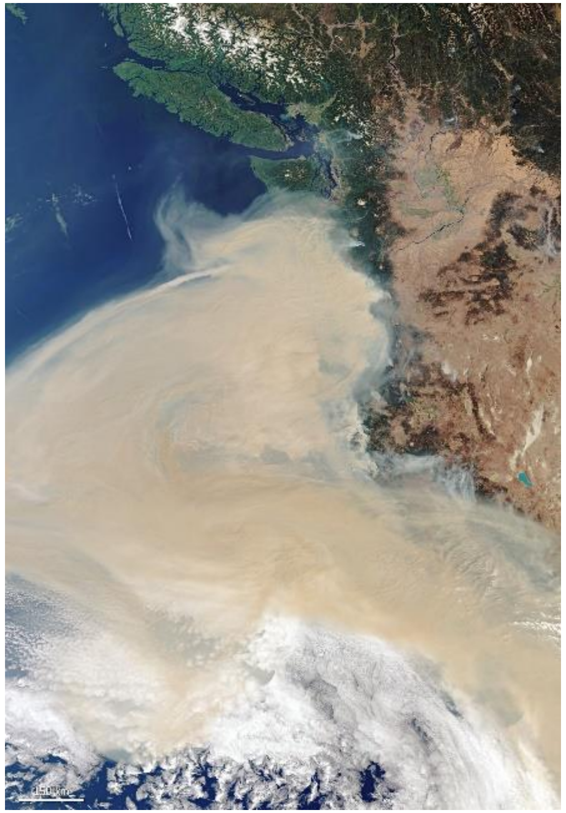
Challenges and opportunities in advancing understanding of soot evolution in fires

Progress in soot modelling and experiments

LLNL-PRES-868608 This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and was supported by the LLNL-LDRD Program under Project No. 23-LW-007.

Wildfires affecting urban/wildland boundaries are becoming a common reality



- Wildfires represent an important environmental and health hazard.
- Understanding the fire rate of spread is important to potentially provide decision-support for wildfire operations, whereas **predicting smoke emissions would help to assess the health effects** and implement related strategies to prevent exposure.
- **Predicting the fire behavior** and its dynamics **along with its emissions** is still an **open challenge**.
- Large-scale wildfire models, such as the coupled fire-weather application WRF-SFIRE-CHEM[1-3], rely on that are **poorly understood** and only **fuel consumption rates and emission factors empirically quantified.**

[1]Kochanski A. K., Jenkins M.A., Yedinak K., Mandel J., Beezley J, and Lamb B. 2015. Toward an integrated system for fire, smoke and air quality simulations, International Journal of Wildland Fire.
[2]Kochanski, A. K., Mallia, D. V., Fearon, M. G., Mandel, J., Souri, A. H., & Brown, T. (2019). Modeling Wildfire Smoke Feedback Mechanisms Using a Coupled Fire-Atmosphere Model With a Radiatively Active Aerosol Scheme. Journal of Geophysical Research: Atmospheres, 124(16), 9099–9116.
[3]Lassman, W., Mirocha, J.D., Arthur, R.S., Kochanski, A.K., Farguell Caus, A., Bagley, A.M, Sospedra, M.C., Dabdub, D., Barbato, M., Using satellite-derived fire arrival times for coupled wildfire-air quality simulations at regional scales of the 2020 California wildfire season. Under Review in JGR-Atmospheres, May 2022.

