Multi-Scale Powder Dispersal Solution using the Extended General Dynamic Equation for Aerosols

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Abstract

In this study, we have extended the aerosol general dynamic equation (GDE), to deal with multi-scale and multi-variable problems relevant to both powders and sprays. As a case study, we examine the dynamics of an extinguishing aerosol or a powder in a reacting flow. The purpose of this application is to find ways to minimize the amount of extinguishing aerosol/powder that is required, using a multi variable approach.

The aim of the first phase of the study, presented here, is to develop a theoretical approach to simulate the dynamics of aerosol particles in a flow field utilizing the GDE. The extended GDE in the case study represents distributions of particle mass, particle temperature and particle velocity.

The case study is the interaction of the aerosol particles with premixed laminar Ozone burning, which has a relatively simple reaction model. We disperse powder at the upstream of the flame zone and find the minimal powder concentration and the initial powder particles diameter distribution required to extinguish the flame.

The simulation considers two known extinguishing mechanisms: homogeneous and heterogeneous mechanisms.

At this paper we don't present results regarding the extinguishing of Ozone burn, as the research hasn't reached this stage, however we will demonstrate the extended GDE on a simple case of evaporating falling water droplets.

Keywords
Aerosols; GDE, powder; dispersal; fire, FFR, extinguishing

Introduction

Fire extinguishing by Alkali Metal salts such as Sodium and Potassium bicarbonate is common as well as the use of water droplets. In this research, we seek ways to enhance the powder extinguishing efficiency by powder dispersal technique or powder diameter distribution. Achieving extended extinguishing efficiency may also minimize residual powder damage to equipment exposed to the powder.

Powder extinguishing mechanism is divided into two groups: Homogeneous and Heterogeneous [1].

The Homogeneous mechanism include: a) Removal of heat from the flame reaction while powder particles are being evaporated and   b) Direct inhibition reaction of the powder evaporation products with the Fire Free Radicals (such as H, O, and OH) which are crucial to chemical reaction propagation. This chemical reaction terminates the reaction and do not allow full oxidation.

The Heterogeneous mechanism includes. a) Mechanical interference of "powder cloud" with the FFR, acting as Flame arrestor, and b) Chemical adsorption of FFR onto particle surface while another FFR is expected to react with the first one and recombine due to particle's surface energy dissipation. The product is desorbed from particle and does not promote completion of oxidation.

The aim of the first phase of the study, presented here, is to develop a theoretical approach to simulate the dynamics of aerosol particles\droplets in a flow field utilizing the GDE. The extended GDE in the case study represents distributions of particle\droplet mass, particle temperature and particle velocity.

1.   General Dynamic Equation (GDE).

1.1 Classical GDE.

"Classic" GDE [2] describes the change in particles number distribution in a fixed volume, $n(m_p,t)$. Namely, particles with mass values between m_p to m_p+dm_p at time t are the particles which gained mass of $m_p - I_{m_p}dt$ at time t-dt

where, $I_{m_p}(m_p,t)$ is the change of particle mass with time due to physical process e.g. evaporation or condensation ($I_{mp}=dm_p/dt$).

Hence:

$$\frac{\partial n}{\partial t} = -\frac{\partial\left(I_{m_p}(m_p,t)*n(m_p,t)\right)}{\partial m_p} + net\ rate\ of\ particle\ addition\ (sorces - sinks) \tag{1}$$

1.2 Extended GDE- Eulerian formulation

In the present study we extended the GDE by defining n, the normalized particle number, as a function not only particle size and time but also particle position (x_p,y_p,z_p), particle velocity (u_p,v_p,w_p) and particle temperature T_p. The n extended definition is such that in order to calculate the number of particles that acquire the same position, velocity, mass and temperature in an infinitesimal 8D generalized space, we should multiply n by $dx_p*dy_p*dz_p*du_p*dv_p*dw_p*dm_p*dT_p$.

Under similar physical principle described above we can say that the particles that acquire, at time t, position x_p,y_p,z_p velocity u_p,v_p,w_p, temperature T_p and mass m_p are those who were at t-dt in position x_p-$I_{xp}*dt$, y_p-$I_{yp}*dt$, z_p-$I_{zp}*dt$, with velocity u_p-Iu_p*dt, v_p-Iv_p*dt, w_p-Iw_p*dt and temperature T_p-IT_p*dt with the addition of new particles added under the same conditions and subtraction of particles deposition.

The mathematical phrase of the principle above is:

$$\left(n + \frac{\partial n}{\partial t}dt\right)dx_p dy_p dz_p du_p dv_p dw_p dm_p dT_p$$
$$= n(t, x_p - Ix_p dt, y_p - Iy_p dt, \dots\dots\dots)J\, dx_p dy_p dz_p du_p dv_p dw_p dm_p dT_p$$
$$+ P\, dx_p dy_p dz_p du_p dv_p dw_p dm_p dT_p dt$$

Where, P is the net number of particles added under the same conditions per unit of time.

