indicating that the hot oxidising zone was propagating along the monolith as predicted. During this time no forced convection was used and therefore no rapid oxidation was promoted. Although it was not clear at this stage to what extent the presence of thermocouples perturbed the localised temperatures in the monolith (see later however) during this experiment a fairly uniform radiant orange glow from the outlet channels of the monolith was clearly seen.

This experiment was repeated with another loaded monolith and a temperature rise from 20°C to 250°C was achieved in 3 seconds and temperatures later reached 950°C.
4.5.3 Forced Convection

The same monolith as above was used (though with some of the particulate oxidised) and a warm flow of air at 85°C was blown through the trap. The particulate at the inlet end reached 165°C in 90 seconds and levelled off. Switching off the flow enabled the temperature to rise to 500°C in 4 minutes. This confirmed that a by-pass pipe (usual on most external energy source trap regeneration systems) would be required.

With the temperature at 750°C the air flow was again switched on and the whole of the monolith outlet channels could be seen to radiate a bright white-orange, indicating very rapid oxidation. The outlet channels reached 950°C during this forced-convection period. It was found the forced-convection stimulated rapid oxidation as long as the particulate remained above 600°C. Below 500°C the relatively cool 85°C incoming air cooled the trap and extinguished the rapid oxidation.

4.6 MORE DETAILED EXPERIMENTS

4.6.1 Bench Test Regenerations

A set of bench test regenerations were conducted before fitting the prototype to an engine. The downstream conical flanged end of the trap casing was removed and a large mesh screen fitted enabling all the monolith outlet channels to be viewed without the microwave energy escaping from the trap cavity. It was found that thermocouples embedded into the particulate in fact acted as 'aerials' focusing the microwave energy and causing high localised heating shown as radiant hot spots and hence they were not used in subsequent tests.
The trap was fitted to a warm air pump which could deliver air at a flow rate of 1112 litres/min at 85°C. This represents an oxygen feed-rate equivalent to that of a 2 litre engine operating at 2250 rpm and 10% exhaust oxygen. The trap was loaded with 44.8g of particulate and with the by-pass open the microwave system was switched on. The initial temperature was 20°C (much lower than that likely in engine operation). The overall microwave system power consumption was 1 kW during a 400 second preheating period at which point the by-pass was closed encouraging forced convection and rapid particulate oxidation. Figure 4.11 shows a sequence of photographs (taken from video pictures) of the monolith outlet channels during regeneration. The bright areas indicate where the particulate contained in the inlet channels is oxidising. The ceramic channel walls are heated by conduction from the hot particulate. Figure 4.11a indicates that the top upstream zone of the monolith is initially regenerated, because this region was nearest the exit of the waveguide. Forced convection caused the hot zone to propagate through the monolith as shown in Figures 4.11a to 4.11j. At 1400 seconds the oxidation ceased and reweighing the monolith revealed that 83% of the particulate had oxidised and no damage to the ceramic was observed.

4.6.2 M.A.R. Prototype on Engine

The prototype was then fitted to a 2 litre DI engine and the trap loaded with 37.1g of particulate. With the engine condition given in Table 4.2 the by-pass valve was opened and microwave preheating initiated. A preheating period of 400 seconds was estimated to be sufficient and at this point the by-pass valve was closed to promote rapid oxidation and the microwave switched off. The trap inlet and outlet gas temperatures are plotted against time in Figure 4.12.
FIGURE 4.11: PHOTOGRAPHS FROM VIDEO PICTURES OF MONOLITH OUTLET END DURING REGENERATION IN M.A.R. SYSTEM
TABLE 4.2: ENGINE OPERATING CONDITIONS DURING REGENERATION

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speed</td>
<td>1508 rpm</td>
</tr>
<tr>
<td>Load (BMEP)</td>
<td>288 kPa</td>
</tr>
<tr>
<td>Flow rate</td>
<td>1230 (N) litres/min</td>
</tr>
<tr>
<td>Exhaust temperature</td>
<td>129-195°C</td>
</tr>
<tr>
<td>Exhaust oxygen content</td>
<td>14% by volume</td>
</tr>
</tbody>
</table>

Inlet and Outlet Gas Temperatures vs Time

FIGURE 4.12: TRAP INLET AND OUTLET GAS TEMPERATURES DURING REGENERATION AFTER THE 400 SECOND MICROWAVE PREHEATING PERIOD
These clearly demonstrate that rapid oxidation was taking place since the outlet temperature rose above the inlet temperature. On removal the monolith was undamaged and 39% of the particulate had been oxidised. The low regeneration efficiency is due to uneven heating of the upstream face of the monolith. This led to some channels being completely regenerated whilst others remained largely unaffected as shown schematically in Figure 4.13.

![Figure 4.13: Schematic of partial regeneration due to uneven heating of inlet end](image)

4.7 CLOSURE

In this chapter the concept of Microwave Assisted Regeneration has been presented, together with its advantages and disadvantages. Preliminary experiments demonstrated its practicability and these led to the building of a prototype, the design of which was described.

The prototype performed well both on bench and engine, consuming only 1 kW of power during a 400 sec particulate preheating time. The bench regenerations were photographed showing that the microwave heating effect is not uniformly spread across the trap inlet face and this resulted in low regeneration efficiencies.
To improve trap regeneration efficiencies, a more even heating is necessary. A modified prototype seeking to improve the heating uniformity is the first subject of the next chapter.
CHAPTER 5

5.1 INTRODUCTION

The M.A.R. prototype required some development to improve the heating symmetry and uniformity of the trapped particulate in the upstream end of the monolith. This Chapter describes the modified prototype design seeking to achieve this, and its subsequent testing. The prototype design and construction was more light-weight than previously since it was intended to fit into a vehicle. The vehicle installation and preliminary testing are also described in this Chapter, together with further bench experiments with the modified prototype.

5.2 MODIFIED PROTOTYPE

The original prototype M.A.R. system performed well but as Figure 4.11 shows the initial heating zone was at the top inlet end of the monolith. Although the electromagnetic field distribution within the cylindrical cavity contributes to this effect [56] it was thought that more even and symmetric heating could be achieved if the microwave energy was introduced axially and the exhaust gas off-axis. The prototype design was modified to incorporate an axial waveguide to demonstrate this and is shown in Figure 5.1.

The design was more light-weight than previously and closer to an envisaged commercial system. The waveguide glass seal is located very near the trap inlet (see thick rectangular flanges, Figure 5.1). This is to stop convective heating from the hot turbulent exhaust gases entering any part of the waveguide. In the original prototype the glass seal was located at the waveguide midpoint. The waveguide itself also has external fins to help it and the magnetron stay cool.
The inlet end of the modified trap could also be used with the original prototype bolted casing which enabled the oxidation process to be photographed and also monolith removal.

5.2.1 Bench Tests

Figure 5.2 shows a sequence of photographs taken during trap regeneration on a test bench as outlined earlier in Chapter 4. The flow conditions were the same as those bench tests and the initial trap loading was 45.8g of particulate. Clearly the initial reaction zone is more central than in the original prototype experiments and although this zone essentially propagated downstream it also spread radially to the peripheral regions of the monolith.
FIGURE 5.2: PHOTOGRAPHS FROM VIDEO PICTURES OF MONOLITH OUTLET END DURING REGENERATION (MODIFIED PROTOTYPE)
During this test a thermal scanning camera was used to measure local temperatures of the monolith outlet channels during regeneration. Although the particulate laden inlet channel surfaces are at a higher temperature because of the oxidation process, the temperatures measured give an indication of thermal gradients and hence radial thermal stresses in the monolith. The temperatures measured ranged from 550 to 595°C with a mean of 577°C and these imply that very high stresses are unlikely.

Removing the monolith revealed that it was undamaged and that 60% of the particulate had been oxidised.

5.2.2 Engine Tests
The modified prototype loaded with 50.0g of particulate was fitted to the 2 litre D.I. engine. The engine was operated at the condition shown in Table 5.1 and after opening the by-pass valve, a 500 second microwave preheating period was initiated.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Speed</td>
<td>1481 rpm</td>
</tr>
<tr>
<td>Load (BMEP)</td>
<td>234 kPa</td>
</tr>
<tr>
<td>Flow rate</td>
<td>1207 (N) litres/min</td>
</tr>
<tr>
<td>Exhaust temperature</td>
<td>50-140°C</td>
</tr>
<tr>
<td>Exhaust oxygen content</td>
<td>14.5% by volume</td>
</tr>
</tbody>
</table>

TABLE 5.1: ENGINE OPERATING CONDITIONS DURING REGENERATION (MODIFIED PROTOTYPE)

After this period the microwave system was switched off and the by-pass valve closed. The resulting exhaust gas temperatures entering and exiting the trap are shown in Figure 5.3. Clearly the temperature
excursion (often termed 'exotherm') indicates rapid oxidation of the particulate. On removal, the monolith was undamaged and 43% of the particulate had been oxidised. Again this is a fairly low regeneration efficiency due to some channels being fully regenerated but others are unaffected because of the uneven heating of the particulate in the upstream end of the trap. Other regeneration systems have also exhibited this situation during their early development (the electrical resistance system described by Barris and Rocklitz, 1989 [8] for example).