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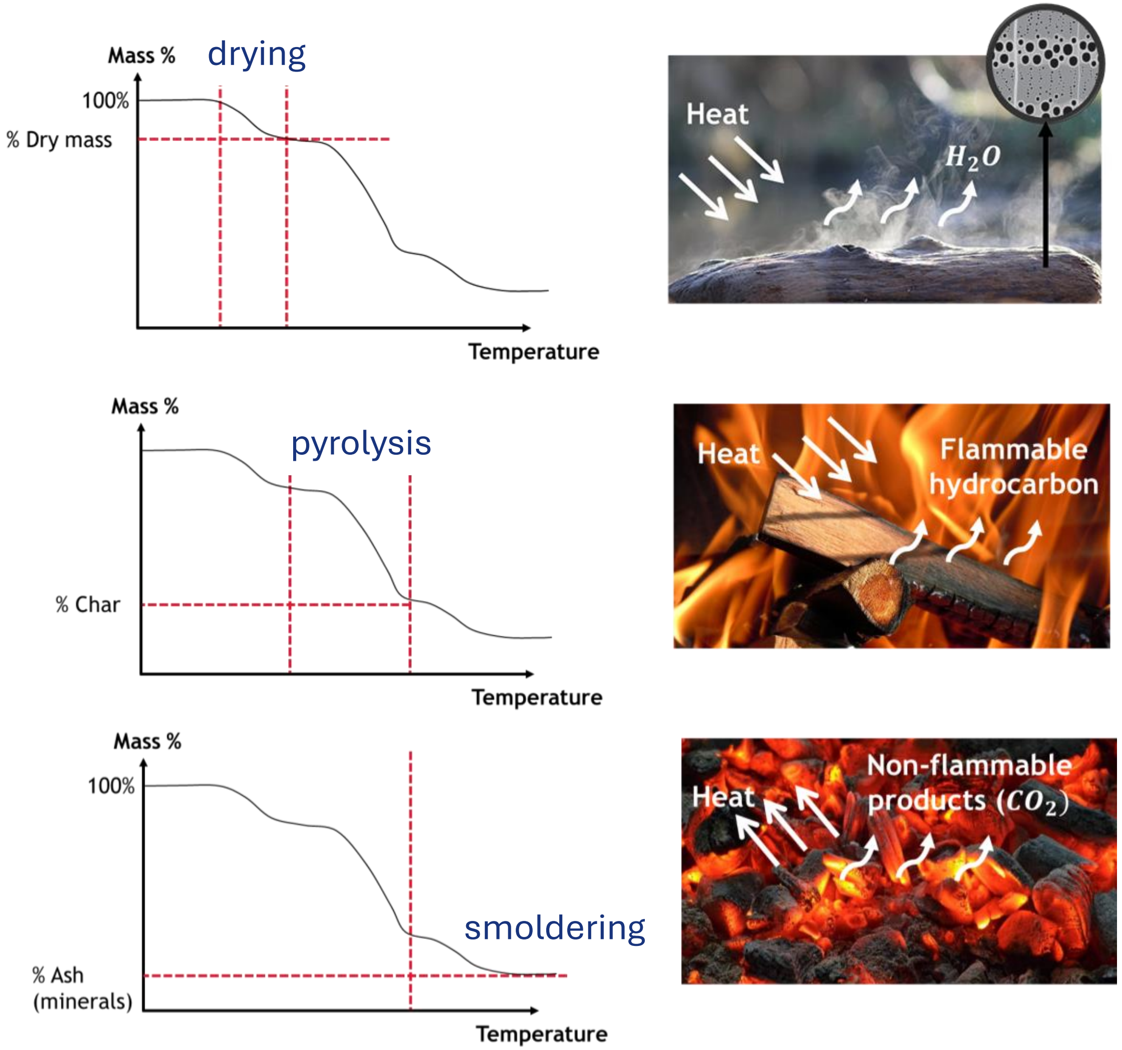
Flame Spread in Wildland Fires

- Flame spread in wildland fires is a repeated process of:
  1) heating of the solid biomass fuel
  2) release of gaseous volatiles (**drying and pyrolysis**)
  3) combustion of the gaseous volatiles with ambient oxygen (**flaming**)
  4) Combustion of the residual char with ambient oxygen (**char oxidation or smoldering**)



