MODELLING OF TWO PHASE ROCKET EXHAUST PLUMES AND OTHER PLUME PREDICTION DEVELOPMENTS

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Abstract

Combustion processes result in the creation of an exhaust flow. The exhaust is released into the atmosphere creating a plume. A knowledge and understanding of the exhaust plume flowfield can be important for a number of reasons such as thermal or aerodynamic loading from impingement, infrared signature prediction or environmental considerations (e.g. diesel particulates). Software exists for the prediction of plume flowfields from a number of powerplant types. This software has been developed over several years and uses PHOENICS as the core solver. This paper describes recent developments of the plume prediction software carried out to enhance its capabilities and applications. The particular areas that are described in this paper are 1/ the implementation of a limited two phase capability, 2/ the application of the PHOENICS enhancements to the parabolic capability for underexpanded flows, 3/ the feasibility of using parallel PHOENICS for plume predictions, 4/ the prediction of transient phenomena within plumes.

Computer: Pentium 233-400mHz
Operating system: Windows NT4
Compiler: Digital FORTRAN
PHOENICS version: 3.1

Contents

Introduction

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Software exists for the prediction of plumes. This software has been developed over a number of years and uses PHOENICS as the core solver. This paper describes recent developments of the plume prediction software carried out to enhance its capabilities and applications.

The exhaust plumes from rocket motors, gas turbines and diesel engines can contain significant quantities of particles. The presence of particles within the plume may be a very important aspect which cannot be ignored. For example, the presence of the particles may modify the overall momentum of the exhaust flow producing a different core length, the particles may dominate the infrared signature of exhaust plume, or the particles may be the most significant pollutant present in the exhaust flow.

In rocket exhaust flows, aluminium oxide particles can be present in large numbers according to the propellant type. Although the particles are small in size (being typically less than 10micron) they can still affect the momentum and heat capacity of the exhaust flow. Also because they emit as grey bodies they may have a significant influence on radiative heat transfer from the plume. Further influence may come from changes in phase, with particles forming from condensation, or evaporation taking place.

This paper describes an enhancement to the existing PLUMES prediction software, aimed at providing an efficient way of modelling the effects of particles within exhaust plumes.

Modelling of three dimensional exhaust plumes when considering the transport of a large number of chemical species and reactions can be a very time consuming process. Two methods of increasing the speed of analysis have been examined and are described here. One is the use of the new PHOENICS parabolic capabilities for underexpanded rocket exhausts and the other is the feasibility of using parallel PHOENICS.

Most rocket exhaust flows are highly transient phenomena lasting only a couple of seconds. Whilst modelling these flowfields as steady state provides useful information, far more insight into the real phenomena is obtained by modelling the flowfield transiently from ignition to burn-out. The issues surrounding this approach are also described in this paper.

1. Two-phase modelling

1.1 Modelling strategy

Some of the existing PHOENICS two phase modelling techniques were considered – i.e. IPSA, ASM = algebraic slip model, GENTRA. The need to be able to model a 3D rocket exhaust plume, with typically upwards of 12 chemical species and 18 chemical reactions poses a significant constraint upon adding complexity to the modelling approach. There was concern that IPSA, with the need to model a second set of momentum equations, might make the solution time excessive. It is believed that the particles with rocket exhaust plumes are very small – typically less than 10micron – and that they follow the gas flow very closely. The difference between the particle and gas velocity is believed to be relatively small (for the majority of the particles present). The use of IPSA would only allow a single particle size to be considered. In practice, any need to consider separate particle velocities would probably only be worthwhile if several different diameters could be considered. Such a requirement might be met through the use of GENTRA, but this would require large numbers of particle tracks to be considered if the bulk effect was to be correctly simulated.

For this reason, a new modelling approach was developed in which only the gas phase momentum was modelled (i.e. assuming the particles are 'lazy') but the influence of the particles upon bulk density was calculated.

1.2 Particle influence on momentum and energy

Particulate species at the nozzle exit plane are specified as mole fractions in the same way as the gaseous species. Particulates are inert in this version.

The gas density is calculated as normal from the ideal gas law, using the mean molecular weight of the gaseous species.

An overall particulate mass fraction is calculated as the sum of the particulate concentrations times the species molecular weight:

$$m_f = \Sigma \ (M_{fi} * smw/mmw) \qquad\qquad (1)$$

where M_{fi} is the mole fraction of any particulate species, *smw* is the species molecular weight and *mmw* is the overall mixture molecular weight.

and the mean particulate species density as:

$$\rho_p = m_f / \Sigma (M_{fi} / \rho_i) \qquad (2)$$

the particulate volume fraction is then:

$$V_f = (m_f/\rho_p) / [(1-m_f)/\rho_g + m_f/\rho_p] \qquad (3)$$

where ρ_g is the gas mixture density and the overall mean density is:

$$\rho = V_f \cdot \rho_p + (1-V_f) \cdot \rho_g \qquad (4)$$

Wherever the pressure is calculated, the gas density is used, including the pressure force contribution to the thrust. However, the mixture density is used in any momentum calculations.

An extra variable, PVOL, is stored which is the particulate volume fraction. Species boundary conditions are prescribed in exactly the same way as for single phase plumes.