Further ideas to improve the heating field are discussed later in this Chapter, but first the vehicle installation is described.
5.3 VEHICLE INSTALLATION

The modified prototype was developed with the intention of fitting it to a vehicle. This was to establish the practicality of a vehicle system and to reveal any unforeseen difficulties and problems requiring solving.

5.3.1 The Vehicle

The vehicle used was a 2.5 litre direct injection diesel engined (1986 specification) short wheelbase Ford Transit minibus as shown in Figure 5.4. This engine was ideal for the trap sizes being investigated. Also, Ford the manufacturers, were keen to investigate particulate control equipment for this size of engine in view of the strict Swiss diesel engine emission standards to be implemented in 1991 which are as strict as the imminent US regulations.

5.3.2 The Installation

The M.A.R. unit was fitted into the engine bay as shown in Figure 5.5. (The waveguide and magnetron can be seen in the engine bay just next to the radiator). No structural modifications were necessary although obviously the exhaust pipe required some changes to incorporate the trap and provide a by-pass. The front and rear silencer boxes were left as standard. In the design of a production system however one box could have been omitted since as Barris and Rocklitz, 1989 [8] show, the monolith acts as a very effective silencer. Figure 5.6 shows the M.A.R. unit in the engine bay. Beneath the exhaust manifold a standard turbocharger wastegate valve was used to allow the gas flow to by-pass the trap during preheating. This valve was air-operated (at 0.8 bar gauge pressure) but a 12V solenoid operated valve could have equally been utilised and this would have negated the need for a small on-board compressed air cylinder.

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The controller key pad to operate the magnetron was situated next to the driver’s seat as shown in Figure 5.7. The power supply shown in Figure 4.10 (Chapter 4) was mounted under the seat. Although an inverter powered from the vehicle’s battery providing the crude 3 kV DC for the magnetron was one power supply option (as has been used in luxury coaches to power microwave ovens for cooking food) it was
FIGURE 5.5: M.A.R. MODIFIED PROTOTYPE INSTALLED IN FORD TRANSIT (FRONT GRILLE REMOVED)
FIGURE 5.6: M.A.R. (MODIFIED PROTOTYPE) IN ENGINE BAY ON NEAR SIDE

FIGURE 5.7: M.A.R. CONTROLLER KEY PAD NEXT TO DRIVER'S SEAT
decided to keep the original 240V AC (input) system, and concentrate development on the M.A.R. unit itself. Having decided this, three ways of providing 240V AC on-board were explored:

i) 12V DC to 240V AC inverter;
ii) special engine alternator to deliver 12V DC and 240V AC; or
iii) 240V AC petrol generator.

The first option was attractive since it did not require the engine to be running at all times. However, on trying a suitable proprietary system the trapezoidal AC waveform output, although of 240V rms, gave a peak-to-peak voltage about 50V too low for the existing power supply. The inverter could have been easily modified but the manufacturers required some lead time to do this.

The second (very attractive) option (ii) was to use a special alternator. A proprietary alternator system comprising a standard automotive alternator casing incorporating an extra winding is available. The output can be either 12V DC or 240V AC by just operating a switch. The makers have sold these for use on yachts to power microwave ovens for cooking food. One drawback is that they need to rotate with an engine speed of 1600 rpm to provide the full 240V AC and since idle speed is 800 rpm a doubling of drive pulley size would be required. In our particular application the alternator installed in the vehicle also had the servo-brake vacuum pump attached to its rear (since there is negligible inlet depression in a diesel engine) and the special alternator manufacturers had no direct exchange unit of this type. Longer term this would not be a problem.
It was finally decided, for rapidity, to install a small 240V AC petrol generator in the rear of the minibus; it had its own exhaust pipe routed out of the vehicle. A 2 kW unit was chosen which was ample and could also power some of the on-board instrumentation.

The trap was instrumented with inlet and outlet thermocouples and pressure tappings. The temperatures and pressures could be read from inside the vehicle whilst in motion.

5.3.3 Vehicle Tests

These began by driving the vehicle to load up the trap with particulate. During this period (115 miles), the installation was checked out. There were no problems: the wastegate (by-pass valve), exhaust piping, trap installation and microwave system etc all worked as they should.

The first on-vehicle regeneration was carried out with the vehicle stationary and the engine at idle with a trap inlet gas temperature of 100°C. The wastegate valve was opened and a 500 second microwave preheat time initiated. After preheating, the wastegate valve was closed and the trap outlet gas temperature rose to a maximum of 232°C before falling again. This temperature excursion demonstrated that preheating had occurred and the trap pressure drop at idle fell from 9.0 cm of mercury to 8.1 cm. This indicated that some particulate had been oxidised. A clean pressure drop at idle should have been less than 1 cm of mercury and this indicated that although some particulate had been oxidised it was very little. It appeared that the problem was due to some low temperature exhaust gas entering the trap during microwave heating limiting this heating effect significantly. Although oxygen availability helps the rapid heating as previously discussed, the convective cooling of this flow was thought to be too high. The
wastegate (by-pass) valve was causing a resistance to exhaust gas flow forcing some of the flow to enter the trap. A valve of finite size always provides some resistance hence it would be a requirement on a future installation to provide a second valve at the trap inlet to stop cooling flow entering during preheating. Ambient atmospheric air could be made available to help promote rapid heating.

In an attempt to overcome this problem the microwave preheating was initiated with the vehicle engine switched off. The engine was started up after the preheat period and idled. The trap inlet temperature was 100°C and the outlet gas temperature rose from 87°C to 120°C and then rose very rapidly to 924°C before falling back to below 100°C. During the phase from 120°C to 924°C the engine speed was increased to about 1500 rpm. The trap back pressure fell from 52 cm mercury to 21 cm (at maximum engine speed).

The high outlet gas temperatures (924°C) indicate very high interior monolith temperatures. Pattas and Samaras, 1989 [68] as mentioned in Chapter 3 conclude that outlet temperature is a very poor indicator of trap temperature and the difference is typically some 400°C. Thus the reduction in pressure drop was either due to the monolith melting or regenerating. The only non-destructive way to check this was to drive the vehicle to try and reload the trap with particulate. No increase in trap back pressure was observed and hence melting or severe cracking was strongly suspected. The vehicle was driven a further 700 miles (approximately) in poor conditions (snow, sleet, heavy rain etc) but the M.A.R. system was unaffected and still functioned well.
The trap was removed and cut open. On extracting the monolith the outlet end was accidentally damaged, but there had already been substantial melting of the channels as shown in Figure 5.8. The monolith was then axially sawn in half and Figure 5.9 clearly shows significant melting of the interior channels - mostly at the downstream end. This is in accordance with other investigators findings [37] and is due to a cumulative rise in gas temperature as it flows through the reactive particulate. The black sooty deposits are due to particulate being deposited in the monolith after the catastrophic regeneration failure.
FIGURE 5.9: MONOLITH AXIALLY SAWN IN HALF SHOWING MELTED CHANNELS AT OUTLET END (RIGHT HAND SIDE). OUTLET END WAS DAMAGED CAUSING CERAMIC TO CRUMBLE AWAY ON REMOVAL FROM STEEL TRAP CASING
5.3.4 Important Conclusions from Vehicle Tests

The vehicle tests revealed a very significant amount of useful information. Firstly, it clearly demonstrated the practicality of fitting an M.A.R. unit to a real vehicle. The installation itself was completely reliable and this augurs well for longer term durability of the magnetron etc. Secondly, it showed how difficult it is to ascertain the trap condition before, during or after regeneration. It is almost certain that the catastrophic failure occurred due to the trap being too heavily loaded with particulate, and poor control of gas flow rate. Chapter 3 showed how high mass loadings lead to very high temperatures. Measurement of trap particulate loading has been a major problem encountered by many investigators and its solution often ignored. Pressure drop has been used by several investigators (e.g. MacDonald and Simon, 1988 [54]) but it is not directly a good measure since it relies on exhaust gas flow rate. Therefore engine speed needs to be measured in addition to the pressure drop and some further calculation (by a microprocessor) is required. M.A.R. has an inherent feature which can be used to assess trap loading regardless of engine speed.