J is the Jacobian that is the ratio between the 8D generalized space occupied by the particles at time t-dt to the space occupied at time t.

$$J = \det\left[\frac{\partial(x_p, y_p, z_p, u_p, v_p, w_p, m_p T_p)}{\partial(x_{p_0}, y_{p_0}, z_{p_0}, u_{p_0}, v_{p_0}, w_{p_0}, m_{p_0} T_{p_0})}\right] = 1 - \frac{\partial I_{x_p}}{\partial x_p}dt - \frac{\partial I_{y_p}}{\partial y_p}dt - \frac{\partial I_{z_p}}{\partial z_p}dt - \frac{\partial I_{u_p}}{\partial u_p}dt \dots \tag{2}$$

Incorporating the phrases above, gives the Eulerian formulation of the Extended GDE:

$$\frac{\partial n}{\partial t} = -\frac{\partial\left(nI_{x_p}\right)}{\partial x_p} - \frac{\partial\left(nI_{y_p}\right)}{\partial y_p} - \frac{\partial\left(nI_{z_p}\right)}{\partial z_p} - \frac{\partial\left(nI_{u_p}\right)}{\partial u_p} - \frac{\partial\left(nI_{v_p}\right)}{\partial v_p} - \frac{\partial\left(nI_{w_p}\right)}{\partial w_p} - \frac{\partial\left(nI_{m_p}\right)}{\partial m_p} - \frac{\partial\left(nI_{T_p}\right)}{\partial T_p} \tag{3}$$

We solve this equation for n at specific position, velocity, mass and temperature as a function of time.

The I's functions in equation (3) are time derivative of each of the eight characteristics; i.e. they are function of time and of each of the eight properties as well. These functions are derived from physical laws:
- I_{xp}, I_{yp}, I_{zp} – are the particle velocities: u_p, v_p, w_p
- I_{up},I_{vp},I_{wp} – are derived from Newton's second law
- I_{mp} - is derived from evaporation\ condensation laws
- I_{Tp} – is derived by the first law of Thermodynamics.

1.3 Extended GDE - Lagrangian formulation

With the Lagrangian approach we follow a parcel of particles with the same initial conditions (position, velocity, temperature and mass) as it flows downstream. The physical principle here is that the number of particles in the parcel remains constant with the exception of particle removal or production. Therefore, the extended GDE Lagrangian formulation is:

$$\frac{D(n*J)}{Dt} = P * J \tag{4}$$

$\frac{D()}{Dt}$ - is the material derivative, which is the time derivative along the particle's parcel trajectory in the X-Y-Z coordinate system.

As opposed to the Eulerian formulation, here J is function of the time solely.

Though the implicit expression for the extended GDE (4) can be complex, it is an ODE with a simple solution:

$$n = \frac{n_0}{J(t)} + \frac{\int_0^t P*J(t')*dt'}{J(t)} \tag{5}$$

The solution can be verified by substituting it in equation (4).

Solving equation (3) along particle parcel trajectory (which is equivalent to (4)), will give us extended phrase similar to that given in [2]. Comparing between (5) to this phrase leads us to (6).

$$J(t) = e^{\int_0^t \left(\frac{\partial I u_p}{\partial u_p} + \frac{\partial I v_p}{\partial v_p} + \frac{\partial I w_p}{\partial w_p} + \frac{\partial I m_p}{\partial m_p} + \frac{\partial I T_p}{\partial T_p}\right)*dt'} \tag{6}$$

2. Extended GDE Demonstration

2.1 Problem description

We considered a problem of hemispherical water droplets\aerosol with initial velocity which falls under the influence of gravity in an ambient humid air in rest.

During the fall the droplets continuously change their velocity due to the evaporation process (and hence their terminal velocity) that decreases their diameter and therefore, changing the drag force exerted on them [9]. We consider an isothermal dilute flow thus, one-way coupling is applied.

$$I_{up} = a_{droplet} = \frac{m_{droplet}*g - \frac{1}{2}*\rho_{air}*u_{droplet}^2*A_{droplet}*C_d}{m_{droplet}} = g - 0.75*\frac{\rho_{air}*u_{droplet}^2*C_d}{\rho_{water}*d_{droplet}} \qquad (7)$$

$$C_d = [\left(\frac{24}{Re}\right)^{0.52} + 0.32^{0.52}]^{\frac{1}{0.52}} \qquad\qquad 0 \le Re \le 10^4 \qquad (8)$$

$$I_{dp} = \frac{d(d_{droplet})}{dt} = -4*\frac{M_{w_L}*D_v*P_{sat}*(1-RH)}{d_{droplet}*\rho_{water}*R_u*T_f}*(1 + 0.276\,Re^{0.5}*Sc^{0.33}) \qquad (9)$$

Where M_{w_L} is water molecular weight, D_v is the average diffusion coefficient for vapour molecules in the saturated film around the droplet, T_f is the average absolute temperature in that film (which equal in our case to the surroundings temperature), Re is Reynolds' number, Sc is Schmidt's number, P_{sat} is saturation pressure at the droplet temperature, RH is the relative humidity of the air (that is constant in our model), R_u is the universal gas constant, $d_{droplet}$ is the water droplet diameter, $u_{droplet}$ is the droplet velocity ρ_{water} and ρ_{air} are water and air densities respectively. The thermophysical properties are temperature dependent in our model [9].

