

# Gasification of Single Wood Particles: Experiment and Simulation

**B. Wilmes, U. Kuhlmann, F. Behrendt**

Berlin University of Technology  
Institute of Energy Engineering  
Berlin, Germany  
birgit.wilmes@tu-berlin.de

## Introduction

Due to the increasing use of renewable energy sources the thermochemical gas generation from solid biomass represents an economically attractive technology with good prospects. High efficiency and low emissions are important goals requiring a detailed understanding of all physical and chemical effects involved. Based on experimental investigations and detailed modelling of single particles a systematic description of the gasification process can be achieved. In this paper such an experiment as well as a new detailed single-particle model describing the gasification of a single porous fuel-particle and corresponding numerical results are presented.

## Experimental Setup

Spherical wood particles (15 mm dia.) were put into the exhaust gas of a flat-flame burner (McKenna, stoichiometric methane-air mixture) or alternatively into a flow of hot argon. The gases escaping the wood particle during pyrolysis were monitored near the stagnation point ( $\approx 0.6$  mm in front of particle) by Rayleigh-Raman spectroscopy. The spectra were obtained by using a 300 mm spectrograph (Acton Research) together with an intensified CCD camera (LaVision-Nanostar). As Raman excitation source a Spectra Physics LAB 150 Nd:YAG laser with 10 Hz repetition rate and 300 mJ pulse energy at 532 nm was used. Simultaneous to the Raman spectra the temperature at the center of the particle and near the particle was measured by thermocouples and the weight loss of the particle was determined (Fig. 1).

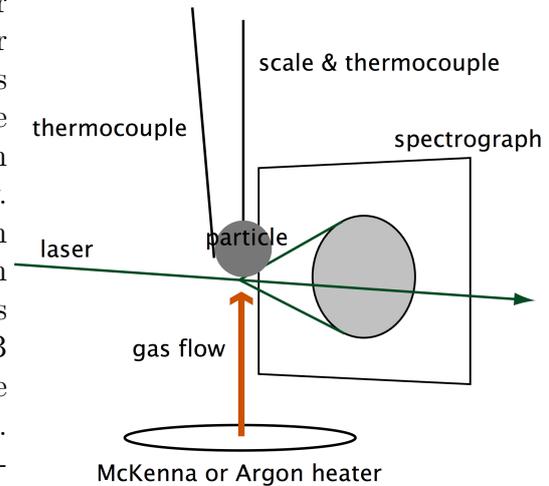


Figure 1: Experimental setup

## Experimental Results

A preliminary result of our experiments is displayed in Fig. 2, showing the temporal evolution of the Rayleigh-Raman spectra during pyrolysis. After drying of the wood particle (initial humidity  $\approx 7$  weight-%) the onset of the pyrolysis is marked by the evolution of a strong signal of supposedly fluorescence origin. We tentatively assign this signal to  $C_2^*$ -LIF [1]. These well known Swan bands are prominent in the spectra of carbon stars as well as in sooting flames. The strong signal at 589 nm which comes in somewhat later can be attributed to the Na-D doublet. Sodium was found in the particles with a concentration of 180 ppm.

Additional Raman lines of the major species of the pyrolysis gases are probably hidden by the strong fluorescence.

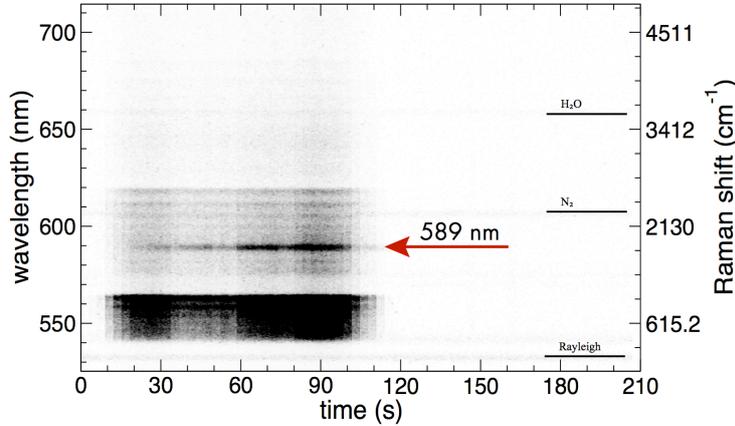


Figure 2: Time evolution of the Rayleigh-Raman spectra from an outgassing wood particle during pyrolysis.

