

Numerical simulation of devolatilization of wood LOGs and pressure generation in the wood log center

I. Haberle¹, Ø. Skreiberg², N.E.L. Haugen^{1,2}

¹ Department of Energy and Process Engineering, Norwegian University of Science and Technology, NTNU, Kolbjørn Hejes vei 1b, 7491 Trondheim, Norway, Tel.: +47 73 593697, E-mail: inge.haberle@ntnu.no

² Department of Thermal Energy, SINTEF Energy Research, Postboks 4761 Torgard, 7465 Trondheim, Norway

ABSTRACT: A transient model for devolatilization of a dry or wet cylindrical wood log is developed. The model is mesh-based and 1D even though the extension to 2D or 3D can easily be done. The stiff solid matrix of porous wood contains the gas phase (non-condensable gases, condensable gases and air). The gas is assumed to be ideal and Darcy's law is applied to define the gas phase motion within the pores. Devolatilization is described with a primary three independent competitive reactions model which is followed by secondary tar cracking and re-polymerization reactions. Overall good agreement between measurements and modeling results was found. This model can accurately predict the solid mass loss behavior, temperature history at the surface and in the wood log center. The model was applied to predict the pressure in the wood log center with respect to time. Special focus is on the identification of parameters that influence the pressure peak formation in the center of the wood log.

Keywords: drying, pressure, tar, thermochemical conversion, wood

1 INTRODUCTION

Intensified research within the field of numerical modeling of thermal conversion, including thermochemical degradation of wood logs, has been done during the last two decades [1]–[7]. Numerical modeling can significantly support a gain in new knowledge concerning chemical and physical processes occurring during devolatilization.

Overall the main challenge is the complex coupling of these physical and chemical phenomena. Mainly 1D models are therefore developed [3]–[6], since they are computationally fast and less complex.

However, in 1D models the anisotropy of wood (e.g.; different thermal conductivities and permeability depending on fiber orientation) cannot be precisely accounted for, which however, can be done in multi-dimensional models. Still, multi-dimensional models do not necessarily contribute to a deeper understanding of the fundamental processes related to wood devolatilization, even though they do increase a model's accuracy and also consider the combined influence of direction-dependent wood properties. Therefore, it is assumed that 1D models are a suitable starting point for obtaining fundamental understanding of devolatilization related processes including pressure generation during devolatilization. These models still need to be extended to multi-dimensional models if highly accurate results are the main modeling criteria.

Reviewing the current state-of-the-art revealed that only limited research has yet been done on internal pressure evolution in the wood log during devolatilization. Park et al. [8] modeled and experimentally tested a spherical wood particle ($D=25.4$ mm) and investigated heat and mass transfer processes during pyrolysis reactions. They were able to show that a pressure peak (up to 1.6 atm) in the center of the spherical wood particle was formed. This pressure peak is dependent on the temperature history in the particle [8].

In this work, a 1D mesh-based devolatilization model for dry or wet cylindrical wood logs is developed. The model can predict the pressure throughout the wood log including the pressure peak in the center of the wood log.

It is assumed that accurate pressure prediction is highly relevant, as the pressure gradient is the driving force of the convective term of the gas phase equation. In addition a high internal pressure can result in splitting of the wood log, which was also found by Park et al. [8]. Furthermore it is assumed that accurate pressure prediction is required since the internal pressure can influence char conversion reactions as well as secondary tar reactions. This suggests that accurate pressure prediction is required for accurate gas species predictions. Besides the relevance of accurate pressure predictions during devolatilization, it has also been mentioned in the literature, that drying is expected to be influenced by the internal pressure evolution. Due to an increased pressure in the wood log, which exceeds ambient pressure, evaporation of the water in the porous wood structure is expected to occur at higher temperatures than 373 K [9]. This makes accurate pressure prediction also essential during drying. This work investigates some of the most influencing input parameters of the model on pressure prediction.

2 METHODOLOGY

The cylindrical wood log is fully discretized in 1D, even though the model development is done in such a manner that extension to 2D or 3D can easily be done in the future. The applied governing equations and boundary conditions were taken from Lu et al. [10]. Re-condensation of liquid free water, considered in the work by Lu et al. [10], was not considered in this work. Furthermore, movement of liquid free water was modeled as suggested by Grønli [11]. Devolatilization was modeled by three independent competitive reactions followed by tar cracking and re-polymerization reactions. The IDA solver included in SUNDIALS [12] was used for solving the evolution equations. In this solver the backward differentiation formula is used. This implicit method is a suitable choice for very stiff equations which are expected when thermal conversion of wet wood is modeled. Validation of the model was done against experiments by Lu et al. [10], where differently wet wood logs were dried and thermochemically degraded.