Early tests with this approach showed that the technique produced changes in exhaust plume mixing when particles where present. This was as a result of the influence of the higher density on momentum – see Figure 1.

This approach was extended to allow the particles to influence the temperature of the plume through the Cp. Again, it was felt that the small particles had a very little temperature lag compared to the gas. A typical result is shown in Figure 2.

The mixture Cp and enthalpy are calculated including the particulate species in exactly the same way as the gaseous ones – i.e. assuming that mixture stagnation enthalpy is conserved and calculating Cp using a ninth order polynomial the coefficients of which are based on data from the JANAF tables. In addition, a separate Cp for the gaseous species only is calculated. This and a mixture gas constant (for the gaseous species only) are used to calculate γ - the ratio of specific heats. This is based on the assumption that the compressibility of the particulate species is negligible, and that their overall volume fraction is small.

A new subroutine calculates and stores the particulate volume fraction on a slabwise basis. The $d\rho/dp$ calculation in GROUND uses only the gas properties, as does the Mach number calculation at the end of the run.

Overall the above approach allows solid and liquid particles within the rocket plume to influence the momentum and temperature distribution without the overhead of a second set of equations being solved.

1.3 Phase change source terms

The temperature changes within a rocket exhaust plume are large. This occurs for the following reasons.

1. The plume starts from a combustion chamber with very high stagnation temperature (typically 3000K).
2. The acceleration through the convergent/divergent nozzle which usually continues in the atmosphere, reduces the local static temperatures within the gas to below 1000K. At these temperatures many of the reactions may cease.
3. Shock waves within the exhaust decelerate the flow (sometimes to subsonic values) raising the static temperatures back towards the stagnation values.
4. The mixing of atmospheric oxygen with the exhaust plume and the increases in local static temperature can result in secondary combustion occurring within the plume raising the temperatures still higher.

As particles travel through these regions of temperature variation, changes in phase can occur. Gas concentrations of, say, aluminium oxide may condense forming liquid particles. Liquid particles may freeze to form solid ones, and vice-versa. These changes in phase may have a significant influence on both the gas momentum and on the plume temperature as well as determining the overall level of particulates within the plume.

Without solving for a separate phase, the above techniques have been extended to allow particle phase changes to be taken into account. These are described below.

a) liquid-solid phase change

A mass transfer source term has been written to allow a liquid-to-solid phase change to take place for particulate species modelled within the PLUMES code.

The rate of phase change within each droplet or particle is controlled by the rate at which heat transfer between the particle and the gas phase can take place. This in turn is dependent on the temperature lag and relative velocity between the particle and the gas.

This version of the PLUMES code (5.1) does not model the particle velocity or temperature lag explicitly, consequently the formulation of a source term requires some assumptions to be made about the particle-to-gas phase heat transfer.

For pure substances, the liquid-to-solid phase change is isothermal, and the melting point temperature (Tmp) is effectively constant. It can then be assumed that the particle temperature remains at Tmp as long as the phase change is taking place. A temperature difference then exists between the bulk fluid at temperature T and the particle temperature Tmp. (Strictly speaking the

gas temperature rather than the bulk temperature should be used.)

The rate of heat transfer from the particle to the gas is then given by:

$$Q = K_h.A_s.(T_{mp}-T) \qquad (5)$$

where K_h is a heat transfer coefficient and A_s is the surface area.

For a spherical particle in a flow at a low Reynolds' number, the Nusselt number Nu is approximately 2. If the particle velocity lag is small, the heat transfer coefficient is then:

$$K_h = Nu*\lambda/D_p \qquad (6)$$

where λ is the gas thermal conductivity and D_p the particle diameter.

If $T < T_{mp}$, the liquid-to-solid transfer rate for each particle is then:

$$S_p = Q/H_{fs} = K_h.A_s.(T_{mp}-T)/H_{fs} \qquad (7)$$

where H_{fs} is the latent heat of fusion in J/kmol.

The number of particles of a particular species and phase per unit volume is given by;

$$n_p = r_p /(\pi D_p^3/6) \qquad (8)$$

where r_p is the liquid species volume fraction

The liquid-to-solid transfer rate per unit volume (in kmol/s/m^3) is then

$$S_{vol} = S_p * n_p$$
$$= K_h.6/D_p.(T_{mp}-T) \, r_p/H_{fs} \qquad (9)$$

and

$$r_p = (C_l)*smw*\rho/\rho_p \qquad (10)$$

where C_l is the species concentration (in kmol/kg) of the liquid species, ρ is the bulk mean density and ρ_p is the particle density.

It is assumed that there is no difference in density between the liquid and solid phases for a given species, and that the particle size does not change.

This transfer rate can be linearised for inclusion as a PHOENICS source term in the following way:

The source term for each phase i, $S = cell \, vol.Co.(Val - C_i)$ (11)

$$where \; Co = K_h.6/D_p/H_{fs}.|T_{mp}-T|*smw*\rho/\rho_p \qquad (12)$$

and if $T < T_{mp}$,
for the liquid phase   Val = 0
for the solid phase   Val = C_l +C_s

This gives equal and opposite sources for the liquid and solid phases, in units of kmol/s. The source term drops to zero when the liquid phase concentration is zero.