As part of the problem boundary conditions we chose two-dimensional water droplets distribution (droplets number per unit volume as function of velocity and droplets diameter) at Xp=0.

The water droplets distribution as a function of Xp (distance from the droplet\aerosol source) was solved, with the currently extended GDE. Results are presented in section 4.1.

3. Combustion.

3.1 Ozone laminar combustion.

As stated above, our aim is to demonstrate the use of the extended GDE to achieve fire extinguishing by applying powder dispersal on ozone laminar combustion according to the chemical kinetics that is described in [3]. The advantage of ozone combustion is that we deal only with three species (O, O_2, O_3) and three chemical reactions:

$$O_3 + M \rightleftarrows O + O_2 + M \qquad\qquad (R1)$$

$$O + O_3 \rightleftarrows O_2 + O_2 \qquad\qquad (R2)$$

$$O + O + M \rightleftarrows O_2 + M \qquad\qquad (R3)$$

M is a "third body" component that does not participate in the reaction, but rather catalyse it. In this case, M can be one of the three species. Later, when we will introduce the extinguishing powder, M can also be evaporated gas from the powder.

Heimeri and Coffee [3] solve a 1D, constant pressure, steady-state combustion and find the flame (or burning) velocity for an initial value of Ozone Mole Fraction (IOMF) of 0.2, 0.25, 0.75 and 1. The velocity of the unburnt zone is changed until a steady-state flame front is obtained.

3.2 Modifications in Ozone Laminar Combustion model.

In the present study, we modified the model presented in [3] so it can be used to analyse the powder-extinguishing problem:

   a. We added a *theoretical* extinguishing powder with similar thermophysical properties to Potassium (K) according to [4],[5].
   b. For simplicity, we decided that the gas that is released from the powder acts as the third body (M) in chemical reactions R1, R3.
   c. We introduced a two-phase flow with a gaseous volume fraction ε(x). As aforementioned, we consider a dilute flow so that ε values should be higher than 0.9.
   d. The FFR in this set of reaction is O radical. Enhancing R3 reaction rate, by adding dependency on evaporated extinguishing powder mole fraction, will cause fire extinguishing (reaction termination).
   e. We also added to R3 a dependency on the particle concentration (1-ε) which account for the FFR destruction by the heterogeneous mechanisms.

3.3 Modified model governing equations
 <u>Gas Phase</u>:

a. The continuity equation:

$$\varepsilon \rho u(x) = (\varepsilon \rho u)_0 + \int_0^x \dot{w}_{evap}(x)_K \, dx \tag{10}$$

 - where $\dot{w}_{evap}(x)_K$ is the evaporation rate per volume of *all* the particles at the specified position. Since the particle Thermodynamic properties follow Potassium, evaporation will occur above its melting point, 338 [K]. The particle temperature doesn't exceed the evaporation temperature 1032 [K]. (The suffix K represents the Potassium)

$$\dot{w}_{evap}(x)_k = \iiint_{m_p \, u_p \, T_p} \rho_{K_g}(T_p)(u + V_K - u_p)A_p \, n \, dT_p du_p dm_p \tag{11}$$

 - V_K is the potassium diffusion velocity.
 - We take the evaporation velocity as $u + V_K - u_p$ which agrees with the "d-square law" for the evaporation rate [6]
 - $\rho_{K_g}(T_p)$ is the vapor density for liquid Potassium at temperature T_p, taken from Heimel [4]
 - A_p is the particle surface area which is a function of its mass, assuming perfect spherical particles.
 Note that n is function of x_p, u_p, m_p, T_p
 Equation (10) is used in order to calculate the gas velocity at every position x, while we know from other equations: ρ(x) (19), ε(x) (24), $\dot{w}_{evap}(x)_k$ (13).

b. Species Equations:
 For O\O₂:

$$(\varepsilon \rho)\frac{\partial Y_j}{\partial t} = -(\varepsilon \rho u)\frac{\partial Y_j}{\partial x} - \frac{\partial (Y_j \varepsilon \rho V_j)}{\partial x} + \dot{w}_{ch}(x)_{o\backslash o_2} - Y_j \dot{w}_{evap}(x)_k \tag{12}$$

