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## Effects of Radiation on Predicted Flame Temperature and Combustion Product of a Burning Liquid Fuel Spray

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### ABSTRACT

The effects of radiative heat transfer calculations on the predicted temperature rise in a burning liquid-fuel spray, are studied. The adiabatic temperature rise resulting from a comprehensive spray combustion model is adjusted for heat transfer to the chamber cooling water by incorporating a radiation model using the Discrete Transfer Technique. The spray combustion model used is of the 'mixed-is-burnt' type where combustion is treated as a post process event. The data needed for the combustion post-processor are obtained from an effective property Locally Homogeneous CFD flow model, incorporating a droplet evaporation model to account for the liquid phase. The combustion model itself is based on the minimisation of Gibbs free energy and incorporates kinetic sub-modules for soot formation and oxidation. The results from the combustion model are fed into a radiation sub model for calculating cell emissivities. These are used to calculate corrective terms for incorporation within the energy balance employed by the combustion model resulting in corresponding temperature (and, subsequently, composition) corrections. The convergence of this iterative process yields results of product concentrations and of temperature throughout the combustion chamber. The predicted results are compared with existing experimental result in a case study. The results are also compared with those obtained from the combustion model with no radiation correction and also with ones obtained with empirical corrections.

### INTRODUCTION

The ability to predict spatial and temporal variations of flow properties, chemical species, temperature and soot concentrations in burning liquid fuel sprays is of great importance in the design of many practical combustion systems. These systems are continuously required to meet ever increasing stringent demands for cleaner exhaust. The use of reliable mathematical models capable of simulating the operation of any of these combustion systems enables various design improvements aimed at cleaner combustion and safer and more efficient operation to be tested at a relatively low cost. However, the processes involved in spray combustion are varied and extremely complex rendering a full analysis of the problem very difficult. This has prompted researchers into employing simplifying assumptions and/or limiting their analysis to one aspect of the problem (such as the mixing analysis or the evaporation process). Attempts at full analysis from injector to exhaust were also made but with certain assumption regarding some aspects of the problem such as the atomisation process, the evaporation process and the combustion process.

The Locally Homogeneous Flow (LHF) approach was adopted by most workers to describe the flow field resulting from the two-phase flow spray. This was thought to be more applicable to dense sprays than the more

advanced Separated Flow (SF) type models in their present form (Faith (1987), Wu *et al* (1983)). The basic premise of the LHF approach is that the transfer processes between the two phases are fast in comparison to the rate of development of the flow field as a whole. The evaporation from the spray, generally speaking, is not accounted for directly in this approach; instead the fuel vapour fraction in each control volume is calculated from the saturation vapour pressure in the volume. LHF type models can be made more effective by incorporating a droplet evaporation sub-model within the formulation. This allows droplet properties with the most significant effects on the gas-phase to be accounted for while maintaining the essential characteristics of the LHF type formulation. A model of this type was developed by Nazha *et al* (2000) and was used in a parametric study to investigate the effects of pressure, temperature and droplet size on the behaviour of a burning spray. The same model was also adapted to be applicable to burning water-in-diesel fuel emulsions (Nazha *et al* (1999)). The model was initially developed for a spray burning adiabatically in a confined space. No heat transfer effects were considered and the flame temperature was either left at the predicted adiabatic value or corrected (for particular case studies) by removing from the input energy a fraction equivalent to that found to be absorbed by the cooling water experimentally. This model has been developed further by the inclusion of a thermal radiation module within the analysis.

### MODEL FORMULATION

As stated above, the LHF type approach was adopted in the development of the 2-D, steady state finite volume model (Rajakaruna (1997)). This model is capable of describing the behaviour of a reacting two-phase flow. Fuel and air are assumed to enter a cylindrical combustion chamber co-axially through two concentric tubes. The dimensions of the chamber and the diameters of the two tubes can be varied. The fuel type can also be varied by supplying the programme with the relevant fuel properties. Evaporation from the liquid fuel is accounted for via a droplet evaporation sub-model that runs in parallel with the mixing analysis and exchanges data with it. The programme is modular in structure enabling the addition of new modules and the omission or replacement of existing ones. In addition to the evaporation module, a flame temperature module, a combustion module and a soot production module are included in the code. Recently, a thermal radiation module has been added to account for the heat transfer effects. The original model has been described previously (Nazha *et al* (2000)), therefore only a brief description of the main components is presented below with particular emphasis on the new addition, mainly the thermal radiation and the way it is incorporated within the analysis.