The energy absorbed by the particulate is directly proportional to its mass and hence if the microwave field is measured downstream of the monolith (using a cheap voltage standing wave ratio (VSWR) coil) the mass can be assessed. Thus in a vehicle M.A.R. system the magnetron could be energised every, say, 10 minutes (at perhaps a very low power) and the mass measured. Once the mass reaches a certain level a full regeneration can be initiated. This technique has not yet been developed by the author but will be in the future. Both the M.A.R. Patent Application [94] and Garner, 1988 [27] describe this idea in more detail together with a range of other novel ideas related to M.A.R., some of which are discussed later in this thesis.
Poor control of gas flow rate is also a problem encountered by nearly all trap investigators. Control of the flow during the rapid oxidation phase can be accomplished by blowing ambient air through the trap with a suitable fan. Both flow rates and oxygen concentration can therefore be controlled. Barris and Rocklitz, 1989 [8] adopted this approach, as have others, since engine exhaust gas flow and oxygen content are far from predictable. Figure 5.10 shows how the M.A.R. system should be redesigned. The operation procedure is as follows:

<table>
<thead>
<tr>
<th>Normal Operation</th>
<th>Valve A</th>
<th>Valve B</th>
<th>Valve C</th>
<th>Action/Result</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Closed</td>
<td>Open</td>
<td>Closed</td>
<td>Monolith traps particulate</td>
</tr>
<tr>
<td>Preheating</td>
<td>Open</td>
<td>Closed</td>
<td>Closed</td>
<td>Microwave preheats particulate</td>
</tr>
<tr>
<td>Regeneration</td>
<td>Open</td>
<td>Closed</td>
<td>Open</td>
<td>With air fan on, rapid oxidation occurs</td>
</tr>
</tbody>
</table>

![Diagram of M.A.R. System](image)

**FIGURE 5.10: REDESIGN OF M.A.R. SYSTEM**
In reality valves A and B could be rationalised into one special valve. This redesigned system (with other internal modifications) is described in Chapter 6.

5.4 IMPROVING THE MICROWAVE HEATING FIELD

It became clear that the regeneration process must be carefully controlled if it is to be successful. This is dealt with in the next Chapter, but here the important task of providing an even heating of the particulate in the inlet end of the trap is looked at further.

The monolithic wall-flow trap despite its favourable attributes (such as excellent filtration efficiency and high melting temperature) has a deficiency which the author was aware of and Mizrah et al, 1989 [58] recently underlined. Since the inlet channels containing the particulate are separated from each other (a bit like the black squares on a chess board, see Figure 1.9) and that the ceramic is a poor heat conductor, the oxidation zone propagates fairly well axially, but very poorly radially. Thus if the inlet end is not uniformly heated only parts of the trap will be regenerated (as described in Chapter 4) and thermal gradients might be high. This 'channelling' effect is further accentuated since regenerated channels provide a low resistance route for the gas and therefore unregenerated regions of the trap do not receive enough oxygen. As far as the author is aware, to date all other reported regeneration systems using a wall-flow monolith have experienced this to varying degrees. Several ideas to promote even heating were therefore explored.
5.4.1 Assessment of the Electromagnetic Field

Up to now, the electromagnetic field pattern in the trap cavity has been assessed by observing radiation from the monolith outlet channels during regeneration. This is a very instructive method but has the disadvantage that it generally takes two days to mount, load and demount a test monolith. Thus testing various field shaping techniques would take a long time. Probes to measure the electromagnetic field are available but the whole cavity would require traversing and the pattern subsequently plotted. Again this would take time.

It was found that neon bulbs light up if placed in a microwave oven. This is due to the electromagnetic field establishing a voltage gradient across the electrodes and the neon gas is electrically excited and illuminates. In a microwave oven one can observe the neon bulbs turning on and off as the turntable moves them from nodes and antinodes in the microwave field.

One hundred and fifty seven 16 mm long x 6 mm diameter neon bulbs with their 'legs' removed were stuck on to a perspex disc of 150 mm diameter. This disc was placed in the trap cavity and the magnetron switched on. A typical result is shown in Figure 5.11. Clearly there are zones of high and low intensity. This assessment of the field pattern although only qualitative, takes only seconds to carry out.

This technique in representing the actual field pattern during heating of a particulate loaded monolith is given some validity if one observes the actual pattern of the oxidation (and melting) of the monolith removed from the vehicle. Before it was cut in half the monolith was seen to have the same shape as found with the neon bulbs,
see Figure 5.8. Using this technique a rapid assessment of the field could be made.

FIGURE 5.11: NEON BULBS ILLUMINATING INSIDE M.A.R CAVITY AND SHOWING MICROWAVE HEATING FIELD PATTERN

5.4.2 Waveguide Lens

From Figure 5.11 it can be seen that the left and right edges of the field are not very energetic and poor heating results. This type of mode pattern is common in a cylindrical cavity (i.e. the $TM_{11n}$ mode) as described by Metaxas and Meredith, 1984 [56].
Since at the waveguide exit a piece of special glass is mounted to stop magnetron damage, it was thought that maybe this glass could be shaped as a divergent lens to spread the microwave beam out. Microwave 'lenses' are usually parallel metal plates [19] but it was reasoned that if light can refract through glass, so should the electromagnetic microwaves. Appendix 4 provides some theoretical basis for this.

A fairly crude diverging lens shape was machined into a test glass waveguide seal. The neon bulb matrix disc was placed inside the cavity and a series of photographs of the energised neons were taken at different axial distances from the waveguide exit. Photographs of two such positions are shown in Figure 5.12. Even though the lens was crude and results would probably be better with an improved lens, these results showed that it was probably not worth pursuing the idea further; the cavity shape itself dominated the final field pattern and the lens had little effect.

5.4.3 Aerial Focusing
Early in the M.A.R. system development programme, thermocouples were found to focus the microwave energy around them if they were embedded in the monolith and high localised temperatures were measured (see Section 4.6.1). This precluded their further use in measuring trap temperature. However, it was thought that the aerial focusing effect might be put to use if many aerials were embedded in the front face of the monolith in the regions where the heating effect was a minimum (i.e. at the periphery and, left and right sides).
FIGURE 5.12: EFFECT OF WAVEGUIDE LENS ON MICROWAVE HEATING FIELD AS DEPICTED BY NEON BULB MATRIX. (DISTANCES ARE THOSE FROM WAVEGUIDE EXIT TO NEON BULB MATRIX)
Sixty four metal staples of dimension 13 mm wide with leg length 7 mm were put into a loaded monolith (as shown in Figure 5.13) which was regenerated in the M.A.R. system. Results showed that these 'aerials' did indeed attract the heating effect to the periphery but only in patches. A photocopy of the outlet end of the monolith (Figure 5.14) shows definite white patches where the high temperature zones oxidised the peripheral traces of soot at the outlet end. (Full video pictures are available of this regeneration). This also demonstrates the channelling effect characteristic of the wall-flow monolith where some channels become dominant. The aerial technique was not considered to be good enough to warrant further work.

FIGURE 5.13: MONOLITH WITH METAL AERIALS (STAPLES) TO ENCOURAGE MICROWAVE HEATING TO PERIPHERY AND SIDES
FIGURE 5.14: OUTLET END OF MONOLITH REGENERATED WITH M.A.R. USING AERIAL INSERTS
5.4.4 Even Heating - Conclusions

The above experiments, although of interest, did not produce results good enough to warrant further effort. The cavity itself appeared to assume its 'natural' mode shape. Thus two directions could be chosen.

Firstly, given that the heating shape is an ellipse, why not use a monolith of elliptical cross-section and mount it in the vertical plane? The monolith manufacturers were contacted and suitable elliptical wall-flow monoliths were found to be available. These have been obtained and at the time of writing a suitable cavity has just been completed to test out this idea, see Figure 5.15. Results with this elliptical monolith and cavity will be reported at a later date.

FIGURE 5.15: THE AS YET UNTESTED ELLIPTICAL MONOLITH AND CAVITY DESIGN ATTACHED TO MODIFIED M.A.R. PROTOTYPE FRONT END. (LARGE CIRCULAR FLANGES ARE TO ENABLE THE SEPARABLE CAVITY TO BE INTERCHANGED WITH EXISTING SYSTEM). AN ELLIPTICAL WALL-FLOW MONOLITH IS SHOWN IN THE FOREGROUND
The second answer is to modify the cavity such that heating is more even for the existing circular cross-section monoliths. This is the first subject of Chapter 6.

5.5 CONCLUDING REMARKS

In this Chapter, a modified, more commercial M.A.R. unit design has been described. The system has been shown to be rugged enough for vehicle use. Results on bench, engine and vehicle were extremely useful and two key areas where attention is needed were noted.

Firstly the regeneration process itself must be carefully controlled to allow the oxidation zone to propagate whilst keeping trap temperature excursions within safe limits. This is best done by feeding in a controlled flow of ambient air during regeneration.

Secondly, the heating of the upstream end of the particulate loaded monolith must be as even as possible if the inherent 'channelling' effect of the wall-flow monolith is to be alleviated and regeneration efficiencies improved. It was concluded that the cavity itself required modification to achieve this.

Both these requirements are incorporated in the Third-Generation M.A.R. system design discussed in the next Chapter.
CHAPTER 6

6.1 INTRODUCTION

In Chapter 5 it was concluded that an even heating of the particulate was important for good regeneration efficiency. It was also suggested that an ambient air feed during regeneration was desirable since the oxidation could be closely controlled to promote propagation and reduce the risk of trap melting. Here a Third-Generation M.A.R. system incorporating new features based on these recommendations to improve the system is described together with its bench and engine testing. The final engine tests include a description of a 100 regeneration cycle durability programme currently in progress.

