An Interactive Microsoft® Excel Program for Tracking a Single Evaporating Droplet in Crossflow

K.H. Liew, E. Urip, and S.L. Yang
Michigan Technological University, Houghton, Michigan

C.J. Marek
Glenn Research Center, Cleveland, Ohio

July 2004
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The interactive Microsoft® Excel spreadsheet entitled, “An Interactive Microsoft® Excel Program for Tracking a Single Evaporating Droplet in Crossflow” that computes and plots data with and without spray evaporation is available on CD-ROM as a separate document and can also be accessed from the URL’s located on page 17 of this report. The CD-ROM also contains NASA/TM—2002-211710 which includes an interactive spreadsheet that computes and plots data without spray evaporation.
An Interactive Microsoft® Excel Program for Tracking a Single Evaporating Droplet in Crossflow

K.H. Liew, E. Urip, and S.L. Yang
Michigan Technological University
Houghton, Michigan 49931
Ph.: 906–487–2624
Fax: 906–487–2822
E-mail: slyang@mtu.edu

C.J. Marek
National Aeronautics and Space Administration
Glenn Research Center
Cleveland, Ohio 44135
Ph.: 216–433–3584
Fax: 216–433–3000
E-mail: Cecil.J.Marek@nasa.gov

Abstract

Droplet interaction with a high temperature gaseous crossflow is important because of its wide application in systems involving two phase mixing such as in combustion requiring quick mixing of fuel and air. The focus of this work is to investigate dispersion of a two-dimensional evaporating spray into a crossflow.

An interactive Microsoft® Excel program for tracking a single droplet in crossflow that has previously been developed was modified to include droplet evaporation computation. In addition to the high velocity airflow, the injected droplets are also subjected to increased combustor temperature and pressure that affect their motion in the flow field. Six ordinary differential equations (namely the time rate of change of $x$, $z$, $u_d$, $w_d$, $D$, and $T_s$) are then solved by 4th-order Runge-Kutta method using Microsoft® Excel software.

Visual Basic programming and Excel macrocode are used to calculate the data and plot the droplet’s motion in the flow field. This program computes and plots the data sequentially without forcing the user to open other types of plotting programs. A user’s manual on how to use the program is included.
## Symbol List

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_d$</td>
<td>Projected area of the droplet</td>
</tr>
<tr>
<td>$B_M$</td>
<td>Mass transfer number</td>
</tr>
<tr>
<td>$B_T$</td>
<td>Heat transfer number</td>
</tr>
<tr>
<td>$C_{exp}$</td>
<td>Expansion coefficient</td>
</tr>
<tr>
<td>$C_D$</td>
<td>Drag coefficient</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Specific heat at constant pressure</td>
</tr>
<tr>
<td>$c_{p,A}$</td>
<td>Specific heat of air</td>
</tr>
<tr>
<td>$c_{p,F}$</td>
<td>Specific heat of liquid fuel</td>
</tr>
<tr>
<td>$c_{p,Fv}$</td>
<td>Specific heat of fuel vapor</td>
</tr>
<tr>
<td>$c_{p,g}$</td>
<td>Specific heat of fuel-air mixture</td>
</tr>
<tr>
<td>$D$</td>
<td>Droplet diameter</td>
</tr>
<tr>
<td>$D_{FA}$</td>
<td>Diffusion coefficient of fuel in air</td>
</tr>
<tr>
<td>$D_0$</td>
<td>Initial diameter of droplet</td>
</tr>
<tr>
<td>$F$</td>
<td>Force</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravitational acceleration constant</td>
</tr>
<tr>
<td>$k_A$</td>
<td>Thermal conductivity of air</td>
</tr>
<tr>
<td>$k_{Fv}$</td>
<td>Thermal conductivity of fuel vapor</td>
</tr>
<tr>
<td>$k_g$</td>
<td>Thermal conductivity of fuel-air mixture</td>
</tr>
<tr>
<td>$L$</td>
<td>Latent heat of vaporization</td>
</tr>
<tr>
<td>$L_{Tbn}$</td>
<td>Latent heat at normal boiling point</td>
</tr>
<tr>
<td>$M_A$</td>
<td>Molecular weight of air</td>
</tr>
<tr>
<td>$M_F$</td>
<td>Molecular weight of fuel</td>
</tr>
<tr>
<td>$m_{drop}$</td>
<td>Mass of a droplet</td>
</tr>
<tr>
<td>$\dot{m}$</td>
<td>Evaporation rate</td>
</tr>
<tr>
<td>$\dot{m}^*$</td>
<td>Evaporation rate per unit surface area</td>
</tr>
<tr>
<td>$n$</td>
<td>Exponential constant</td>
</tr>
<tr>
<td>$Nu$</td>
<td>Nusselt number</td>
</tr>
<tr>
<td>$P$</td>
<td>Ambient pressure</td>
</tr>
<tr>
<td>$P_F$</td>
<td>Partial pressure of fuel</td>
</tr>
<tr>
<td>$P_{vap}$</td>
<td>Vapor pressure</td>
</tr>
<tr>
<td>$Pr_A$</td>
<td>Prandtl number of air</td>
</tr>
<tr>
<td>$Q_{act}$</td>
<td>Total heat transfer to droplet</td>
</tr>
<tr>
<td>$Q_{ss}$</td>
<td>Steady-state heat transfer to droplet</td>
</tr>
<tr>
<td>$R_u$</td>
<td>Universal gas constant</td>
</tr>
<tr>
<td>$Re_d$</td>
<td>Reynolds number of droplet</td>
</tr>
<tr>
<td>$r$</td>
<td>Spherical radius of the droplet</td>
</tr>
<tr>
<td>$r_{32}$</td>
<td>$0.5^*(\text{Sauter mean radius})$</td>
</tr>
<tr>
<td>$T_{bn}$</td>
<td>Normal boiling point</td>
</tr>
</tbody>
</table>
$T_{\text{crit}}$ Critical temperature
$T_{\text{drop}}$ Droplet temperature
$T_r$ Reference temperature
$T_s$ Droplet surface temperature
$T_{\infty}$ Ambient temperature
$t_e$ Evaporation time
$U_R$ Relative velocity between the droplet and the gas stream
$u_A$ Velocity of the cross stream (air) in the x-direction
$u_d$ Velocity of the droplet in the x-direction
$V_d$ Droplet Volume
$w_A$ Velocity of the cross stream (air) in the z-direction
$w_d$ Velocity of the droplet in the z-direction
$x$ Horizontal direction (+ equals to the right)
$Y_A$ Mass fraction of air
$Y_F$ Mass fraction of fuel
$Z$ Vertical direction (+ equals up)
$\alpha_g$ Thermal diffusivity of gas
$\lambda$ Evaporation constant
$\mu_A$ Viscosity constant of air
$\rho_A$ Density of the cross stream (air)
$\rho_d$ Density of the droplet
$\rho_{F,288.6K}$ Density of fuel droplet at 288.6K
$\Delta t$ time step-size

**Subscripts**

- A Air
- d Droplet
- F Fuel
- g Mixture of gaseous phase
- r Reference condition
- s Droplet surface
- st Steady state
1. Introduction

A liquid spray injected into a gaseous crossflow with high temperature is important because of its wide application in systems involving two phase mixing. It is important to be able to compute this flow to optimize the mixing strategy.

An existing Excel program (ref. 1) has previously been developed for tracking a single droplet in crossflow computation. This work is focused on producing a quick computational method for determining spray penetration with evaporation. With this spreadsheet, one can investigate the dispersion of an air-blast atomized spray jet into a high temperature crossflow. During the transverse injection of a spray into high velocity airflow, the droplets (carried along in the gaseous stream of co-flowing air) are not only subjected to forces due to the crossflow motion, but also to increases in the combustor temperature and pressure (see fig. 1).

![Figure 1.1](from NASA/CR—2000-210467) (ref. 2)

2. Governing Equations

2.1 Droplet Trajectories and Velocities

The trajectories of the droplets can be tracked by applying a Lagrangian-based analysis to the droplets. The momentum equations for a droplet can be obtained by equating the droplet motion to: (1) The viscosity and pressure-related drag forces, and (2) The pressure gradient and viscous forces related to the fluid surrounding the droplet, and (3) The inertia of the virtual mass, induced when the particle acceleration affects the fluid mass acceleration.

Droplet trajectory and velocity with respect to time can be calculated. Based on these principles along with the following assumptions:

1. The droplets are spherical,
2. No droplet breakup occurs,
3. Vaporization is not considered yet and will be derived separately in section 2.2,
4. Lift, virtual mass, and Basset forces which takes into account the acceleration history of the droplet, are neglected,
5. Chemical reaction is not included,
These assumptions reduce the droplet momentum equation to include only the effects of the drag and body forces. The general momentum equations for a single droplet injected along the positive x-direction, transversely into a downward-flowing air stream in the positive z-direction, as shown in figure 2, is described by

\[ \vec{F}_d = \vec{F}_{\text{drag}} + \vec{F}_{\text{body}} \]  

(1)

where the net force \( \vec{F}_d \) that drives the droplet motion is balanced by the drag force opposing its motion, and the field forces acting on the droplet. The aerodynamic drag force is given by

\[ \vec{F}_{\text{drag}} = -\frac{1}{2} \rho_A \vec{U}_R |\vec{U}_R| A_d C_D \]  

(2)

where \( \rho_A \) is the air density, and \( A_d \) and \( C_D \), the projected area and the drag coefficient of the droplet, respectively. The relative velocity between the droplet and the crossflow has a magnitude of \( U_R \) (see fig. 2). The subscript “\( d \)” refers to the droplet and “\( g \)” the crossflow air.

\[ \left| \vec{U}_R \right| = \sqrt{(u_d - u_A)^2 + (w_d - w_A)^2} \]

The body force, resulting from an equivalent volume of air that buoys the droplet, includes the gravitational and buoyancy forces. It is given by

\[ \vec{F}_{\text{body}} = (\rho_d - \rho_A) V_d \vec{g} \]  

(3)

which says that the body force is equal to the product of relative droplet and air density \((\rho_d - \rho_A)\), the droplet volume \( V_d \), and the gravitational acceleration \( g \).
Substituting equation (2) and equation (3) to equation (1) yields:

\[
\rho_d V_d \frac{du_d}{dt} = -\frac{1}{2} \rho_A (u_d - u_A) \left| \vec{U}_R \right| A_d C_D
\]  

(4)

\[
\rho_d V_d \frac{dw_d}{dt} = -\frac{1}{2} \rho_A (w_d - w_A) \left| \vec{U}_R \right| A_d C_D + (\rho_A - \rho_d) V_d g
\]  

(5)

\[
\frac{dx}{dt} = u_d
\]  

(6)

\[
\frac{dz}{dt} = w_d
\]  

(7)

The drag coefficient of the droplet depends on the droplet Reynolds number and is given by

\[
C_D = \begin{cases} 
\frac{24}{Re_d} \left[1 + \frac{1}{6} Re_d^{2/3}\right] & \text{Re}_d \leq 1000 \\
0.424 & \text{Re}_d > 1000 
\end{cases}
\]  

(8)

where \( \text{Re}_d \) is the droplet Reynolds number and is defined as follows

\[
\text{Re}_d = \frac{2 \rho_d \left| \vec{U}_R \right| r_d}{\mu_g}
\]  

(9)

in which \( r_d \) is the droplet radius and \( \mu_g \) is the gas (air) viscosity.