#### Mixing Analysis

A Navier-Stokes solver based on the SIMPLE algorithm (Patankar (1980)) is used to carry out the mixing analysis. The differences between the two phases within the control volume are neglected in this LHF type formulation and average flow properties are determined for each volume. This is achieved by taking appropriate account of the property value for the liquid fuel, fuel vapour and air present within the volume. Property changes resulting from the evaporation of the liquid fuel are thus allowed to propagate according to the turbulent mixing model affecting the overall mixing process. The generic form of the gas-phase equation set is:

$$\frac{\partial(\rho u \phi)}{\partial x} + \frac{1}{r} \frac{\partial(r \rho v \phi)}{\partial r} - \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \phi}{\partial x} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left( r \Gamma \frac{\partial \phi}{\partial r} \right) = S_\phi$$

Where  $\phi$  is the generalised flow variable and  $S_\phi$  is the source term which is explicitly given in the table below (the lower case  $s_\phi$  term in each source term is there to account for the wall boundary conditions).

| $\phi$        | $S_\phi$   |
|---------------|--|
| 1             | -  |
| $u$           | $-\frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left( \mu_e \frac{\partial u}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \mu_e \frac{\partial v}{\partial x} \right) + s_u$                         |
| $v$           | $-\frac{\partial P}{\partial r} + \frac{\partial}{\partial x} \left( \mu_e \frac{\partial u}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \mu_e \frac{\partial v}{\partial r} \right) - 2 \mu_e \frac{v}{r^2} + s_v$ |
| $T$           | $s_T$  |
| $m\ddot{n}$   | -  |
| $k$           | $G - C_D \rho \varepsilon + s_k$   |
| $\varepsilon$ | $C_1 \frac{\varepsilon}{k} G - C_2 \frac{\rho}{k} \varepsilon^2 + s_\varepsilon$   |

where  $G = \mu_e \left\{ 2 \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial r} \right)^2 + \left( \frac{v}{r} \right)^2 \right] + \left( \frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right)^2 \right\}$

#### Evaporation

Evaporation from the spray is assumed to be represented by the evaporation of a Sauter Mean Diameter droplet travelling along the spray axis. The history of such a droplet is determined via a droplet evaporation sub-model. This sub-model is of the transient, variable property, quasi-steady gas-phase and finite liquid diffusivity type (Rajakaruna and Nazha (1998)). The following equations of heat and mass transfer are solved in the evaporation analysis:

$$\frac{\partial T}{\partial t} = \alpha \left( \frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right)$$

where  $\alpha = \frac{k_L}{C_{p_L} \rho_L}$

subject to the following boundary conditions at the droplet surface and centre respectively,

$$4\pi r^2 k_L \left( \frac{dT}{dr} \right)_s = h_c 4\pi r^2 (T_\infty - T_s) \frac{z}{e^z - 1} + \frac{dm}{dt} L$$

$$\left( \frac{\partial T}{\partial r} \right)_{r=0} = 0$$

$$\frac{dm}{dt} = -A K_c P_{\text{fl}} \alpha_c$$

where;  $k_L$  = liquid thermal conductivity  
 $L$  = enthalpy of evaporation

$r$  = droplet radius  
 $m$  = droplet mass  
 $z$  = factor accounting for mass transfer  
 $\alpha_c$  = correction for mass transfer  
 $T$  = temperature  
 $P$  = pressure