6.2 THIRD-GENERATION M.A.R. SYSTEM DESIGN

6.2.1 Design Concept

The microwave applicator (a waveguide in the previous M.A.R. designs) caused a dominant mode producing an elliptical heating pattern. For the circular cross-section monoliths the heating effect requires spreading out, and as shown in Chapter 5 it was difficult to accomplish this with the existing design.

The microwave applicator cavity could be redesigned so as to produce a different dominant mode shape, but this would still lead to 'patches' receiving little heat and therefore a different approach was required.

In most microwave ovens, a turntable is provided to rotate the food so that it moves in and out of the high and low intensity heating field zones. Clearly in an M.A.R. system a turntable is not a practical
reality so here another technique commonly employed in microwave ovens can be used. This is to use a metallic 'mode stirrer' inside the cavity, a fan-like paddle, which slowly rotates so that the field pattern is perturbed and continually changed. The rotating mode stirrer in an M.A.R. system is best placed upstream of the glass seal so that it is not damaged by the hot exhaust gases. The basic concept is as shown in Figure 6.1.

FIGURE 6.1: SCHEMATIC OF MODE STIRRER IN AN M.A.R. SYSTEM
6.2.2 Design
The upstream end of the M.A.R. system required a redesign so that a suitable mode stirrer could be incorporated upstream of the glass seal. The design of the new unit is shown in Figure 6.2.

The classic waveguide was discarded in favour of a parabolic reflector behind the magnetron (see Figure 6.3) and a large cavity after the magnetron to contain the mode stirrer prior to a large circular glass seal. The parabolic reflector was intended to promote beam spread from the magnetron anode situated at the parabola's focus; its design is described in Appendix 1.

6.2.3 Mode Stirrers
As Metaxas and Meredith, 1984 [56] suggest, mode stirrers are extremely difficult to design theoretically and are therefore usually empirically designed.

Three generic mode stirrers were made as shown in Figure 6.4. These were each tried separately in the Third-Generation M.A.R. system, mounted vertically (in the sense of Figure 6.2), half way along the inside of the mode stirrer cavity.

The mode stirrers were driven by a small electric motor (not shown in Figure 6.2) mounted underneath the stirrer cavity. The motor was geared to give a mode stirrer rotational speed of 6.67 rpm. The speed is not critical from the microwave standpoint (since these propagate at the speed of light) but the slow speed seeks to provide a sufficient heating time for each part of the particulate in the monolith.
FIGURE 6.2: THIRD-GENERATION M.A.R. PROTOTYPE

FIGURE 6.3: UNDERSIDE VIEW OF PARABOLIC REFLECTOR IN THIRD-GENERATION M.A.R. PROTOTYPE
The neon bulb matrix mounted on the perspex disc (as described in Chapter 5) was positioned and energised inside the cavity where the upstream face of the monolith would be situated and Figure 6.5 shows the field pattern without any mode stirrer. Again this is the shape found on the modified prototype described in Chapter 5 and is also the same shape as the melted zones of the failed monolith from the vehicle (Figure 5.8). This confirms the suggestion in Chapter 5 that the cavity itself dominates the resultant mode shape unless otherwise perturbed.
Mode stirrer 1 (Figure 6.4) was simply two brass 'flags' attached to a steel rod. This design was chosen since each flag enters and passes through the dominant mode node positions and helps to reflect the microwave energy elsewhere. Figure 6.6 shows how the neon bulb matrix reacted as the mode stirrer 1 rotated and clearly at some stage during the cycle all the bulbs received enough energy to illuminate.

Mode stirrer 2 (Figure 6.4) was designed so that the three brass plates are at 45° to the rod axis and equally disposed (at 120°) about the rod axis. The idea was that at no time do the brass plates face directly back toward the magnetron; reflected energy can under some circumstances, cause the magnetron to 'mode' (i.e. rapid power fluctuations caused by a collapsing electrical field inside the
magnetron) causing damage. Figure 6.7 shows how the neon bulb field pattern altered with mode stirrer 2. Most bulbs did light, but the overall evenness was inferior to that found with mode stirrer 1.

Mode stirrer 3 (Figure 6.4) was simply a plate which could fill the maximum cross-section of the trap cavity and still rotate. It could also stop the heating directly in the dominant mode position twice per revolution. Results with this were fairly poor as Figure 6.8 shows. Energy reflection straight back to the magnetron was also considered undesirably high.

From the above tests, it appeared that mode stirrer 1 was the best and hence it was used during all the subsequent tests.
FIGURE 6.6: MICROWAVE HEATING PATTERN AS DEPICTED BY NEON BULBS WITH MODE STIRRER 1 (Photographs from Video Pictures)
FIGURE 6.7: MICROWAVE HEATING PATTERN AS DEPICTED BY NEON BULBS WITH MODE STIRRER 2 (Photographs from Video Pictures)
FIGURE 6.8: MICROWAVE HEATING PATTERN AS DEPICTED BY NEON BULBS WITH MODE STIRRER 3 (Photographs from Video Pictures)
6.3 THIRD-GENERATION SYSTEM BENCH TESTS

6.3.1 Reasons for Tests

Bench tests were conducted to establish how even the preheating is in practice using the mode stirrer, plus the following very important parameters:

i) Optimum trapped mass
ii) Optimum heating time
iii) Optimum air flow rate during the regeneration.

The reasons for establishing these were as follows. If the mass is too high, melting can occur, conversely if too low the oxidation zone might die out and not propagate. From a vehicle system viewpoint it is also important to establish how often regenerations are required (which depends on trapped mass prior to regeneration) and whether trap destruction is a possibility if the trapped mass accidently rises too high.

The preheating time should ideally be minimised so that energy consumption is low and the trap by-passing period is kept as short as possible. It is also necessary to establish a minimum preheating time to guarantee a full regeneration.

The air flow rate is also very important. If it is too high a runaway regeneration may occur and the trap may melt. On the other hand, depending on the trapped mass and preheated temperature, the oxidation may die out and not propagate. A low flow rate, however, would generally increase the regeneration time since the oxygen feed-rate is reduced.
Ideally, the best situation would be an infrequent regeneration with rapid preheating, followed by a rapid, complete regeneration without trap damage. To establish these parameters 12 monoliths were loaded with varying amounts (and types) of particulate ready for bench regeneration. Ideally many more bench regenerations under many trapped mass, particulate type, preheat times and air flow rates would have been beneficial. The particulate type was varied by operating the engine at different speeds and loads. This was because, in general, the high load, high speed (i.e. high exhaust gas temperature) particulate is more carbonaceous, has less soluble organic fraction content (SOF) and can be more difficult to oxidise [71].

6.3.2 Bench Tests
The Third-Generation M.A.R. system upstream end was bolted to the original separable trap cavity. An air supply was used to pump air through the trap during regeneration. The velocity of gas was measured with a hot wire flow meter probe mounted in the inlet pipe. The ensuing oxidation was viewed and videoed as in previous tests.

For a given monolith the time was chosen as 10 minutes as a reasonable first iteration. The air flow rate was adjusted so that the oxidation caused visible radiation of the outlet channels and was further adjusted if the radiation was considered to be too bright. (A 'cherry-red' glow was chosen as the acceptable target from previous experience).

Since all the previous tests had considered high trapped mass loadings, the highly loaded monoliths were regenerated first and followed by the monoliths containing decreasing amounts of particulate
Throughout these tests the most recent information gleaned was used to estimate the best conditions for the next test. In Appendix 5 the full results of these tests are tabulated but here the results are summarised graphically in the following section.

6.3.3 Bench Test Results

Each regeneration was videoed in a similar manner to previous bench tests and these demonstrated that the mode stirrer was improving the heating field spread as Figure 6.9 shows (Test No 4, in Appendix 5).

Test No 1 led to trap melting because of the high mass loading (43.6g) and high air flow rate, and Figure 6.10 shows a very radiant central core of the monolith prior to melt-down. This sort of radiant temperature was avoided in all subsequent bench tests by reducing the air flow rate. Figure 6.11 shows the failed trap after sawing it axially in half and clearly the core was severely damaged by melting.

FIGURE 6.9: EVEN HEATING OF MONOLITH. VIEW ALONG OUTLET CHANNELS DURING REGENERATION (Circle is 75% of overall monolith diameter)
(a) Very radiant core

(b) Core begins to melt

(c) After core melt-down

FIGURE 6.10: MELT-DOWN OF MONOLITH (TIMES ARE MINUTES AFTER AIR-FEED STARTED)
From the results presented in Appendix 5, Figure 6.12 shows how the regeneration efficiency is dependent upon initial particulate mass loading. The lowest mass was too low to sustain a propagating oxidising zone. No propagation also occurred during the first attempt at regenerating the highest loaded trap. The preheating time of 10 minutes was too short to reach a temperature where rapid self-sustaining oxidation could occur. The preheating time was therefore increased to 15 minutes and substantial oxidation occurred.
Figure 6.13 shows how the regeneration efficiency is affected by the air flow rate. A high mass (43.6g) and high flow lead to a melted monolith (discussed above). The second attempt at the 56g load with a low air flow (to avoid melting) was reasonably successful. It became apparent that an inlet pipe air flow velocity of approximately 1 m/s (equivalent to 1.61 g/s) gave the best oxidation of the mid-range mass loadings.