This source term will also function as a melting rate if $T>T_{mp}$, but with Val = C_l+C_s for the liquid, and Val = 0 for the solid.

b) gas-liquid and gas-solid phase change

A mass transfer source term has been written to allow a gas-to-liquid phase change (ie condensation) to take place for species modelled within the PLUMES code. A similar term to allow a gas-to-solid phase change at temperatures below the melting point has also been written.

The rate of phase change at the surface of each droplet or particle is controlled by the rate of diffusion of the species from the bulk fluid to the surface. This is dependent on the difference in species concentration between the bulk and the surface and a mass transfer coefficient in turn dependent on the relative velocity between the particle and the gas. (Whilst a term dependent on the droplet to gas heat transfer rate could be used, this would require the temperature lag to be modelled.)

The PLUMES code does not model the particle velocity explicitly, consequently the formulation of a source term requires some assumptions to be made about the mass transfer coefficient.

If any temperature lag is ignored, the species concentration in the gas at the droplet surface can be assumed to be the saturation value at the bulk temperature.

For each droplet the rate of mass transfer from gas to droplet is then given by:

$$S_p = K_m.A_s.(C_{sat}-C_g).\rho \qquad (13)$$
where K_m is a mass transfer coefficient and A_s is the surface area. C_g is the gas species concentration in kmol/kg, ρ the bulk mean density and $C_g > C_{sat}$ if condensation is taking place.

C_{sat} is proportional to the saturation vapour pressure p_{sat} of the species:
$$C_{sat}*gmw = p_{sat}/p \qquad (14)$$
Where p is the local static pressure and gmw the mean molecular weight of all the gaseous species.

The vapour pressure is a function of temperature and can be estimated as
$$p_{sat} = e^{(a-b/T)} \qquad (15)$$

where a and b are constant for a particular species and can be determined if two points on the saturation line are known [1].

For a spherical particle in a flow at a low Reynolds' number, the Sherwood number Sh is approximately 2 (cf Nu = 2 for heat transfer - a valid analogy if the species concentration is small). If the particle velocity lag is small, the mass transfer coefficient is then:

$$K_m = Sh*D/D_p \qquad (16)$$

where D is the diffusivity of the species in the mixture and D_p the particle diameter.

The number of droplets of a particular species and phase per unit volume is given by equation 8.

The gas-to-liquid transfer rate per unit volume (in kmol/s/m^3) is therefore

$$S_{vol} = S_p * n_p$$
$$= K_m.6/D_p.(C_{sat}-C_g).\rho. \ r_p \qquad (17)$$

where r_p is defined in equation (10)

This transfer rate can be linearised for inclusion as a PHOENICS source term in the following way:

The source term for each phase i, S = cell vol.Co.(Val - C_i) (11)

$$\text{where Co} = K_m.6/D_p.*smw*C_l.\rho^2/\rho_p \qquad (18)$$

and
for the gas phase   Val = C_{sat}
for the liquid phase Val = $C_g-C_{sat}+C_l$

This gives equal and opposite sources for the gas and liquid phases, in units of kmol/s. The source term drops to zero when the liquid phase concentration is zero - ie some droplets must be present in the flow to allow condensation to take place.

There is no mechanism in this implementation to allow the droplet size to vary. The assumption is therefore made that the *number* of droplets increases as the condensed phase volume fraction increases.

This source term will also function as an evaporation rate if $T>T_{sat}$.

The source term for gas-to-solid transfer is identical except that the solid phase concentration is used in place of the liquid phase. Since the solid phase will only come into existence if the temperature dips below the melting point, a cut-off for this source term at T_{mp} is not necessary. Strictly speaking, while both liquid and solid species exist, C_{sat} should be for $T=T_{mp}$, as the

droplet/particle temperature is assumed to remain at that value while the solidification process takes place (see notes on liquid-to-solid phase change.)

c) implementation within GROUND

The Coefficient and Value for the LIQUID-SOLID and GAS-LIQUID phase change source terms are calculated in a new subroutines called from Group 13 of the PLUMES GROUND subroutine.

For the species for which a phase change occurs, the location of the gas, liquid and solid phases in the species list in the input files are specified in a separate file - PHASE.IN. Condensed phase species are solved for if they are expected to form within the plume, even if the exit plane temperature is such that their mole fraction is negligible at that point. The particle diameter for each condensed phase has to be specified by the user.

The latent heat of fusion is calculated from the difference in enthalpies of the solid and liquid phases at Tmp. The gas thermal conductivity is assumed to be the same as that of air and varies linearly with temperature.

Very little data is available for the mass diffusivity of individual species in air, so a constant value of 0.1e-3 m^2/s has been assumed. This value is of the same order of magnitude as the diffusivity of a number of binary gas mixtures.

The constants used in the expression for the vapour pressure for each species are read from a new file - PHASED.

d) example calculation using the phase change model

The case studied is a plume which includes all three phases of a metal compound and which includes reactions. The following conditions govern the flow –

exit plane pressure:	1 atm
exit plane temp:	2000K
exit plane velocity	600m/s
free stream velocity	200 m/s

In the absence of available data, the vapour pressure curve for this compound was estimated from 1 known point on the saturation line (the normal boiling point - 2536K at 1atm) and an assumption that the vapour pressure at the melting point (T=1536K) is a small fraction (0.2%) of the value at 2536K.