2.2 Droplet Evaporation

To include the effect of evaporation rate on spray penetration, apply a control volume at droplet surface that will change with droplet radius during evaporation process. For simplicity, consider steady state analysis first.

2.2.1. Steady-State Analysis

A fuel droplet rarely reaches a steady state (ref. 3) during its lifetime. This is because most commercial fuels are multi-component, where different fuel compounds possess its own properties, for example kerosene and gasoline. To simplify analysis, ‘steady state’ term here refers to ‘quasi-steady’, which allows droplet lifetime and evaporation rate to be estimated to an acceptable level of accuracy.
To simplify the analysis, in addition to the assumptions listed in trajectory analysis as shown in section 2.1:

1. there is no radiation,
2. there is no internal circulation and internal convective heating within droplet,
3. consider only single-component fuel (with well-defined boiling point), and
4. it is quasi-steady flow.

Consider a fuel droplet at low fuel injection temperature that is suddenly exposed to a gaseous crossflow at high temperature. Initially, almost all heat supplied to the droplet serves to raise the droplet temperature. As the droplet temperature rises, fuel vapor will form at the droplet surface and has two main effects:

1. a large portion of heat transferred to droplet is used to vaporize the droplet, and
2. the outward flow of fuel vapor impedes the rate of heat transfer to droplet

Eventually, a stage is reached where all heat transferred to droplet is used as the heat of vaporization and the droplet temperature will stabilize at a steady-state temperature.

**Mass Transfer Number**

Assume that the thermal diffusion is negligible. Therefore, the concentration gradient is the only driving force considered for species diffusion in the direction of the diffusion path. Then, the following expression for an evaporating fuel droplet of radius $r$ is described by:

$$
\frac{dY_F}{dr} = -\frac{R_u T}{D_{FA} P} (\dot{m}_{F}^* Y_A)
$$

where $D_{FA}$ diffusion coefficient of fuel in air

$\dot{m}_{F}^*$ mass rate of diffusion per unit area (mass flux)

$P$ ambient air pressure

$R_u$ universal gas constant

$T$ ambient air temperature

$Y_F(r)$ fuel mass fraction

$Y_A$ air mass fraction at range $r_s < r < \infty$ at any time

$$
Y_A = 1 - Y_F
$$

(10a)

From the continuity equation applied on the control surface surrounding a droplet, one obtains

$$
\dot{m}_{F}^* = \dot{m}_{F,\infty} \left(\frac{r_s}{r}\right)^2
$$

(11)
where $\dot{m}_{F,s}$ – mass flux at droplet surface

$r_s$ – radius of droplet

$r$ – radius of control surface at time $t$

Substituting equation (10a) and (11) into (10) yields:

$$\frac{dY_F}{dr} = -\frac{R_u T}{D_{F_A} P} \dot{m}_{F,s} \left( \frac{r_s}{r} \right)^2 \left( 1 - Y_{F,s} \right)$$

(12)

where $Y_{F,s}$ - fuel mass fraction at droplet surface

Assume the ideal gas relation ($\rho = \frac{P}{R_u T}$), separating variables, integrating, and rearranging equation (12) yields:

$$\dot{m}_{F,s} = -\frac{\rho D_{F_A}}{r_s} \cdot \ln(1 - Y_{F,s})$$

(13)

where $\rho$ – fuel density

Multiplying by droplet surface area ($A_s = 4\pi r_s^2$) and for $D = 2r_s$,

$$\dot{m}_{F,s} = -2\pi D \cdot \rho D_{F_A} \cdot \ln(1 - Y_{F,s})$$

(14)

where $D$ – diameter of evaporating droplet
**Unity Lewis Number (Le)**

Assume $Le = 1$, it implies that the mass transfer rate is equal to the heat transfer rate, i.e.

$$D_{FA} = \alpha_g$$

(15)

where

$$\alpha_g = \left( \frac{k}{\rho c_p} \right)_g$$

(15a)

where $\alpha_g$ – thermal diffusivity of gas
$k$ – thermal conductivity
$c_p$ – specific heat at constant pressure

Then,

$$\rho_g D_{FA} = \left( \frac{k}{c_p} \right)_g$$

(16)

Define the mass transfer number, $B_M$:

$$B_M = \frac{Y_{F,s} - Y_{F,\infty}}{Y_{F,drop} - Y_{F,s}}$$

(17)

Since $Y_{F,\infty} \approx 0$ and $Y_{F,drop} = 1$, equation (17) is simplified as:

$$B_M = \frac{Y_{F,s}}{1 - Y_{F,s}}$$

(18)

$$Y_{F,s} = \left[ 1 + \left( \frac{P}{P_{F,s}} - 1 \right) \left( \frac{M_A}{M_F} \right) \right]^{-1}$$

(19)

where $M_F$ – molecular weight of fuel [kg/kg-mol]
$M_A$ – molecular weight of air [kg/kg-mol]
$P$ – ambient pressure [kPa]
$P_{F,s}$ – fuel vapor pressure at droplet surface [kPa]

Rearranging $ln(1-Y_F)$ in term of $B_M$ yields:

$$\ln(1-Y_F) = -\ln(1 + B_M)$$

(20)
Substituting (16) and (20) into (14) yields the rate of evaporation of a fuel drop at the surface:

\[
\dot{m}_{F,s} = 2\pi D \left( \frac{k}{c_p} \right)_g \ln(1 + B_M) \tag{21}
\]

**Reference Conditions**

For better accuracy, the choice of values of \( k_g \) and \( c_{p,g} \) are evaluated at the following reference temperature and composition using the “one-third rule”:

\[
T_r = T_s + \frac{1}{3}(T_\infty - T_s) \tag{22}
\]

\[
Y_{F,r} = Y_{F,s} + \frac{1}{3}(Y_{F,\infty} - Y_{F,s}) \tag{23}
\]

Since \( Y_{F,\infty} = 0 \),

\[
Y_{F,r} = \frac{2}{3} Y_{F,s} \tag{24}
\]

\[
Y_{A,r} = 1 - Y_{F,r} \tag{25}
\]

**Fuel-air Mixture**

Therefore, the reference thermal conductivity and specific heat at constant pressure are estimated as:

\[
k_g = Y_{A,r} \cdot k_A(T_r) + Y_{F,r} \cdot k_{Fv}(T_r) \tag{26}
\]

\[
c_{p,g} = Y_{A,r} \cdot c_{p,A}(T_r) + Y_{F,r} \cdot c_{p,Fv}(T_r) \tag{27}
\]

All properties for air and different fuels are provided in *Appendix A* and *B*.

**Evaporation Constant**

At steady-state period, the droplet diameter \( D \) at any instant may be related to its initial diameter \( D_0 \) by \( D^2 \)-law:

\[
D_0^2 - D^2 = \lambda_{st} t \tag{28}
\]
where $\lambda_{st} \left[ \frac{m^2}{s} \right]$ is the steady state evaporation constant

$$\lambda_{st} = \left( \frac{k}{c_p} \right)_g \frac{8 \ln(1 + B_M)}{\rho_f}$$

(28a)

The $D^2$-law states that the square of droplet diameter is a linear function of time where the evaporation constant apparently represents the slope of the equation. The larger the $\lambda_{st}$, the shorter the time it takes for the droplet to vaporize completely.

**Heat Transfer Number**

Consider conductive and convective heat fluxes across a thin shell surrounding the evaporating droplet, the heat transfer number is defined as the ratio of enthalpy available in the surrounding gas to the energy required to vaporize the fuel:

$$B_T = \frac{c_{p,g} (T_m - T_s)}{L + c_{p,drop} (T_s - T_{drop})}$$

(29)

where $L$ – latent heat of fuel vaporization corresponding to fuel surface temperature \[ \frac{kJ}{kg} \]

For simplicity, one can neglect the energy required to raise the droplet temperature to the surface temperature. Then, equation (29) becomes:

$$B_T = \frac{c_{p,g} (T_m - T_s)}{L}$$

(30)

When heat transfer dominates the evaporation process, the rate of evaporation of a fuel droplet at the surface is then described by:

$$\dot{m}_{F,s} = 2 \pi D \left( \frac{k}{c_p} \right)_g \ln(1 + B_T)$$

(31)

**B_T versus B_M**

Estimation of rate of fuel evaporation using equation (31) is only good for steady-state conditions. Nevertheless, equation (21) applies under all conditions, including the heat-up process of droplet (ref. 6).
However, under steady state conditions, \( B_M = B_T = B \) and equation (21) and (31) are identical. Therefore, droplet evaporation rate can be written as:

\[
\dot{m}_{FS} = 2\pi D \left( \frac{k}{c_p} \right) \ln(1 + B) \quad (32)
\]

### 2.2.2 Heat-up Process

According to Chin\(^6\), serious error may be incurred in the calculation of fuel evaporation rate and droplet lifetime if the transient heat-up process is neglected. In fact, for many fuels at high ambient pressure and temperature, the transient heat-up process constitutes a significant portion of the droplet evaporation time.

At the steady-state period, the heat used in vaporizing the fuel is given by:

\[
Q_{ss} = \dot{m}_F L \quad (33)
\]

Substituting equation (14) into (33) yields,

\[
Q_{ss} = 2\pi D \left( \frac{k}{c_p} \right) \ln(1 + B_M) L \quad (34)
\]

Including the heating process, the actual heat transfer is estimated as:

\[
Q_{act} = 2\pi D (T_\infty - T_S) \left( \frac{\ln(1 + B_M)}{B_M} \right) \quad (35)
\]

Then, the rate of change of the droplet surface temperature is given by:

\[
\frac{dT_s}{dt} = \frac{Q_{act} - Q_{ss}}{c_p,F m_{drop}} \quad (36)
\]

Substituting equation (34) and (35) into (36) and rearranging gives,

\[
\frac{dT_s}{dt} = \frac{\dot{m}_F L}{c_p,F m_{drop}} \left( \frac{B_T}{B_M} - 1 \right) \quad (37)
\]

where

\[
m_{drop} = \frac{\pi}{6} \rho_F D^3 \quad (37a)
\]
Note that
\[ \dot{m}_F = \frac{d}{dt} \left( \frac{\pi}{6} \rho_F D^3 \right) \]  
(38)

Equating equation (14) and (38) and rearranging gives the rate of change of droplet size:
\[ \frac{dD}{dt} = \frac{4 \ln(1 + B_M)}{\rho_f D} \left( \frac{k}{c_p \gamma} \right) \]  
(39)

### 2.2.3 Droplet Lifetime

Since the rate of chemical reactions in many practical combustion systems are so high, the burning rate is mainly controlled by the fuel evaporation process. Therefore, droplet lifetime is important in such situations because it determines the residence time needed to ensure completion of combustion.