FIGURE 6.12: EFFECT OF INITIAL PARTICULATE LOADING ON REGENERATION EFFICIENCY
Figure 6.14 demonstrates that the total regeneration time (preheat time plus air-only rapid oxidation phase) is only dependent on particulate loading at high masses. This was because a very low flow rate was used with these high masses to avoid trap melting. At the lower masses the total regeneration time was fairly constant at approximately 20 minutes. The rapid (20 minute) regeneration of 43.6g led to melting. The result that the total regeneration is not a strong function of trapped mass is in accordance with the modelled results in Chapter 3.
From the above results it was evident that a mass loading of between 15 and 25g, a preheat time of 10 minutes, a flow rate of 1 m/s (1.61 g/s) and an air-only time of 10 minutes, would provide a reliable and reasonably effective regeneration. This operating envelope was therefore used as a target in the durability programme discussed later in this Chapter.

6.3.4 Further Comments

It was noted earlier in this thesis that the actual design of the wall-flow monolith inherently encourages an axial 'channelling' of the oxidation zone. During the above bench tests it also became increasingly apparent that the design also may promote difficulties in
the axial oxidation zone propagation which, if only partially successful, can lead to poor regeneration. The low regeneration efficiencies in the bench tests could not be solely due to radially uneven heating.

Referring to Figure 3.1 in Chapter 3 it can be seen that if the particulate at the upstream (left hand) end of the channel is oxidised, gas flow will readily flow through the wall there and the propagating oxidation zone upstream face would receive an ever decreasing oxygen-feed to sustain the reaction and under some circumstances might die out prematurely. This effect is highly unpredictable and requires further investigation if it is to be fully understood. Huthwohl et al, 1987 [41] studied the oxidation (flame) travel inside a monolith and showed that propagation could be enhanced if precious metal catalysts were used. Despite the author's reservations of the use of catalysts in traps, these could certainly be employed to improve the propagation in the M.A.R. system. Both the channelling and propagation problems might be overcome however if a ceramic foam trap substrate was used. This is discussed further in Chapter 7.

Another small observation from the above bench tests was that the oxidation of the carbonaceous particulate might not be purely a reaction of \(
\text{C} + \text{O}_2 \rightarrow \text{CO}_2
\)
, as assumed by all the investigators reviewed in Chapter 3. During Test No 3 (see Appendix 5) the monolith outlet channels showed a slight blue glow in the gas phase. This colour is usually associated with the homogeneous oxidation of carbon monoxide and was probably due in part to the low air flow rates (0.15 to 0.6 m/s) during this particular regeneration. Thus for convective transport limited oxidation, the process might be more closely represented in future modelling work by the relations:
6.4 DURABILITY TEST PROGRAMME

To establish the longevity of a monolith in an M.A.R. system a durability test programme consisting of an attempted 100 regenerations on one monolith has just been embarked upon.

The Third-Generation M.A.R. system containing a standard 5.66" dia x 6" long 17/100 wall-flow monolith was fitted to the Perkins Prima engine on a transient dynamometer (as used in the engine tests described in Chapters 4 and 5). The valve arrangement was similar to that shown in Figure 5.10 although valves B and C were actually rationalised into a very compact unit consisting of a wastegate valve and an elliptical balanced butterfly valve. Valve A could have been another wastegate valve but a standard gate valve was used in this instance.

The transient dynamometer has closed loop control for constant speed, load, or a 'power-law' and thus by moving the fuelling rack by a microprocessor controlled stepper motor drive, the engine condition can be cycled to give a reasonable spread of different types of particulate throughout the trap loading period. Figure 6.15 shows the drive-cycle path on the engine load-speed map. Each point is operated for an equal amount of time. The 550°C shaded region was avoided since thermal regeneration might occur. During regeneration the inlet and outlet exhaust gas temperatures are data-logged.
6.5 CLOSURE

The Third-Generation M.A.R. system described in this Chapter provides a more even heating than previous designs by employing a mode stirrer.

Fourteen bench regenerations revealed a significant amount of further data to establish the optimum 'operating window' for an effective regeneration. These results are being used as a basis for the 100 regeneration cycle durability test programme currently in progress.
CHAPTER 7

This Chapter presents short discussions of some wider aspects of the work in this thesis. Firstly, the commercialisation of M.A.R. is discussed with respect to its cost, safety, performance and current industrial interest it has aroused. A brief discussion of the limitations of the wall-flow monolith is then presented and finally some comments on microwave assisted chemical reactions, together with notes on recently published work on the subject are given.

7.1 COMMERCIALISATION OF M.A.R.

At the very conception of M.A.R., the author considered it important that the system be commercially viable with respect to cost, safety performance and reliability. At the feasibility study stage (referred to in Chapter 4) the attributes of M.A.R. in these areas appeared favourable and having since developed three working prototypes more definitive estimates can now be made.

7.1.1 Cost

Cost is a favourable advantage of M.A.R. over other trap-regeneration systems. The individual components of M.A.R. are drawn from existing technology and hence parts are relatively cheap. Domestic microwave ovens retail at below £150 and contain parts unnecessary to M.A.R. Since a steel trap casing is required on any trap-regeneration system the marginal cost of the microwave circuit hardware is small. The one-off retail cost of the magnetrons used in this study were £32 which for an ignition source is at least an order of magnitude cheaper than fuel-burners. The magnetron production cost is probably about £5. The
power-supply cost depends upon the envisaged installation. Domestic microwave oven power supplies are inexpensive and the price of proprietary replacement alternators to provide 240V AC (mentioned in Chapter 5) would probably be 25% more than standard alternators (currently £180) if supplied in numbers of more than 1000, according to the manufacturers. However, a dedicated supply from 24V DC to the magnetron voltage might be cheaper than unnecessarily stepping via 240V AC.

The monoliths used here cost approximately £60 and obviously this is a cost for all wall-flow monolith trap systems. (Similarly sized catalysed monoliths incidentally cost more than £200).

Other components include the special glass seal (less than £10) and valves and actuators which are unlikely to be prohibitively expensive since turbocharger wastegates and exhaust brakes are suitable, and are in common usage in the automotive industry.

The overall price is sensitive to the numbers to be produced, but the above discussion does suggest an inexpensive system mainly because individual components are commercially available and relatively cheap.

7.1.2 Safety
This too was addressed at the feasibility study stage. Several authors, including Copson, 1975 [18] and Stuchly and Stuchly, 1983 [79] have addressed safety issues concerning microwaves. The main conclusions were that microwaves are not sufficiently energetic from a quantum energy standpoint to be called 'ionising radiation', and if suitably contained they present no danger. Hazards with domestic microwave ovens appear to be minimal and should not be viewed in the
same light as military use of microwaves which involve massive concentrations of power in open space.

Microwave ovens are already fitted to many coaches for cooking food and some truck operators are calling for their use. Current legislation is generally no tighter than that for microwave oven use [95][96] and the M.A.R. system proposed here is inherently safer than these ovens since it has no opening doors and therefore door interlocks etc are unnecessary. In the vehicle system described in Chapter 5, no measurable levels of microwave energy leakage from the exhaust pipe were detected (using an "Apollo" microwave test meter). However, any production system would obviously require full Radio Frequency Interference (RFI) and Electro-magnetic Capability (EMC) testing within a vehicle.

General safety is very important and safeguards with respect to misuse and accidental damage must be addressed. For the latter, "g-force" switches may be incorporated which electrically isolate the M.A.R. unit if subject to a large impact.

7.1.3 Performance and Reliability
The M.A.R. system offers a low power (1 kW), direct, non-contact ignition-source which works well. A magnetron life of 4000 hours is now a reasonable period for many heating applications [18]. For the U.S. Environmental Protection Agency target 290,000 vehicle mile trap life requiring 1000 regenerations each involving up to, say, a 10 minute microwave preheating time, the magnetron will only be in operation for a total of 167 hours. However, since the cost of the magnetrons is low, replacement if necessary would be inexpensive. Reliability in general is likely to be high since few moving parts are
required and the microwave heating method does not rely on a special ignition system.

The M.A.R. system, however, is still not perfect and requires more development effort. The main problem appears to be low regeneration efficiencies caused in part by the use of wall-flow monoliths which exhibit unique characteristics which lead to poor radial and axial oxidation zone propagation. This point is returned to later in Section 7.2.

Preheating times of typically less than 10 minutes are either the same or an improvement on electrical resistance heaters of the same trap size requiring at least 30% more power and catalysts [4]. Although reliability of the M.A.R. microwave units so far have been 100%, it is not known whether there are any significant longer-term durability problems.

7.1.4 World-Wide View of M.A.R.

The M.A.R. system has attracted interest from both sides of the Atlantic and currently discussions with companies from the UK, Continental Europe and USA are taking place with a view to the systems development and commercialisation.