No data was available for the mass diffusivity, so a value of 0.1e-3 m^2/s was assumed - this is of the same order of magnitude as the diffusivity of a number of binary gas mixtures.

Figures 3-6 show the effect including phase change for a reacting plume. A comparison between Figures 3 and 4 shows that the influence of including

condensation of the metal particles is significant. The downstream plume temperatures are much higher for the case when the metal particles are allowed to evaporate and the gaseous phase then reacts. This result is quantified in Figure 6. Figure 5 shows the effect of condensation and solidification in the shear layer of the plume.

No significant changes in run time were noticed when including the effects of condensation and solidification within the plume model in addition to reaction source terms. Furthermore, the stability of the plume calculation was not impaired by adding these extra source terms.

1.4 Validation

The above approach makes a number of assumptions with regard to particle size and loading and the lags in velocity and temperature. Very little data is available to validate the predictions in order to justify these assumptions. Recently, work has been carried out to measure particle velocity and particle size distributions within rocket exhaust plumes (see references 2 and 3). This work has been primarily aimed at establishing the viability of the laser based measurement techniques. However, some information about particle size and velocity has come from these measurements. This information indicates that there are a very large range of particle sizes with the largest number being in the 0 –30 micron range and small quantities of particles up to 100 micron. The measurements have also shown a large range of velocities with particles velocities over 2000m/s being measured.

The indications are that the techniques for modelling the flowfields described above may be appropriate for some of the particles found within the plume but that there are almost certainly areas where the simplifications will not capture the full nature of the flowfield. There is very little data at this stage on exactly what the impact of the particles is on the shock wave distribution and temperature of the flowfield.

2. Application of the parabolic solver

CHAM has carried out work to extend the parabolic capabilities of PHOENICS (see reference 4). The IPARAB=5 setting can now be used to successfully model underexpanded free jets. This capability has been implemented within the plumes code in order to enhance the speed of exhaust plumes in 2D and 3D when the flowfields are clearly going to be parabolic in nature.

To implement this new feature, the IPARAB=5 setting is made along with the value of LITER - the number of iterations. A value of 50-100 is generally required for this parameter. The variable RSG(40) should be set > 1 (typically 100); this a factor which is used to multipy the influence coefficients ($\partial u/\partial p$

and $\partial v/\partial p$) in the pressure correction equation in the sub-sonic regions. The use of the PARPHI or PARADA files needs to be implemented. Similar levels of under-relaxation are required as for the elliptic solver although these may need to be higher (tighter) if the initial part of the flowfield is difficult to resolve. The variable PBAR is set to the free stream pressure.

For flows with a supersonic free stream, a different coefficient is set for pressure at the outer boundaries of the jet to prevent shock reflections at these boundaries.

For non-reacting plumes with weak to moderate (but not strong)shocks, the parabolic solver can provide results which match the results of the elliptic solver but at a much faster speed – typically 8 times faster when predicting 3D plumes.

With regard to reacting plumes, it has been found that the initial changes in the flowfield in the first slab or two cannot be adequately resolved using the parabolic solver even with a high number of iterations. For this reason, development work is presently underway to allow the results from the final slab of an elliptic plume calculation to be used as the boundary conditions for a parabolic calculation – thus making optimum use of both solver capabilities. Such a technique would also be useful for plumes with base regions, plumes which are not on axis to start with but are turned by the free stream, plumes with strong shocks in the near field, and plumes which may need to solved with a BFC grid to start with (e.g. where the nozzle is included).

3. Parallel PHOENICS

A brief study has been made to investigate the feasibility of using the parallel version of PHOENICS (see reference 5) for enhancing the speed of solution of the PLUMES software. It was not clear at the start whether the parallel version could be used to enhance the speed of solution of a case with such a predominant flow direction in the slabwise orientation which is the same direction as the domain decomposition.

The work was carried out using a Silicon Graphics Origin 200 machine with 4 processors and running under IRIX6.5. The PHOENICS version was 3.1.

Initially a simple, inert, 2D axisymmetric jet test case was carried out. This showed approximately 2.5 times speed up in execution for the 4 processors.

The satellite and ground coding of the plumes software were then compiled and linked to the parallel version of PHOENICS. A test case for a rocket exhaust plume with combustion was run successfully under the parallel version. The speed up was again approximately 3 times for 4 processors and seemed almost linear with number of processors.

Overall the indications were that the parallel version of PHOENICS could be used to speed up calculations of rocket exhaust plume predictions.

4. Transient calculations of rocket exhaust plumes

As stated above, most rocket motor exhaust plumes last for only a few seconds. The build up of pressure and temperature in the combustion chamber from ambient to around 100 atmospheres and 3000K within a fraction of a second make the plume development a highly transient and violent phenomenon. Transient calculations of plume flowfields are now being carried out. Some success has been achieved with realistic results being produced – see Figure 7.