3 RESULTS AND DISCUSSION

The model showed good agreement with experiments, for both low and high moisture contents. The validated results for the high moisture content test case (40 wt% wet basis) are shown in Fig. 1 to Fig. 3. The different experimental results of Lu et al. [10] were all done for the same setup. This means that the spread in the experimental results gives an indication of the error-bars associated with the experiments.

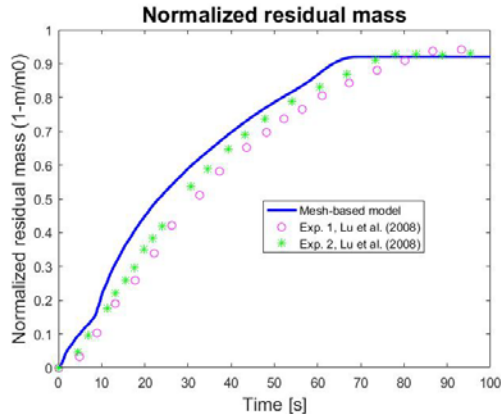


Figure 1: Normalized residual solid mass of a cylindrical wood particle (40 wt% wet basis).

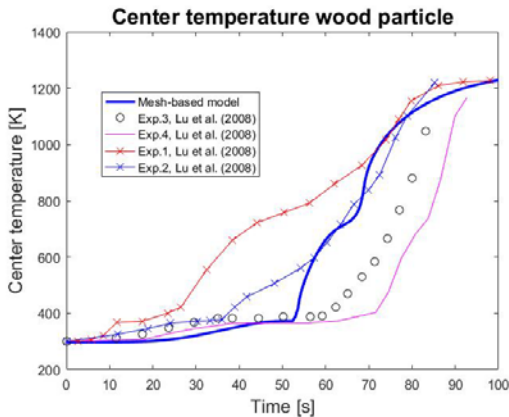


Figure 2: Center temperature prediction of a cylindrical wood particle (40 wt% wet basis).

Drying was modeled with the thermal drying model and evaporation occurred at 373 K.

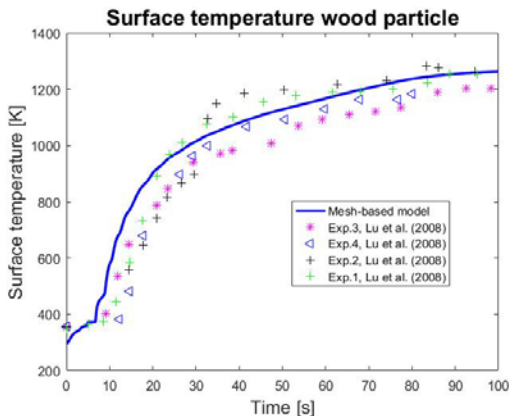


Figure 3: Surface temperature prediction of a cylindrical wood particle (40 wt% wet basis).

Lower moisture content model predictions (6 wt% wet

basis) showed even better agreement with experiments. Subsequent to validation of the model, the internal pressure development during dry wood log devolatilization was tested. Firstly, only the permeability of char was changed, while the permeability of wood was kept constant at $\kappa_{\text{wood}} = 10^{-16} \text{ m}^2$. In the model the permeability only changed with the degree of conversion. The degree-of-conversion-dependent effective permeability was calculated such that

$$\kappa_{\text{eff}} = (X) \kappa_{\text{wood}} + (1-X) \kappa_{\text{char}} \quad (1)$$

$$X = M_{\text{wood}} / M_{\text{wood initial}} \quad (2)$$

was fulfilled [10], with (1-X) being the degree of conversion depending on the actual mass of wood (M_{wood}) and the initial wood mass ($M_{\text{wood initial}}$). The effective permeability weighted the influence of the permeability of wood κ_{wood} and the permeability of char κ_{char} . All applied permeabilities are listed in Table I.

Table I: List of permeabilities applied in the devolatilization model.