Assume the final droplet diameter, \( D_0 \), equal to zero and rearranging the \( D^2 \)-law, the steady state droplet lifetime is readily obtained by:
\[ t_{c, st} = \frac{D_0^2}{\lambda_{st}} \]  
(40)

### 2.2.4 Convective Effect

All derivations shown above are only good for droplet at stationary condition. In addition, it is known that convection may enhance both mass and heat transfer during the evaporation process. Moreover, to include the convective effect into the evaporation rate equation is straightforward. Equation (23) is then modified by replacing the coefficient with the Nusselt number correlation (ref. 5):
\[ \dot{m}_F = Nu \pi D \left( \frac{k}{c_p \gamma} \right) \ln(1 + B_M) \]  
(41)

where
\[ Nu = 2 + 0.6 \text{Re}_d^{0.5} \Pr_A^{0.33} \]  
(41a)
\[ \text{Re}_d = \frac{P_A \cdot U_r \cdot D}{\mu_A} \]  
(41b)
All physical properties should be evaluated at the reference temperature, \( T_r \), except for \( \mu_A, Pr_A, \) and \( \rho_A \). Please refer to Appendix B for air properties.

3. Numerical Method

Six ordinary differential equations are to be solved for the six dependent variables \( x, z, u_d, w_d, D, \) and \( T_s \). The droplet trajectory is defined by the set of \( x \) and \( z \) values. A 4th-Order Runge-Kutta explicit method\(^8\) was used to solve these equations. The Runge-Kutta explicit method is an ideal numerical scheme for solving ordinary differential equations using Microsoft® Excel software. It is a self-starting method with good stability characteristics. The time step-size can be changed as desired without any complications for higher-order schemes.

There are totally six sets of coupled equations, namely the time rate change of \( x, z, u_d, w_d, D, \) and \( T_s \), along with their solutions, as shown below: (subscript \( n \) stands for the \( n^{th} \) time step)

[1]  
\[
\frac{dx}{dt} = u_d = f_1(u_d) \\
\tag{1}
\]
\[
x_{n+1} = x_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\
\tag{1a}
\]

where

\[
k_1 = \Delta t \cdot f_1(u_{d,n})
\]
\[
k_2 = \Delta t \cdot f_1(u_{d,n} + \frac{l_1}{2})
\]
\[
k_3 = \Delta t \cdot f_1(u_{d,n} + \frac{l_2}{2})
\]
\[
k_4 = \Delta t \cdot f_1(u_{d,n} + l_3)
\]

[2]  
\[
\frac{dz}{dt} = w_d = f_2(w_d) \\
\tag{2}
\]
\[
z_{n+1} = z_n + \frac{1}{6}(kz_1 + 2kz_2 + 2kz_3 + kz_4) \\
\tag{2a}
\]

where
\[ k_{z1} = \Delta t \cdot f_2(w_{d,n}) \]
\[ k_{z2} = \Delta t \cdot f_2(w_{d,n} + \frac{l_{z1}}{2}) \]
\[ k_{z3} = \Delta t \cdot f_2(w_{d,n} + \frac{l_{z2}}{2}) \]
\[ k_{z4} = \Delta t \cdot f_2(w_{d,n} + l_{z3}) \]  

\[ \frac{du_d}{dt} = \frac{-\frac{1}{2} \rho_g \left( u_d - u_g \right) \left[ \bar{U}_g \right] A_d C_D}{\rho_d V_d} = f_3(u_d, w_d, D, T_s) \]  

\[ u_{d,n+1} = u_{d,n} + \frac{1}{6}(l_1 + 2l_2 + 2l_3 + l_4) \]  

where

\[ l_1 = \Delta t \cdot f_3(u_{d,n}, w_{d,n}, D_n, T_{s,n}) \]
\[ l_2 = \Delta t \cdot f_3(u_{d,n} + \frac{l_1}{2}, w_{d,n} + \frac{l_{z1}}{2}, D_n + \frac{md_1}{2}, T_{s,n} + \frac{mt_1}{2}) \]
\[ l_3 = \Delta t \cdot f_3(u_{d,n} + \frac{l_2}{2}, w_{d,n} + \frac{l_{z2}}{2}, D_n + \frac{md_2}{2}, T_{s,n} + \frac{mt_2}{2}) \]
\[ l_4 = \Delta t \cdot f_3(u_{d,n} + l_3, w_{d,n} + l_{z3}, D_n + md_3, T_{s,n} + mt_3) \]  

\[ \frac{dw_d}{dt} = \frac{-\frac{1}{2} \rho_g \left( w_d - w_g \right) \left[ \bar{U}_g \right] A_d C_D + \left( \rho_g - \rho_d \right) \bar{V}_g}{\rho_d V_d} = f_4(u_d, w_d, D, T_s) \]  

\[ w_{d,n+1} = w_{d,n} + \frac{1}{6}(l_{z1} + 2l_{z2} + 2l_{z3} + l_{z4}) \]  

where

\[ l_{z1} = \Delta t \cdot f_4(u_{d,n}, w_{d,n}, D_n, T_{s,n}) \]
\[ l_{z2} = \Delta t \cdot f_4(u_{d,n} + \frac{l_1}{2}, w_{d,n} + \frac{l_{z1}}{2}, D_n + \frac{md_1}{2}, T_{s,n} + \frac{mt_1}{2}) \]
\[ l_{z3} = \Delta t \cdot f_4(u_{d,n} + \frac{l_2}{2}, w_{d,n} + \frac{l_{z2}}{2}, D_n + \frac{md_2}{2}, T_{s,n} + \frac{mt_2}{2}) \]
\[ l_{z4} = \Delta t \cdot f_4(u_{d,n} + l_3, w_{d,n} + l_{z3}, D_n + md_3, T_{s,n} + mt_3) \]
\[
\frac{dD}{dt} = -\frac{\lambda}{2D} = f_5(D, T_s) 
\]  
(5)

\[D_{n+1} = D_n + \frac{1}{6}(mD_1 + 2mD_2 + 2mD_3 + mD_4) \]  
(5a)

where

\[mD_1 = \Delta t \cdot f_5(D_n, T_{s,n})\]
\[mD_2 = \Delta t \cdot f_5(D_n + \frac{mD_1}{2}, T_{s,n} + \frac{mt_1}{2})\]
\[mD_3 = \Delta t \cdot f_5(D_n + \frac{mD_2}{2}, T_{s,n} + \frac{mt_2}{2})\]
\[mD_4 = \Delta t \cdot f_5(D_n + mD_3, T_{s,n} + mt_3)\]  
(5b)

\[
\frac{dT_s}{dt} = \frac{\dot{m}_F L}{c_{p,F} m_{drop}} \left( \frac{B_T}{B_M} - 1 \right) = f_6(u_d, w_d, D, T_s) 
\]  
(6)

\[T_{s,n+1} = T_{s,n} + \frac{1}{6}(mt_1 + 2mt_2 + 2mt_3 + mt_4) \]  
(6a)

where

\[mt_1 = \Delta t \cdot f_6(u_{d,n}, w_{d,n}, D_n, T_{s,n})\]
\[mt_2 = \Delta t \cdot f_6(u_{d,n} + \frac{l_1}{2}, w_{d,n} + \frac{l_2}{2}, D_n + \frac{mD_1}{2}, T_{s,n} + \frac{mt_1}{2})\]
\[mt_3 = \Delta t \cdot f_6(u_{d,n} + \frac{l_2}{2}, w_{d,n} + \frac{l_3}{2}, D_n + \frac{mD_2}{2}, T_{s,n} + \frac{mt_2}{2})\]
\[mt_4 = \Delta t \cdot f_6(u_{d,n} + l_3, w_{d,n} + l_3, D_n + mD_3, T_{s,n} + mt_3)\]  
(6b)

Only every nth cycle (as specified by the user) is saved for plotting. This greatly saves on storage and increases the speed of post processing. We have chosen to enter the data in SI units in the unlocked cells. The required conversions are done in the locked cells. When the user becomes familiar with the spreadsheet, the spreadsheet can be unlocked as there is no password and the user can adapt the spreadsheet as required.
The report can be accessed on the web at:
along with the interactive Microsoft® Excel spreadsheet¹ that computes and plots
data with and without spray evaporation can be accessed through hyperlinks located on the back
of the title page and on page 17, or directly on the web at:

The interactive Microsoft® Excel spreadsheet is also available on CD-ROM as a separate
document. Additional copies of the Microsoft® Excel spreadsheet can be requested by e-mailing:
Dan.L.Bulzan@nasa.gov.

The CD-ROM also contains NASA/TM—2002-211710 and supplemental Microsoft® Excel
interactive spreadsheet that computes and plots data without spray evaporation.

¹To access the interactive spreadsheet, Microsoft® Excel 2002 or higher is recommended to view the file and for
proper functionality. It can be opened through your browser, however, saving to the hard drive is recommended. If
you cannot access this file, please contact: Dan.L.Bulzan@nasa.gov.
4. Equations Summary for Tracking an Evaporating Spray in a Crossflow

**Inputs**

**Droplets**
- Properties: \( R_{32}, A_d, V_d, \rho_d, 288.25K, T_{crit}, T_{bn}, C_{exp}, L_{Thn}, MW_d, a, b \)
- Initial conditions: \( X_0, U_{d0}, Z_0, W_{d0}, T_{ini} \)

**Crossflow**
- Properties: \( M_g, U_g, W_g \)

**Ambient conditions:** \( T_{\infty}, P, g \)

**Numerical method:** \( \Delta t, n \) (total cycle number), \( n_{data}, \epsilon \)

**Outputs**

**Ballistics:** \( X, U_d, Z, W_{d0}, C_{dt} \)

**Evaporation:** \( D, T_{surf} \)
Equations

Mass Transfer Number:

If (Group 1 fuel\(^2\)) then

\[
P_{F,s} = P_{vap}(T_s) = \exp\left( a - \frac{b}{T_s - 43} \right) \text{[kPa]} \tag{1}
\]

else

\[
\log_{10} P_{vap} = A + \frac{B}{T_s} + C \log_{10} T_s + DT_s + ET_s^2
\]

\[
P_{F,s} = P_{vap}(T_s) \text{[mmHg]} \tag{3}
\]

End if

\[
Y_{F,s} = \left[ 1 + \left( \frac{P}{P_{F,s}} - 1 \right) \left( \frac{M_A}{M_F} \right) \right]^{-1} \tag{4}
\]

\[
B_M = \frac{Y_{F,s}}{1 - Y_{F,s}} \tag{5}
\]

Reference Conditions:

\[
T_r = T_s + \frac{1}{3}(T_\infty - T_s)[\text{K}] \tag{6}
\]

\[
Y_{F,r} = \frac{2}{3} Y_{F,s} \tag{7}
\]

\[
Y_{A,r} = 1 - Y_{F,r} \tag{8}
\]

Thermal Properties of Air

\[
k_A = 2 \cdot 10^{-11} T_r^3 - 5 \cdot 10^{-8} T_r^2 + 0.0969 \cdot 10^{-3} T_r + 0.8289 \cdot 10^{-3} \left[ \frac{W}{m \cdot K} \right] \tag{9}
\]

\(^2\text{Group 1 fuels – DF 2, JP 4, JP 5 and n-Heptane}

Group 2 fuels – Jet-A (C\(_{12}\)H\(_{23}\)) and Water (H\(_2\)O) (please refer to Appendix A for more details.)
\[ c_{p,A} = -5 \cdot 10^{-11} T_r^3 + 2 \cdot 10^{-7} T_r^2 - 1 \cdot 10^{-5} T_r + 1.004 \left[ \frac{kJ}{kg} \right] \] (10)

\[ \mu_A = (7 \cdot 10^{-8} T_\infty^3 - 0.0003 T_\infty^2 + 0.6227 T_\infty + 18.761) \cdot 10^{-7} \left[ \frac{Ns}{m^2} \right] \] (11)

\[ \text{Pr}_A = 2 \cdot 10^{-13} T_\infty^4 - 10^{-9} T_\infty^3 + 2 \cdot 10^{-6} T_\infty^2 - 0.0009 T_\infty + 0.8632 \] (12)

\[ \rho_A = 355.91 T_\infty^{-1.0032} \left[ \frac{kg}{m^3} \right] \] (13)