Where j is either O/O₂.
For K (Powder evaporated gas):

$$(\varepsilon \rho)\frac{\partial Y_K}{\partial t} = -(\varepsilon \rho u)\frac{\partial Y_K}{\partial x} - \frac{\partial (Y_K \varepsilon \rho V_K)}{\partial x} + (1 - Y_K)\dot{w}_{evap}(x)_k \tag{13}$$

$$Y_{o_3} = 1 - Y_{o_2} - Y_o - Y_K \tag{14}$$

 - V_K, V_o, V_{o2}, V_{o3} are the species diffusion velocities calculated by Multicomponent Diffusion Equation [6], with negligible thermal, body forces and pressure induced diffusion.
 - 6 diffusion coefficients as a function of flow temperature which are needed to calculate the diffusion velocities are taken from [3] and [5].

c. Energy Equation:

$$(\varepsilon \rho)\sum_i Y_i C_{p_i}\frac{\partial T}{\partial t} = -(\varepsilon \rho u)\sum_i Y_i C_{p_i}\frac{\partial T}{\partial x} - (\varepsilon \rho)\sum_i Y_i V_i C_{p_i}\frac{\partial T}{\partial x} + \frac{\partial\left(\lambda \varepsilon \frac{\partial T}{\partial x}\right)}{\partial x} - \sum_i h_i \dot{w}_{ch}(x)_i - A1(x) + A2(x) - A3(x) \tag{15}$$

 - C_{p_i} the constant pressure specific heat is taken for each species from [3], [4].
 - λ is the species weighted conduction heat transfer coefficient (function of temperature) which is taken from [3], [4].
 - $\dot{w}_{ch}(x)_i$ is the chemical production rate through chemical reactions R1 – R3 [3]. The potassium was considered only as a Third body (M).
 - A1 (x) is the energy per volume taken from the gas flow to all particles in x position due to heat convection:

$$A1(x) = \iiint_{m_p \, u_p \, T_p} H_c A_p(T - T_p)n * dT_p * du_p * dm_p \tag{16}$$

   - H_c is the heat convection coefficient

 - A2(x) is the energy per volume gained by the flow due to the evaporation of all particles at position x (enthalpy +kinetic energy):

$$A2(x) = \iiint_{m_p \, u_p \, T_p} (h_{K_l}(T_p) + \frac{(u+V_k-u_p)^2}{2})\rho_{K_g}(T_p)(u + V_K - u_p)A_p \, n * dT_p * du_p * dm_p \tag{17}$$

   - $h_{K_l}(T_p)$ is the Potassium specific enthalpy for the liquid phase taken from [4] (it is assumed that substantial evaporation occurs only when Potassium is in the liquid phase).

- A3(x) is the energy per volume taken from the flow in order to bring the evaporated gas to the same energy of the gas flow (temperature and kinetic energy):

$$A3(x) = (h_{K_g}(T) + \frac{u^2}{2}) \, \dot{w}_{evap}(x)_k \tag{18}$$

  - $h_{K_g}(T)$ is gas phase Potassium specific enthalpy, at the bulk flow temperature [4].

d. Equation of State:

$$\rho(x) = \frac{P_a}{R_U * T(x) * (\frac{Y_O}{M_{wo}} + \frac{Y_{O2}}{M_{wo_2}} + \frac{Y_{O3}}{M_{wo_3}} + \frac{Y_K}{M_{wK}})} \tag{19}$$

- It is assumed that the gaseous phase is an ideal mixture at one atmosphere, and that each gas follow the ideal gas law.

Particles (solid and liquid phase):
We solve here the extended GDE (2) – Eulerian formulation, with the following defined functions:

$$I_{x_p} \triangleq \frac{dx_p}{dt} = u_p \tag{20}$$

$$I_{u_p} \triangleq \frac{du_p}{dt} = \frac{3\rho(x)(u(x) - u_p)^2 C_D}{4\rho_{K_l} d_p} \frac{(u(x) - u_p)}{|u(x) - u_p|} \tag{21}$$

- d_p is the particle diameter which can be calculated from particle mass (m_p) and particle density ρ_{K_l} .
- C_D is the particle drag coefficient.

$$I_{m_p} \triangleq \frac{dm_p}{dt} = \rho_{K_g}(T_p)(u + V_K - u_p)A_p \tag{22}$$

- For temperature lower than 338 [K] I_{m_p} is zero because there is no substantial evaporation.
- In our formulation we replaced I_{m_p} with I_{d_p}.

$$I_{T_p} \triangleq \frac{dT_p}{dt} = \frac{H_c A_p(T - T_p) + I_{m_p} h_{K_l}(T_p)}{m_p C_{p_{K_{S\backslash l}}}(T_p)} \tag{23}$$

- $C_{p_{K_{S\backslash l}}}(T_p)$ is the Potassium constant pressure specific heat at particle temperature T_p (particle can be in solid or in liquid phase therefore we added the suffix s\l) taken from [4].