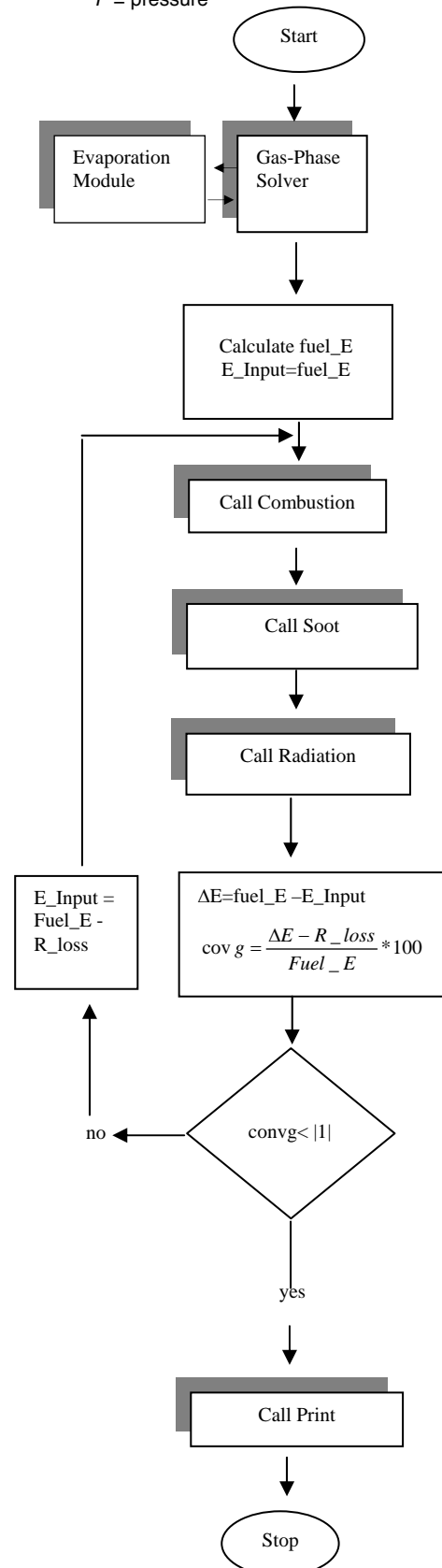


Fig. 1 Flow diagram of the overall model

### Combustion

The mixed is burnt approach is adopted for this analysis. This in effect assumes that evaporation and mixing are the controlling factors enabling the combustion analysis to be carried out as a post process activity. The relevant local data from the mixing analysis are passed to the combustion module where the gaseous products soot concentrations and flame temperature are calculated. The gaseous products are assumed to attain their equilibrium values which are evaluated by minimising the total Gibbs free energy of the system. The technique used for this is based on the approach developed by Nazha (1983) and described by Crookes and Nazha (1990). Kinetics models for soot formation and oxidation are used to predict the concentration of soot inside the burning spray. The approach developed by Narasimhan (1964) for Methane and modified by Nazha (1983) to account for liquid fuels is used to predict the rate of soot formation while soot oxidation rate is accounted for by adopting the approach of Appleton (1973). The flame temperature is calculated using the adiabatic temperature rise initially. This is then corrected, where appropriate, by a correction factor derived from the radiation calculations or from the experimental values of the heat transfer to the cooling water if known.

### Thermal Radiation Sub-Model:

The radiation model uses the Discrete Transfer Method developed by Lockwood and Shah (1981). The method is based on the direct solution of the radiation transport equation given below.

$$\frac{dI}{ds} = K_g \frac{\sigma T^4}{\pi} - K_g I$$

Where  $I$  &  $s$  are the radiant intensity and the distance respectively in the direction of  $\Omega$ , where  $\Omega$  is a direction vector;  $K_g$  is the gas absorption coefficient  $\sigma T^4$  is the black body emissive power of the gas ( $E_b$ ) and  $\sigma$  is the Stefan-Boltzmann constant. The gas absorption coefficient can be related to the cell emissivity by:

$$\varepsilon_g = 1 - e^{-K_g L}$$

Where  $L$  is the path length; and the total emissivity of a cell is obtained by using a mixed grey gas model (Truelove (1976)). The solution procedure is based on an iterative ray tracing technique, which is applied to the integrated form of the radiation transport equation. Further details of this procedure are given in (Carvalho *et al* (1991), Malalsekera and James (1993)). In the current analysis the radiation module is run in parallel with the combustion module as a post process event.

### Global Convergence Procedure:

The method used in the current analysis differs from other radiation modelling methods by the technique used for global convergence. The overall convergence is achieved by sequentially iterating the three sub models (flame temperature, product formation & radiation) until a global convergence criteria based on the overall energy balance within the chamber is achieved via controlled reduction of the fuel energy input. A flow diagram depicting this process is shown in fig. 1.