The transient predictions can be more difficult to converge than their steady state equivalents. In steady state plumes the usual practice is to provide initial fields in the expected location of the plume; these initial fields usually specify the exit plane temperature, velocity and chemical composition of the plume and are found to allow gradual and stable development of the plume flowfield. However in the case of transient flowfields, such initial fields are inappropriate and only free stream values can be specified in the domain. As the exhaust emerges, very high temperature and pressure gradients develop between the exhaust front and the free stream – hence the requirement for very small time steps with slightly increased under-relaxation values. Also, the phenomena occur extremely rapidly requiring initial time steps typically of the order of 100 micro-seconds to resolve the phenomena. Often the under-relaxation can be reduced as the flow develops and the number of sweeps reduced as the plume progresses.

Conclusions

Further development work has been carried out on exhaust plume prediction software based on PHOENICS. A major development has been the ability to provide limited two phase rocket motor exhaust plume predictions. Within this enhancement, a second set of momentum and energy equations are not solved but the presence of solid and liquid particles within the plume are allowed to influence the density of the flow and thus modify the jet momentum. Also, source terms have been provided to allow limited phase changes to be modelled. Work to evaluate the validity of this approach has commenced.

Plume predictions often involve the transport of a significant number of chemical species and the provision of source terms to describe the associated chemical kinetics. In 3D, the computational run times associated with such calculations can be significant. CHAM's recent parabolic solver enhancements have been incorporated into the plumes prediction software in order to provide large savings in run time and memory. The application of the parabolic solver has highlighted the need to provide an elliptic/parabolic interface in the future in order to optimise the use of these capabilities. The feasibility of using parallel PHOENICS to provide further run-time improvements for the elliptic solver has been examined. The parallel version of PHOENICS has been successfully applied to 2D axisymmetric plume predictions in which the flow direction is predominantly slabwise (z-direction) and in which reaction source terms are being calculated. If a cost effective

installation of the parallel solver can be provided (both in terms of hardware and software), then significant speed improvements are viable.

Many exhaust plumes, in particular those from rocket motors, are highly transient in nature. Work on predicting the development of the plume has been carried out. Some successful results have been obtained for 2D and 3D plumes with and without reactions, although careful choice of the time step size and under-relaxation is required because the initial fields can no longer be used to aid convergence.

Acknowledgements

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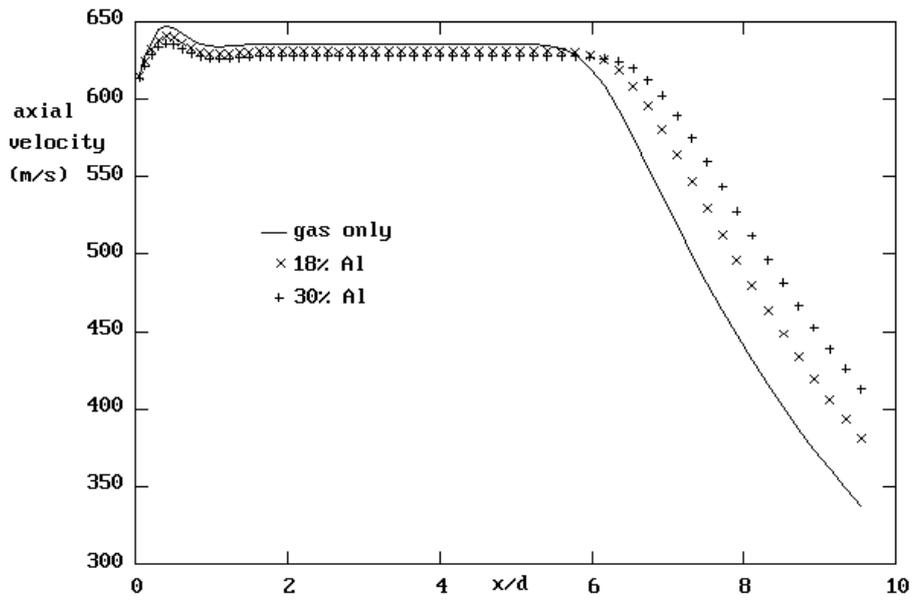
Figure 1 Influence of particle loading on exhaust plume centreline velocity decay
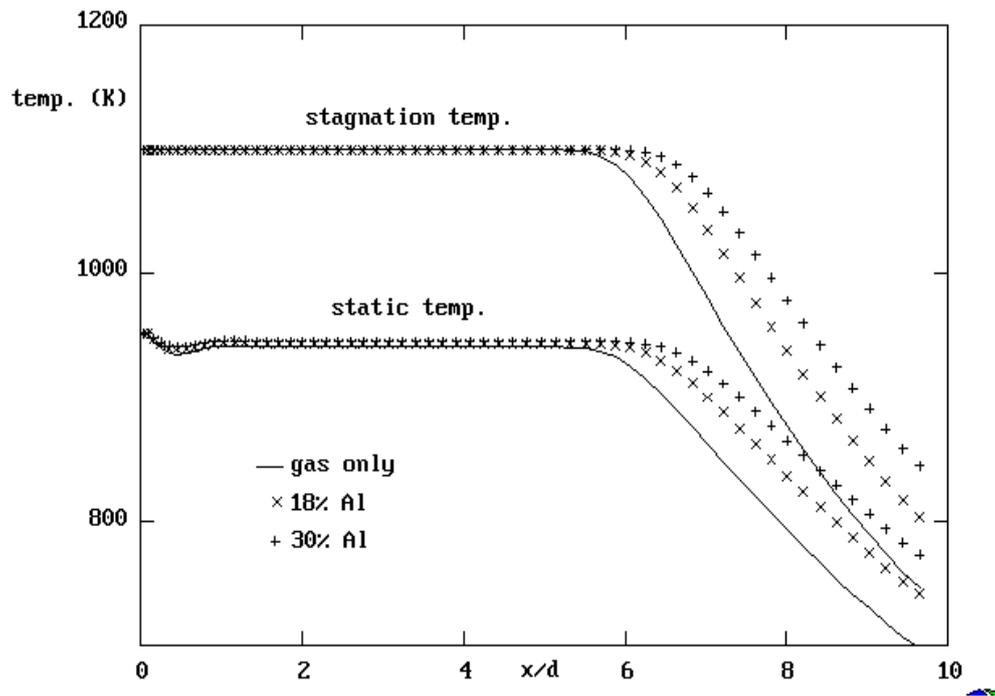