**Thermal properties of hydrocarbon fuel:**

If (Group 1 fuel) then

\[ \rho_F = \rho_{F,288.6K} \left[ 1 - 1.8 C_{e_0} (T - 288.6) - 0.09 \left( \frac{T - 288.6}{T_{crit} - 288.6} \right)^2 \right] \left[ \frac{kg}{m^3} \right] \] (14)

\[ c_{p,Fv} = \left( 0.363 + 0.000467 T_r \right) \left( 5 - 0.001 \rho_{F,288.6K} \right) \left[ \frac{kJ}{kgK} \right] \] (15)

\[ c_{p,F} = \left( 0.76 + 0.00335 T_{drop} \right) \left( 0.001 \rho_F \right)^{0.5} \left[ \frac{kJ}{kgK} \right] \] (16)

\[ n = 2 - 0.0372 \left( \frac{T_r}{T_{bn}} \right)^2 \] (17)

\[ k_{Fv} = 10^{-6} \left[ 13.2 - 0.0313(T_{bn} - 273) \right] \left( \frac{T_r}{273} \right)^n \left[ \frac{W}{m \cdot K} \right] \] (18)

\[ L = L_{bn} \left( \frac{T_{crit} - T_z}{T_{crit} - T_{bn}} \right)^{0.38} \left[ \frac{kJ}{kg} \right] \] (19)

Else

\[ \rho_F = AB \left( \frac{1}{T_{drop}} \right)^n \left[ \frac{g}{cm^3} \right] \] (20)
\[ k_{Fv} = A + BT + CT^2 \left( \frac{W}{m \cdot K} \right) \]  
(21)

\[ C_{p,Fv} = A + BT + CT^2 + DT^3 + ET^4 \left( \frac{J}{mol \cdot K} \right) \]  
(22)

\[ C_{p,F} = A + BT_{drop} + CT_{drop}^2 + DT_{drop}^3 \left( \frac{J}{mol \cdot K} \right) \]  
(23)

\[ L = A \left( 1 - \frac{T_{drop}}{T_c} \right)^n \left( \frac{kJ}{mol} \right) \]  
(24)

End if

**Thermal properties of fuel-air mixture:**

\[ k_g = Y_{A,r} \cdot k_A(T_r) + Y_{F,r} \cdot k_v(T_r) \]  
(25)

\[ c_{p,g} = Y_{A,r} \cdot c_{p,A}(T_r) + Y_{F,r} \cdot c_{p,v}(T_r) \]  
(26)

**Droplet trajectories:**

\[ \bar{U}_R = \sqrt{(u_d - u_g)^2 + (w_d - w_g)^2} \]  
(27)

\[ \text{Re}_d = \frac{2 \rho_A |\bar{U}_R| r_{d,s}}{\mu_A} \]  
(28)

\[ C_D = \begin{cases} 
\frac{24}{\text{Re}_d} \left[ 1 + \frac{1}{6} \text{Re}_d^{2/3} \right] & \text{Re}_d \leq 1000 \\
0.424 & \text{Re}_d > 1000
\end{cases} \]  
(29)

\[ \rho_d V_d \frac{du_d}{dt} = -\frac{1}{2} \rho_g \left( u_d - u_g \right) |\bar{U}_R| A_d C_D \]  
(30)

\[ \rho_d V_d \frac{dw_d}{dt} = -\frac{1}{2} \rho_g \left( w_d - w_g \right) |\bar{U}_R| A_d C_D + \left( \rho_g - \rho_d \right) V_d g \]  
(31)
\[ \frac{dx}{dt} = u_d \]  
\[ \frac{dz}{dt} = w_d \]  

Convective effect:

\[ Nu = 2 + 0.6 \text{Re}^{0.5} \text{Pr}_{air}^{0.33} \]  
\[ \dot{m}_F = Nu\pi D \left( \frac{k}{c_p g} \right) \ln(1 + B_M) \]  

Heat transfer number:

\[ B_T = \frac{c_{p, g} (T_\infty - T_s)}{L} \]  

Evaporation constant:

\[ \lambda = \left( \frac{k}{c_p g} \right) \frac{8 \ln(1 + B_M)}{\rho_F} [\frac{m^2}{s}] \]  
\[ m_{drop} = \frac{\pi}{6} \rho_F D^3 [\text{kg}] \]  

Heat-up process:

\[ \frac{dT_s}{dt} = \frac{\dot{m}_F L}{c_{p,F} m_{drop}} \left( \frac{B_T}{B_M} - 1 \right) [\frac{K}{s}] \]  
\[ \frac{dD}{dt} = -\frac{\lambda}{2D} [\frac{m}{s}] \]  

Evaporation time:

\[ t_{e,\text{st}} = \frac{D_0^2}{\lambda} [s] \]
5. User’s Manual


‘CoverPage’ sheet
Relevant information about authors is provided in this sheet. If there are any questions or comments regarding this program, please feel free to contact us.

‘Instruction’ sheet
The instruction sheet contains a description of each sheet in the program, as well as the user’s manual.

![Figure 5.1 – ‘Process’ sheet](image)
**‘Process’ sheet**
The process sheet contains all user-inputs necessary for performing computations. First of all, the user needs to choose a fuel type from the pull down menu. This program contains built-in a database of properties of each listed fuel necessary for evaporation computations (see *Appendix A – Fuel Properties*). Other than that, the user can specify any hydrocarbon fuel not listed here, provided that the properties of each specified fuel are available.

The cells highlighted in **light-brown** are the user inputs. The cells highlighted in **pink** contain computed values associated with the light-brown cells; therefore, they are locked to prevent the user from modifying their values. When values are entered into the formula cells, the formulas are erased and linkages to other cells are interrupted. That is why for this version we chose to lock the closed cells without a password.

One feature added to the previous work (ref. 1) is the ‘Evaporation ON/OFF’ switch. If the user chooses to turn off the ‘Evaporation switch’, the Microsoft® Excel program will run as if there is no evaporation and will give the solution for the droplet ballistics only.

If the ‘Evaporation switch’ is turned on, one main concern is the computational time because it is considered very computation-intensive to use Runge-Kutta method in a Microsoft® Excel spreadsheet for tracking a single evaporating droplet in crossflow. The computational time varies mostly with the CPU power available and the total cycle number as well as the time step size. To remedy this problem, four options have been proposed and it is up to the user to select one of the four options before running the code:

a. **Option 1** – Properties are calculated four times each cycle (more accurate but very slow)
b. **Option 2** – Properties are calculated one time each cycle (less accurate but fast)
c. **Option 3** – Properties are calculated four times during droplet heating. After droplet reaches steady state temperature, properties are not calculated any more. The values are used from the last cycle of droplet heating. This option requires user to input a constant value of epsilon, $\varepsilon$. It defines the condition when the steady state temperature will occur. $(dT/dt = \varepsilon)$
d. **Evap time estimate** – Before computation, it's always good to estimate the steady state evaporation time (droplet lifetime) of the droplet of size $r_{32}$. Click the **Update** button to start the estimation. The computational speed depends mostly on the droplet size $r_{32}$ and ambient conditions. For example, a Jet-A droplet of 50-micron diameter ($r_{32}=25$ micron) is estimated to completely vaporize within 0.004s. Using $\Delta t=1.0e-7s$, at least $n=40,000$ cycles are required.

4th-Order Runge-Kutta method calculates temperature derivative $(dT/dt)$ four times in each cycle. **Option 3** will force the program to check all four temperature derivatives in each cycle. If one of the temperature derivatives in a cycle is less than the constant epsilon, properties calculation will not be performed afterward. Based on the experiment, epsilon between 0.1 and 1 is good enough. For instance, a case has been performed using two constant epsilons, say 0.0001 and 0.1. Solutions from both epsilons yield similar results. Note that this may not apply to cases with fuel with properties highly sensitive to temperature.
From figure 4, the last two user inputs, **Total Cycles (C32)** and **Data taken every ## cycles (C33)** are the important features that were added for monitoring the amount of output data. *The number assigned in pink cell “E34”must be kept below 65,536; the cell will turn red if this condition is not satisfied.* Keeping the value below the limit can be done by changing the value in the cell “C33”.

After all the inputs have been specified, clicking the **Update** button will instruct the program to update the data in the ‘Data’ sheet as well as all plots in the ‘Trajectory’ and ‘Evap’ sheets.

In summary, the user needs to do the following steps to run the program:

1. Go to the ‘Process’ Sheet ➔ click on the **Process** tab.
2. Enter input values in the light-brown cells.
3. Adjust the value in the cell C33 so that the computed value in cell E34 is less than 65,536.
4. Choose the fuel type from the ‘Fuel’ option menu.
5. Choose the **ON/OFF** evaporation switch from the evaporation option menu.
6. If Evaporation is **ON**, choose one of the four options: *Option 1, 2, 3 or Evap time estimate.*
7. If ‘Evap time estimate’ is selected in step 6, click the **Update** button. The code will estimate evaporation constant and time.
8. Based on the estimated value of \( t_{\text{est},\text{evap}} \) (droplet lifetime), adjust and input appropriate 'Time step \( \Delta t \)' and 'Total cycles \( n \)'.
9. Click the **Update** button.
10. Observe the droplet profiles on the solution plots at both ‘Trajectory’ and ‘Evap’ sheets.
11. Repeat step 1 through step 10 for different input values
12. Click the **Clear Data** button to clear the data (Optional).

An additional feature in this program is the option to store the computed data into a **TecPlot** format file. This feature provides the user a flexibility to plot the data using other software such as **TecPlot**. In summary, user needs to do the following steps to save the data into TecPlot format file:

1. Select "Yes" to save the data into a file
2. Specify the path and the filename to save into a file (e.g. C:\Document\result.dat)
3. Select the unit length (i.e. meter or millimeter)
4. Click the **Update** button

Other than computational time, another concern is the computer memory usage because the code needs a lot of memory space for those six variables arrays to be solved. As discussed above, the feature of estimating the steady state droplet lifetime enables us to predict the total cycle number \( n \) required to complete a whole evaporation process for each fuel droplet. By making use of this advantage, a so-called ‘**dynamic array size**’ is added to the existing code such that the allocated memory space for each computation will closely follow the total cycle number \( n \) entered by user. Using the example in ‘Evap Time Estimate’ option where \( n=40,000 \), each variable array size will be set to \( n+2=40002 \).
‘Data’ sheet

This sheet contains the solution data computed by the program. All the solution data will be listed separately at eight columns A to H for plotting. Table 1 shows the corresponding variables of each column:

<table>
<thead>
<tr>
<th>Column</th>
<th>Variable</th>
<th>Units</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Time</td>
<td>sec</td>
<td>Time</td>
</tr>
<tr>
<td>B</td>
<td>X</td>
<td>m</td>
<td>Droplet trajectory in x-direction</td>
</tr>
<tr>
<td>C</td>
<td>Z</td>
<td>m</td>
<td>Droplet trajectory in z-direction</td>
</tr>
<tr>
<td>D</td>
<td>Uₜ</td>
<td>(\frac{m}{s^2})</td>
<td>Droplet velocity in x-direction</td>
</tr>
<tr>
<td>E</td>
<td>Wₜ</td>
<td>(\frac{m}{s^2})</td>
<td>Droplet velocity in z-direction</td>
</tr>
<tr>
<td>F</td>
<td>C_D</td>
<td>n/a</td>
<td>Drag coefficient</td>
</tr>
<tr>
<td>G</td>
<td>D/D₀</td>
<td>µm</td>
<td>Normalized droplet diameter square</td>
</tr>
<tr>
<td>H</td>
<td>Tₛ</td>
<td>K</td>
<td>Droplet surface temperature</td>
</tr>
</tbody>
</table>

Table 5.1 – Variables with their corresponding column in ‘Data’ sheet

‘Trajectory’ sheet

As shown in figure 5, there are five graphs on this sheet, namely droplet trajectory, droplet velocity profile, drag coefficient, C_D, as a function of time, droplet velocity profiles as a function of time, and droplet trajectory profiles as a function of time.
Figure 5.2 – ‘Trajectory’ sheet
‘Evap’ sheet

There are two graphs on this sheet, as shown in figure 6, namely droplet size and surface temperature histories. It also shows the values of the estimated steady-state evaporation constant and evaporation time.

