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Application of Smooth particle hydrodynamics simulation on biomass burning

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INTRODUCTION

Biomass burning includes both decisive and accidental clearing of forests, savannas, and agricultural fields [1]. Today population overpasses the 6.5 billons [2], and growing, as well the demands for natural resources, this deterioration in the environments is taken place all over the world. The biomass burning it is a significant contributor to air pollution around the world[3,4,10].The mass transport of primary particles generated by biogenic process enter the atmosphere directly as particles, from the biomass burning e.g., soot, fly ash, sea salt, pollen, fungi, soil, polycyclic hydrocarbons aromatics (PAH), hydrophobic organic pollutants (HOCs)[5,6,11,12,13]. The size (aerodynamic diameter) of these particles is from 10 μm to 100 μm [7,8].

The atmospheric boundary layers (ABL) represent the lower part of the troposphere extends 100 to 3000m [9]. Chemical analysis provided a more accuracy or a better understanding of this phenomenon. Since techniques from different fields of sciences are taking a more multidisciplinary role, this allows a variation of methods to be employed.

The use of ABL is essential for studying this connection, between pollutants and the complex behavior of winds, therefore the air is the major carrier of chemicals, in vapor or particulate forms [14,15,16,17].

However, in this paper a different approach is mentioned. The smooth particles hydrodynamics (SPH) models were used first in astrophysics, specially the one developed by Lucy, SPH is a Lagrangian approach for computational fluid dynamics, where the flow is modeled as a collection of particles that move under the influence of hydrodynamic and gravitational forces [18], also the technique is a mesh-free, make possible the simulation involving fluid masses moving arbitrarily in three dimensions in absence of boundaries [19-21]. The use of SPH allows resolving problems such as galaxy and star formation, binary star interactions, comet, self gravitating impacts, and much more. Different implantations were used in free surface flows by Monaghna [22-27].

Using factors like wind speed, momentum, and artificial viscosity along with temperatures gradient will determine the stability of the atmosphere. As long the atmosphere is stable, high mixing occurs, however unstable atmosphere, low mixing occurs, therefore turbulent conditions increase the degree of uncertainty, vortex, eddies, etc. [28,29,30]

The use of advection-convection model of Comsol was used to simulate point sources (dust particles) of high concentration to a low concentration zone. With a wind flow of constant speed, variation in the pollutant concentration are related to the equations provided by Comsol, but they are not mention, since the idea was to explain the mesh results in a mesh-free approach, however my lack of knowledge was the Galilean invariant. Even Thought Comsol is a mesh platforms, it was used to as a sources of information in the behavior of two different particles with SPH equations. Therefore there is no real solution, nor natural explanation in the simulation.

Continuity Equations:

Since SPH works in a meshless platform, increasing the amounts of assumption, as well the interpretation or analogy of the results to come. The dusty gas is included as two interpenetrating fluids which interacts via pressure and drag conditions. The stress tensor of the dust fluid is negligible, also dust grains do not evaporate and the gas does not condensate [31, 32,33]. The continuity equation, for gas is equation (1) and the equation (2) for dust. In both, equations the mass densities per unit volume of the dusty gas are related to actual density in equation (3).

$$\frac{d\hat{\rho}_g}{dt} = -\hat{\rho}_g \nabla \cdot (v_g) \tag{1}$$

$$\frac{d\hat{\rho}_d}{dt} = -\hat{\rho}_d \nabla \cdot (v_d) \tag{2}$$

$$\hat{\rho}=\theta\,\rho\,. \tag{3}$$

Here θ is the void fraction which satisfies the condition, Eq (4).

$$\theta_g + \theta_d = 1. \tag{4}$$

Since the gas density ρ_d of the dust grain is known, it is possible to determine θ_d once $\hat{\rho}_d$ is known from the dust continuity equation. Is possible to calculate θ_g and from the gas continuity equation, we can determine $\hat{\rho}_g$ then it is possible to locate ρ_g which is needed for the gas pressure. The SPH equations for the gas particles subscripts are; a, and b. In the case for the dust particles subscripts j, and k, from this continuity equations becomes

$$\frac{d\hat{\rho}_a}{dt} = \sum m_b\, v_{ab} \cdot \nabla_a W_{ab}. \tag{5}$$

$$\frac{d\hat{\rho}_j}{dt} = \sum_k m_k\, v_{jk} \cdot \nabla_j W_{jk}. \tag{6}$$

equation (5) for the gas and equation (6) for the dust, therefore if there is a need to include more fluids, one approach is by adding continuity equations and void fraction for each. In absence of viscous effect the acceleration equations for gas is (7) and (8) for dust. In equations (7) and (8), the drag factor K depends on the gas and dust θ density, also on the geometry of the dust grains SPH particles. The continuity equations are transforms in; equation (9) for gas and equation (10) for dust.

