

# Modeling biomass particle drying, devolatilization and combustion in a grate fired combustor

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**Abstract** The paper presents the application of a numerical model to describe the evolution of a particle in a grate fired combustion system. Due to the particle dimensions, important temperature gradients exist inside the particles and reactions occur within the particles. A model using layers is used to describe the processes inside the particles. The biomass composition is expressed as fractions of moisture, unreacted biomass, char and ash. Biomass conversion is described by a competitive reaction model leading to the formation of light volatiles, tars and char. Tar is subject of secondary reactions inside the particles forming either light gases or char. Transport equations are solved for the gases within the particle including oxygen from the environment that reacts with gases or char. The model is applied to different heating rates leading to different amounts of tars and char in accordance with data from the literature. The model is also applied to simulate the combustion of a single trunk standing in a heated gas stream and comparisons are done for the temperature and mass loss.

**1. Introduction** – Grate fired combustion although being the oldest biomass combustion systems are complex to represent through numerical models. There are a large number of reasons for this, namely i) the motion of the biomass, ii) the gas flow through the bed, iii) the large size of the biomass. The representation of these processes can be done using several degrees of complexity and detail. For the solids motion a Discrete Element Model can be used but it requires large computational resources and the introduction of simplifications in solid-solid interaction. An alternative approach was considered [1] assuming a continuous solid phase that is converted due to reactions and is moved as a consequence of the grate vibration that is one of the mechanisms to move the solids. The gas flow through the bed is modeled considering a Forchheimer equation [2] that considers the pressure drop in the gas flow through the bed with a viscous and inertial term.

Based on the hydrodynamic description of the gas and solid phases, the model requires the solution of gas species mass balances and energy balances both for the solid particles and for the gas phase. The conversion of the particle can be calculated at each time step as a function of the gas phase conditions surrounding the particle and the previous particle conditions. For the overall grate fired combustion model the particle composition is also influenced by particle mixing that is accommodated in the layer model by averaging the compositions knowing the mixing between neighbouring elements.

The present paper presents the formulation of the mass and energy balances for a single large particle in the following section. A layer model to calculate the energy balance that was previously tested for heat transfer [2] is extended to include biomass conversion into light gases and tars. These are then transported within the particle where tar may decompose into light gases and char and light gases may react with oxygen that may enter the particle. The oxygen within the particle reacts also with char. To validate the model formulation the biomass decomposition products are compared with literature data for different heating rates. Section 3 presents data on mass loss and temperature of a trunk that burns in a hot gas stream simulating combustion conditions. Section 4 presents the main conclusions.

**2. Numerical model** – This section describes the numerical model that was developed to represent the evolution of the particle properties along conversion. The model is based on a discretization in layers for arbitrary shapes that are applied to cylindrical particles (Pellets)[4]. The conversion of biomass is described by devolatilization models and due to the large particle sizes, gas flow and reactions are considered within the particle. To describe the products resulting from the devolatilization an important contribution presented in the paper is the formulation of elemental mass and energy balances to characterize the biomass products.

**2.1 Particle layer model** - Due to the large size of the particles present in the grate fired combustion system, it is necessary to consider the variation of the properties inside them. This can be done through different approaches, discretizing the particles. For a spherical particle due to symmetry the problem reduces to one dimensional approach, while for cylindrical and parallelepiped the problem becomes two or three dimensional. As the calculation of these require much more computational effort than one dimensional situations, the layer model suggested by Thunman et al [3] is considered. For heat transfer it was shown that the calculation time is reduced by a factor of 80 for a cylindrical geometry. For the development of the mass balances, the particle is discretized in layers as represented in figure 1.