Figure 2 Effect of particle loading on exhaust plume centreline temperature decay

Temperature contours - reacting plume

Figure 3

Temperature contours - reacting plume with condensation and solidification
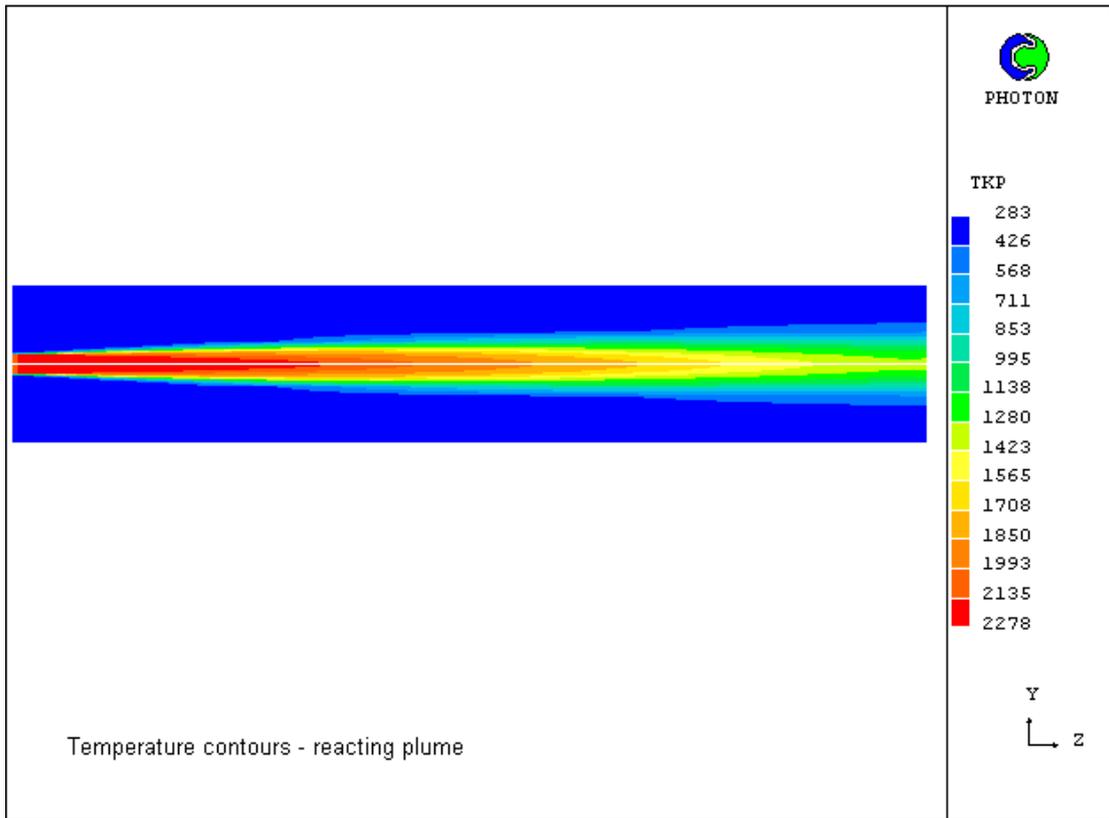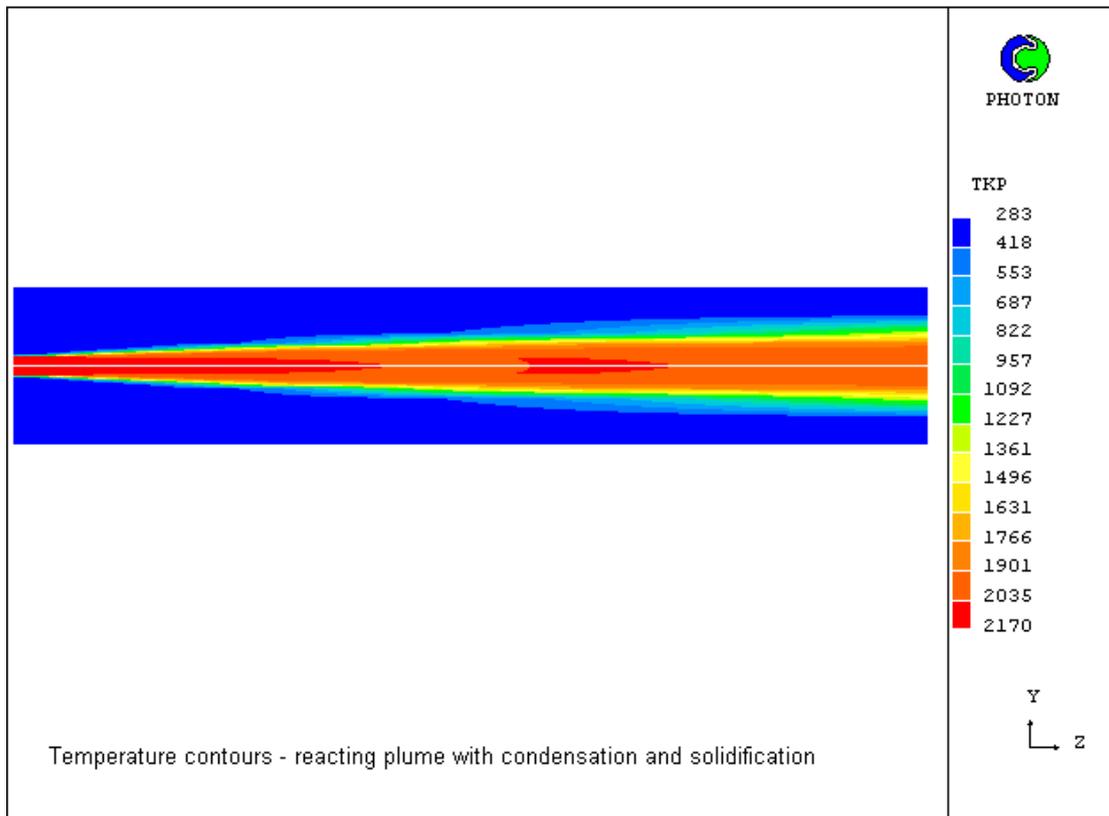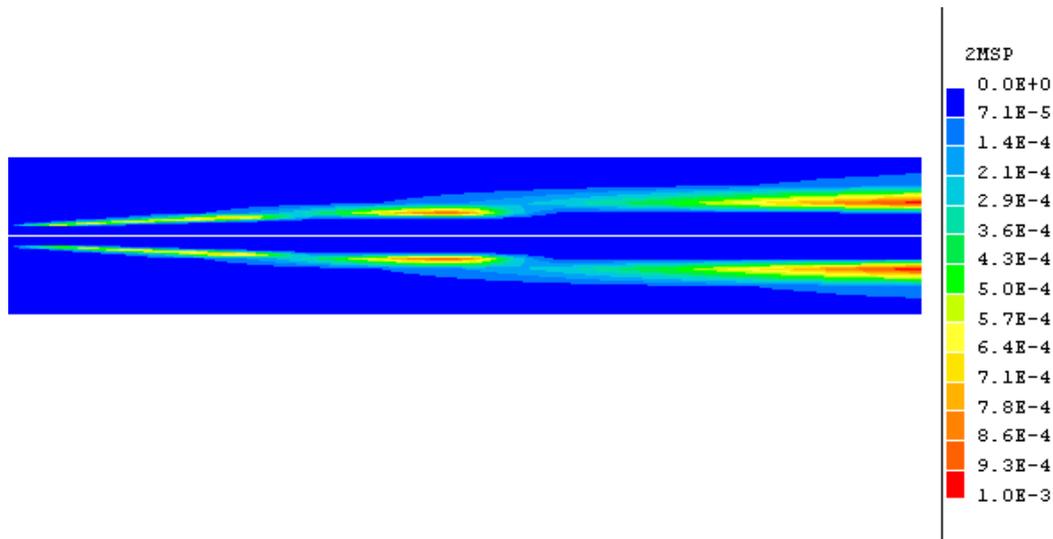
Figure 4

