SAND2022-9296C

Sandia National Laboratories

# Verification and Validation of 1D Peat Smoldering Model

Raquel S.P. Hakes[1,*], Matthew W. Kury[1], Rory M. Hadden[2], Sara S. McAllister[3], Sarah N. Scott[1]

[1] Sandia National Laboratories, Livermore, CA, USA, *Email: rshakes@sandia.gov

[2] School of Engineering, University of Edinburgh, Edinburgh, UK

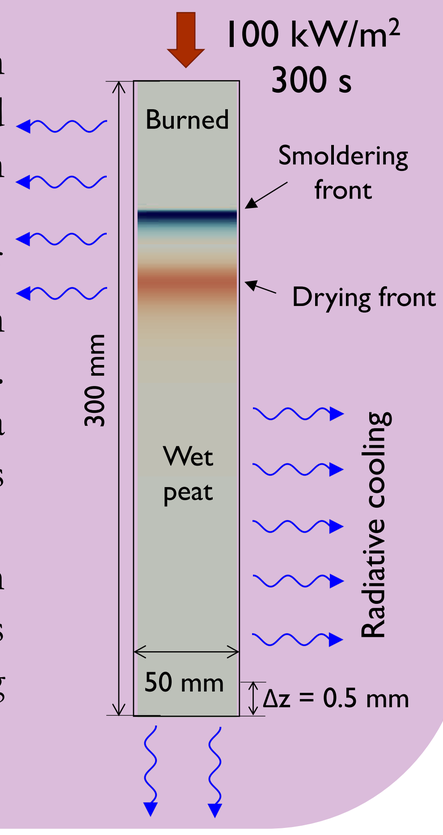
[3] United States Forest Service, Missoula, MT, USA

## BACKGROUND

Peat fires are a major contributor to greenhouse gas emissions, which are expected to increase with climate change. Estimates of the $CO_2$ released by peat fires contain large uncertainties, driven by **overwhelming uncertainty** in the mass of peat consumed in these fires. This project aims to expand current peat smoldering models to 2D and 3D. Here, we show **0D verification** against existing literature and **1D validation** against experiments.

## COMPUTATIONAL MODEL

- The model is based on an existing 1D peat smoldering model [1-3]. We recreate this model in Gpyro, in which it was developed, and implement it in Sierra Thermal/Fluids: Aria.
- We consider the **0D case** to verify model implementation with TGA at 20 K/min, presented in [1].
- We consider the **quasi-1D case** for an initial validation against lateral and downward spread experiments, shown schematically.
- The model solves conservation of mass, species, and energy equations in both the condensed and gas phases. We use Darcy's law for flow through a porous media to calculate the gas phase velocity.
- A 5-step reaction mechanism developed in [2] for Scottish peat is used to describe the peat smoldering process.




## 0D VERIFICATION

We conduct a verification of the 0D Aria model against Gpyro and literature results [1] for TGA conducted on Scottish peat (Figure 1).

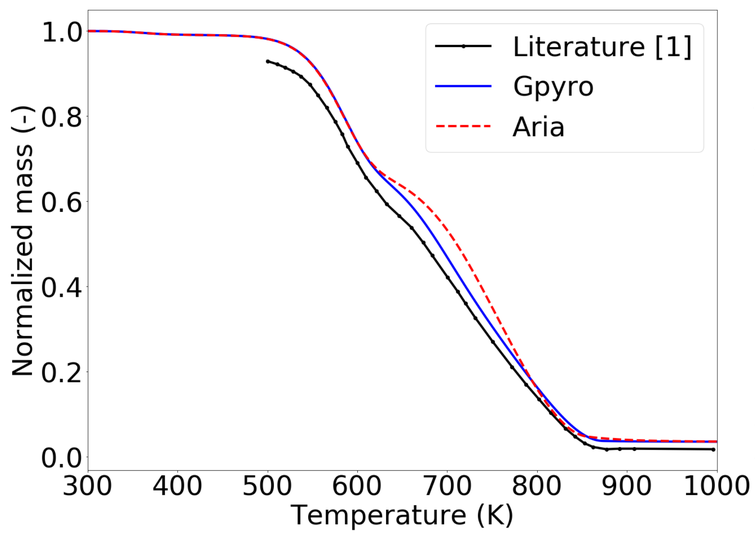



Figure 1: Temperature vs mass loss shows good comparison between literature model and our Gpyro and Aria implementations.

Our Aria and Gpyro show good agreement with the simulated literature results, with some differences in the 650-800 K range where oxidation occurs. To explore potential causes of these differences, bulk densities of each solid species were compared, as shown in Figure 2. Agreement is quite good in the pyrolysis region. Tests exhibit differences in the amount of char produced (by pyrolysis vs oxidation) at higher temperatures.