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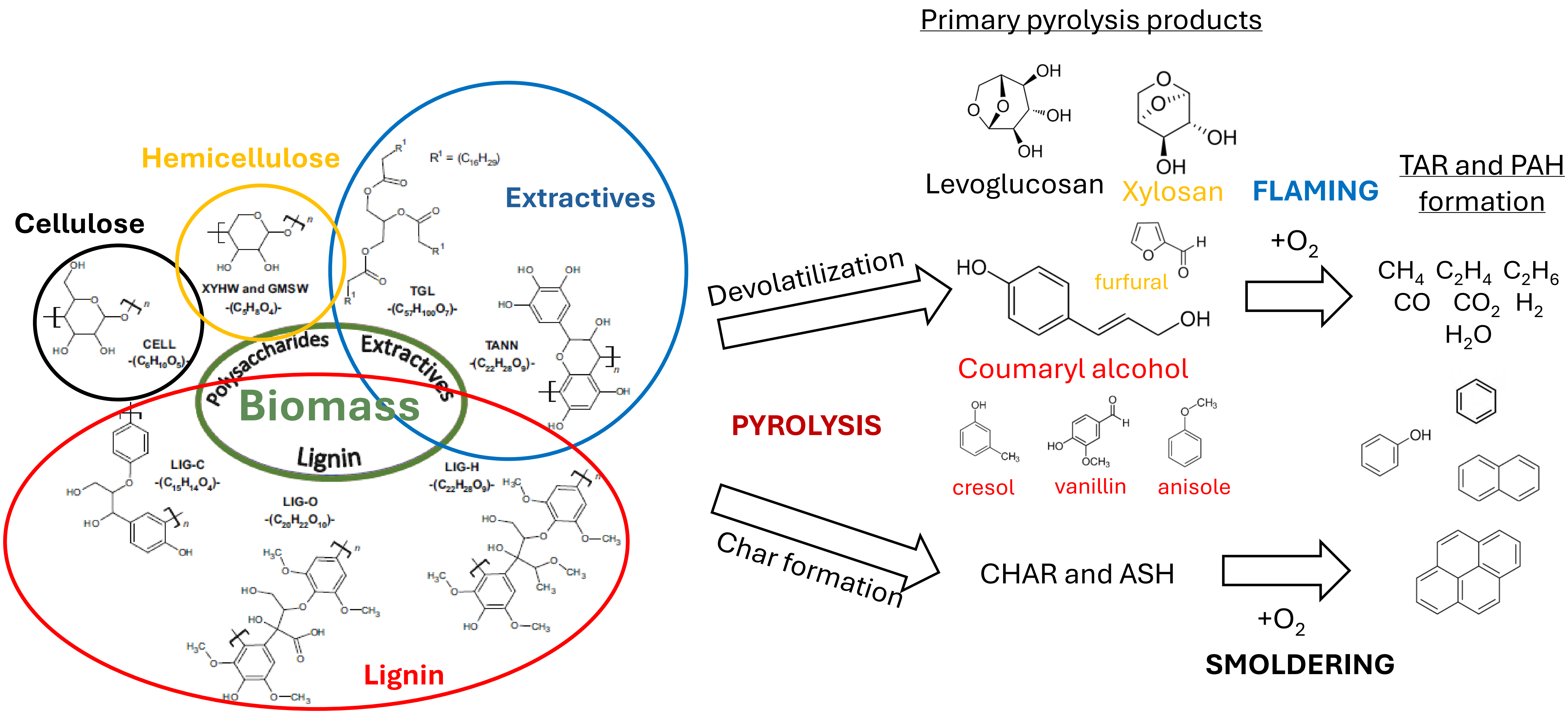
Emissions in Wildland fires