ε(x) is calculated after we solve the GDE:

$$1 - \varepsilon(x) = \iiint_{m_p \, u_p \, T_p} n \frac{m_p}{\rho_{K_l}} \, dT_p du_p dm_p \tag{24}$$

3.4 Principle algorithm
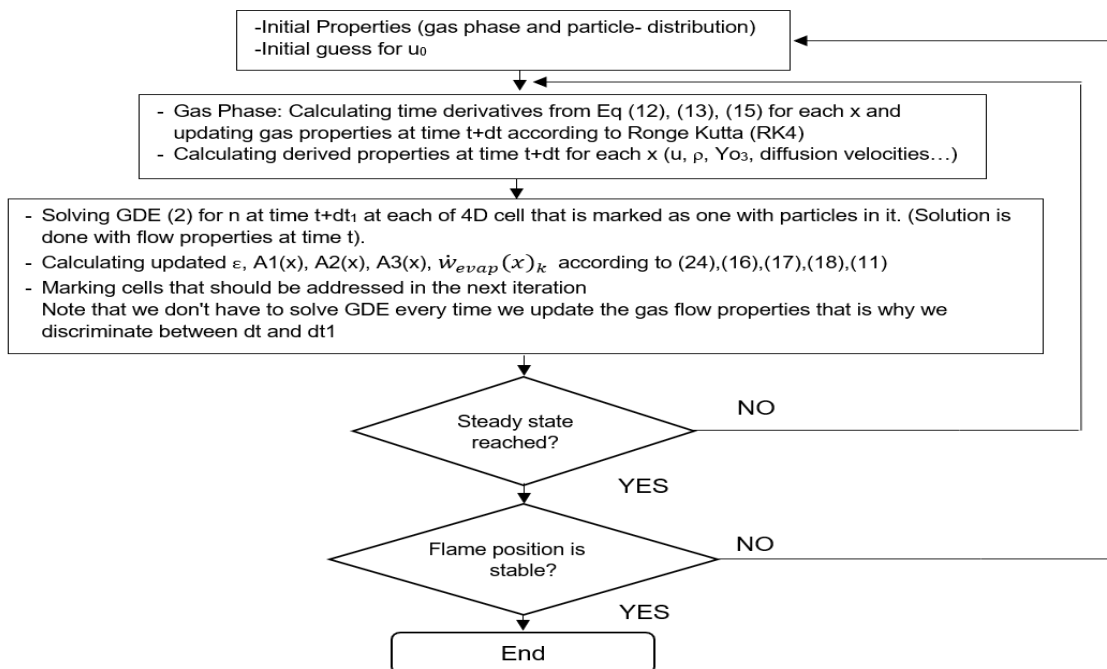Fig 1 illustrate the principle algorithm of the Matlab computer program made in order to analyze the problem:

Figure 1. Problem analysis principle Algorithm.

4. Results and discussion

4.1 Results regarding water droplets\aerosol evaporating while free falling

The parameters chosen for demonstration: Water droplets and air temperature of 300[K], Air relative humidity (RH) of 40%. Boundary conditions- droplet source which provides water droplets\aerosol at a constant rate with diameter between 97-100 [micron] and velocity of 10 [m/sec]. The calculation was made with 300 Xp elements, Δxp, of 2.5 mm, (0<Xp<0.75 [m]), 50 elements of water droplet velocity with Δup=0.2[m/sec]
(0.1< Up<10[m/sec]) and 100 elements of water droplets diameter Δdp=1micron (1 <dp<100 micron) total of 1.5 million 3D elements.