### Mathematical Model of the Gasification of a Single Porous Fuel-Particle

A one-dimensional mathematical model of the gasification of single porous fuel-particles is presented. The porous particle is modelled as a homogeneous three-phase mixture consisting of a solid, a liquid and a gas mixture.

In the case of thermally large particles (Biot number  $> 0.1$ ) it is known that intra-particle heat and mass transfer needs to be solved. The microkinetic processes during gasification to be considered are drying, pyrolysis, gas phase reactions of the volatiles, and heterogeneous reactions at the inner and outer surfaces. Those processes interact in a complex way with mass transfer in the pores and, in addition, with mass transfer into the surrounding of the particle.

Drawing differential balances for energy, mass, momentum, and mass of the chemical species leads to a one-dimensional, transient system of partial differential conservation equations.

In this model the kinetic scheme for the pyrolysis is taken from Miller et al. [2]. They suggested a biomass pyrolysis-model based on superimposed cellulose, hemicellulose, and lignin reactions enabling the simulation of different biomass feedstock. The reactions are modelled with first-order Arrhenius kinetics.

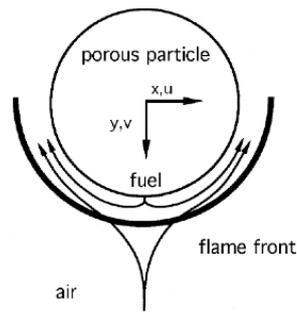


Figure 3: Configuration of the model

The gas phase reactions in the pores are calculated with a detailed gas-phase reaction mechanism (39 species) [3]. More complicated is the description of heterogeneous reactions as well as adsorption and desorption reaction steps. Elemental chemical processes of the combustion / gasification of char are analyzed by [4] leading to a detailed reaction mechanism for adsorption, reaction, and desorption. This mechanism is used in our model.

Regarding the mass and heat transfer in the surrounding of the particle it is important to define proper boundary conditions. For that reason the surrounding gas phase is also modelled and simulated. The behavior of the gas is characterised by a directional flow towards the surface of the wood particle (Fig. 3). This kind of flow is known as stagnation-point flow [5]. The governing equations can be found in [6]. Those sets of equations have to be coupled by means of conservation equations for the interface. The resulting system of differential equations is solved together with appropriate initial and boundary conditions using the solver LIMEX [7].

## Results

Results of the pyrolysis of dried beech spheres are presented. Following conditions are used. The diameter of the particle is  $d_{\text{sphere}} = 15$  mm. The initial temperature is  $T_0 = 293$  K. The temperature in the surrounding is  $T_{\text{surrounding}} = 923$  K, which is here used to calculate the heat flux to the particle. So, following calculations neglect the informations of the stagnation-point flow. The concentrations at the border of the particle are given by means of the mass flux.

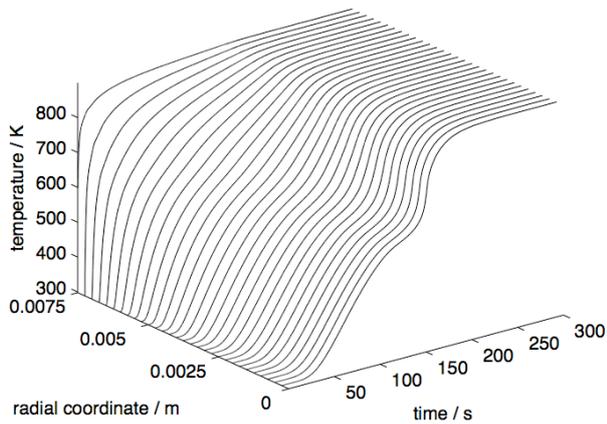


Figure 4: Development of temperature in the particle

Fig. 5 shows a comparison of experimental and simulation results for mass as well as temperature at the center and border of the particle. Simulations and experimental data are shown as solid and dashed lines, respectively.