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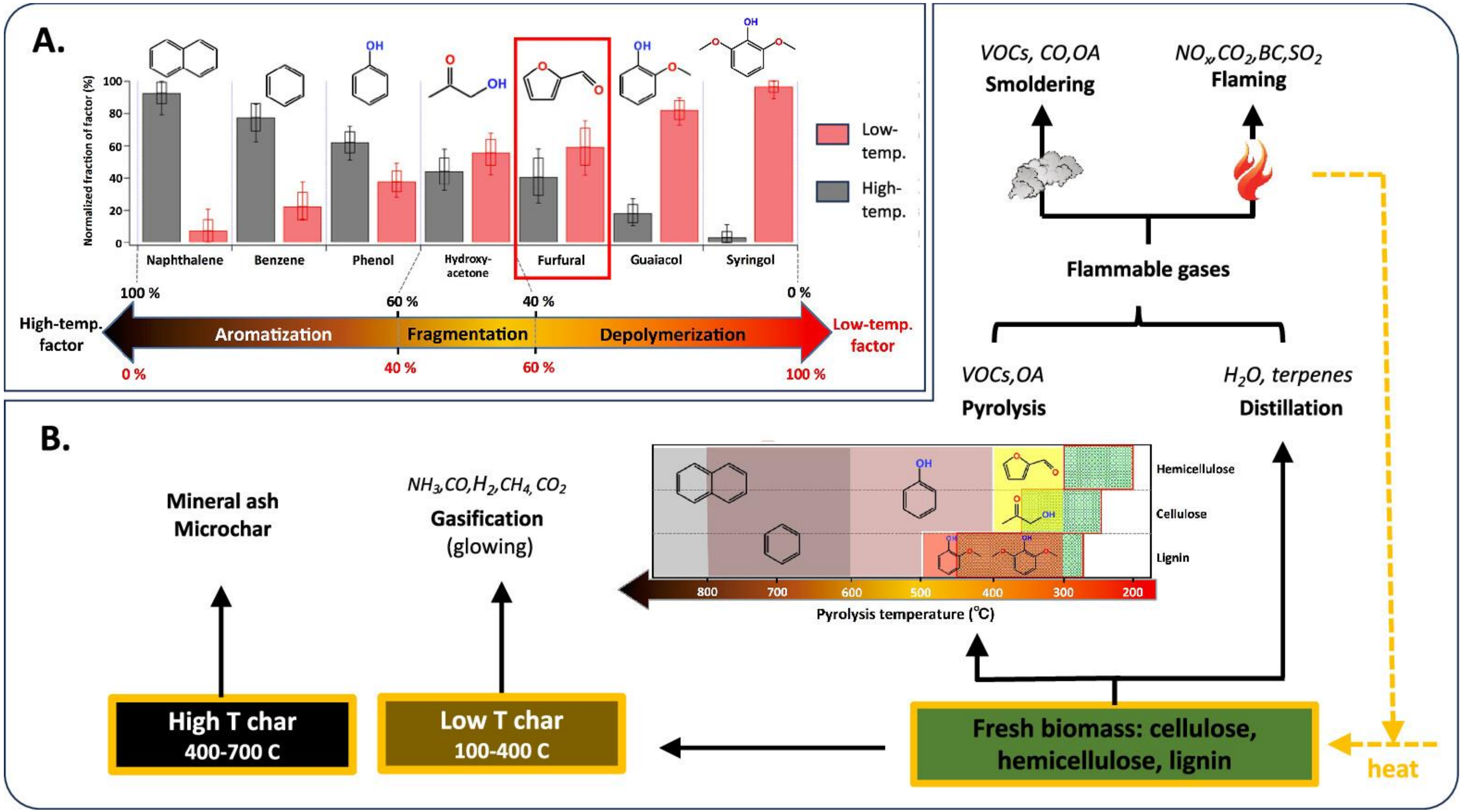
Emissions from fires – biomass burning VOCs



Romanias, M.N., Coggon, M.M., Al Ali, F., Burkholder, J.B., Dagaut, P., Decker, Z., Warneke, C., Stockwell, C.E., Roberts, J.M., Tomas, A. and Houzel, N., 2024. Emissions and atmospheric chemistry of furanoids from biomass burning: Insights from laboratory to atmospheric observations. *ACS Earth and Space Chemistry*, *8*(5), pp.857-899.

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Emission factors

In large-scale wildfire models, the emissions are estimated using the following equation to estimate **emission fluxes**:

$$E_i = A(x,t) \times B(x) \times FB \times ef_i$$

Emission factor of species i (mass of i emitted (g) / mass of biomass burned(kg))

- E_i: emission of species i (mass of i emitted)
- $A(x,t)$: area burned at time t and location x
- $B(x)$: biomass loading at location x
- FB: fraction of that biomass that is burned in the fire

Emission factors from observations:
CO_2: 500- 1700 g/kg
CO: 60- 120 g/kg
CH_4: 2-6 g/kg
Non-methane organic gases (or VOC): 28-55 g/kg
PM2.5: 7-20 g/kg
PM10: 7-20 g/kg

Table 4: Emission factors (g kg^{-1}) for FINNv2.5.

