CHAPTER 6

CONCLUSIONS AND SCOPE FOR FUTURE WORK

Conclusions

A comprehensive unsteady, spherically symmetric, single component gas phase droplet combustion model has been developed first by solving time dependent conservation equations of energy and species numerically with one initial and three boundary conditions. Results indicate that flame first moves away from the droplet surface then towards it, and flame stand off ratio (flame to droplet diameter ratio) increases throughout the burning period. These results are in conformity with the experimental observations. Other authors have developed droplet combustion models that utilise three or four time dependent conservation equations together with phase equilibrium relations and three to four initial and boundary conditions. These equations are then non dimensionalised and solved either analytically or numerically and come up with the same results as in the present work. Present results being closer to the experimental observations. The present gas phase model was then used to quantify effects of ambient temperature, pressure and composition on important droplet burning parameters like flame temperature and flame location, $F/D$ ratio, burning rate, burning constant, droplet lifetime etc. and further extended to include effects of forced convection and droplet heating and for exploring effects of droplet size (including homogeneous, transition and heterogeneous burning regimes) and different fuels (alkanes, alcohols and biodiesel) on important combustion characteristics. It is observed that dimensionless flame diameter $F/D_0$ is influenced primarily by the fuel boiling point.

Literature review reveals that there is lack of information on thermophysical/transport properties and subsequently combustion and emission data of biodiesel fuels. Present study has tried to overcome this deficiency.

For multicomponent droplet evaporation/combustion, present study suggests that: (i) a realistic multicomponent droplet model should take into account the mixing of air and fuel vapour by employing proper mixing rules as it greatly affects the vaporisation characteristics, (ii) diffusion limit model with convection of the present work (developed by solving numerically liquid phase transient-diffusive equations of
species and energy) can be used in spray analysis as it can serve better than the multicomponent $d^2 - \text{law}$ model or the infinite conductivity model, (iii) effect of Lewis number (a very important parameter in MC analysis) on evaporation behaviour of a MC droplet has been obtained.

For high pressure droplet evaporation/combustion, present work offers a relatively simple yet accurate model with (i) considerations of high pressure liquid-vapour equilibrium, real gas effects, absorption of ambient gas in a thin layer at the droplet surface and pressure dependent properties which are analysed using Newton-Raphson method, (ii) two different high pressure systems with widely different properties; n-heptane-N$_2$ and LOX-H$_2$ (employed in liquid rockets) are investigated. It is observed that critical mixing temperature variation with pressure is different for the two systems while solubility of nitrogen and hydrogen in liquid n-heptane and oxygen respectively increases with an increase in temperature in the supercritical regime for both systems. Mass fraction of n-heptane and oxygen vapours at the droplet surface increases with droplet temperature for a given pressure, and decreases with an increase in ambient pressure for a fixed droplet temperature, (iii) it is observed that $d^2 - \text{law}$ is valid at high pressures, (iv) effect of convection on the vaporisation of a LOX droplet in H$_2$ environment has been quantified.

Emission data for a spherically symmetric single and multicomponent fuel droplets with respect to CO, NO, CO$_2$ and H$_2$O concentrations is obtained and effect of temperature on these concentrations quantified by using the Olikara and Borman code in conjunction with the gas phase code of the present work. The present approach is simpler and rapidly calculates the equilibrium combustion products providing a general trend of species variation.

It is well established that modelling results are dependent on proper estimation of properties which may be a function of temperature, pressure and composition. Therefore much attention has been focussed on this aspect and details of various methods used for evaluating properties are provided in Appendix A.

The above sub models developed in the present work are simple but preserve the essential physics and are represented by computer programmes that require less CPU time which is important in spray analysis where CPU economy plays a vital role.

The development of each code is based on the choice of mathematical technique which is simple, accurate and numerically efficient. This is also a unique feature of
the present study. The details regarding the mathematical aspects of the problem are provided in the chapter on Problem Formulation and Solution Technique.

**The present study provides following contributions/recommendations to our understanding of droplet combustion**

1. A comprehensive transient gas phase model has been evolved and tested for effects of variation in ambient pressure, temperature, composition, fuels, droplet size, convection and droplet heating on important combustion characteristics.
2. A realistic high pressure model is developed for two different systems and investigated with respect to critical mixing temperature, solubility of ambient gas into liquid, droplet surface temperature variation, forced convection and $d^2$-law behaviour.
3. Multicomponent droplet vaporisation and combustion models for the case when $d^2$-law is followed are formulated and effects of air-fuel vapour mixing and Lewis number are obtained on droplet vaporisation behaviour. A realistic MC diffusion limit model with convection has been evolved and compared with other models.
4. Gasohol and Diesohol show that they are better fuel blends than Gasoline and Diesel oil respectively with respect to NO and CO emissions.
5. The results of the present work have been compared with the available experimental and modelling data and are found to be in a fairly good agreement.
6. The submodels developed in the present study are quite accurate and can be incorporated in spray codes.

**Scope for Future Work**

(i) The present gas phase model can be extended to include the effects of biodiesel and diesel/alkanes mixtures for droplet combustion characteristics and can be compared with the experimental data of Long Pan et al.[156] who conducted microgravity droplet combustion experiments using different biodiesel-diesel/alkane fuel blends.

(ii) Multicomponent model of the present work can be modified to include high pressure, high temperature effects and different liquid fuel mixtures.
(iii) There is a need to develop a computer code for predicting thermophysical and transport properties for the range of pressures and temperatures prevailing in practical combustion devices. Experimental and modelling data for only a narrow range of pressure and temperature and that too for limited fuels and properties are available in literature. Recently, Derevich [157] has developed a thermodynamic model for viscosity calculations for pure hydrocarbon fuels and their mixtures in wide range of pressure, temperature and concentrations. Present work can be used to develop a detailed thermodynamic model for estimating properties in varying conditions using the relations provided in Appendix A.

(iv) Current understanding of how droplet clouds and sprays burn is still limited. It is questionable whether study of simple arrays will yield much insight into the burning of practical clouds and sprays. A review on this subject is provided by Lee et al.[158]. It is felt that more experimental and analytical effort is needed for understanding of issues related to group combustion and spray burning. The present model can be extended in this direction.

(v) Since modern approach is to make combustion systems more environmental friendly, a serious consideration to control exhaust emissions at a fundamental level (on the scale of single droplet) is required. Present model can be made more realistic so that it not only provides a general behaviour but a quantitative variation in emission spectrum as well.