Figure 5.3 – ‘Evap’ sheet
6. Results and Discussions

To understand the performance of this Excel code, several results have been obtained and displayed in the following pages using the input parameters as shown in Table 6.1. Only the trajectory and the time variation of normalized droplet size and surface temperature are selected as the results to be discussed.

6.1(a) Normalized diameter square vs time

6.2(a) Normalized diameter square vs time

6.1(b) Droplet surface temperature vs time

6.2(b) Droplet surface temperature vs time

6.1(c) Trajectory of fuel droplet after injection

6.1(c) Trajectory of fuel droplet after injection

Figure 6.1 – Injection of fuel droplet at T=500K and P=1atm

Figure 6.2 – Injection of fuel droplet at T=500K and P=10atm
Figure 6.3 – Injection of fuel droplet at T=500K and P=1atm

Figure 6.4 – Injection of fuel droplet at T=500K and P=10atm
In figure 6.1(a), water droplet of diameter 50 micron at 500K 1 atm takes a much longer time to reach complete vaporization i.e. around 0.13s than Jet-A and DF 2 do. As shown in figure 6.2(a), increasing the ambient pressure to 10 atm further extends its droplet lifetime to around 0.16s, as known from the general physics results. Similar conclusions will be obtained when comparing figure 6.3(a) with 6.4(a) except that each fuel droplet lifetime is much shorter at such a high ambient temperature (T=1000K).

Figures 6.1(b) and 6.2(b) show the time variation of droplet surface temperature at the same ambient temperature i.e. 500K and two different ambient pressures, i.e. 1 atm and 10 atm respectively. In figure 6.1(b), each droplet reaches its steady state temperature and it never goes beyond its normal boiling point. While at high pressure as shown in figure 6.2(b), the boiling point increases with pressure and consequently the steady state temperature is higher. These observations also apply to figures 6.3(b) and 6.4(b).

The droplet trajectory after injection and before complete vaporization for each droplet is shown in figures 6.1(c), 6.2(c), 6.3(c) and 6.4(c). Due to the decreasing droplet mass (as a result of vaporization) followed by the momentum loss, the downward crossflow forces the evaporating droplet to drop almost vertically (or in z-direction) at the very end of its drop life. Water, with a higher heat capacity, therefore penetrates deepest across the crossflow among all the fuels.

<table>
<thead>
<tr>
<th>Input</th>
<th>Value (unit)</th>
<th>Input</th>
<th>Value (unit)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r_{32}$</td>
<td>25 $\mu$m</td>
<td>$W_g$</td>
<td>-38 m/s</td>
</tr>
<tr>
<td>$X_o$</td>
<td>0 m</td>
<td>$T_\infty$</td>
<td>1000 K</td>
</tr>
<tr>
<td>$U_{do}$</td>
<td>-2.4 m/s</td>
<td>$P$</td>
<td>1010 kPa</td>
</tr>
<tr>
<td>$Z_o$</td>
<td>0 m</td>
<td>$g$</td>
<td>0 m/s$^2$</td>
</tr>
<tr>
<td>$W_{do}$</td>
<td>0 m/s</td>
<td>$\Delta t$</td>
<td>1.00E-07 sec</td>
</tr>
<tr>
<td>$T_{init}$</td>
<td>300 K</td>
<td>$n$</td>
<td>100000 Cycles</td>
</tr>
<tr>
<td>$M_g$</td>
<td>28.97 kg/kmol</td>
<td>$\varepsilon$</td>
<td>1 K</td>
</tr>
<tr>
<td>$U_g$</td>
<td>0 m/s</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 6.1 – Input parameters used in discussion
Appendix A—Fuel Properties

In this code, two different groups of fuels are considered. The reason is because the thermal properties for these two groups of fuels are referring to different sources as shown below.

<table>
<thead>
<tr>
<th>Group</th>
<th>Source</th>
<th>Fuels</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Chin (refs. 3 and 6)</td>
<td>DF 2 (diesel oil)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>JP 4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>JP 5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Heptane</td>
</tr>
<tr>
<td>2</td>
<td>Yaws (ref. 7)</td>
<td>Jet-A (C_{12}H_{23})</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water (H_{2}O)</td>
</tr>
</tbody>
</table>

Table A.1 – two groups of fuels

<table>
<thead>
<tr>
<th>Fuel/properties</th>
<th>DF 2</th>
<th>Jet-A (C_{12}H_{23})</th>
<th>JP 4</th>
<th>JP 5</th>
<th>n-Heptane</th>
<th>Water (H_{2}O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_{d,288.6K}$ (kg/m$^3$)</td>
<td>846</td>
<td>915.91</td>
<td>773</td>
<td>827</td>
<td>687.8</td>
<td>1036</td>
</tr>
<tr>
<td>$T_{\text{crit}}$ (K)</td>
<td>725.9</td>
<td>737.0</td>
<td>612</td>
<td>648.8</td>
<td>540.17</td>
<td>647.3</td>
</tr>
<tr>
<td>$T_{\text{bn}}$ (K)</td>
<td>536.4</td>
<td>529.0</td>
<td>420</td>
<td>495.3</td>
<td>371.4</td>
<td>373.16</td>
</tr>
<tr>
<td>$C_{\text{exp}}$ (1/K)</td>
<td>0.00046</td>
<td>n/a</td>
<td>0.000557</td>
<td>0.000485</td>
<td>0.000715</td>
<td>n/a</td>
</tr>
<tr>
<td>$L_{\text{Tbn}}$ (kJ/kg)</td>
<td>254</td>
<td>341.200</td>
<td>292</td>
<td>266.5</td>
<td>317.8</td>
<td>2191</td>
</tr>
<tr>
<td>$M_d$ (kg/kmol)</td>
<td>198</td>
<td>181.321</td>
<td>125</td>
<td>169</td>
<td>100.16</td>
<td>18.02</td>
</tr>
<tr>
<td>a*</td>
<td>15.5274</td>
<td>n/a</td>
<td>15.2323</td>
<td>15.16</td>
<td>14.2146</td>
<td>n/a</td>
</tr>
<tr>
<td>b*</td>
<td>5383.59</td>
<td>n/a</td>
<td>3999.66</td>
<td>4768.77</td>
<td>3151.68</td>
<td>n/a</td>
</tr>
</tbody>
</table>

*Clusius-Clapeyron constants

Table A.2 – Physical properties of fuels (Group 1 and 2)

All fuel properties are calculated in subroutines $\text{transfernumber}(Ts)$ and $\text{fuel_thermal_prop}(Ts)$ where Ts refers to surface temperature of a fuel droplet.
Group 1 Fuels: DF 2 (diesel oil), JP 4, JP 5, and n-Heptane

At any given droplet surface temperature, $T_s$, fuel vapor pressure at droplet surface, $P_{F,s}$, is approximated by Clasius-Clapeyron equation (or called Antoine equation (ref. 4)) [kPa]:

$$P_{F,s} = P_{vap}(T_s) = \exp\left(a - \frac{b}{T_s - 43}\right) \quad (A.1)$$

where $a$ and $b$ are constants for certain fuels (provided in Table A.2 shown above).

$T_s$ – droplet surface temperature [K]

Meanwhile, variation of $k_{Fv} \left[ \frac{W}{m \cdot K} \right]$ and $c_{p,Fv} \left[ \frac{kJ}{kg} \right]$ of fuel vapors with temperature are given by Chin (ref. 3):

$$k_{Fv} = 10^{-6}\left[13.2 - 0.0313(T_{bn} - 273)\right]\left(\frac{T_r}{273}\right)^n \quad (A.2)$$

$$c_{p,Fv} = (0.363 + 0.000467T_r)(5 - 0.001\rho_{F,288.6K}) \quad (A.3)$$

where

$$n = 2 - 0.0372\left(\frac{T_r}{T_{bn}}\right)^2 \quad (A.3a)$$

$\rho_{F,288.6K}$ - fuel density in kg/m$^3$ at 288.6K.

Liquid fuel density$^3 \left[ \frac{kg}{m^3} \right]$ is needed to calculate $\lambda_{si}$:

$$\rho_F = \rho_{F,288.6K}\left[1 - 1.8C_{ex}(T_{drop} - 288.6) - 0.09\left(\frac{T_{drop} - 288.6}{T_{crit} - 288.6}\right)^2\right] \quad (A.4)$$

where $C_{exp}$ is the expansion coefficient (provided in Table A.2).
Latent heat of fuel vaporization \( \frac{kJ}{kg} \) corresponding to fuel surface temperature is estimated by:

\[
L = L_{bn} \left( \frac{T_{crit} - T_T}{T_{crit} - T_{bn}} \right)^{0.38}
\]  
(A.5)

\( L_{Tbn} \) – Latent heat of fuel vaporization at normal boiling point \( \frac{kJ}{kg} \)

Specific heat at constant pressure of fuel liquid is given by \( \frac{kJ}{kgK} \):

\[
e_{p,F} = (0.76 + 0.00335T_{drop})(0.001\rho_F)^{0.5}
\]  
(A.6)
Group 2 Fuels: Jet-A (C_{12}H_{23}) and Water (H_2O)

All equations for the fuel properties can be found in Yaws (ref. 7), as shown below:

*Fuel liquid density* $[\frac{g}{cm^3}]$:

\[ \rho_F = AB \left(1 - \frac{T_{drop}}{T_c}\right)^n \]  
(A.7)

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Jet-A (C_{12}H_{23})</th>
<th>Water (H_2O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.29292</td>
<td>0.3471</td>
</tr>
<tr>
<td>B</td>
<td>0.26661</td>
<td>0.274</td>
</tr>
<tr>
<td>n</td>
<td>0.298</td>
<td>0.2857</td>
</tr>
</tbody>
</table>

Table A.3 – Coefficients for *Fuel Liquid Density* $[\frac{g}{cm^3}]$ in Group 2 fuel.