Chemical Species	Generic Vegetation Index and Type						
	1	2	3	4	5	6	9
	Savanna Grasslands[1]	Woody Savanna/ Shrubs	Tropical Forest	Temperate Forest[2]	Boreal[3]	Temperate Evergreen Forest[2]	Crops[4]
Carbon Dioxide (CO2)	1686	1681	1643	1510	1565	1623	1444
Carbon Monoxide (CO)	63	67	93	122	111	112	91
Methane (CH4)	2	3	5.1	5.61	6	3.4	5.82
Non-methane Organic Gases (NMOG)[5]	28.2	24.8	51.9	56	48.5	49.3	51.4
Hydrogen (H2)	1.7	0.97	3.4	2.03	2.3	2	2.59
Nitrogen Oxides (NOXasNO)	3.9	3.65	2.6	1.04	0.95	1.96	2.43
Sulfur Dioxide (SO2)	0.9	0.68	0.4	1.1	1	1.1	0.4
Particulate Matter with Diameters less than 2.5 µm (PM25)	7.17	7.1	9.9	15	18.4	17.9	6.43
Total Particulate Matter (TPM)	8.3	15.4	18.5	18	18.4	18	13
Total Particulate Carbon (TPC)	3	7.1	5.2	9.7	8.3	9.7	4
Particulate Organic Carbon (OC)	2.6	3.7	4.7	7.6	7.8	7.6	2.66
Particulate Black Carbon (BC)	0.37	1.31	0.52	0.56	0.2	0.56	0.51
Ammonia (NH3)	0.56	1.2	1.3	2.47	1.8	1.17	2.12
Nitrogen Oxide (NO)	2.16	0.77	0.9	0.95	0.83	0.95	1.18
Nitrogen Dioxide (NO2)	3.22	2.58	3.6	2.34	0.63	2.34	2.99
Non-methae Hydrocarbons (NMHC)	3.4	3.4	1.7	5.7	5.7	5.7	7
Particulate Matter with Diameters less than 10 µm (PM10)	7.2	11.4	18.5	16.97	18.4	18.4	7.02

Emission factors are mostly known in flaming conditions, while estimates of smoldering emission factors are still scares.

Wiedinmyer, C., Kimura, Y., McDonald-Buller, E. C., Emmons, L. K., Buchholz, R. R., Tang, W., Seto, K., Joseph, M. B., Barsanti, K. C., Carlton, A. G., and Yokelson, R.: The Fire Inventory from NCAR version 2.5: an updated global fire emissions model for climate and chemistry applications, *EGUsphere*, https://doi.org/10.5194/egusphere-2023-124, 2023.