At the time of writing the author is unaware of a fully developed, cost effective vehicle trap-regeneration system being available. The future of M.A.R. depends on many factors including future engine technology and legislation, but it is a considered personal view that the system should at least find a small niche in the market.
7.2 THE WALL-FLOW MONOLITH

In Chapter 1 the wall-flow monolith was shown to be a good filter medium for a particulate trap system. It exhibits a good trapping efficiency and thermal strength but in practical applications has proved to exhibit some unique characteristics leading to regeneration problems. These are not unique to M.A.R. but have also become apparent on other systems, including the electrical resistance face heater types [4][8]. As described in previous chapters, the monolith channels promote poor radial and axial propagation of the oxidation zone leading to poor regeneration efficiencies. Another problem is that it only takes one channel wall to fracture for the trapping effectiveness to be lost almost completely.

These problems might be overcome if new ceramic foams being developed [58] are used in M.A.R. With ceramic foams the particulate is not separated into discrete channels but is more homogeneously distributed and thus oxidation propagation is better. Since foams are depth filters, the concentration gradient of particulate is an exponential-decay function from the upstream to the outlet and this ideally lends itself to upstream preheating used in M.A.R. One final characteristic is that if melting causes a 'pocket' somewhere in the foam, trapping effectiveness is not substantially lost. It is the author's intention to investigate ceramic foams with M.A.R. in the future.

7.3 MICROWAVE ASSISTED CHEMICAL REACTIONS

When it was found that microwaves rapidly heat up diesel particulate, the phenomenon was quickly applied to trap regeneration. However, at that stage little was known about the mechanisms involved. Recently there has been work published showing that microwave energy can speed up a variety of chemical reactions. These are not to be confused with
earlier work with high temperature plasmas enhanced with microwave energy such as described by Groff and Krage, 1984 [32].

Many people have assumed that microwaves can only excite water molecules but this is not the case as shown, for example, in this thesis. Gedye et al, 1988 [29] reported some fundamental studies of increasing the synthesis of organic compounds with microwave energy of 560W at 2450 MHz (the same frequency as the M.A.R. systems here). Reaction rates were up to 1240 times faster with microwaves than by conventional techniques. Gedye et al showed that the reaction rate depended on how polar the molecules were. In Chapter 4 it was suggested that the polar compounds in the particulate were responsible for its high reactivity when exposed to microwave energy.

Baghurst and Mingos, 1988 [5] in similar experiments with microwave ovens showed that inorganic oxides could be synthesised in 30 minutes compared to a whole day using conventional heating. Again the polarity of the molecules was considered the key to these rapid reaction rates.

The author is not aware of published research work, outside that of this present thesis, on the combustion of material assisted by microwave energy. During this study some very basic experiments were conducted and these included placing various combinations of substances (coal dust, charcoal 'flour', diesel fuel, isopropylalcohol, petrol and engine sump oil) into a standard microwave oven (see Appendix 6). Only diesel particulate exhibited visible combustion, all the others merely warmed up slowly. It would be of benefit to conduct detailed fundamental experiments in this new area of combustion.
Emsley, 1988 [22] in his review article of the work of Gedye et al and Baghurst and Mingos pointed out that chemistry with microwaves is in its infancy and a lot of fundamental research is required if it is to be understood.

With respect to M.A.R., it appears that, as in many other instances, there is an engineering application of a physical phenomenon prior to a full scientific understanding of the basic mechanisms involved.
CHAPTER 8

8.1 CONCLUSIONS

The work of this thesis has sought to provide a better understanding of the regeneration characteristics of monolithic wall-flow diesel particulate traps and has presented the concept and development of a new regeneration technique using low power microwave energy.

It has been shown that the imminent diesel particulate emissions legislation will make it necessary for future engines to be fitted with exhaust after-treatment devices and the monolithic wall-flow trap was shown to exhibit the most favourable characteristics for after-treatment in terms of filtration efficiency and thermal strength. Since traps of any kind retain the trapped particulate, they eventually become blocked and therefore require regenerating, i.e. in-situ 'cleaning' by oxidation of the particulate.

Various regeneration techniques were explored and none were shown to be wholly satisfactory in terms of both cost and efficiency. The prime requirement of an ideal trap regeneration system was identified as being that the trapped particulate itself should be specifically and primarily heated if external power requirements are to be minimised. It was proposed that low-power microwave energy be used to accomplish this since the ceramic monolith was found to be virtually transparent to this energy but diesel particulate was found to be highly responsive to it and rapidly heated up to radiant temperature.
A greater understanding of trap behaviour during thermal regeneration was derived from a new mathematical model. The model was shown to be in good agreement with published experimental results. It showed that to avoid failure by melting the trap should be regenerated at mid to low particulate mass loadings.

The concept of using microwave energy to promote trap regeneration was discussed further and experiments leading to the development of the first Microwave Assisted Regeneration (M.A.R.) prototype were described. The prototype was bench and engine tested and was shown to perform encouragingly well but uneven heating of the particulate resulted in incomplete regeneration.

A modified prototype improved the heating pattern and this unit was also fitted to a vehicle. These tests demonstrated the practicality of the M.A.R. system in a real environment. The vehicle installation highlighted some improvements which could be made to the system to control the oxidation process by using externally fed air during the rapid regeneration phase.

Further experiments on some new ideas to provide a more even microwave heating field were conducted and a novel method of assessing the microwave heating field was proposed and used. This method employed a matrix of small neon bulbs which illuminated where the field was most intense.

It was concluded that the microwave heating field pattern could only be spread out if the field was continually perturbed by a metallic mode stirrer. A Third-Generation prototype system incorporating this feature was designed, tested and shown to be reasonably successful.
This prototype was extensively bench tested to provide an indication of the ideal conditions for regeneration in terms of initial trapped particulate mass, pre-heating time and air feed rate. A trap durability programme involving many regeneration cycles has been embarked upon which use these data.

Throughout the experimental stages of this work the wall-flow monolith was found to have inherent features which discouraged complete regeneration of the monolith. These include the cellular channel structure of the monolith which inhibits radial heat flow and can cause poor axial propagation of the oxidation zone. It was suggested that new ceramic foams might be a better trap material for improved regeneration.

The novel M.A.R. technique has been shown to be commercially attractive from power, cost and size considerations. The use of microwave energy to assist chemical reactions is still in its infancy and it was suggested that further fundamental studies of these processes, especially combustion, would be of significant interest.

8.2 OUTLINE OF FUTURE WORK

The body of this thesis has already stated areas where future work will be concentrated. The following sections mention these and other related areas of interest.

8.2.1 M.A.R. Development

The M.A.R. system merits further development and future work should seek to take it to the production stage. Specific areas of development include: a dedicated and cheap power supply for the on-vehicle M.A.R. unit; microwave sensing of particulate trapped mass

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(by measuring the downstream microwave field) and a control system for sequencing valves, magnetron and fan prior to and during regeneration. Modelling work, extended to the entire trap, would be useful and help future M.A.R. design. This could include microwave field modelling and maybe a three-dimensional heat flow and thermal stress model.

Other filter materials including ceramic foams should be investigated with a view to improving regeneration efficiency. In addition, testing of various filter shapes (including the oval monoliths) would be of benefit.

8.2.2 Other Related Areas
Related applications of microwave energy in engine exhaust after-treatment systems include preheating or activating of exhaust catalysts, and this could be a possible spin-off technology.

The whole area of chemistry, and especially combustion, with microwaves is of significant interest. There are still many unknowns, especially identifying the prime constituents of diesel particulates which make them particularly responsive to microwave energy, and therefore fundamental work in this area would be beneficial.
REFERENCES


This Appendix outlines the microwave applicator designs chosen for the M.A.R. prototypes. The first section considers the design of the rectangular waveguide used on both the first prototype (Chapter 4) and the modified prototype (Chapter 5). The second section considers the design of the parabolic reflector used in the Third-Generation prototype (Chapter 6).

Al.1.1 Rectangular Waveguide

Electrical current may be passed through metal wires. If the frequency is increased then it becomes necessary to shield this wire by a metal sheath to stop the electromagnetic energy radiating to the surroundings. This would be wasteful and might cause radio interference or be in some way dangerous. Sheathed wires of this kind are termed 'coaxial'. At high frequencies the central wire may be dispensed with since the energy may be regarded purely as an electromagnetic wave and only the outer hollow tube is required for wave propagation. Barrow, 1936 [9] was the first to publish the concept of using a hollow waveguide to transmit electromagnetic waves. Here the waveguide is used to direct the microwave energy with maximum efficiency into the cavity containing the wall-flow monolith.

A generalised rectangular waveguide can be represented as shown in Figure Al.1.
The electromagnetic pattern is shown schematically in Figure A1.2.