TEST CASE	κ_{wood}	κ_{char}
1	10^{-16} m^2	10^{-16} m^2
2	10^{-16} m^2	10^{-15} m^2
3	10^{-16} m^2	10^{-14} m^2
4	10^{-16} m^2	10^{-13} m^2

Besides the permeability, also the assumed molecular weights of the modeled gas species have an influence on the internal pressure prediction. The molecular weight of tar was assumed to be 0.110 kg/mol and the molecular weight of the lumped-together-non-condensable gas species was assumed to be 0.038 kg/mol. Both molecular weights were taken from Park et al. [8]. These molecular weights were kept constant when investigating the influence of char permeability. It is outlined that the classification “permanent gases” and “non-condensable gases” can be used interchangeably.

As shown in Fig. 4 to Fig. 5, the char permeability significantly influences the pressure predictions, which suggests that model accuracy is closely linked to the applied char permeability values.

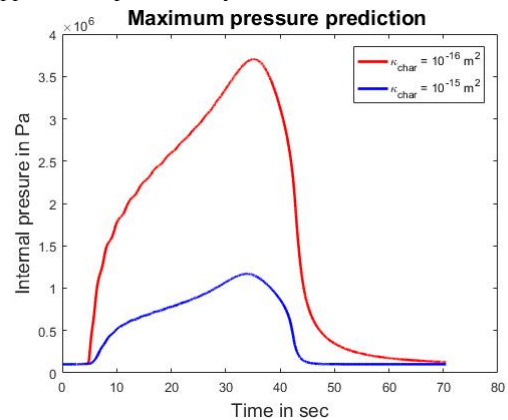


Figure 4: Pressure prediction in the center of the wood log with char permeability being 10^{-16} m^2 in red and 10^{-15} m^2 in blue.

Model predictions with the lowest char permeability of 10^{-16} m^2 led to an unphysically high maximum pressure of 37 bar, while a char permeability of 10^{-13} m^2 (Fig. 5)

resulted in a significantly lower pressure peak of approximately 1.5 bar.

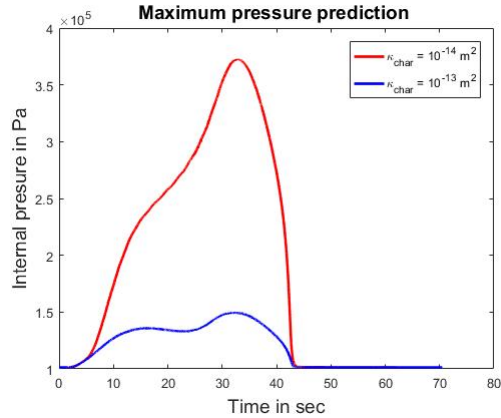


Figure 5: Pressure prediction in the center of the wood log with char permeability being 10^{-14} m^2 in red and 10^{-13} m^2 in blue.

For permeabilities between the minimum (10^{-16} m^2) and the maximum (10^{-13} m^2) value assumed, the pressure peak predictions were also within the limits of what was found for those permeabilities.

For a char permeability of 10^{-14} m^2 the maximum pressure was 3.75 bar, while for a char permeability of 10^{-15} m^2 the internal pressure was significantly higher reaching 12 bar.

It can be concluded that by assuming incorrect permeabilities, also the gas phase velocity prediction can be highly inaccurate.

In Fig. 6 it is shown how significant the dependency of pressure prediction on char permeability is.

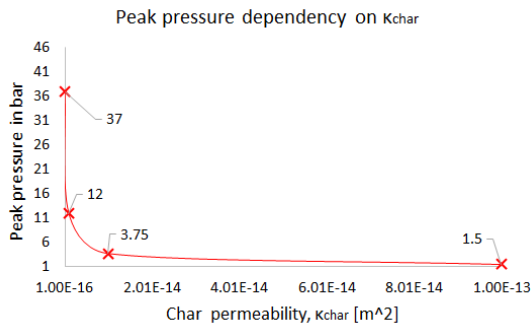


Figure 6: Peak pressure drop with increasing char permeability.

One can explain this significant drop of maximum pressure related to increasing char permeabilities (see Fig. 6) by considering the convective term of the gas phase continuity equation, where gas phase velocity is modeled by Darcy's law. Darcy's law links the velocity of the gas phase to the pressure gradient, the effective permeability and the dynamic viscosity of the gas. Assuming a lower char permeability results in a lower gas phase velocity and therefore reduced transportation of the gas phase outwards. Gases are, however, still being formed due to devolatilization. Consequently, a pressure peak can build up to a higher extent. Since splitting or cracking are not yet included in the model, the pressure continuously keeps building up, as there is no structural change occurring that can result in sudden pressure reduction. The consequence is the unphysically high internal pressure. A higher permeability, however, results

in facilitated outwards flow of the gas phase. Therefore, the internal pressure in the center of the wood log cannot build up as significantly.