The energy balance considering the gas motion within the particle can be written as:

$$\left(\rho_s c_{p,s} + \rho_g c_{p,g} \varepsilon\right) \frac{\partial T}{\partial t} + \frac{1}{A(r)} \frac{\partial}{\partial r} \left(\rho_g c_{p,g} T u_g A(r)\right) = \frac{1}{A(r)} \frac{\partial}{\partial r} \left(A(r) k \frac{\partial T}{\partial r}\right) + S_E \quad (1)$$

where the first term represents the energy accumulation both in the solid and gas that are considered at the same temperature. The second term represents the energy transport by the gas moving inside the particle. The right hand side is the variation of the heat flux and the energy sources due to reactions. The equation is written in one dimensional form as this is the approximation considered in the particle layer model. The area for the cylindrical geometry, represented in figure 1, is represented as a function of the radius by:

$$A(r)_{cil} = 2\pi r(3r + L - D) \quad (2)$$

The gas velocity is calculated from the continuity equation where the gas mass sources are the result of the particle conversion.

$$\frac{\partial(\rho_g)}{\partial t} + \frac{1}{A(r)} \frac{\partial}{\partial r} \left(\rho_g u_g A(r)\right) = S_g \quad (3)$$

This equation is used to calculate the pressure distribution considering the gas velocity proportional to the pressure gradient, according to the Darcy law:

$$u_g = \nabla P \frac{K}{\mu_g} \quad (4)$$

where K is the permeability coefficient in the biomass.

The gas velocity is important to evaluate the gas composition within the particle that is calculated based on mass balances to individual gas species written as:

$$\frac{\partial(\rho X_{gi})}{\partial t} + \frac{1}{A(r)} \frac{\partial}{\partial r} \left(\rho_g c_{p,g} X_{gi} u_g A(r)\right) = \frac{1}{A(r)} \frac{\partial}{\partial r} \left(A(r) \mathcal{D} \frac{\partial X_{gi}}{\partial r}\right) + S_{gi} \quad (5)$$

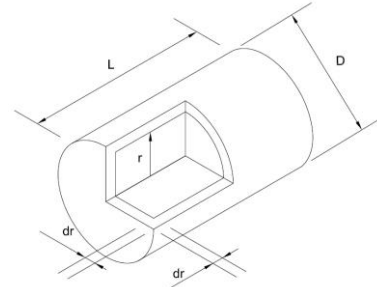
All the equations are discretized using the hybrid scheme and are applied in particle layers. The actual size of the particles has a small variation due to shrinkage that produces a velocity of the solid phase. This velocity was neglected but the dimensions of the layers were changed accordingly to the shrinkage.

The mass balances to individual species are applied to: moisture, the light gas components considered, tars, oxygen and combustion products. Due to space restrictions the gas phase reactions are not presented but they use literature data on rates and for tar they include secondary reactions.

**2.2 Biomass decomposition model** - There are several models to describe the biomass conversion that includes drying, volatilization and char burnout. Biomass drying can be described: i) as a kinetically controlled process through an Arrhenius expression [5]; ii) occurring at the boiling temperature for the local pressure or iii) with a thermodynamic equilibrium model between the water vapor and the liquid bound water [6]. For high drying temperatures all models produces similar results.

After complete drying, biomass is heated and the decomposition can be represented by different types of models. The two most popular approaches are: i) the consideration of parallel reactions for specific products (PRP) that have a prescribed total yield and ii) the use of parallel competitive reactions (PCR). The PRP model is the easier to consider since the yield of final products are pre-defined according to the biomass composition and heating value so the global balances are guaranteed. The main drawback from the PRP model is that it leads to the same amount of products irrespectively of the final temperature and heating rate. Therefore the application is limited to the conditions of the tests from where it was derived.

The PCR model considers that biomass is converted in light gases, tars and char by three competitive reactions (1 to 3 in figure 2) that are all first order on the mass fraction of unconverted biomass. The final yield of the three main products and their composition is a result of the temperature time history. The tars are large molecular mass species that are liquid at room temperature and have secondary reactions that



**Figure 1.** Discretization of a cylindrical particle in layers.

were considered within the particle to form further light gases or char in equation (5). This is an extension of the PCR model that is illustrated in figure 2 through reactions 4 and 5. Tars may also be oxidized if oxygen is available within the particle or outside the particles.