Acceleration Equations:

$$\frac{dv_g}{dt} = \boxed{-\frac{\nabla P}{\rho_g}} + \frac{K}{\hat{\rho}_g}(v_d - v_g) + g \qquad (7)$$

$$\frac{dv_d}{dt} = \boxed{-\frac{\nabla P}{\rho_d}} - \frac{K}{\hat{\rho}_d}(v_d - v_g) + g. \qquad (8)$$

In order to build SPH equations which conserve linear and angular momentum the pressure term needs to be writing in the form of equation (7).

$$\boxed{\frac{\nabla P}{\rho_g} = \nabla\left(\frac{P\theta_g}{\hat{\rho}_g}\right) + \frac{P\theta_g}{\hat{\rho}_g^2}\nabla\hat{\rho}_g - \frac{P}{\hat{\rho}_g}\nabla\theta_g.} \qquad (9)$$

Avoiding the details of the processes, equation (10) is used, if the drag term is required and conserves both linear and angular momentum.

$$K(r)\,(v_g(r) - v_d(r)) = \sigma\int K(r,r')\left(\frac{\Delta v' \cdot \Delta r'}{(\Delta r')^2 + \eta^2}\right)\Delta r' W(|r - r'|)dr' \qquad (10)$$

Where, η^2 is a clipping constant which prevents singularities in the numerical work, and σ is a constant equal to 0.5 for 2-D, and 0.3 for 3-D. Equation (10) is compose by equations (11) and (12) both factors are inside the integral of equation (10).

$$\Delta v' = v_g(r) - v_d(r') \qquad (11)$$

$$\Delta r' = r - r' \qquad (12)$$

The equation (10) for a gas particle is obtained by replacing the integral for a summation on dust particles as show in equation (13).

$$\sigma\sum_j m_j \frac{K_{aj}}{\hat{\rho}_j}\left(\frac{v_{ja}\cdot r_{ja}}{r_{ja}{}^2 + \eta^2}\right) r_{ja} W_{ja} \qquad (13)$$

The drag coefficient K depends on the gas SPH and on the dust SPH particle. Therefore the drag coefficient for volcanic dust gas in this case, may have the following K_{aj} value [31];

$$K_{aj} = \frac{\rho_a \, \theta_j \, C_D}{r_d} \left| v_{ja} \right| \qquad (14)$$

The r_d is the radius of a dust grain (assumed spherical) and C_D depends, in Reynolds number calculated from the relative velocity of the grain as well as the gas and size of the grains [34] .Now the momentum equation for the gas particle (*a)* from equations (7), (8) and (10), are calculated with SPH rules. This is allowing equation (4) parameter replacement from $\Delta\theta_g$ to $-\Delta\theta_d$, after this validate $-\Delta\theta_d$ with the summation over the dust particles equation (13). The application of these steps generates the acceleration of (a) particles.

$$\frac{dv_a}{dt} = -\sum_b m_b \left(\frac{P_a \theta_a}{\rho_a^2} + \left(\frac{P_b \theta_b}{\rho_b^2} \right) + \prod_{ab} \right) \nabla_a W_{ab} - \sum_j m_j \frac{P_a \theta_j}{\hat{\rho}_a \, \hat{\rho}_j} \nabla_a W_{aj} + \sigma \sum_j m_j \frac{K_{aj}}{\hat{\rho}_a \, \hat{\rho}_j} \left(\frac{v_{ja} \, r_{ja}}{r_{ja}^2 + \eta^2} \right) r_{ja} W_{aj} + g_a \qquad (15)$$

The acceleration equation for the dust particles may be writing as,

$$\frac{dv_j}{dt} = -\theta_j \sum_a m_a \frac{P_a}{\hat{\rho}_j \hat{\rho}_a} \nabla_j W_{ja} - \sigma \sum_a m_a \frac{K_{aj}}{\hat{\rho}_a \hat{\rho}_j} \left(\frac{v_{ja} \cdot r_{ja}}{r_{ja}^2 + \eta^2} \right) r_{ja} W_{ja} + g_j \qquad (16)$$