At resonance the length $d_c$ (which is the distance from the magnetron anode to the waveguide outlet) can be calculated by taking three half wavelengths $\lambda$ i.e.

$$d_c = \frac{3}{2} \lambda$$

* i.e. Transmission Electrical mode in x direction and n integer multiples in z direction.
For a frequency of 2450 MHz, taking the velocity of light as $2.9979 \times 10^8$ m/s gives

$$\lambda = 122.36 \text{ mm therefore, } d_c = 183.54 \text{ mm}$$

The dimensions $a$ and $b$ may be calculated by considering Maxwell's equations for electromagnetic wave propagation in the $z$ direction and boundary conditions for the $TE_{10n}$ mode.

The actual solution of Maxwell's equations is presented in standard texts [7][73] but adopting the internationally recommended waveguide dimensions quoted by Metaxas and Meredith, 1983 [56] (his Appendix VII) the dimensions chosen were:

$$a = 86.36 \text{ mm}$$
$$b = 43.18 \text{ mm}$$

i.e. $a = 2b$.

These sizes are ideal for exhaust systems and traps. The chosen frequency of 2450 MHz is internationally recognised for domestic and industrial applications (except in the USSR and some Eastern Block countries who adopt the slightly lower frequency of 2375 MHz). Other frequencies commonly available e.g. 915 MHz would require unacceptably large waveguides and trap cavity sizes.

1.1.2 Parabolic Reflector

This was used in the Third-Generation M.A.R. prototype. To improve the field distribution the intent was to excite as many modes as possible in the cavity and a mode stirrer was adopted. Since the applicator itself (i.e. the cavity connecting the magnetron to the main heating
cavity) was not intended to resonate at a single frequency (2450 MHz) but at as many as possible the classic waveguide shape was discarded.

In an attempt to help spread the electromagnetic field a parabolic reflector behind the magnetron was incorporated, with the magnetron anode at its focus. This approach was described by Puschner, 1966 [73] for heating wide items at the mouth of a parabolic shaped applicator.

The parabolic applicator for the Third-Generation M.A.R. prototype was calculated as follows. Figure A1.3 shows a parabola given by \( y^2 = 4ax \)

\[ \begin{align*} 
\text{FIGURE A1.3: PARABOLA FOR THIRD-GENERATION M.A.R. PROTOTYPE} 
\end{align*} \]
The maximum total width of the parabola mouth which could be connected to the circular mode stirrer cavity was $2 \times 70.3 \, \text{mm} = 140.6 \, \text{mm}$.

The minimum distance between the focus $a$ and the outlet was 52 mm (due to the physical size of the magnetron) and the focal distance was set at 17.7 mm. Thus the dimensions in Figure A1.2 could be found from the above equation. The internal depth of the parabolic cavity was the same as the dimension $b$ given in Section A1.1 above, i.e. 43.18 mm.
APPENDIX 2

A2.1 POWER REQUIREMENTS OF M.A.R.

The following is an edited extract of the "Microwave Assisted Regeneration (M.A.R.) Initial Feasibility Study", by Gamer, 1987, pp 8-10 [26]. It shows that even a power delivery of 1.3 kW is feasible from a vehicle's electrical system.

"An M.A.R. unit requires electrical power. The microwave oven used for the experiment described previously had a microwave output power of 650W; the input power of such an oven is less than 1.3 kW. Although these ovens need some power for the turntable, the internal light and extractor fan etc, here we can assume that the magnetron (the microwave producer) is approximately 50% efficient. Barber, 1983 suggests a constant efficiency of 55% for a magnetron.

In the experiment the microwave oven promoted burning of the particulate so we could assume that input power requirements may be in the range of up to 1.3 kW.

To put this amount of electrical power in perspective a bus or truck has the following:

* Alternator power 2 to 3 kW continuous at 28V and can produce >60A when engine speed is just above idle.
* Battery set 150-200A Hours, 24V.
* Headlights 55W each main beam.

For a car:

* Alternator 40A (max) at 14V
* Battery 30-60A Hours, 12V
* Headlights 55W each main beam
* Heated rear window consumes 15-20A (180-240W at 12V)

Ref [7]
The battery size is usually set by the size of engine it needs to start and the alternator replaces this energy and provides the power for the auxiliaries. It is not envisaged that an M.A.R. unit would be used continuously - regeneration frequencies of typical ceramic traps are every 50 to 100 miles and the actual regeneration time is a matter of minutes. Therefore the M.A.R. unit would probably be powered by the battery during regeneration and at other times switched off.

Assuming a transformer efficiency of typically 90%, an M.A.R. unit drawing 1.3/(0.9) kW (= 1.4 kW) in the worst case would need 60A at 24V and 120A at 12V. A bus or truck could run this continuously on the alternator (assuming no auxiliaries switched on) and up to 2.5 hours solely on a 150A hour battery pack. A car could run an M.A.R. unit for up to 1/2 an hour continuously solely on a 60A hour battery and up to 3/4 of an hour with alternator assistance.

For M.A.R. applications with diesel-generator sets the electrical power can obviously be fed back from the generator as necessary.

At this stage it is somewhat premature to go into further detail since the above calculations demonstrate the feasibility of using even a high power M.A.R. unit under continuous conditions. Required powers an order of magnitude lower than 1.3 kW may be sufficient, and the M.A.R. unit will almost certainly not be operated continuously."
A3.1 GLASS SEAL

An important component in each of the M.A.R. prototypes described in this thesis is the glass seal which needs to transmit microwave energy but not allow hot exhaust gases to reach the microwave hardware. This glass must withstand temperatures up to a possible 700°C.

A proprietary glass material exhibiting the necessary characteristics was used.

A3.1.1 Thermal Strength

The glass had the following thermal properties:

- Maximum continuous working temperature: 950°C
- Maximum short-term temperature: 1200°C
- Softening point: 1600°C
- Coefficient of linear expansion: 0.59 x 10⁻⁶/°C (5% of steel)

The glass was placed in a furnace at 800°C for 3 hours with no resulting damage. It also performed well on the vehicle installation (Chapter 5) with no damage.

A3.1.2 Microwave Characteristics

The dielectric properties of materials are usually expressed in complex form:

\[ e^* = e' - j\varepsilon_{\text{eff}} \]
where $e^*$ is the relative complex permittivity

$e'$ is the relative dielectric constant

$e_{\text{eff}}$ is the relative effective loss factor

and $j$ is the complex operator.

At high frequencies, the complex coefficient of this expression is the important measure of the "lossiness" of the material. It is often expressed as the dielectric loss angle tangent

$$\tan \delta_{\text{eff}} = \frac{e''}{e'}$$

and this is the measure of how much the material absorbs microwave energy. For the glass used here the loss angle tangent data provided by the manufacturers was as given in Table A3.1.

<table>
<thead>
<tr>
<th>Frequency (Hz)</th>
<th>Clear Glass</th>
<th>Opaque Glass</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^3$</td>
<td>$&lt; 5 \times 10^{-4}$</td>
<td>$6-20 \times 10^{-4}$</td>
</tr>
<tr>
<td>$10^6$</td>
<td>$&lt; 1 \times 10^{-4}$</td>
<td>$5-15 \times 10^{-4}$</td>
</tr>
<tr>
<td>$10^7$</td>
<td>$&lt; 1 \times 10^{-4}$</td>
<td>$4-12 \times 10^{-4}$</td>
</tr>
<tr>
<td>$10^8$</td>
<td>$&lt; 1 \times 10^{-4}$</td>
<td>$4-12 \times 10^{-4}$</td>
</tr>
<tr>
<td>$10^9$</td>
<td>$&lt; 1 \times 10^{-4}$</td>
<td>$4-12 \times 10^{-4}$</td>
</tr>
<tr>
<td>$3 \times 10^{10}$</td>
<td>$4 \times 10^{-4}$</td>
<td>-</td>
</tr>
</tbody>
</table>

**TABLE A3.1:** DIELECTRIC LOSS ANGLE TANGENTS FOR GLASS SEAL MATERIALS
(M.A.R. uses at frequency of $2.45 \times 10^9$ Hz)
The effect of temperature on loss angle tangent was described in the manufacturers literature with the following words:

"Tan $\delta_{\text{eff}}$ is practically constant at a frequency of $10^6$ Hz up to 200°C, but then increases as the temperature rises; at $10^{10}$ Hz, tan $\delta_{\text{eff}}$ falls off slowly with rising temperature up to 350°C, but then, as the temperature rises still further, it begins to climb again slightly".

Detailed measurements of the glass properties with respect to M.A.R. were not possible but a series of basic experiments demonstrated that the material was suitable.

A3.1.3 Microwave Experiments

To establish how well the glass could transmit microwave energy sheet samples were attached to the inside of a domestic microwave oven over the waveguide outlet. A Pyrex beaker containing 75 ml of water was placed in the oven and the time taken to boil fiercely was measured. Table 3.2 shows preliminary results.