The PCR model was used in the present work with kinetic parameters from Thurner and Mann [7] and from Font and Wagennar as reviewed by Hong and Lu [8] for the primary reactions (1 to 3). The parameters were obtained for different types of biomass that may explain part of the differences. The particle size, heating rate and final temperature are other factors influencing the results. For the case of wood pellets, the conditions from Font using sawdust with diameter from 0.3 to 0.5 mm and higher temperature of 600 °C are the most similar. The PCR model is tested considering different heating rates and the results are compared with results from experiments used to develop PRP models, namely from Nunn et al [9] for 1000°C/s with peak temperature of 1100°C/s and from Grieco [10] with heating rates of 0.05 and 1°C/s. Figure 3 presents a comparison of the final yield of light gases, tars and char.

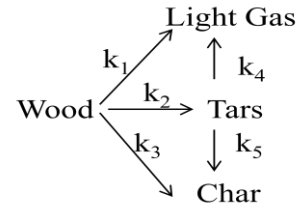


Figure 2. Parallel Competitive Reaction model for biomass decomposition.

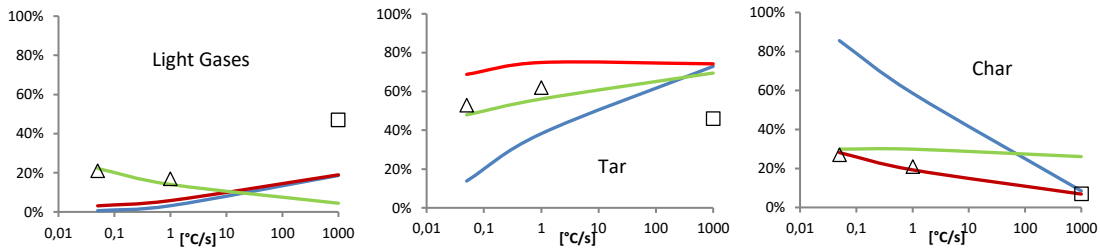


Figure 3. Comparison of the fractions of biomass decomposition products with measured values. Kinetic parameters: Thurner and Mann (Green) Wagennar (Blue), Font (Red), Experimental values Nunn et al (Square), Grieco et al (Triangles).

From the figure it can be observed that the kinetics from Font is the one that represents the results more closely, although with higher tar content and lower light gases. It should be mentioned that the kinetics from secondary reactions present similar activation energy but the pre-exponential of reaction 4 is 43 times larger than for reaction 5 meaning that in secondary reactions tar is mainly converted in light gases. This may explain the lower tar content in the experimental results due to some secondary reactions [9].

The kinetic parameters of Thurner and Mann obtained for wood, 0.65 mm diameter, lead to better results for the lower heating rate possibly because they were obtained for a low peak temperature (400°C).

Apart from the yield of products another very important component of the biomass decomposition model is the composition of light gas species and tar. As can be observed from figure 3 the amount of char changes with the heating rate and therefore the heating value of light gases and tar will change. For some PRP models the amount of light gases species and properties of tars were characterized [9]. Based on these results the composition of light gas species was specified as H<sub>2</sub>O, CO, CO<sub>2</sub> and C<sub>i</sub>H<sub>j</sub>O<sub>k</sub> representing hydrocarbons and acetaldehydes. Based on the measured light gas composition observed by Nunn et al [9] the composition can be estimated with mass fractions of 42%, 15%, 12% and 31% and i=1.8; j=4.1 and k=0.7. The heating value of the equivalent C<sub>i</sub>H<sub>j</sub>O<sub>k</sub> is 34 MJ/kg and of the light gas mixture is 14.7 MJ/kg. Tar is considered as another general molecule C<sub>a</sub>H<sub>b</sub>O<sub>c</sub> and char is considered to retain only carbon and ash. The tar elemental composition can be derived from the elemental mass balances or if experimental values [9] are used the previous j and k parameters can be adjusted to 7.8 and 2.3. The global energy balance can be used to calculate the heating value of tar. The results of the application of this model lead to the results presented in table 1. The differences are a direct consequence of the results in figure 3 due to the lower fraction of light gases predicted.