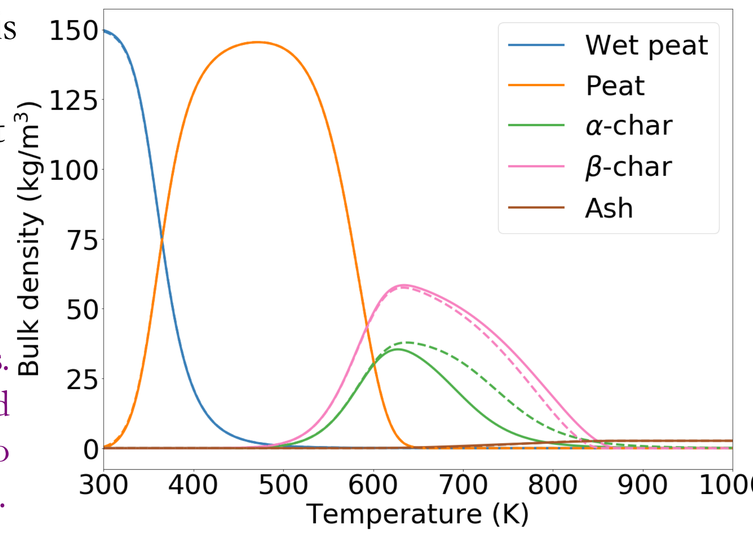
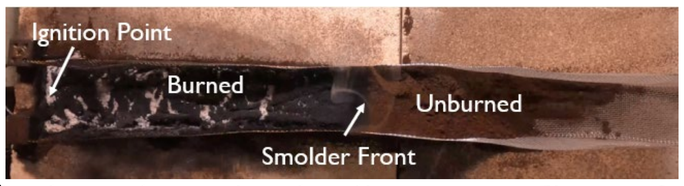



Figure 2: Temperature vs. bulk density for all solid species comparing Gpyro (dashes) and Aria (solid line).

## EXPERIMENTAL VALIDATION

Initial validation experiments used commercially harvested sphagnum moss peat at higher bulk densities (300-400 kg/m$^3$) than those in the literature. Figure 2 shows a comparison between measured and simulated mass loss. Although there is qualitative agreement in trends and the total mass lost, experiments exhibit much higher mass loss rates than simulations. Differences may be due to the higher density of peat used here compared to that used in validation experiments in the literature [1-3].



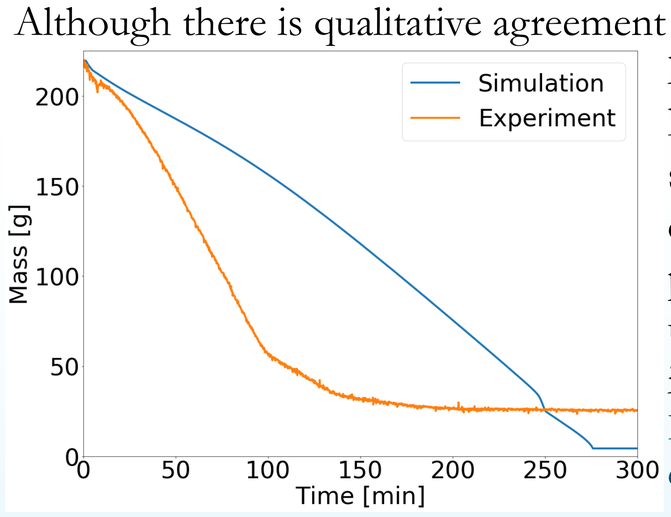




Figure 3: Mass loss over time for experiments and simulations.

## FUTURE WORK

- 0D verification shows good agreement with literature. Future work will look at causes of differences in oxidizing reactions.
- Understanding the 0D model will be leveraged for 1D verification. Expanding peat models to higher dimensions will decrease uncertainty in mass consumed and emissions.
- Bulk density of the peat has a key effect on material properties and kinetics, which will be explored in future work.

**Acknowledgements** Funding for the modeling portion of this work was provided by the Sandia LDRD program. The authors would like to acknowledge Hamish Allan and Da Ke for conducting experiments, and Sagar Gautam, Mark Lara, and Umakant Mishra for discussions.

## REFERENCES

[1] X Huang and G Rein, *Combust Flame* 161 (2014) 1633-1644.
[2] X Huang et al., *Proc Comb Inst* 35 (2015) 2673-2681.
[3] X Huang and G Rein, *Int J Wildland Fire* 24 (2015) 798-808.

U.S. DEPARTMENT OF ENERGY
National Nuclear Security Administration

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
SAND No. _____
Funding for the modeling portion of this work was provided by the Sandia LDRD program.

Sandia National Laboratories