## RESULTS AND DISCUSSION

As stated earlier, the versatility of the model was demonstrated previously in a parametric study, on diesel fuel and on emulsified fuels (Nazha *et al* (2000) and (1999)). Radiation did not form part of those studies and

the flame temperature was based on adiabatic temperature rise and corrected for the heat transfer to the chamber cooling water by deducting the amount of energy removed by the water (arrived at experimentally) from the total energy input into the chamber. The objective of the present study is to investigate the effects of adding the thermal radiation sub-model on the predictive capability of the model as a whole. This is best demonstrated by a case study for which experimental results are known. The experimental results against which the predicted ones are to be compared have been obtained by Nazha (1983) and described by Nazha & Crookes (1984). The model was run for diesel fuel at a pressure of 650 kPa and an input equivalence ratio of 1.085 (conditions for which the experimental results were obtained). The relevant parameters of chamber dimension, fuel injection, ..etc. were also similar to those of the experimental tests.

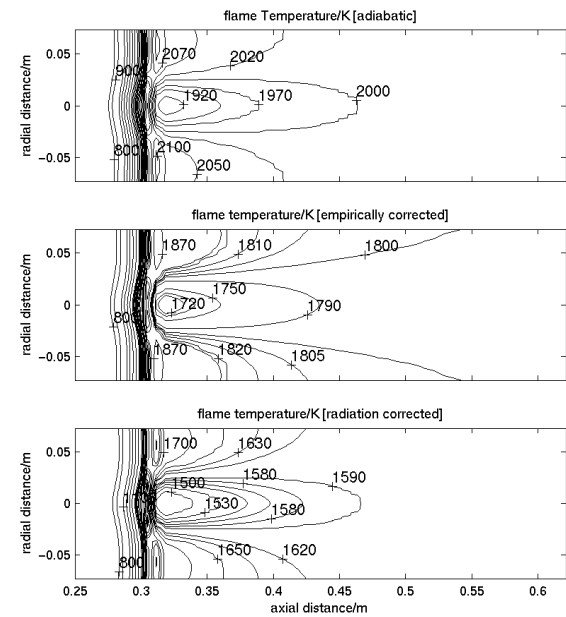


Fig. 2 Predicted iso-thermal contours

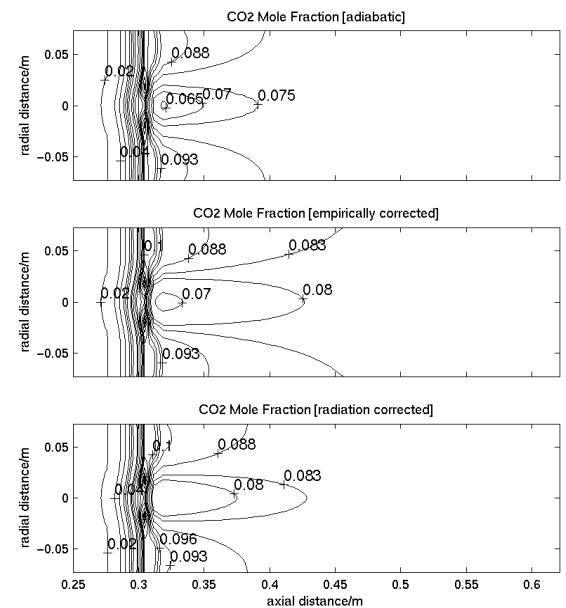


Fig. 3 Predicted iso-concentration contours for CO<sub>2</sub>

The effect of thermal radiation calculations on flame temperature within the chamber is evident in fig.2. This figure shows the predicted isothermal contours obtained from adiabatic calculations and those with empirical correction as well as those with the new thermal radiation correction. Taking radiation into account appears to result in approximately 20% reduction in flame temperature indicating that 20% of the fuel energy is removed by the chamber cooling water. Although this figure is consistent with general expectations, the empirically corrected flame temperature contours show a lower figure of 12 – 15% only; giving flame temperature values closer to the experimental ones (described later).