<table>
<thead>
<tr>
<th>Test Condition</th>
<th>Time to Boil (seconds)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) No glass</td>
<td>61</td>
</tr>
<tr>
<td>b) &quot;HSQ&quot; Type (6 mm thick)</td>
<td>85 ) 39% longer</td>
</tr>
<tr>
<td>c) &quot;BQ&quot; Type (6 mm thick)</td>
<td>85 )</td>
</tr>
<tr>
<td>d) &quot;7940&quot; Type (6 mm thick)</td>
<td>85 )</td>
</tr>
</tbody>
</table>

TABLE 3.2: INCREASE IN HEATING TIME WITH VARIOUS GLASS SEAL MATERIALS
These results showed that the glass was attenuating the microwave energy by 39%. Another alternative glass material was also tested in a similar manner and Table 3.3 shows that the increase was 9.7%. However, the sample was 5 mm thick compared to 6 mm in Table 3.2 results and allowing for this, 32% would be representative for this BQ-B glass. This highlighted that glass thickness should be minimised to allow maximum microwave energy transmission.

<table>
<thead>
<tr>
<th>Time to Boil (seconds)</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>Mean</th>
<th>Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td>No glass</td>
<td>54.59</td>
<td>62.53</td>
<td>57.01</td>
<td>58.04</td>
<td></td>
</tr>
<tr>
<td>&quot;BQ-B&quot; glass (5 mm thick)</td>
<td>62.47</td>
<td>60.51</td>
<td>68.02</td>
<td>63.67</td>
<td>9.7%</td>
</tr>
</tbody>
</table>

TABLE 3.3: INCREASE IN HEATING TIME FOR "BQ-B" TYPE GLASS SEAL MATERIAL

For the prototypes the following thicknesses and types of glass were used:

- Original Prototype: "7940" type 6 mm thick
- Modified Prototype: "HSQ" type 5.67 mm thick
- 3rd-Generation System: "HSQ" type 5.67 mm thick

A3.1.4 Effect of Particulate on Glass Seal

It was not clear to what extent particulate contaminated glass would attenuate the microwave energy. To assess this a 5.67 mm thick glass sample covered on one side by a layer of particulate (accumulated over several hours with the engine operated on the cycle given in Figure 6.15) was placed over the waveguide exit in a domestic microwave oven. The time for 75 ml of water to boil was measured with the following results (Table A3.3).
| Clean Glass ("HSQ")          | 73.93 |
| Particulate Contaminated Glass ("HSQ") | 74.38 (0.6% increase) |

TABLE A3.3: INCREASE IN HEATING TIME FOR PARTICULATE CONTAMINATED GLASS

The particulate layer would not be expected to be any thicker even after many hundreds of hours (due to the shearing effect of the exhaust gas flow) and hence this negligible increase indicates that contamination is not a problem.
APPENDIX 4

A4.1 MICROWAVE LENS

This Appendix outlines the design of a lens (Section 5.4.2) made from the waveguide glass seal material to help spread out the microwave energy. This lens simultaneously acts as the waveguide seal.

A4.1.1 Theoretical Basis

Jenkins and White, 1957 [43] on p.483 show that as the electromagnetic wavelength approaches infinity, the refractive index, \( n = (e_r)^{1/2} \), where \( e_r \) is the relative dielectric constant of the transparent material. Also the refractive index decreases nonlinearly with wavelength.

From the glass seal manufacturer's data

\[
e_r = 3.81 \text{ at } 30 \text{ GHz, and } e_r = 3.77 \text{ at } 900 \text{ MHz}
\]

Thus for a frequency of 2.45 GHz

\[ e_r = 3.8 \text{ (2 significant figures) and therefore } n_{\text{max}} = (3.8)^{1/2} = 1.95 \]

(The maximum refractive index \( n_{\text{max}} \) is defined since wavelength \( \neq \) infinity).

The refractive index of the glass at visible light frequencies is 1.46 and hence a lens of this material would have a refractive index (at microwave frequencies) of somewhere between 1.46 and 1.95. It would therefore be more effective at refracting microwaves than visible light.
Using refractive indices between these ranges a divergent lens was designed, the dimensions being subject to trap design constraints and calculated from basic geometric optics. The shape is shown in Figure A4.1.
The material manufacturers were unable to supply this cheaply enough, however they could supply a more crude 'lens' as shown in Figure A4.2 free of charge.

This shape had the restrictions that the centre portion is not curved and the curvatures at the sides were only in a single dimension. Despite these limitations it was considered that the crude lens would provide some basis as to whether or not the lens concept warranted further investigation.

![Crude Lens Design](image-url)

**Figure A4.2: Crude Lens Design Used in Experiments (Chapter 5)**
APPENDIX 5

A5.1 THIRD-GENERATION SYSTEM BENCH REGENERATIONS

Here the full set of results of the 14 bench regenerations described in Chapter 6 are tabulated. See Table A5.1 overleaf.
<table>
<thead>
<tr>
<th>DATE</th>
<th>TEST NUMBER</th>
<th>MONOLITH NUMBER</th>
<th>MONOLITH TYPE (thick)</th>
<th>PARTICULATE SIZE</th>
<th>REGENERATION SEQUENCE</th>
<th>TIMING (mins)</th>
<th>REGENERATION EFFICIENCY (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Cell size</td>
<td>Initial Temp</td>
<td>Weight</td>
<td>Load Weight</td>
<td>Gas Load Weight</td>
</tr>
<tr>
<td>7.8.89</td>
<td>1</td>
<td>11</td>
<td>12/200</td>
<td>43.6</td>
<td>95</td>
<td>1502-1510</td>
<td>5.04-5.47</td>
</tr>
<tr>
<td>8.8.89</td>
<td>2</td>
<td>15</td>
<td>17/100</td>
<td>56.0</td>
<td>149</td>
<td>1501-1509</td>
<td>5.04-5.62</td>
</tr>
<tr>
<td>8.8.89</td>
<td>3</td>
<td>15</td>
<td>17/100</td>
<td>56.5</td>
<td>1501-1509</td>
<td>5.04-5.62</td>
<td>(See Test 2 above)</td>
</tr>
<tr>
<td>11.8.89</td>
<td>4</td>
<td>10</td>
<td>12/200</td>
<td>25.2</td>
<td>52</td>
<td>1502-1510</td>
<td>5.42-5.75</td>
</tr>
<tr>
<td>14.8.89</td>
<td>5</td>
<td>16</td>
<td>17/100</td>
<td>20.6</td>
<td>43</td>
<td>1505-1510</td>
<td>5.33-5.52</td>
</tr>
<tr>
<td>15.8.89</td>
<td>6</td>
<td>17</td>
<td>17/100</td>
<td>14.3</td>
<td>53</td>
<td>1401-1511</td>
<td>5.27-5.57</td>
</tr>
<tr>
<td>16.8.89</td>
<td>7</td>
<td>12</td>
<td>17/100</td>
<td>12.1</td>
<td>25</td>
<td>1509-1510</td>
<td>5.56-5.69</td>
</tr>
<tr>
<td>16.8.89</td>
<td>8</td>
<td>13</td>
<td>12/200</td>
<td>6.4</td>
<td>43</td>
<td>3002-3013</td>
<td>4.84-5.38</td>
</tr>
<tr>
<td>17.8.89</td>
<td>9</td>
<td>3</td>
<td>12/200</td>
<td>1.9</td>
<td>30</td>
<td>2509-2525</td>
<td>1.83-2.19</td>
</tr>
<tr>
<td>27.10.89</td>
<td>10</td>
<td>13</td>
<td>12/200</td>
<td>9.6</td>
<td>77</td>
<td>3909-4063</td>
<td>3.35-4.45</td>
</tr>
<tr>
<td>30.10.89</td>
<td>11</td>
<td>13</td>
<td>12/200</td>
<td>8.5</td>
<td>38</td>
<td>8009-8025</td>
<td>1.43-2.19</td>
</tr>
<tr>
<td>1.11.89</td>
<td>12</td>
<td>12</td>
<td>12/200</td>
<td>11.7</td>
<td>64</td>
<td>2000-2009</td>
<td>1.49-1.54</td>
</tr>
<tr>
<td>1.11.89</td>
<td>13</td>
<td>12</td>
<td>12/200</td>
<td>9.9</td>
<td>64</td>
<td>2000-2009</td>
<td>1.49-1.54</td>
</tr>
<tr>
<td>2.11.89</td>
<td>14</td>
<td>13</td>
<td>12/200</td>
<td>6.0</td>
<td>99</td>
<td>2000-2009</td>
<td>1.49-1.54</td>
</tr>
</tbody>
</table>
APPENDIX 6

A6.1 MICROWAVE ASSISTED CHEMICAL REACTIONS

During this study some very basic experiments were conducted to investigate how various organic substances responded to microwave energy.

The following substances in Pyrex beakers were placed in a standard 650W (maximum output) microwave oven and the results qualitatively assessed.

1. Charcoal 'flour'
2. Diesel fuel
3. Isopropylalcohol
4. Engine sump oil
5. Petrol
6. Coal dust
7. Diesel particulate (loose)
8. Diesel particulate (compressed into a pellet).

(Number 8 was 'diesel particulate' obtained by collecting soot on a metal plate held above a burning wick (orange flame) dipped in diesel fuel).

Table A6.1 shows the various combinations of substances tried.
This it was found in this limited survey that only diesel particulate was highly responsive to microwave energy.