*Latent heat of vaporization of fuel liquid* $[\frac{kJ}{mol}]$:

\[ L = A \left(1 - \frac{T_{drop}}{T_c}\right)^n \]  
(A.8)

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Jet-A (C_{12}H_{23})</th>
<th>Water (H_2O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>73.509</td>
<td>52.023</td>
</tr>
<tr>
<td>n</td>
<td>0.347</td>
<td>0.321</td>
</tr>
</tbody>
</table>

Table A.4 – Coefficients for *Latent Heat of Vaporization of fuel liquid* $[\frac{kJ}{mol}]$ in Group 2 fuel.
Specific heat at constant pressure of fuel liquid $\left[ \frac{J}{mol \cdot K} \right]$: 

$$C_{p, F} = A + BT_{drop} + CT_{drop}^2 + DT_{drop}^3 \quad (A.9)$$

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Jet-A (C_{12}H_{23})</th>
<th>Water (H_2O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>142.238</td>
<td>92.053</td>
</tr>
<tr>
<td>B</td>
<td>1.5261</td>
<td>-0.039953</td>
</tr>
<tr>
<td>C</td>
<td>-0.0034477</td>
<td>-0.00021103</td>
</tr>
<tr>
<td>D</td>
<td>0.0000032968</td>
<td>0.0000005347</td>
</tr>
</tbody>
</table>

Table A.5 – Coefficients for Specific Heat at constant pressure of fuel liquid $\left[ \frac{J}{mol \cdot K} \right]$ in Group 2 fuel.

Specific heat at constant pressure of fuel vapor $\left[ \frac{J}{mol \cdot K} \right]$: 

$$C_{p, Fv} = A + BT_r + CT_r^2 + DT_r^3 + ET_r^4 \quad (A.10)$$

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Jet-A (C_{12}H_{23})</th>
<th>Water (H_2O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>-128.032</td>
<td>33.933</td>
</tr>
<tr>
<td>B</td>
<td>1.4622</td>
<td>-0.0084186</td>
</tr>
<tr>
<td>C</td>
<td>-0.00086193</td>
<td>0.000029906</td>
</tr>
<tr>
<td>D</td>
<td>0.000000018462</td>
<td>-0.00000017825</td>
</tr>
<tr>
<td>E</td>
<td>0.00000000036227</td>
<td>3.6934E-12</td>
</tr>
</tbody>
</table>

Table A.6 – Coefficients for Specific Heat at constant pressure of fuel vapor $\left[ \frac{J}{mol \cdot K} \right]$ in Group 2 fuel.

Thermal conductivity of fuel vapor $\left[ \frac{W}{m \cdot K} \right]$: 

$$k_{Fv} = A + BT_r + CT_r^2 \quad (A.11)$$

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Jet-A (C_{12}H_{23})</th>
<th>Water (H_2O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>-0.01184</td>
<td>0.00053</td>
</tr>
<tr>
<td>B</td>
<td>0.0000061839</td>
<td>0.000047093</td>
</tr>
<tr>
<td>C</td>
<td>0.00000025082</td>
<td>0.00000049551</td>
</tr>
</tbody>
</table>

Table A.7 – Coefficients for Thermal Conductivity for fuel vapor $\left[ \frac{W}{m \cdot K} \right]$ in Group 2 fuel.
Vapor pressure [mmHg]:

\[
\log_{10} P_{\text{vap}} = A + \frac{B}{T_s} + C \log_{10} T_s + D T_s + E T_s^2
\]  
(A.12)

Then, let

\[
P_{F,s} = P_{\text{vap}}(T_s) 
\]  
(A.12a)

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Jet-A (C_{12}H_{23})</th>
<th>Water (H_{2}O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>-50.5512</td>
<td>29.8605</td>
</tr>
<tr>
<td>B</td>
<td>-2705.3</td>
<td>-3152.2</td>
</tr>
<tr>
<td>C</td>
<td>28.273</td>
<td>-7.3037</td>
</tr>
<tr>
<td>D</td>
<td>-0.045702</td>
<td>0.00000024247</td>
</tr>
<tr>
<td>E</td>
<td>0.000020443</td>
<td>0.000001809</td>
</tr>
</tbody>
</table>

Table A.8 – Coefficients for Vapor Pressure [mmHg] in Group 2 fuel.
Appendix B—Air Properties

Variation of air properties with temperature (range 100K through 2000K) can be obtained from correlation provided in Incorpera. Air properties are all calculated in subroutine air().

Thermal conductivity \( \frac{W}{m \cdot K} \):

\[
k_A = 2 \cdot 10^{-11} T_r^3 - 5 \cdot 10^{-8} T_r^2 - 0.0969 \cdot 10^{-3} T_r + 0.8289 \cdot 10^{-3}
\]  
(B.1)

Specific heat at constant pressure \( \frac{kJ}{kg} \):

\[
c_{p,A} = -5 \cdot 10^{-11} T_r^3 + 2 \cdot 10^{-7} T_r^2 - 1 \cdot 10^{-5} T_r + 1.0041
\]  
(B.2)

Viscosity \( \frac{Ns}{m^2} \):

\[
\mu_A = (7 \cdot 10^{-10} T_\infty^3 - 0.0003 T_\infty^2 + 0.6227 T_\infty + 18.761) \cdot 10^{-7}
\]  
(B.3)

Prandtl number:

\[
Pr_A = 2 \cdot 10^{-13} T_\infty^4 - 10^{-9} T_\infty^3 + 2 \cdot 10^{-6} T_\infty^2 - 0.0009 T_\infty + 0.8632
\]  
(B.4)

Density \( \frac{kg}{m^3} \):

\[
\rho_A = 355.91 T_\infty^{-1.0032}
\]  
(B.5)
Appendix C—Microsoft® Visual Basic Code

In the Microsoft® Excel spreadsheet, select ‘Tools ➔ Macro ➔ Visual Basic Editor’, a new window will open showing all the numerical codes in different sheets or modules.

Main Code

Private Sub CommandButton3_Click()
'Declare ballistics variables

    Dim n As Long, nn As Double, nnn As Long, speedup As Long
    Dim Cdm As Double, Rems As Double
    Dim dtt As Double
    Dim k1 As Double, k2 As Double, k3 As Double, k4 As Double, l1 As Double, l2 As Double, l3 As Double, l4 As Double
    Dim kz1 As Double, kz2 As Double, kz3 As Double, kz4 As Double, lz1 As Double, lz2 As Double, lz3 As Double, l4 As Double
    Dim Urm As Double
    Dim a As Double, b As Double
    Dim location
    Dim sf
    Dim a1, b1, c1, d1, e1, f1, g1, h1
    Dim unitconv

    'Adding these inputs for drop evaporation ' (3/26/03)
    Dim md1 As Double, md2 As Double, md3 As Double, md4 As Double
    Dim mt1 As Double, mt2 As Double, mt3 As Double, mt4 As Double
    Dim evap As Double

    'Variable time
    Dim begin, last, switch
    begin = Second(Time) + Minute(Time) * 60 + Hour(Time) * 3600
    switch = 0
    Call Macro2
    Halt = False
    Msg = "Do you want to continue ?"
    Style = vbYesNo
    Style1 = vbOKOnly
    Title = "Jet Flow in CrossFlow"
    Title1 = "Evaporation Time Estimate"
    Msg3 = "Drop vaporizes completely!"
    Msg_size = "Please reduce droplet size!"
    Msg_size1 = "Can't estimate. Drop size too big!"
    Call taperd

    'Dynamic array size
    asize = kl + 2
    ReDim xx(0 To asize) As Double, xp(0 To asize) As Double
    ReDim zz(0 To asize) As Double, zp(0 To asize) As Double
    ReDim D(0 To asize) As Double, Ts(0 To asize) As Double
'Sheets("Process").Cells(9, 10) = kl
'Sheets("Process").Cells(10, 10) = asize
If flag = 4 And r > 0.0001 Then
    Response = MsgBox(Msg_size, Style1, Title1)
    Cells(5, 3).Select
    GoTo 50
End If

Pi = 22# / 7#

Worksheets("Process").CommandButton1.Width = 0
Worksheets("Process").CommandButton1.Visible = True

n = 0    ' used for array value index
nn = -1  ' used for writing data into cell
nnn = 2  ' used for writing into sequence cell
dt = 0
evap = 0#
nl = 0   ' used to keep track the time level recorded when drop vaporizes completely
ss = 0   ' used to turn on/off switch if temperature has reached steady
sst = 0  ' used to print steady state time
speedup = Int(kl / 50) ' used to update the percentage bar

' Initial position and velocity
xx(n) = xxi
xp(n) = xpi
zz(n) = zzi
zp(n) = zpi

' Assume uniform temperature within the drop
Ts(n) = Tinit

D(n) = 2# * r
D02 = D(n) ^ 2

If flag = 3 Or flag = 4 Then Sheets("Process").Cells(18, 10) = "Temperature is not steady"

'Determine fuel type then select one of two approach to calculate fuel properties
' 0 - Lebefvre's, 1 - Yaws'
fuel_type = Sheets("Process").ComboBox1.Value
Select Case fuel_type
Case "DF 2"
    otherfuel = 0
Case "Jet-A (C12H23)"
    otherfuel = 1
    Apv = -50.5512
    Bpv = -2705.3
    Cpv = 28.273
    Dpv = -0.045702
    Epv = 0.000020443
    Arho = 0.29292
    Brho = 0.26661
    nrho = 0.298
    ...
Akfv = -0.01184
Bkfv = 0.000061839
Ckfv = 0.000000025082

Acpf = -128.032
Bcpf = 1.4622
Ccpf = -0.00086193
Dcpf = 0.00000018462
Ecpf = 3.6227E-13

Alat = 73.509
nlat = 0.347

Case "JP 4"
  otherfuel = 0
Case "JP 5"
  otherfuel = 0
Case "n-Heptane"
  otherfuel = 0
Case "Water"
  otherfuel = 1
  Apv = 29.8605
  Bpv = -3152.2
  Cpv = -7.3037
  Dpv = 0.00000024247
  Epv = 0.000001809

  Arho = 0.3471
  Brho = 0.274
  nrho = 2#/7#

  Akfv = 0.00053
  Bkfv = 0.000047093
  Ckfv = 0.000000049551

  Acpf = 33.933
  Bcpf = -0.0084186
  Ccpf = 0.000029906
  Dcpf = -0.00000017825
  Ecpf = 3.6934E-12

  Alat = 52.023
  nlat = 0.321
Case Else
  otherfuel = 0
End Select
If onoff_flag = 0 Then
  Tref = Tinit + (Tinf - Tinit) / 3#
  'air: viscosity
  mu = 0.000000007 * Tref^3 - 0.0003 * Tref^2 + 0.6227 * Tref + 18.761
  mu = mu * 0.0000001 'Ns/m^2
Else
  'air: viscosity
  Tdocrit = Tinit / Tcrit
  rhof = 1000# * Arho * Brho ^ ((-1#) * (1# - Tdocrit) ^ nrho) 'convert g/cm^3' to 'kg/m^3
End If

If otherfuel = 0 Then
  'fuel: liquid density
  rhof = rhofr * (1# - 1.8 * cexp * (Tinit - 288.6) - 0.09 * ((Tinit - 288.6) / (Tcrit - 288.6)) ^ 2#) 'kg/m^3
Else
  'fuel: liquid density
  Tdocrit = Tinit / Tcrit
  rhof = 1000# * Arho * Brho ^ ((-1#) * (1# - Tdocrit) ^ nrho) 'convert g/cm^3' to 'kg/m^3
End If