Energy Equations:

The equation relates rate of kinetic energy to five terms involving double summations, equation (17).

$$\sum_a m_a v_a \cdot (Eq15) + \sum_j m_j v_j \cdot (Eq16) \qquad (17)$$

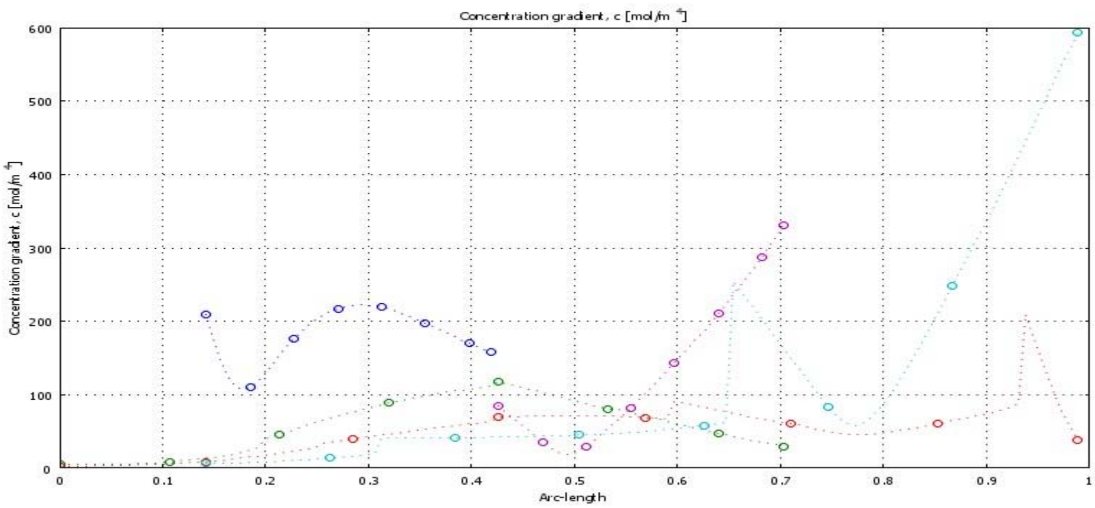
The equation (18) gives the rate of change of the gravitational energy.

$$\sum_a m_a v_a \cdot g_a + \sum_j m_j v_j \cdot g_j \qquad (18)$$

Is imperative to assume that all the drag dissipation goes into gas thermal energy, therefore the rate of change of thermal energy of gas SPH particle *(a)* is presented on equation (19).

In Figure.1, represented by a large set particles, each particles (a) is described by mass (M_a), a position vector (X_a), and a velocity (v_a). This is needed for calculate the total kinetic energy of the system as the sum of the products of particle masses by the amount of energy accumulated per unit mass, as well depend on the deformation, density or other constitutive parameters. In Figure, 2. Solids-Total Lagrangian formulation, allow that internal energy per unit mass given by the elastic strain energy which is a function of the deformation gradient tensor. In which the internal energy is simply a function of the density of the fluid [35,36,37] .

Figure.1. the point sources (dust gas) is at (0, 0), a large set of particles, with mass, position, and velocity are emitted at different rates.



$$\frac{du_a}{dt} = \frac{1}{2}\sum_b m_b\left(\frac{P_a\theta_a}{P_a^2} + \frac{P_b\theta_b}{P_b^2} + \prod_{ab}\right) v_{ab}\cdot\nabla_a W_{ab} + \sum_j m_j \frac{\theta_j P_a}{\hat{\rho}_a\hat{\rho}_j} v_{aj}\cdot\nabla W_{aj} + \sigma\sum_j m_j \frac{K_{aj}}{\hat{\rho}_a\hat{\rho}_j}\frac{\left(v_{ja}\cdot r_{ja}\right)^2}{r_{ja}^2+\eta^2} W_{ja} \quad (19)$$

The first two summations in equation (19) represent SPH expressions for,

$$-\frac{P_g}{\hat{\rho}_g}\nabla\cdot\left(\theta_g v_g + \theta_d v_d\right) \quad (20)$$

These represent the standard expression for the compressibility contribution to the thermal energy of the gas. The thermal energy of the dust remains constant unless there is thermal energy transport between the two phases [31] .In the case for wildfire there is an energy transport factors. The radiation for each phase and heat conduction term which involves the Prandtl number, in a heat transport term which is to be added to the energy equation for the gas, in equation (21).