Table 1. Calculated light gas yield, fraction of elements in tar, heating value of tar and closure with heating value of wood. HHV in [MJ/kg]

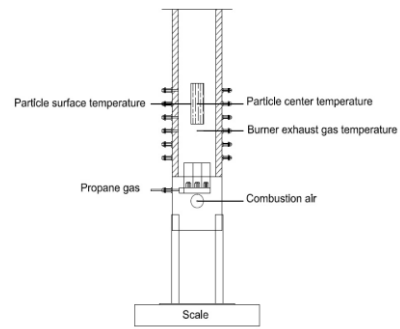
	Conditions	Y <sub>LG</sub>	HHV <sub>LG</sub>	Y <sub>C,tar</sub>	Y <sub>H,tar</sub>	Y <sub>O,tar</sub>	HHV <sub>Tar</sub>	Y <sub>char</sub>	HHV <sub>char</sub>	HHV <sub>wood</sub>
Measured [9]	1000 °C/s	41	14,6	26	3,7	16,3	26,7	7	32	19,5
Calculated	1000 °C/s	19,4	14,7	35,4	5,2	30,8	20,7	9,2	32	19,5
	1 °C/s	6,7	14,7	29,2	5,7	38,9	15,3	19,5	32	19,5

**3. Results and Discussion** - To test the model an experiment was prepared consisting on the suspension of a trunk of acacia wood with 5 cm diameter, 15 cm long that is fixed to the reactor tube supported in a weight scale. Combustion products from a gas burner are supplied in the reactor to promote the trunk heating and combustion.

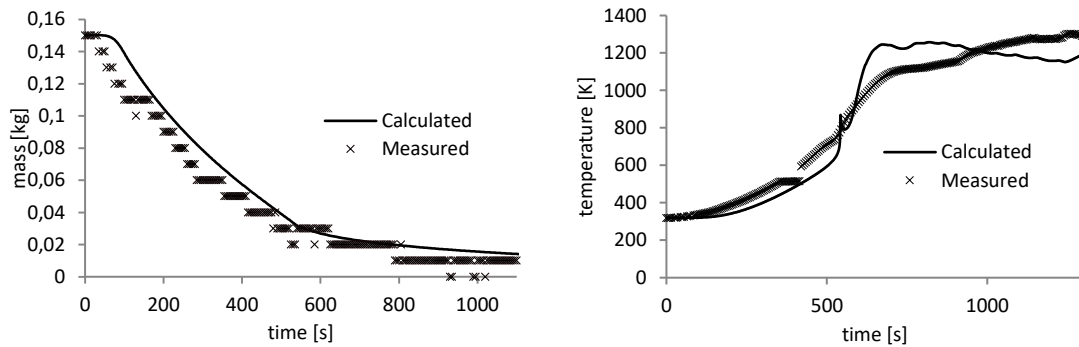
Thermocouples are installed in the gas upstream to the sample and at the centre of the sample. Further gas species were collected at the surface of the trunk but for space reasons data is not presented in the present paper.

The model for conversion of biomass and reaction was applied considering layers of 0,5 mm and the calculations were carried out with a time step of 0,05 s.

Figure 5 presents the comparison between the measured mass loss history and the temperature measured at the centre of the trunk. It can be observed that there are two main stages, the initial one until approximately 500 s that corresponds to most of the mass loss due to volatile release and the temperature profile is well predicted as it results mainly from heating. At the transition time a sudden increase of temperature is calculated due to the oxygen becoming available within the particle burning volatiles. Afterwards the char combustion is associated with a lower rate of mass change and increase in temperature that tends to an asymptotic value. The resolution of the scale can not characterize the final combustion stages corresponding to charred combustion when part of the trunk breaks apart.



**Figure 4.** Sketch of the experiment used to study the large particle combustion



**Figure 5.** Comparison between measured and calculated mass and temperature (at the centre of the trunk) evolution along time.

**4. Conclusions** – A particle layer model for biomass conversion was developed using the parallel competitive reaction (PCR) model. It is shown that the PCR model describes the influence of operating conditions in the biomass decomposition. The application of the layer model with mass and energy balances within the particle is shown to represent the evolution of mass loss and temperature of a 5cm diameter trunk. This model seems appropriate to include in a grate fired combustion model.

## 5. References

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