'air: density
rhog = 355.91 * Tref ^ (-1.0032) 'kg/m^3
End If

Sheets("Process").Cells(14, 12) = "Calculating"
20
  dtt = dtt + dt
  If flag = 1 Or flag = 2 And onoff_flag = 1 Then Call driver_for_runge(Ts(n))
  If flag = 3 And ss = 0 And onoff_flag = 1 Then Call driver_for_runge(Ts(n))
  If flag = 4 And ss = 0 And onoff_flag = 1 Then Call driver_for_runge(Ts(n))
  Call Runge(xp(n), zp(n), D(n), Ts(n))

  If (SuperExit) Then GoTo 50
  k1 = dt * xp(n) 'replaced xp(n) 3/26/03
  l1 = dt * A_x
  kz1 = dt * zp(n) 'replaced zp(n) 3/26/03
  lz1 = dt * A_z
  If onoff_flag = 1 Then
    md1 = dt * (-0.5) * lambda / D(n) '3/28/03
    mt1 = dt * ct
    If ((D(n) + 0.5 * md1) < 0.000000001) Then
      evap = 1#
      nl = n
      GoTo 15
    End If
  End If
  End If

  If flag = 1 And onoff_flag = 1 Then Call driver_for_runge(Ts(n) + 0.5 * mt1)
  If flag = 3 And ss = 0 And onoff_flag = 1 Then Call driver_for_runge(Ts(n) + 0.5 * mt1)
  Call Runge(xp(n) + lz1 / 2#, zp(n) + lz1 / 2#, D(n) + 0.5 * md1, Ts(n) + 0.5 * mt1)

  If (SuperExit) Then GoTo 50
  k2 = dt * (xp(n) + l1 / 2#) 'replaced xp(n) 3/26/03
  l2 = dt * A_x
  kz2 = dt * (zp(n) + lz1 / 2#) 'replaced zp(n) 3/26/03
  lz2 = dt * A_z
If onoff_flag = 1 Then
    md2 = dt * (-0.5) * lambda / (D(n) + 0.5 * md1) '3/28/03
    mt2 = dt * ct
    If ((D(n) + 0.5 * md2) < 0.00000001) Then
        evap = 1#
        nl = n
        GoTo 15
    End If
End If
If flag = 1 And onoff_flag = 1 Then Call driver_for_runge(Ts(n) + 0.5 * mt2)
If flag = 3 And ss = 0 And onoff_flag = 1 Then Call driver_for_runge(Ts(n) + 0.5 * mt2)
Call Runge(xp(n) + l2 / 2#, zp(n) + lz2 / 2#, D(n) + 0.5 * md2, Ts(n) + 0.5 * mt2)

If (SuperExit) Then GoTo 50
k3 = dt * (xp(n) + l2 / 2#)'replaced xp(n) 3/26/03
l3 = dt * A_x
kz3 = dt * (zp(n) + lz2 / 2#)'replaced zp(n) 3/26/03
lz3 = dt * A_z
If onoff_flag = 1 Then
    md3 = dt * (-0.5) * lambda / (D(n) + 0.5 * md2) '3/28/03
    mt3 = dt * ct
    If ((D(n) + md3) < 0.00000001) Then
        evap = 1#
        nl = n
        GoTo 15
    End If
End If
If flag = 1 And onoff_flag = 1 Then Call driver_for_runge(Ts(n) + mt3)
If flag = 3 And ss = 0 And onoff_flag = 1 Then Call driver_for_runge(Ts(n) + mt3)
Call Runge(xp(n) + l3, zp(n) + lz3, D(n) + md3, Ts(n) + mt3)

If (SuperExit) Then GoTo 50
k4 = dt * (xp(n) + l3)'replaced xp(n) 3/26/03
l4 = dt * A_x
kz4 = dt * (zp(n) + lz3)'replaced zp(n) 3/26/03
lz4 = dt * A_z
If onoff_flag = 1 Then
    md4 = dt * (-0.5) * lambda / (D(n) + md3) '3/28/03
    mt4 = dt * ct
    End If
If flag = 3 Or flag = 4 And ss = 0 And onoff_flag = 1 Then
    If Abs(ct) < sstemp Then ss = 1
End If
If flag = 3 And ss = 1 And sst = 0 And onoff_flag = 1 Then
    Sheets("Process").Cells(18, 10) = "Temperature is steady at t = " & dtt * 1000# & "milliseconds"
sst = 1
End If
xp(n + 1) = xp(n) + (1# / 6#) * (l1 + 2# * l2 + 2# * l3 + l4)
zp(n + 1) = zp(n) + (1# / 6#) * (lz1 + 2# * lz2 + 2# * lz3 + lz4)
xx(n + 1) = xx(n) + (1# / 6#) * (k1 + 2# * k2 + 2# * k3 + k4)
zz(n + 1) = zz(n) + (1/6) * (kz1 + 2 * kz2 + 2 * kz3 + kz4)

If onoff_flag = 1 Then
    D(n + 1) = D(n) + (1/6) * (md1 + 2 * md2 + 2 * md3 + md4) '3/28/03
    Ts(n + 1) = Ts(n) + (1/6) * (mt1 + 2 * mt2 + 2 * mt3 + mt4)
End If
DoEvents
If (Halt) Then
    DoEvents
    Halt = False
    Response = MsgBox(Msg, Style, Title)
    If Response = vbNo Then
        evap = 2#
        nl = n
        GoTo 15
    End If
End If
End If

If 0 = (n Mod speedup) Or n >= kl Then
    Worksheets("Process").CommandButton1.Width = ((n / kl) * 165.75)
    Worksheets("Process").CommandButton1.Caption = ((n / kl) * 100) & "%"
    Worksheets("Process").CommandButton1.Height = 20.25
End If

If flag = 4 And ss = 1 And onoff_flag = 1 Then
    Sheets("Process").Cells(14, 12) = "Estimation done"
    Sheets("Process").Cells(18, 10) = "Temperature is steady at t = " & dtt & " seconds"
    Sheets("Process").Cells(6, 10) = D02 / lambda
    Sheets("Process").Cells(5, 10) = lambda
    dt_temp = dt
    dt = dt_old
    'Sheets("Process").Cells(9, 10) = n
    'Sheets("Process").Cells(10, 10) = kl
    'Sheets("Process").Cells(7, 10) = dt '9/10/03
    'Sheets("Process").Cells(8, 10) = dt_temp
    GoTo 50
Else
    If flag = 4 And n >= kl And ss = 0 Then
        Response = MsgBox(Msg_size1, Style1, Title1)
        dt_temp = dt
        dt = dt_old
        GoTo 50
    End If
End If
End If

If (D(n + 1) < 0.00000001) And onoff_flag = 1 Then
    evap = 1#
    nl = n
    GoTo 15
End If
n = n + 1
If n <= kl Then
  GoTo 20
End If

15
Sheets("Process").Cells(14, 12) = "Writing data into cells"
If evap = 1# Then
  nf = nl - 1
ElseIf evap = 2# Then
  nf = nl - 1
ElseIf evap = 0# Then
  nf = kl
End If
n = 0
ttldata = Sheets("Process").Cells(35, 5)
sd = Sheets("Process").Cells(35, 5)
speedup = Int(sd / 10)

25
Urm = (((xp(n) - ug) ^ 2) + ((zp(n) - wg) ^ 2)) ^ 0.5
If onoff_flag = 1 Then Rems = rhog * Urm * D(n) / mu
If onoff_flag = 0 Then Rems = rhog * Urm * D(0) / mu

If Rems <= 1000 Then
  If Rems = 0# Then
    Cdm = 0#
  Else
    Cdm = (((Rems ^ (2# / 3#)) / 6#) + 1#) * 24# / Rems
  End If
Else
  Cdm = 0.424
End If
Sheets("Data").Cells(nnn, 1) = n * dt
Sheets("Data").Cells(nnn, 2) = xx(n)
Sheets("Data").Cells(nnn, 3) = zz(n)
Sheets("Data").Cells(nnn, 4) = xp(n)
Sheets("Data").Cells(nnn, 5) = zp(n)
Sheets("Data").Cells(nnn, 6) = Cdm
If onoff_flag = 1 Then
  Dplot = (D(n) / D(0)) ^ (2#)
  Sheets("Data").Cells(nnn, 7) = Dplot
  Sheets("Data").Cells(nnn, 8) = Ts(n)
End If

If 0 = (nnn Mod speedup) Or n >= nf Then
  Worksheets("Process").CommandButton1.Width = (((nnn - 1) / ttldata) * 165.75)
  Worksheets("Process").CommandButton1.Caption = (((nnn - 1) / ttldata) * 100) & ":%
  Worksheets("Process").CommandButton1.Height = 20.25
End If

DoEvents
If (Halt) Then
  DoEvents
  Halt = False
  Response = MsgBox(Msg, Style, Title)
If Response = vbNo Then
    GoTo 10
End If
End If

n = n + userchoice
nnn = nnn + 1
If n > nf Then
    GoTo 10
Else
    GoTo 25
End If

10
last = Second(Time) + Minute(Time) * 60 + Hour(Time) * 3600
Sheets("Process").Cells(16, 10) = last - begin
If onoff_flag = 1 Then
    Sheets("Evap").Cells(4, 10) = D02 / lambda
    Sheets("Evap").Cells(3, 10) = lambda
End If
If (evap = 1#) Then
    nnn = nnn + 1
    Sheets("Data").Cells(nnn, 1) = (nf + 1#) * dt
    Sheets("Data").Cells(nnn, 7) = 0#
    Response = MsgBox(Msg3, Style1, Title)
End If
Macro1 'plot data on chart
'sd = Sheets("Process").Cells(35, 5)
'print variables in a file (Tecplot format)
If Sheets("Process").Cells(46, 9) = "YES" Then
    location = Sheets("Process").Cells(23, 11)
    Sheets("Process").Cells(14, 12) = "Writing data into file : " + location
    Open location For Output As #1
    Print #1, "TITLE = "; Spc(2); "Spray Jet In CrossFlow"; ";
    If onoff_flag = 1 Then
        If Sheets("Process").Cells(47, 9) = "millimeter" Then
            unitconv = 1000#
        Else
            unitconv = 1#
        End If
        Print #1, "Variables ="; Spc(2); "Time(sec)"; Spc(2); "X(mm)"; Spc(2); "U(mm/s)"; Spc(2); "Cd"; Spc(2); "D(Normalized)"; "T(K)"
    Else
        unitconv = 1#
        Print #1, "Variables ="; Spc(2); "Time(sec)"; Spc(2); "X(meter)"; Spc(2); "U(m/s)"; Spc(2); "Cd"; Spc(2); "D(Normalized)"; "T(K)"
    End If
Else
    If Sheets("Process").Cells(47, 9) = "millimeter" Then
        unitconv = 1000#
        Print #1, "Variables ="; Spc(2); "Time(sec)"; Spc(2); "X(mm)"; Spc(2); "U(mm/s)"; Spc(2); "Cd"; Spc(2); "D(Normalized)"; "T(K)"
    Else
        unitconv = 1#
        Print #1, "Variables ="; Spc(2); "Time(sec)"; Spc(2); "X(meter)"; Spc(2); "U(m/s)"; Spc(2); "Cd"; Spc(2); "D(Normalized)"; "T(K)"
'plot data in a file (Tecplot format)
Print #1, "ZONE I ="; nnn - 2 & ","; Spc(2); "F = POINT"
nnn = nnn - 1
For sf = 2 To nnn
    a1 = Sheets("Data").Cells(sf, 1)
    b1 = Sheets("Data").Cells(sf, 2)
    b1 = b1 * unitconv
    c1 = Cells("Data").Cells(sf, 3)
    c1 = c1 * unitconv
    d1 = Cells("Data").Cells(sf, 4)
    d1 = d1 * unitconv
    e1 = Cells("Data").Cells(sf, 5)
    e1 = e1 * unitconv
    f1 = Cells("Data").Cells(sf, 6)
    If onoff_flag = 1 Then
        g1 = Cells("Data").Cells(sf, 7)
        h1 = Cells("Data").Cells(sf, 8)
    End If
    If onoff_flag = 1 Then
        Print #1, a1; Spc(2); b1; Spc(2); c1; Spc(2); d1; Spc(2); e1; Spc(2); f1; Spc(2); g1; Spc(2); h1
    Else
        Print #1, a1; Spc(2); b1; Spc(2); c1; Spc(2); d1; Spc(2); e1; Spc(2); f1
    End If
Next sf
Close #1
End If
Sheets("Process").Cells(14, 12) = "Completed"
SuperExit = False
End Sub
Other Subroutines