$$R = \frac{Q_{dg}}{\hat{\rho}_g}(T_d - T_g) \tag{21}$$

Where Q_{dg} is a coefficient that depends on the properties of the gas and the dust, and T is temperature, the SPH form of (22) is for a gas particle.

$$R_a = \sum_j \frac{m_j Q_{aj}}{\hat{\rho}_j \hat{\rho}_a}(T_j - T_a) W_{aj} \tag{22}$$

$$R_j = -\sum_a \frac{m_a Q_{ja}}{\hat{\rho}_j \hat{\rho}_a}(T_j - T_a) W_{aj} \tag{23}$$

In equation (23) is evaluated for dust particle *(j)*, therefore thermal energy equation for the gas in equation (24), and equation (25) is for the dust thermal energy.

$$\frac{du_g}{dt} = -\frac{P_g}{\hat{\rho}_g}\nabla \cdot \left(\theta_g v_g + \theta_d v_d\right) + \frac{Q}{\hat{\rho}_g}\left(T_d - T_g\right) + \frac{K}{\hat{\rho}_g}\left(v_g - v_d\right)^2 \tag{24}$$

$$\frac{du_d}{dt} = -\frac{Q}{\hat{\rho}_d}(T_d - T_g). \tag{25}$$

If the heat transport between the phases is due to radiation then $\left(T_d - T_g\right)$ is replaced by $\left(eT_d^4 - aT_g^4\right)$.

Validation:

Figure 2,
time (s) vs. convective flux

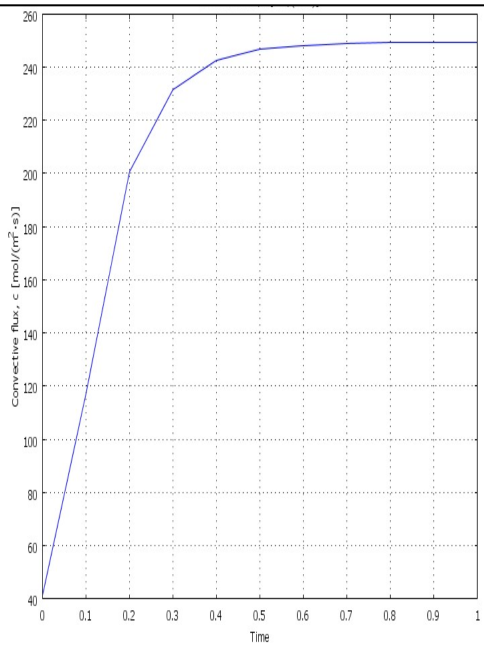


Figure 3,
concentration [CO2] vs. convective flux

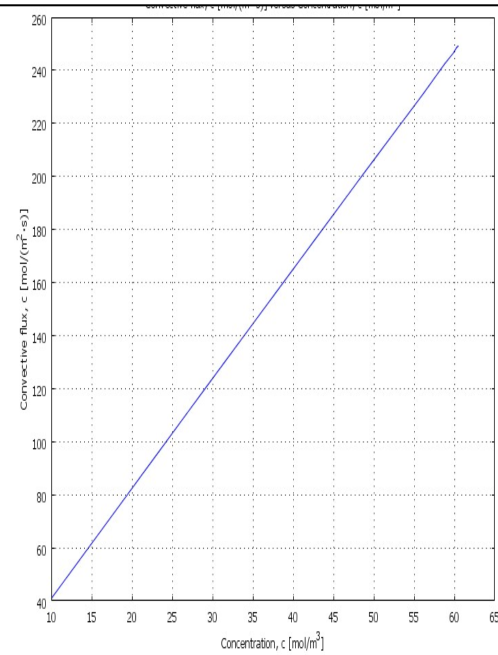


Figure 4,
total flux vs. concentration flux

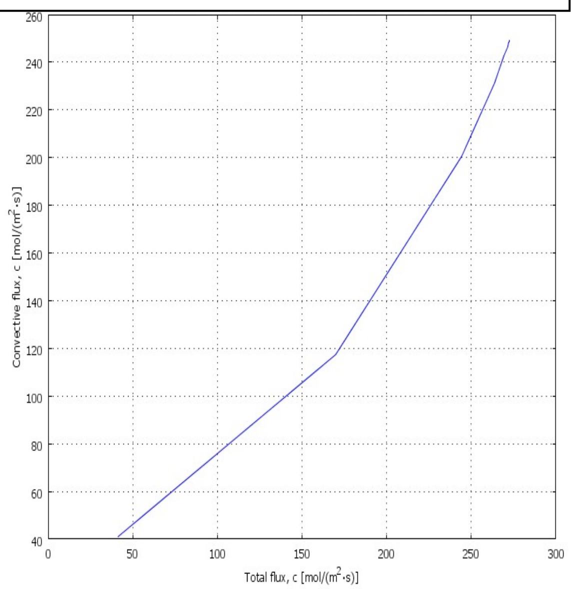


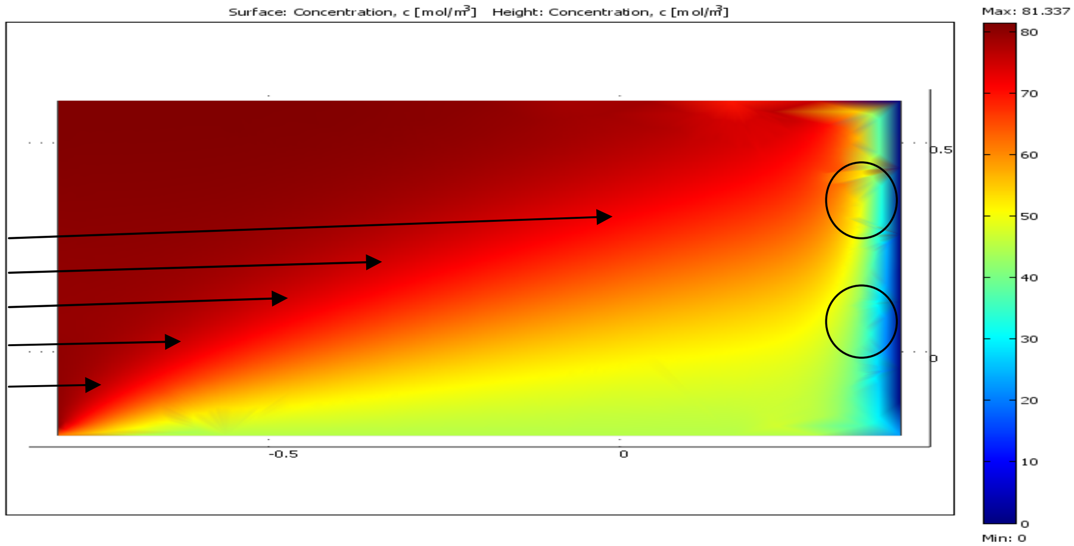
Figure 2; show the equilibrium of the system at certain point in time.

Figure 3, demonstrate that equilibrium has a linear correlation, between concentration of CO_2 [mol/m³] vs. the convective flux, [mol/(m²·s)].

Figure 4, there is an inflection point. This point occurs approximately at 118 [mol/ (m²·s)] convective flux vs. 170 [mol/ (m²·s)] total flux.

Results and Conclusion:

Figure. 5. Represent the particles of figure 1, by internal energy unit mass given by elastic strain energy [35]. Arrows are wind flow, and circles are vortices.



In figure 5, is the outcomes of Comsol application model, which are interpreted as follow, wildfire propagation, the red represent higher concentration of pollutants i.e, dust particles interacting with the (a) particles from the gas. The arrows show the wind flow.

The x-axis represents the solid fuel, vegetation; leaves, twigs, grass, etc. Fresh air is entrained laterally; in these cases are the (a) particles. Previously studies illustrate that downstream from the fire front, is a shear flow between the hot gas column (plume, dust particles) and the aspiration of the fresh air at the base of the combustion zone (red) periodically induced the formation of vortices[38,39]. These vortexes play a significant role in the preheating of the solid fuel (collision particle-solid) during fire propagation, increasing or inducing secondary ignition (**point's sources, Figure.1**) a piloted ignition of gases [40]. Since the SPH is a mesh-free model, it may help in the prediction of where the next point sources occurs during a biomass- burning, However each wildfire is completely different, the reason for these case are difference in physical vegetation as well atmospheric environments. SPH is a multidisciplinary tool. Always reinventing and it may be that the next generation of SPH interface is very well related to the ***Plasmonics methods*** as well as the combustion zones, and industrial boilers.

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