In the literature a broad range of different permeabilities of char is commonly used, e.g. [3], [6], [13], which leads to the conclusion that the choice of char permeability is one of the most significant uncertainties of current modeling.

The molecular weights of tar and non-condensable gases were adjusted in the second step of the work in order to investigate the influence of the assigned molecular weights on the pressure prediction. The applied molecular weights are listed in Table II.

Table II: List of molecular weights, MW in kg/mol, tested for tar and non-condensable gases.

TEST CASE	MW _{Tar}	MW _{Gases}
1	0.11	0.038
2	0.11	0.016
3	0.11	0.029
4	0.128	0.038

In test case 2, the molecular weight of non-condensable gases was set equal to the molecular weight of methane, while in test case 3, the molecular weight of non-condensable gases was set equal to the molecular weight of air. This suggests that air and non-condensable gas phase products of devolatilization were lumped together, while in test case 2, it was assumed that methane is the main representative of the permanent gases. It has to be pointed out, that methane is never the main gas species within the group of permanent gases, but is rather present in a lower quantity compared to CO and CO₂ [14]. However, this test case was still investigated to determine how significant the change in molecular weight of permanent gases has to be in order to see effects on the maximum pressure prediction. In test case 4, the molecular weight of tar was set equal to molecular weight of naphthalene, which was assumed to be representative of the tar fraction.

During the investigation of the influence of the molecular weights on pressure predictions, the char permeability was set to 10^{-14} m^2 .

When reducing the molecular weight of permanent gas species from 0.038 kg/mol to 0.016 kg/mol, the pressure peak increased from approximately 3.75 bar to approximately 4.85 bar. A significant influence on pressure prediction is given, if the molecular weight of non-condensable gases is approximately divided in half.

When reducing the molecular weight of permanent gas species from 0.038 kg/mol to 0.029 kg/mol, the peak pressure only increased from approximately 3.75 bar to approximately 4 bar, which is a comparably minor effect. Changing the molecular weight of tar from 0.110 kg/mol to 0.128 kg/mol only resulted in minor reduction of the maximum pressure, as it only dropped from 3.75 bar to approximately 3.65 bar.

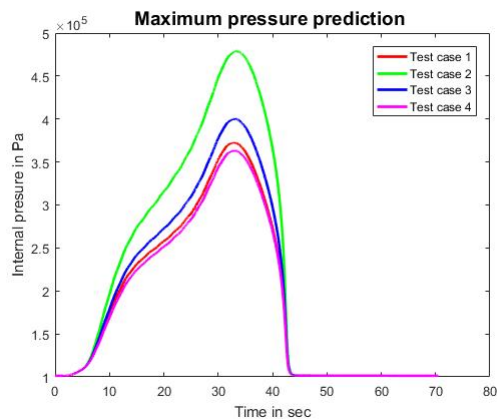


Figure 7: Pressure prediction when applying a char permeability of 10^{-14} m^2 , and the test cases; Test Case 1 in red, Test Case 2 in green, Test Case 3 in blue and Test Case 4 in magenta.

This dependency of dropping pressure peaks when increasing the molecular weights and increasing pressure peaks when reducing the molecular weights, can easily be explained by considering the ideal gas law, which is used to calculate the internal pressure. The pressure is obtained by dividing gas phase density, ideal gas constant and temperature by the mixed molecular weight of the gas phase. As a consequence, it is rather obvious that increasing the molecular weight of one of the gas phase species, will result in an increase in the mixed molecular weight, which therefore leads to a reduced pressure. This happens vice-versa if the mixed molecular weight is reduced.

It was found that the molecular weights of tar and non-condensable gases have an influence on the internal pressure prediction, but the influence is less significant than the influence of char permeabilities. Only in case of assuming pure methane, and the corresponding molecular weight, a significant influence on internal pressure prediction was found. However, since devolatilization will never result in pure methane representing the permanent gases, assuming such a low molecular weight is unphysical and therefore, such a significant influence of molecular weights on internal pressure predictions will not be seen in realistic models.