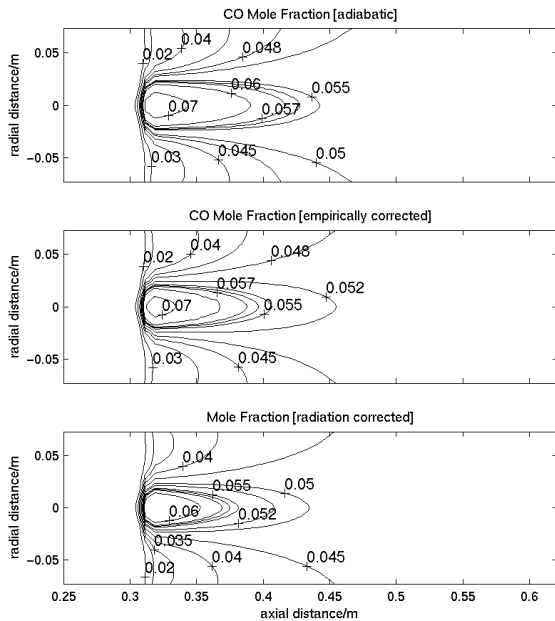


Fig. 4 Predicted iso-concentration contours for CO

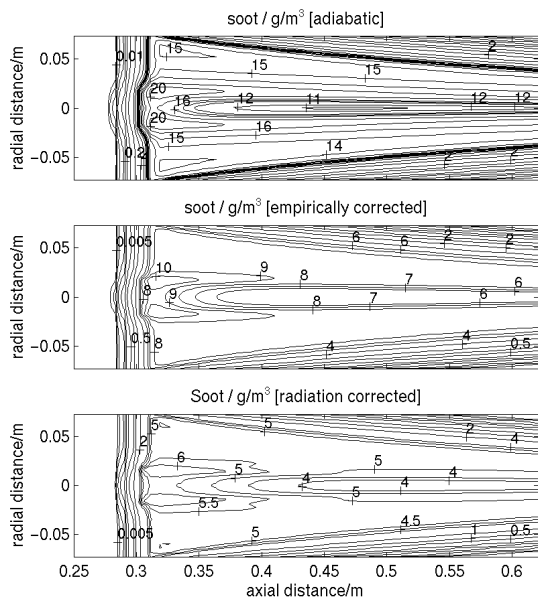


Fig. 5 Predicted iso-concentration contours for soot

Since the flame temperature has an effect on product formation, iso-contours of CO<sub>2</sub>, CO and soot are presented in figures 3-5. The effects on CO<sub>2</sub> and CO concentrations are consistent with dissociation, with the former increasing (by about 5-10%) as the temperature is

reduced while the opposite can be observed for the latter. Soot is highly dependant on temperature and this is reflected in the massive reduction in soot concentration levels (about 70% of the ones obtained with adiabatic temperature).