Droplets of 1[micron] are totally evaporated. The steady state conditions are obtained when the number of entering droplets to the calculation domain is equal to the average number of 1-micron droplets that are eliminated.
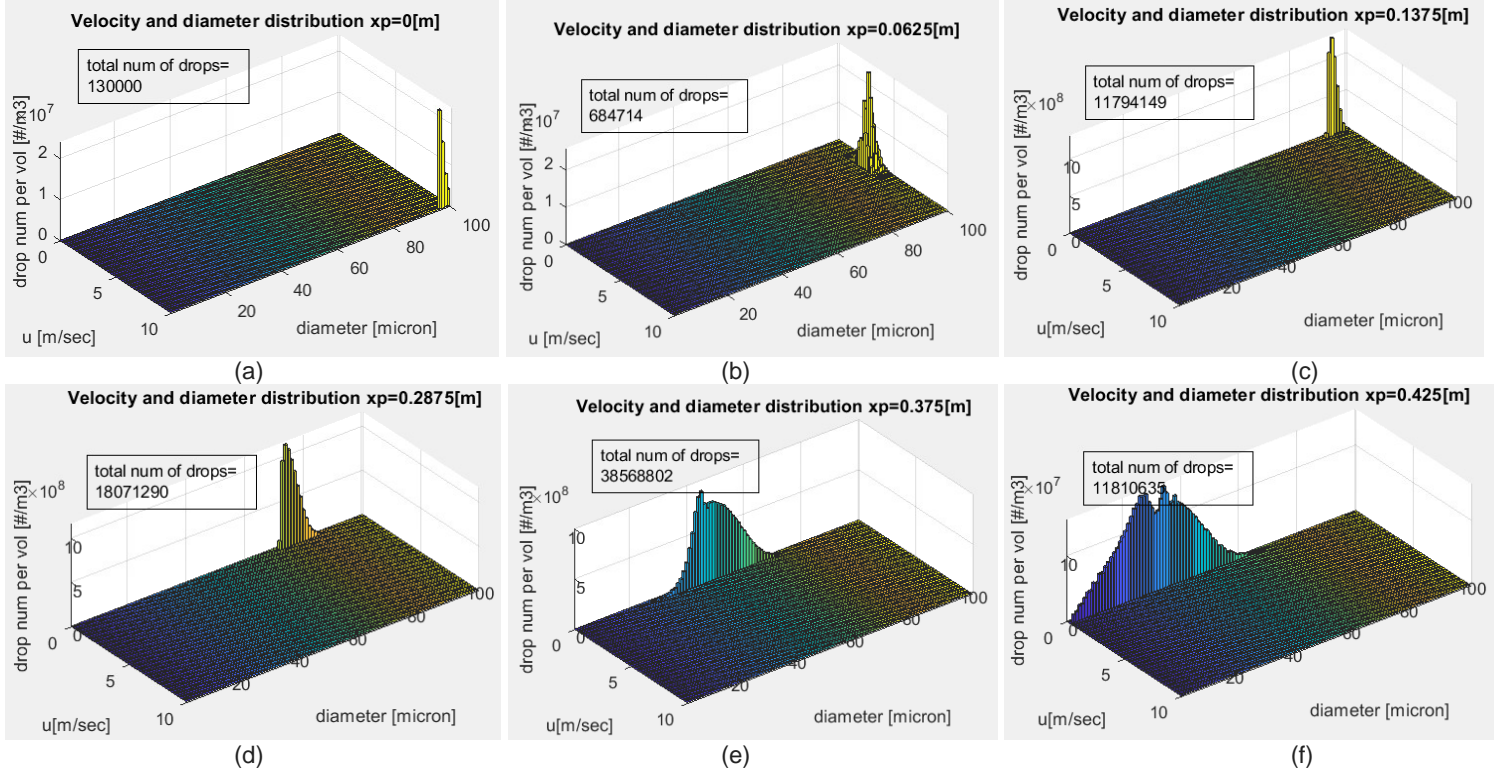

(a)   (b)   (c)

(d)   (e)   (f)

Figure 2. Droplet number per m³ distribution as a function of droplet velocity and diameter at various distances from source
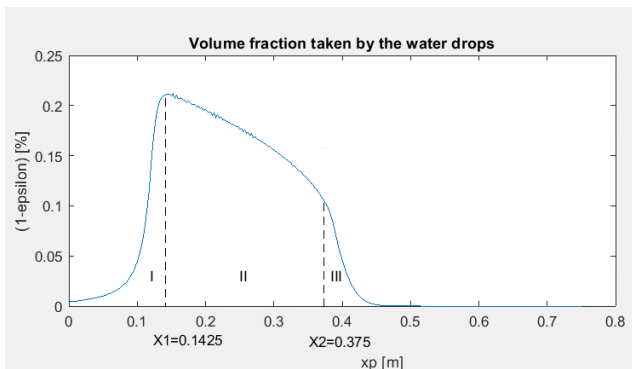

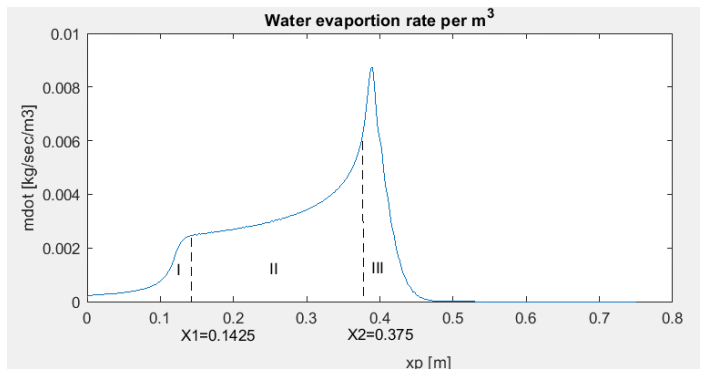**Figure 3.** Volume fraction taken by the water droplets

Figure 4. Water evaporation rate per volume

The water droplets distribution at the source is shown in Fig 2(a). Fig 2(a)-(f) presents the water droplets velocity and diameter distribution as a function of distance from the source (Xp)

Fig 3. shows the volume fraction (1- ε(xp)) taken by the water droplets as a function of Xp in percent, calculated according to (24). Fig 4 presents the water droplets evaporation rate per volume, calculated according to (11)

The problem solution shows 3 distinct regions (Fig 3,4):

- I (See also Fig 2(a), (b)): The water droplets emerge from the source at relative high velocity, as compared to the carrier gas and reduce velocity towards the terminal velocity. As a result, the droplets accumulate and the initial volume fraction taken by the droplets (1-ε) is increased. No significant evaporation occurs at this stage.