Sub driver_for_runge(Ts)

Call transformnumber(Ts)
Call reference_cond(Ts)
Call air
Call fuel_thermal_prop(Ts)

'fuel-air mixture
kg = yar * ka + yfr * kfv
cpg = yar * cpa + yfr * cpfv
BT = cpg * (Tinf - Ts) / lat

'evaporation contant
lambda = 8# * Log(1# + BM) * kg / (cpg * rhof)
End Sub

Sub transformnumber(Ts)

If (otherfuel = 1) Then
   Log10T = Log(Ts) / Log(10#)
   Log10P = Apv + Bpv / Ts + Cpv * Log10T + Dpv * Ts + Epv * Ts * Ts
   pfs = 10# ^ (Log10P) * 0.13333 'convert 'mmHg' to 'Kpa'
   pfs = Application.WorksheetFunction.Min(p, pfs)
Else
   pfs = Exp(acc - bcc / (Ts - 43#)) 'unit='Kpa'
   pfs = Application.WorksheetFunction.Min(p, pfs)
End If

yfs = 1# / (1# + (p / pfs - 1#) * (m wg / m wd))
BM = yfs / (1# - yfs)
End Sub

Sub reference_cond(Ts)

Tref = Ts + (Tinf - Ts) / 3#
yfr = 2# * yfs / 3#
yar = 1# - yfr
End Sub

Sub air()

'air: density
rhog = 355.91 * Tref ^ (-1.0032) 'kg/m^3

'air: viscosity
mu = 0.00000007 * Tref ^ 3 - 0.0003 * Tref + 0.6227 * Tref + 18.761
mu = mu * 0.0000001 'Ns/m^2

'air: prandtl number
\[ \text{Pra} = 0.0000000000002 \cdot \text{Tref}^4 - 0.000000001 \cdot \text{Tref}^3 + 0.000002 \cdot \text{Tref}^2 - 0.0009 \cdot \text{Tref} + 0.8632 \]

'air: thermal conductivity
\[ \text{ka} = 0.00000000002 \cdot \text{Tref}^3 - 0.00000005 \cdot \text{Tref}^2 + 0.0000969 \cdot \text{Tref} + 0.0008289 '\text{W/(mK)} \]

'air: specific heat
\[ \text{cpa} = -0.00000000005 \cdot \text{Tref}^3 + 0.0000002 \cdot \text{Tref}^2 - 0.00001 \cdot \text{Tref} + 1.0041 '\text{kJ/kg} \]
\[ \text{cpa} = \text{cpa} \cdot 1000# '\text{multiply by 1 kilo} \Rightarrow \text{J/(kgK)} \]

End Sub

-----------------------------------------------------------------------------------------------------------------------------

Sub fuel_thermal_prop(Ts)
If (otherfuel = 1) Then
'fuel: liquid density
\[ \text{Tdocrit} = \text{Ts} / \text{Tcrit} \]
\[ \text{rhof} = 1000# \cdot \text{Arho} \cdot \text{Brho} ^ ((-1#) \cdot (1# - \text{Tdocrit}) ^ \text{nrho}) '\text{convert g/cm}^3' \text{to 'kg/m}^3 \]

'fuel: vapor thermal conductivity
\[ \text{kfv} = \text{Akfv} + \text{Bkfv} \cdot \text{Tref} + \text{Ckfv} \cdot \text{Tref} ^ 2 \cdot \text{Tref} '\text{W/(mK)} \]

'fuel: vapor specific heat at constant pressure
\[ \text{cpfv} = \text{Acpfv} + \text{Bcpfv} \cdot \text{Tref} + \text{Ccpfv} \cdot \text{Tref} ^ 2 + \text{Dcpfv} \cdot \text{Tref} ^ 3 + \text{Ecpfv} \cdot \text{Tref} ^ 4 \]
\[ \text{cpfv} = \text{cpfv} \cdot 1000# / \text{mwd} '\text{convert to J/(kgK)} \]

'fuel: liquid specific heat at constant pressure
\[ \text{cpf} = \text{Acpf} + \text{Bcpf} \cdot \text{Ts} + \text{Ccpf} \cdot \text{Ts} ^ 2 + \text{Dcpf} \cdot \text{Ts} ^ 3 \]
\[ \text{cpf} = \text{cpf} \cdot 1000# / \text{mwd} '\text{J/(kgK)} \]

'fuel: liquid latent heat of vaporization
\[ \text{lat} = \text{Alat} \cdot (1# - \text{Tdocrit}) ^ \text{nlat} \]
\[ \text{lat} = \text{lat} \cdot 1000000# / \text{mwd} '\text{J/kg} \]
Else
'fuel: liquid density
\[ \text{rhof} = \text{rhofr} \cdot (1# - 1.8 \cdot \text{cexp} \cdot (\text{Ts} - 288.6) - 0.09 \cdot ((\text{Ts} - 288.6) / (\text{Tcrit} - 288.6)) ^ 2#) '\text{kg/m}^3 \]

'fuel: vapor thermal conductivity
\[ \text{nkfv} = 2# - 0.0372 \cdot (\text{Tref} / \text{Tbn}) ^ 2 \]
\[ \text{kfv} = 0.0000001 * (13.2 - 0.0313 \cdot (\text{Tbn} - 273#)) \cdot (\text{Tref} / 273#) ^ \text{nkfv} '\text{W/(mK)} \]

'fuel: vapor specific heat at constant pressure
\[ \text{cpfv} = (0.363 + 0.000467 \cdot \text{Tref}) \cdot (5# - 0.001 \cdot \text{rhofr} \cdot \text{rho} \cdot \text{Tref} \cdot \text{Tref}) '\text{kJ/(kgK)} \]
\[ \text{cpfv} = \text{cpfv} \cdot 1000# '\text{J/(kgK)} \]

'fuel: liquid specific heat at constant pressure
\[ \text{cpf} = (0.76 + 0.00335 \cdot \text{Ts}) \cdot (0.001 \cdot \text{rho} \cdot \text{Tref}) '\text{kJ/(kgK)} \]
\[ \text{cpf} = \text{cpf} \cdot 1000# '\text{J/(kgK)} \]

'fuel: liquid latent heat of vaporization
\[ \text{lat} = \text{latbn} \times ((\text{Tcrit} - \text{Ts}) / (\text{Tcrit} - \text{Tbn})) \times (0.38) '\text{kJ/kg} \]
\[ \text{lat} = \text{lat} \times 1000# '\text{J/(kgK)} \]
End If
End Sub

-----------------------------------------------------------------------------------------------------------------------------
Sub taperd()

    fl = Sheets("Process").ComboBox2.Value
    If fl = "Option 1" Then flag = 1
    If fl = "Option 2" Then flag = 2
    If fl = "Option 3" Then flag = 3
    If fl = "Evap time estimate" Then flag = 4

    fl = Sheets("Process").ComboBox3.Value
    If fl = "ON" Then onoff_flag = 1
    If fl = "OFF" Then onoff_flag = 0

    'Getting the input
    r = Sheets("Process").Cells(5, 3)
    r = r / 1000000#
    rhofr = Sheets("Process").Cells(8, 3)
    Tcrit = Sheets("Process").Cells(9, 3)
    Tbn = Sheets("Process").Cells(10, 3)
    cexp = Sheets("Process").Cells(11, 3)
    latbn = Sheets("Process").Cells(12, 3)
    mwd = Sheets("Process").Cells(13, 3)
    acc = Sheets("Process").Cells(14, 3)
    bcc = Sheets("Process").Cells(15, 3)
    xxi = Sheets("Process").Cells(17, 3)
    xpi = Sheets("Process").Cells(18, 3)
    zzi = Sheets("Process").Cells(19, 3)
    zpi = Sheets("Process").Cells(20, 3)
    Tinit = Sheets("Process").Cells(21, 3)
    mwg = Sheets("Process").Cells(23, 3)
    ug = Sheets("Process").Cells(24, 3)
    wg = Sheets("Process").Cells(25, 3)
    Tinf = Sheets("Process").Cells(27, 3)
    p = Sheets("Process").Cells(28, 3)
    g = Sheets("Process").Cells(29, 3)
    dt = Sheets("Process").Cells(31, 3)
    kl = Sheets("Process").Cells(32, 3)
    If flag = 4 And onoff_flag = 1 Then
        dt_old = dt
        dt = 0.000001
        kl = 400000
        If r > 0.00005 Then kl = 800000
    End If
    userchoice = Sheets("Process").Cells(33, 3)
    sstemp = Sheets("Process").Cells(34, 3)

    area_noevap = Sheets("Process").Cells(6, 3)
    volume_noevap = Sheets("Process").Cells(7, 3)

End Sub
References


**An Interactive Microsoft® Excel Program for Tracking a Single Evaporating Droplet in Crossflow**

K.H. Liew, E. Urip, S.L. Yang, and C.J. Marek

**National Aeronautics and Space Administration**
John H. Glenn Research Center at Lewis Field
Cleveland, Ohio 44135–3191

**Droplet interaction with a high temperature gaseous crossflow is important because of its wide application in systems involving two phase mixing such as in combustion requiring quick mixing of fuel and air with the reduction of pollutants and for jet mixing in the dilution zone of combustors. Therefore, the focus of this work is to investigate dispersion of a two-dimensional atomized and evaporating spray jet into a two-dimensional crossflow. An interactive Microsoft® Excel program for tracking a single droplet in crossflow that has previously been developed will be modified to include droplet evaporation computation. In addition to the high velocity airflow, the injected droplets are also subjected to combustor temperature and pressure that affect their motion in the flow field. Six ordinary differential equations are then solved by 4th-order Runge-Kutta method using Microsoft® Excel software. Microsoft® Visual Basic programming and Microsoft® Excel macrocode are used to produce the data and plot graphs describing the droplet's motion in the flow field. This program computes and plots the data sequentially without forcing the user to open other types of plotting programs. A user's manual on how to use the program is included.**

**Droplet; Evaporation; Trajectory; Microsoft® Excel spreadsheet; Jet-A; Water; Diesel; JP-4; JP-5; N-heptane**


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