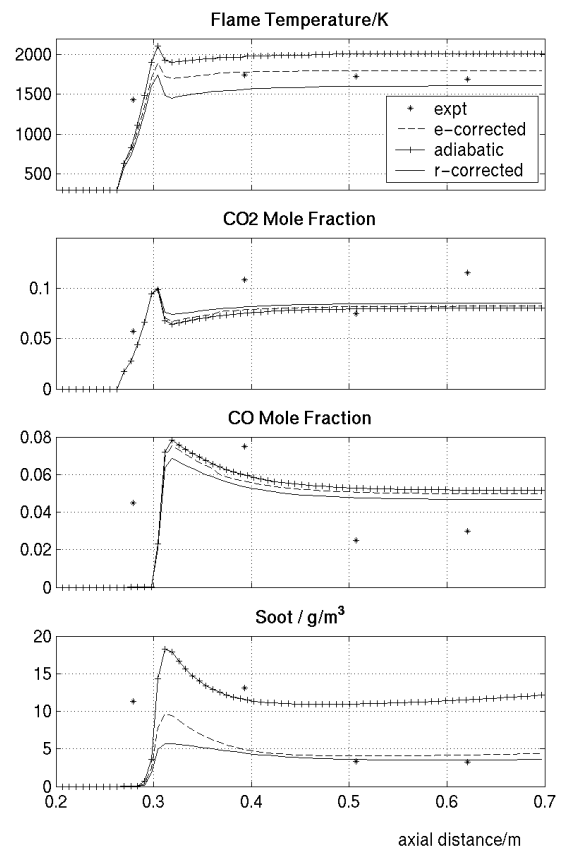


Fig. 6 Predicted & experimental axial distributions

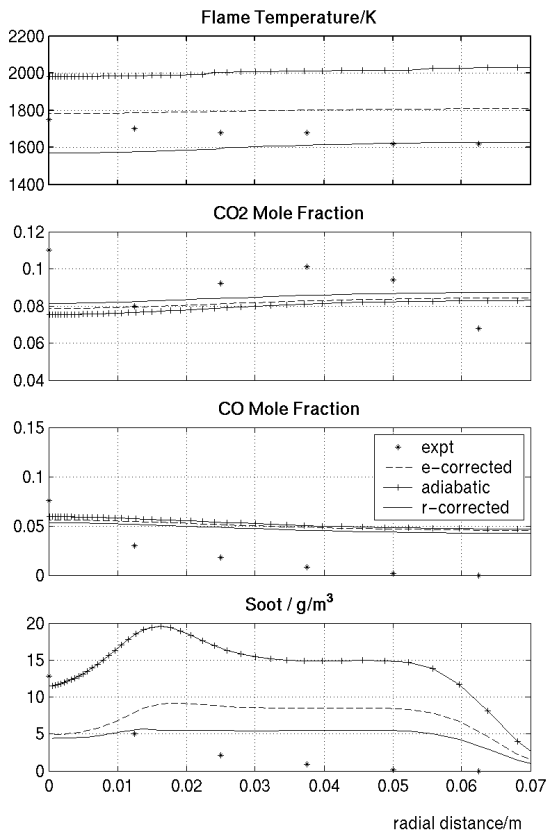


Fig. 7 Predicted & experimental radial distributions

The above effects are quantified further in fig.6 and fig.7. These figures show axial and radial plots with the relevant experimental results superimposed on the predicted ones. It is clear that the thermal radiation brings the axial trace of the temperature closer to the experimental values, particularly near the chamber end. The correction is not as effective as the empirical one however; this is due to the simplified method adopted for this study. The overall energy transfer to the cooling water is subtracted from the overall energy input to the chamber. This results in a higher rate of energy loss in the early part of the chamber than is the case in reality (fig.8). Furthermore, the loss from the various volumes in any one cross-section is not the same, and if the differences were to be taken into account lower losses on the axis will be found with probably higher losses near the wall. Taking these into consideration the model can be improved to give better prediction of the temperature and subsequently of product concentrations, particularly soot. Implementing these modifications is quite involved and work is underway presently to achieve this. Similar trends can be observed for the axial traces of the products, particularly for soot concentrations. These observations are also confirmed in the radial traces presented for cross-section 0.393m from the injector. Again the radial correction brings the temperature and soot concentration closer to the experimental values.

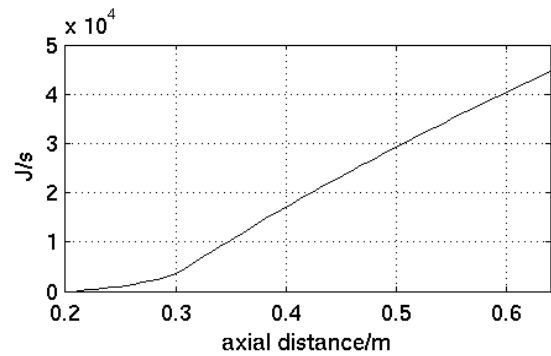


Fig. 8 Accumulated radiative heat transfer to chamber cooling water

#### SUMMARY

- A thermal radiation model has been incorporated successfully within an existing LHF type, 2-D spray combustion model.
- The overall model, with the radiation correction, was run for conditions similar to those for which experimental results are known. The thermal radiation correction was found to bring the predicted results closer to the experimental ones.
- Flame temperature and soot concentration were particularly sensitive to the correction, with the temperature reducing by about 20% from the adiabatic value, and the soot concentration by about 70%.
- Room for improvement in the energy loss due to radiation has been identified and further work is in progress to implement this.

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