- II (See also Fig 2 (c), (d), (e)): The water droplets reached the terminal velocity and start to evaporate, therefore their volume fraction is reduced though their number grows.

- III (See also Fig 2 f): Water droplets are eliminated as they reach diameter of 1 micron, therefore the evaporation rate is enlarged. This region upper limit at about 0.44[m] fits direct calculation of droplet distance until 1 -micron diameter reached. This distance is obtained from ODE solution of equations (7), (9) with initial conditions of

dp(t=0) =100[micron], u_p(t=0) =10[m/sec].
At this region we also notice that the diameter distribution interval grows larger as the evaporation is intensified.

4.2 Ozone powder extinguishing

Ozone combustion [3] in its laminar form was modified in order to demonstrate the problem of powder extinguishing including:
- Equation modification for a two-phase flow.
- Embedding into the model the homogenous and heterogeneous extinguishing mechanisms.
- Theoretical extinguishing powder based on Potassium's Thermodynamic properties was defined.

Our discretization of x for the gas phase contains 1500 spatial intervals, each with Δx of 6.66 microns.

For x_p we took 300 intervals of 5* Δx each. u_p was taken between u_0 (flow initial velocity) to 10*u_0 with Δu_p of 0.2u_0 (45 intervals). Particle diameter was taken between 0.357 Δx to 5 Δx (15 intervals) and particle temperature was taken between 298 [K] to 1032[K] with ΔT_p of 2 [K] (368 intervals) – all sums up to 74,520,000 4D cells (x_p,u_p,d_p,T_p) for the Particle calculation domain.

At this stage we verified our model with the example of Ozon combustion given at [3]. Fig 5 (a)-(d) presents example of such results for initial Ozone mole fraction (IOMF) of 0.5. Fig 5 (a) – (c) presents flow temperature, velocity and species mole fraction (O, O2, O3) as function of x. Fig 5 (d) presents the burning front location Vs time which indicates that the initial flow velocity "guessed" as 2.428 [m/sec] maintains the burning front at a fixed position therefore it is the burning velocity for IOMF of 0.5.
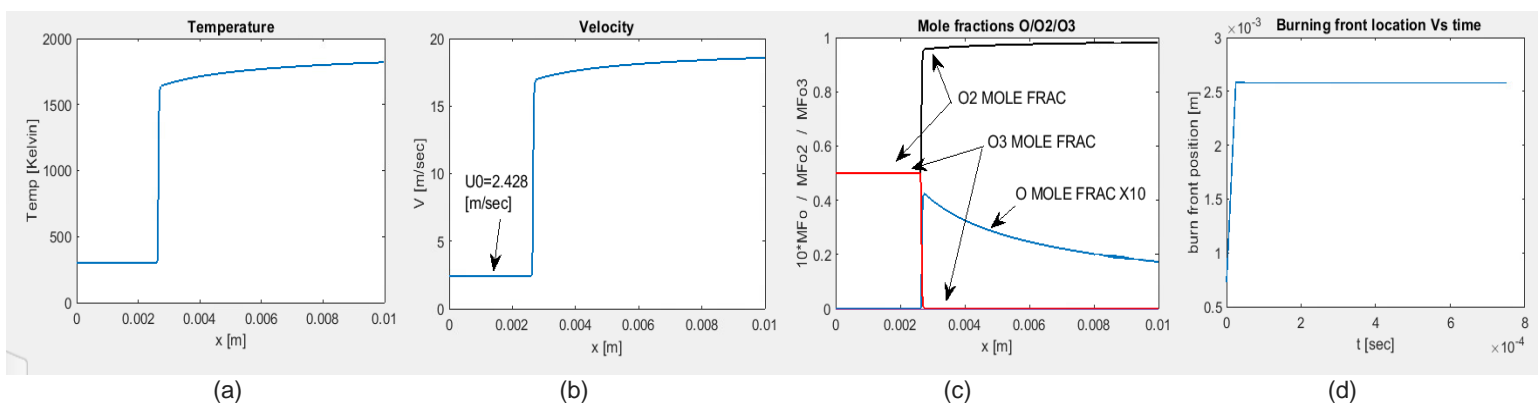

(a)   (b)   (c)   (d)

Figure 5. Burning velocity results for IOMF of 0.5

Conclusions

The aerosol general dynamic equation, known as the "GDE", which is regarded as a function of droplet mass and time is extended here to account also for droplet location, velocity, and temperature. It is applied in the case of spray droplets which are in motion downwards towards the ground while evaporating.
The procedure involves a Eulerian approach which exhibits three main advantages:
- One can easily deal with multiple particle distributions.
- There is no need to solve the particle trajectory equations in order to obtain the particles distribution and location.
- The use of Eulerian grid eliminates the need for transformations between the gas phase and the solid phase.