Differences between experimental and simulation results are mainly due to the assumption of a constant temperature in the surrounding. The real temperature is given by the flame temperature of the McKenna burner.

Fig. 4 shows the calculated temperature field. The center of the sphere is located at  $r = 0$  m. The temperature at the center remains constant for the first 30 seconds. Then the temperature increases slowly and, after the pyrolysis is complete, temperature reaches very fast its maximum. This phenomenon is due to the gases leaving the particle during pyrolysis. This causes a debasement of the heat transfer to the particle.

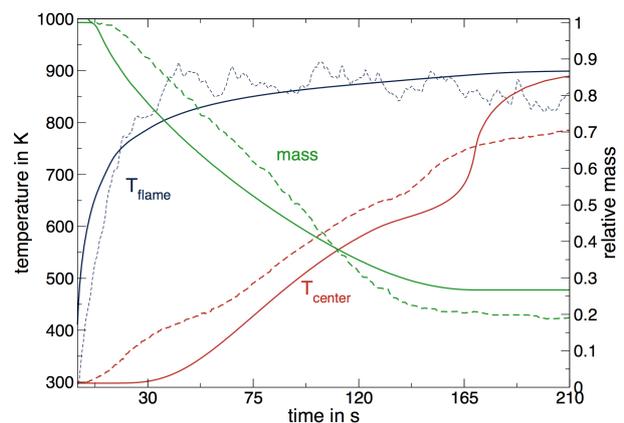


Figure 5: Comparison of experimental and simulation results for mass loss as well as temperature at the center and border of the particle

## Conclusions

A single-particle model is presented providing a simulation tool for calculating the gasification of a porous fuel particle. Discrepancies to experimental results are traced back to the fact that the current results neglect the details of the surrounding flame. Coupled calculation are under way and will improve the overall model.

By simultaneous measurements of mass and temperature of pyrolysed wood particles as well as Rayleigh-Raman spectra during pyrolysis, a correlation could be established between the spectra of the pyrolysis gases, experimental weight loss and the model calculations. The spectra are dominated by strong  $C_2^*$ -LIF which probably mask the expected Raman signal from major pyrolysis species as e.g. CO, CO<sub>2</sub> and others.  $C_2^*$  is currently not included in our model but will be considered in future in order to allow for direct comparison with the spectra.

## References

- [1] BARLOW, R. S. AND MILES, P. C.: A Shutter-Based Line-Imaging System for Single-Shot Raman Scattering Measurements of Gradients in Mixture Fraction, Proc. Combust. Inst., 28, pp. 269-277, 2000.
- [2] MILLER, R. S., BELLAN, J.: A Generalized Biomass Pyrolysis Model Based on Superimposed Cellulose, Hemicellulose and Lignin Kinetics. Combust. Sci. and Tech., 126, pp. 97-137, 1997
- [3] J. WARNATZ, U. MAAS UND R.W. DIBBLE: Combustion. Springer, Heidelberg, 1996.
- [4] MIESSEN, G., BEHRENDT, F., DEUTSCHMANN, O., WARNATZ, J.: Numerical Studies of the Heterogeneous Combustion of Char Particles Using Detailed Chemistry, Chemosphere 41, pp. 609-613, 2001
- [5] KEE, R. J., MILLER, J. A., EVANS, G. H. AND DIXON-LEWIS, G.: A Computational Model of the Structure and Extinction of Strained, Opposed Flow, Premixed Methane-Air Flames. Twenty-Second Symposium on Combustion, The Combustion Institute, pp. 1479-1494, 1988
- [6] BEHRENDT, F., WARNATZ, J.: Simulation of Partially Methane-Air Counterflow-Diffusion Flames and Comparison with Experimental Results, Progress in Astronautics and Aeronautics, 131, pp. 145-160, 1991
- [7] DEUFLHARD, P., HAIRER, E., ZUGCK, J.: One-Step and Extrapolation Methods for Differential-Algebraic Systems. Numer. Math. 51, 501-516, 1987