

## ANALYTICAL MODELING OF OPERATING CHARACTERISTICS OF PREMIXING-PREVAPORIZING FUEL-AIR MIXING PASSAGES

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A model for predicting the distribution of liquid fuel droplets and fuel vapor in premixing-prevaporizing fuel-air mixing passages of the direct injection type is described. This model consists of three computer programs: a calculation of the two-dimensional or axisymmetric air flow field neglecting the effects of fuel; a calculation of the three-dimensional fuel droplet trajectories and evaporation rates in a known, moving air flow; and a calculation of fuel vapor diffusing into a moving three-dimensional air flow with source terms dependent on the droplet evaporation rates. The air flow calculation can treat compressible swirling flows in arbitrary ducts with arbitrary distributions of temperature and velocity as initial conditions. The fuel droplets are treated as individual particle classes each satisfying Newton's law, a heat transfer, and a mass transfer equation. Each particle class has a number density such that summation over all particle classes yields the fuel flow rate. This fuel droplet model treats multicomponent fuels and incorporates the physics required for the treatment of elastic droplet collisions, droplet shattering, droplet coalescence and droplet wall interactions. The vapor diffusion calculation treats three-dimensional, gas-phase, turbulent diffusion processes with the turbulence level determined by the air flow calculations and the source terms determined by the droplet evaporation rates.

The analysis includes two models for the autoignition of the fuel-air mixture based upon the rate of formation of an important intermediate chemical species during the pre-ignition period. This species is produced both within the vicinity of the fuel droplets and throughout the diffusing fuel vapor-air mixture. Since chemical reaction rates may depend upon the local mixture temperature, the local mixture temperature is adjusted for the effect of fuel evaporation. One of these autoignition models is based upon a global chemical reaction rate in which fuel decomposes to form the intermediate species, ethene. Additional chemical reactions result in the oxidation of ethene to carbon dioxide and water vapor. The maximum ethene concentration occurs at approximately the same instant in time in which a sudden rise in gas temperature occurs. The second model is based upon the global chemical reaction rate governing the production of an unknown, but important, intermediate species; autoignition occurs where the concentration of this species reaches a critical value determined by adjusting constants in the global reaction rate expression to give agreement with representative, experimentally-obtained, autoignition times.

Model development has been completed, the computer codes have been delivered to NASA, and the final report has been completed. The final report includes a literature survey conducted to identify the important characteristics that influence the occurrence of autoignition and to aid in the development of auto-ignition models.

## **OBJECTIVES**

- **Develop computer codes to predict 3D distribution of liquid and vapor fuel in moving gas stream**
- **Develop an autoignition model for fuel-air mixtures in LPP passages**

## **COMPUTATIONAL SEQUENCE**

- **Calculate 2D air flow distribution**
- **Calculate 3D fuel droplet trajectories and sources of fuel vapor and autoignition species from droplets**
- **Calculate 3D diffusion of fuel vapor**
- **Calculate 3D diffusion of autoignition species from droplet and vapor sources**
- **Apply autoignition criterion**

## **CALCULATION OF AIR FLOW**

(UTRC ADD code)

- Two dimensional or axisymmetric/swirling
- Arbitrary duct contours
- Arbitrary inlet flow conditions
- Arbitrary perfect gas
- Turbulence model
  - Mixing length free stream turbulence
  - Van Driest wall turbulence
- Streamline coordinates-conformal mapping
- Implicit forward marching numerical integration

## **CALCULATION OF SPECIES**

(UTRC VAPDIF code)

$$\frac{DC}{Dt} - \tilde{\nabla}^2 C = S_g + S_d$$

- 3D binary diffusion equation
  - Fuel vapor into air
  - Autoignition species into air
- Source terms
  - Fuel vapor from droplet evaporation
  - Fuel vapor from evaporation at a wall
  - Autoignition species from droplet evaporation
  - Autoignition species from diffusing fuel vapor
- Turbulent eddy diffusivity

# CALCULATION OF FUEL DROPLET EVAPORATION

(UTRC PTRAK code)

- Air flow field known
- Droplets treated as particle classes
- (3) momentum equations
- Mass transfer equation
- Heat transfer equation
- Fuel liquid and vapor thermodynamics
  - Multicomponent fuel blends
- Droplet shattering, coalescence, and well interactions

## AUTOIGNITION MODEL I

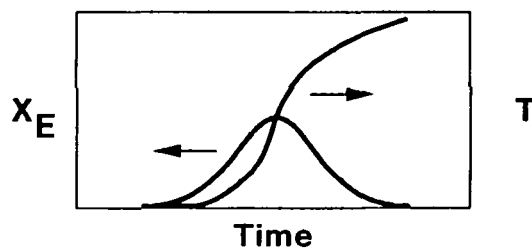
Hautman, Dryer, Shug and Glassman

- Fuel ( $C_nH_{2n+2}$ )

$$\frac{dX_F}{dt} = -K_1 X_{O_2}^{\alpha_1} X_F^{\beta_1} X_E^{\gamma_1}$$

- Ethene ( $C_2H_2$ )

$$\frac{dX_E}{dt} = \frac{n}{2} K_1 X_{O_2}^{\alpha_1} X_F^{\beta_1} X_E^{\gamma_1} - K_2 X_{O_2}^{\alpha_2} X_F^{-\beta_2} X_E^{\gamma_2}$$



## AUTOIGNITION MODEL I - (Cont.)

- Provides general analytical framework
- Requires strong interaction between fuel vapor and autoignition species
- Requires calibration at LPP conditions

## AUTOIGNITION MODEL II

- Autoignition species (?)

$$\frac{d(X_E / X_{E^*})}{dt} = K X_F X_{O_2} \phi \delta T \nu$$

- Criterion

$$\int_0^{\tau} \frac{d(X_E / X_{E^*})}{dt} dt = 1$$

- Correlation

$$\tau = \tau(P, T, \phi, X_F X_{O_2} \dots)$$

- Simple to apply
- Difficult to calibrate