However, a disadvantage of the Eulerian approach, compared with a Lagrangian one, is the need of a larger grid for the particle calculation domain with multidimensional cells (in the case of Ozone fire extinguishing, for example, the domain includes 74,520,000, 4D cells).
The GDE Lagrangian approach is equivalent to the traditional approach of tracking partial parcels paths.
Following/current work:
- Computer program verification
- Running the various cases, we decided on.
- Modification of the program to Methane combustion with realistic extinguishing powders, and comparing the results with actual measurements.

To summarize, the current developed scheme for the description of spray dynamics can serve as a tool for analyzing various spray related problems which may include evaporation and chemical reactions.

Nomenclature

$a_{droplet}$\g	Water droplet acceleration\ gravitational acceleration	$\left[\frac{m}{sec^2}\right]$
A1(x), A2(x), A3(x)	Energy taken from /given to the flow by the particles	$\left[\frac{W}{m^3}\right]$
$A_{p\backslash droplet}$	Particle\droplet surface area	$[m^2]$
C_D	Particle drag coefficient	[-]
$C_{p_o}, C_{p_{o_2}}, C_{p_{o_3}}, C_{p_K}$ or C_{p_i}	Species constant pressure specific heat	$\left[\frac{J}{kgK^0}\right]$

Symbol	Description	Units
$C_{p_{K_{s\backslash l}}}(T_p)$	Potassium constant pressure specific heat (solid or liquid phase)	$\left[\frac{J}{kgK^0}\right]$
$d_{p\backslash droplet}$	Particle\water droplet diameter	$[m]$
D_v	Average diffusion coefficient for vapour molecules in the saturated film around the droplet	$\left[\frac{m^2}{sec}\right.$
H_c	Convection coefficient	$\left[\frac{W}{m^2K^0}\right]$
$h_i \backslash h_{K_g}(T)$	Species specific enthalpy \ Potassium specific enthalpy	$\left[\frac{J}{kg}\right]$
$h_{K_l}(T_p)$	Potassium specific enthalpy –liquid phase	$\left[\frac{J}{kg}\right]$
$I_{x_p}, I_{u_p}, I_{m_p}, I_{T_p}$	Particle rate of change with time of position, velocity, mass and temperature respectively	$\left[\frac{m}{sec}\right], \left[\frac{m}{sec^2}\right], \left[\frac{kg}{sec}\right], \left[\frac{K^0}{sec}\right]$
J	Jacobian	$[-]$
$m_p\backslash m_{droplet}$	Particle\droplet mass	$[kg]$
$M_{w_{o\backslash o_2\backslash o_3\backslash K\backslash L}}$	Species\water molecular weight	$\left[\frac{kg}{kg-mole}\right]$
N	Normalized particle number	$\left[\frac{sec^3}{m^6K^0kg}\right]$ or $\left[\frac{sec}{m^4K^0kg}\right]$ or $\left[\frac{sec}{m^4}\right]$
$P_a\backslash P_{sat}$	Atmospheric pressure -101325 \ water saturation pressure	$\left[\frac{N}{m^2}\right]$
R_u	Gas universal constant -8315	$\left[\frac{J}{kg-mole\,K^0}\right]$
Re	Reynolds number	$[-]$
RH	Air relative humidity	$[-]$
Sc	Schmidt's number	$[-]$
T_p	Particle temperature	$[k]$
T	Flow temperature	$[k]$
t	Time	$[sec]$
u_p, v_p, w_p	Particle 3D velocity	$\left[\frac{m}{sec}\right]$
V_K, V_o, V_{o2}, V_{o3}	Species diffusion velocities	$\left[\frac{m}{sec}\right]$
$\dot{w}_{evap}(x)_k$	Particle evaporation rate (Potassium\water)	$\left[\frac{kg}{m^3sec}\right]$
$\dot{w}_{ch}(x)_i$	Species chemical production rate (relevant only for O, O$_2$, O$_3$)	$\left[\frac{kg}{m^3sec}\right]$
x	Flow location (for 1D flow)	$[m]$
$Y_o, Y_{o_2}, Y_{o_3}, Y_K$ or Y_i	Species mass fraction	$[-]$
x_p, y_p, z_p	Particle 3D position	$[m]$
λ	Flow weighted conduction coefficient	$\left[\frac{W}{mK^0}\right]$
ε	Volume fraction occupied by the gas phase	$[-]$
ρ \ ρ$_a$	Flow density \ Air density	$\left[\frac{kg}{m^3sec}\right]$
ρ_{K_g}	Vapour Potassium density	$\left[\frac{kg}{m^3sec}\right]$
$\rho_{K_l}\backslash\rho_w$	Liquid Potassium density (taken as constant for liquid and solid phase- 828 \ Water density	$\left[\frac{kg}{m^3sec}\right]$

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