4 RECOMMENDATIONS

A 1D mesh-based devolatilization model was developed with the main objective of investigating internal pressure generation during thermochemical degradation of a dry cylindrical wood log. It has been shown that the char permeability and the molecular weights of tar and non-condensable gases influence the internal pressure predictions and using wrong values will therefore cause significant errors. Consequently, future research is encouraged to focus on two main aspects to confront these uncertainties in current models:

1. Gas phase analysis has to be enhanced such that detailed knowledge of gas species in the gas phase is obtained resulting in more accurate molecular weight assumptions for models.
2. It is of interest to experimentally determine char permeabilities and establish a database for char permeabilities of a range of chars derived

from different wood species. It is assumed that hereby more accurate char permeabilities can be assumed in a model and one of the main uncertainties of current thermochemical degradation models can be eliminated.

In addition, extending the investigation of permeability effects to a 2D model should be a focus of future work. Hereby one will also be able to investigate the influence of anisotropy on internal pressure predictions.

5 REFERENCES

- [1] K. Kwiatkowski, K. Bajer, A. Celińska, M. Dudyński, J. Korotko, and M. Sosnowska, "Pyrolysis and gasification of a thermally thick wood particle – Effect of fragmentation," *Fuel*, vol. 132, pp. 125–134, Sep. 2014.
- [2] U. Sand, J. Sandberg, J. Larfeldt, and R. B. Fdhila, "Numerical prediction of the transport and pyrolysis in the interior and surrounding of dry and wet wood log," *Appl. Energy*, vol. 85, no. 12, pp. 1208–1224, 2008.
- [3] J. Larfeldt, B. Leckner, and M. C. Melaaen, "Modelling and measurements of the pyrolysis of large wood particles," *Fuel*, vol. 79, no. 13, pp. 1637–1643, 2000.
- [4] M. J. Hagge and K. M. Bryden, "Modeling the impact of shrinkage on the pyrolysis of dry biomass," *Chem. Eng. Sci.*, vol. 57, no. 14, pp. 2811–2823, 2002.
- [5] K. M. Bryden and M. J. Hagge, "Modeling the combined impact of moisture and char shrinkage on the pyrolysis of a biomass particle," *Fuel*, vol. 82, no. 13, pp. 1633–1644, 2003.
- [6] A. K. Biswas and K. Umeki, "Simplification of devolatilization models for thermally-thick particles: Differences between wood logs and pellets," *Chem. Eng. J.*, vol. 274, pp. 181–191, 2015.
- [7] A. Galgano and C. Di Blasi, "Coupling a CFD code with a solid-phase combustion model," *Prog. Comput. Fluid Dyn.*, vol. 6, pp. 287–302, 2006.
- [8] W. C. Park, A. Atreya, and H. R. Baum, "Experimental and theoretical investigation of heat and mass transfer processes during wood pyrolysis," *Combust. Flame*, vol. 157, no. 3, pp. 481–494, 2010.
- [9] H. Fatehi and X. S. Bai, "A Comprehensive Mathematical Model for Biomass Combustion," *Combust. Sci. Technol.*, vol. 186, no. 4–5, pp. 574–593, 2014.
- [10] H. Lu, W. Robert, G. Peirce, B. Ripa, and L. L. Baxter, "Comprehensive Study of Biomass Particle Combustion," *Energy & Fuels*, vol. 22, no. 4, pp. 2826–2839, 2008.
- [11] M. G. Grønli, "A theoretical and experimental study of thermal degradation of biomass," The Norwegian University of Science and Technology, 1996.
- [12] National Laboratory Lawrence Livermore, "SUNDIALS: SUite of Nonlinear and Differential/ALgebraic Equation Solvers - IDA," 2016. [Online]. Available: <http://computation.llnl.gov/projects/sundials/ida>. [Accessed: 07-Apr-2017].

- [13] K. M. Bryden, K. W. Ragland, and C. J. Rutland, "Modeling thermally thick pyrolysis of wood," *Biomass and Bioenergy*, vol. 22, no. 1, pp. 41–53, Jan. 2002.
- [14] D. Neves, H. Thunman, A. Matos, L. Tarelho, and A. Gómez-Barea, "Characterization and prediction of biomass pyrolysis products," *Prog. Energy Combust. Sci.*, vol. 37, no. 5, pp. 611–630, 2011.

6 ACKNOWLEDGEMENTS

This work has been done within the WoodCFD (243752/E20) project, which is funded by: Dovre AS, Norsk Kleber AS, Jøtulgruppen and Morsø AS together with the Research Council of Norway through the ENERGIX program.

7 LOGO SPACE