Figure 5 Contours of solid particles in rocket exhaust plume for condensation and solidification
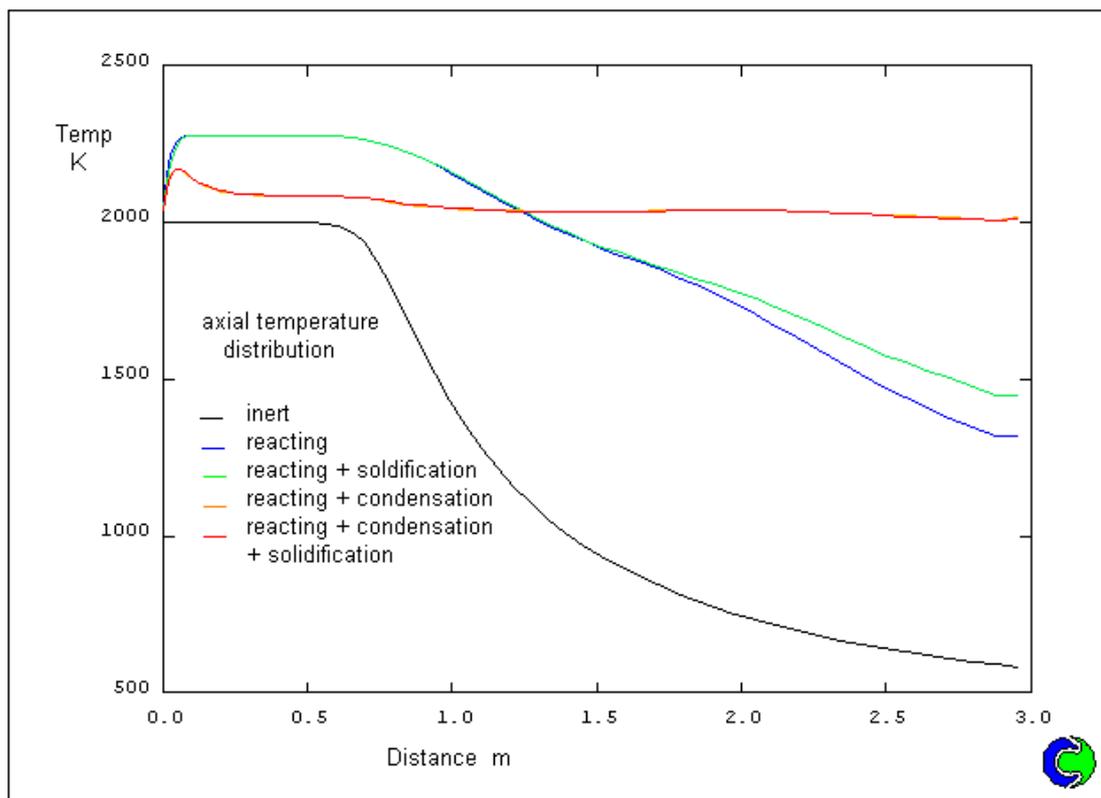
Figure 6 Predicted centreline temperature distribution for multiphase plume
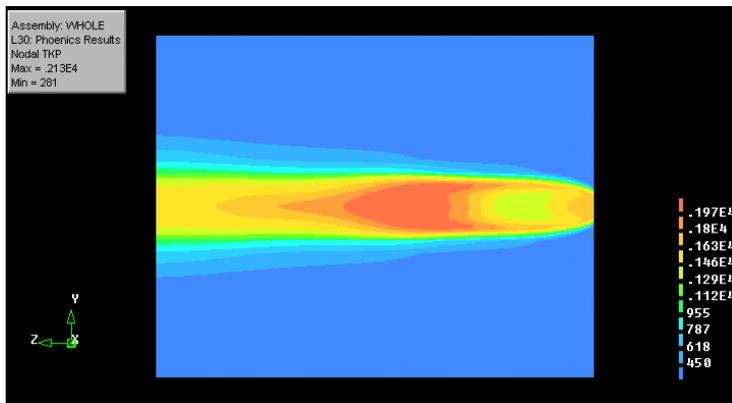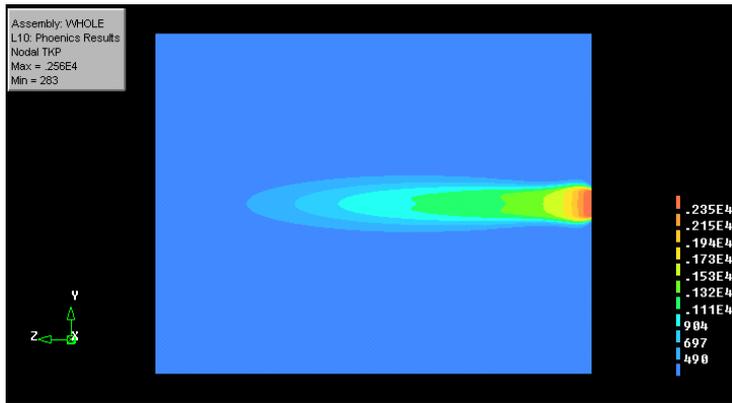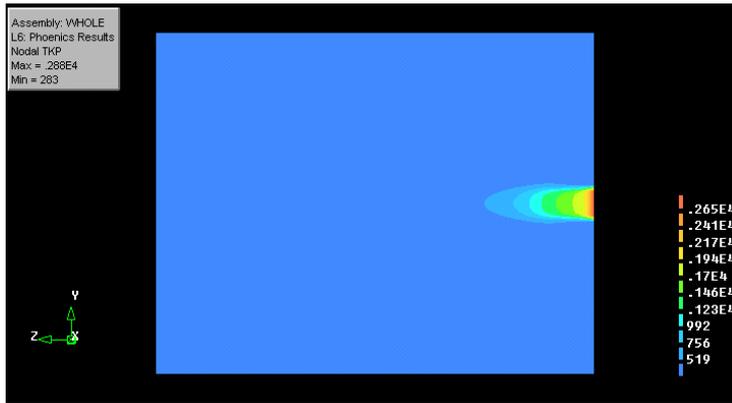
Figure 7 Transient prediction of reacting rocket exhaust plume development