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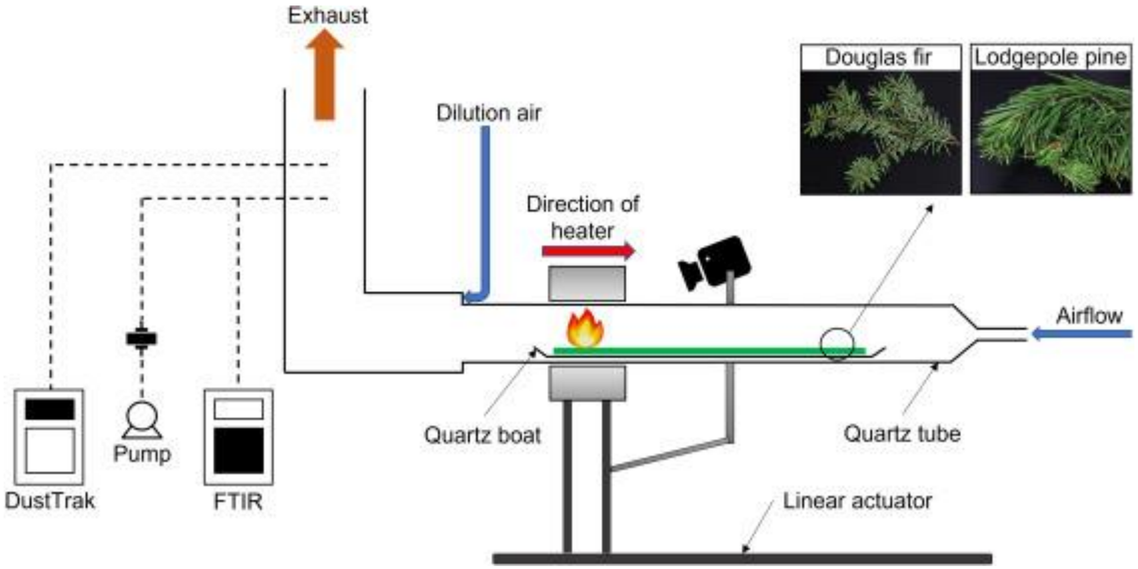
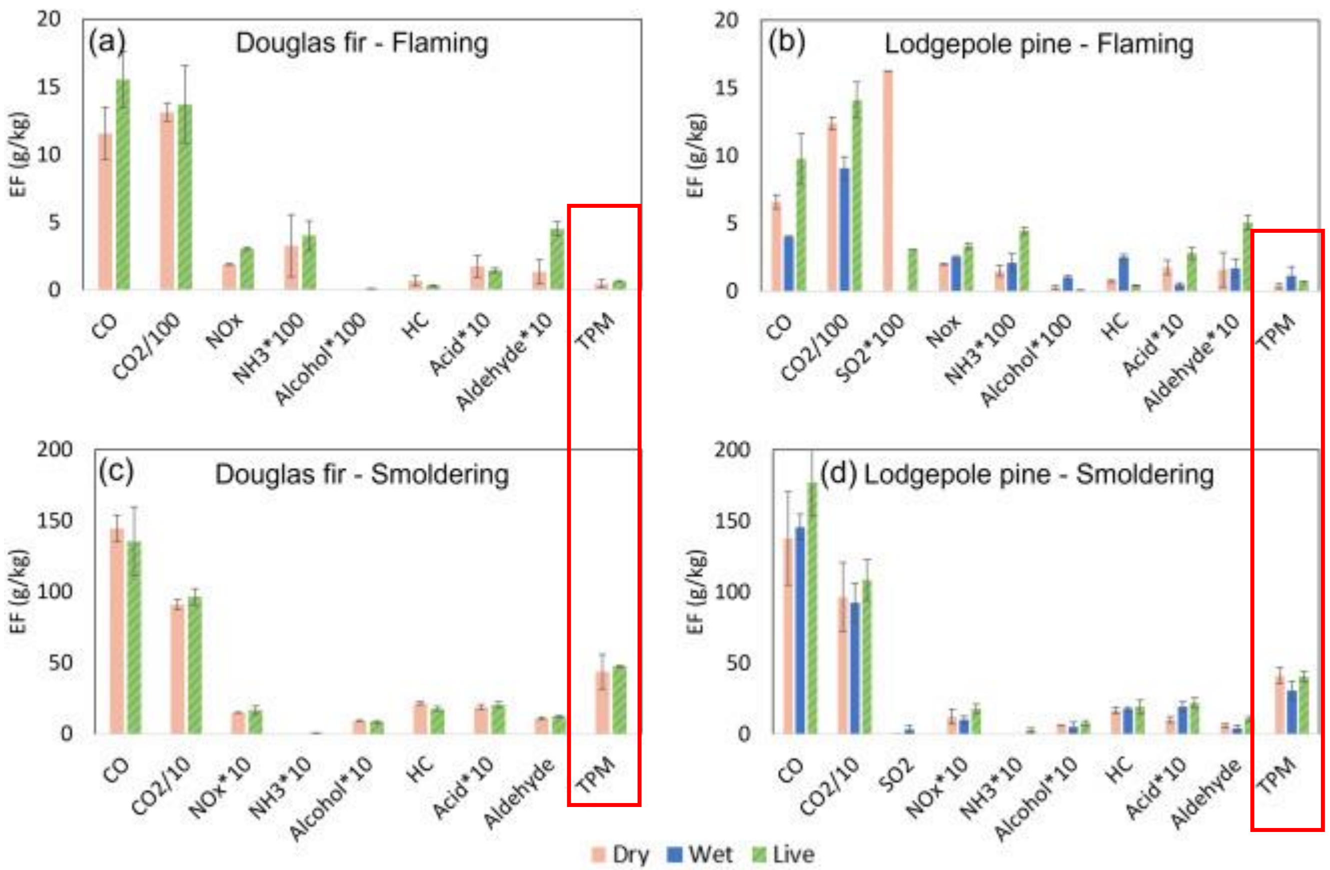
Progress in Experiments 1/2



Emission factors from flaming and smoldering wood combustion



Garg, P., Wang, S., Oakes, J.M., Bellini, C. and Gollner, M.J., 2024. Variations in gaseous and particulate emissions from flaming and smoldering combustion of Douglas fir and lodgepole pine under different fuel moisture conditions. *Combustion and Flame*, *263*, p.113386.

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Presentation: Monday, July 22
IJ05, Room White 2, 12.20 pm

Progress in Experiments 2/2

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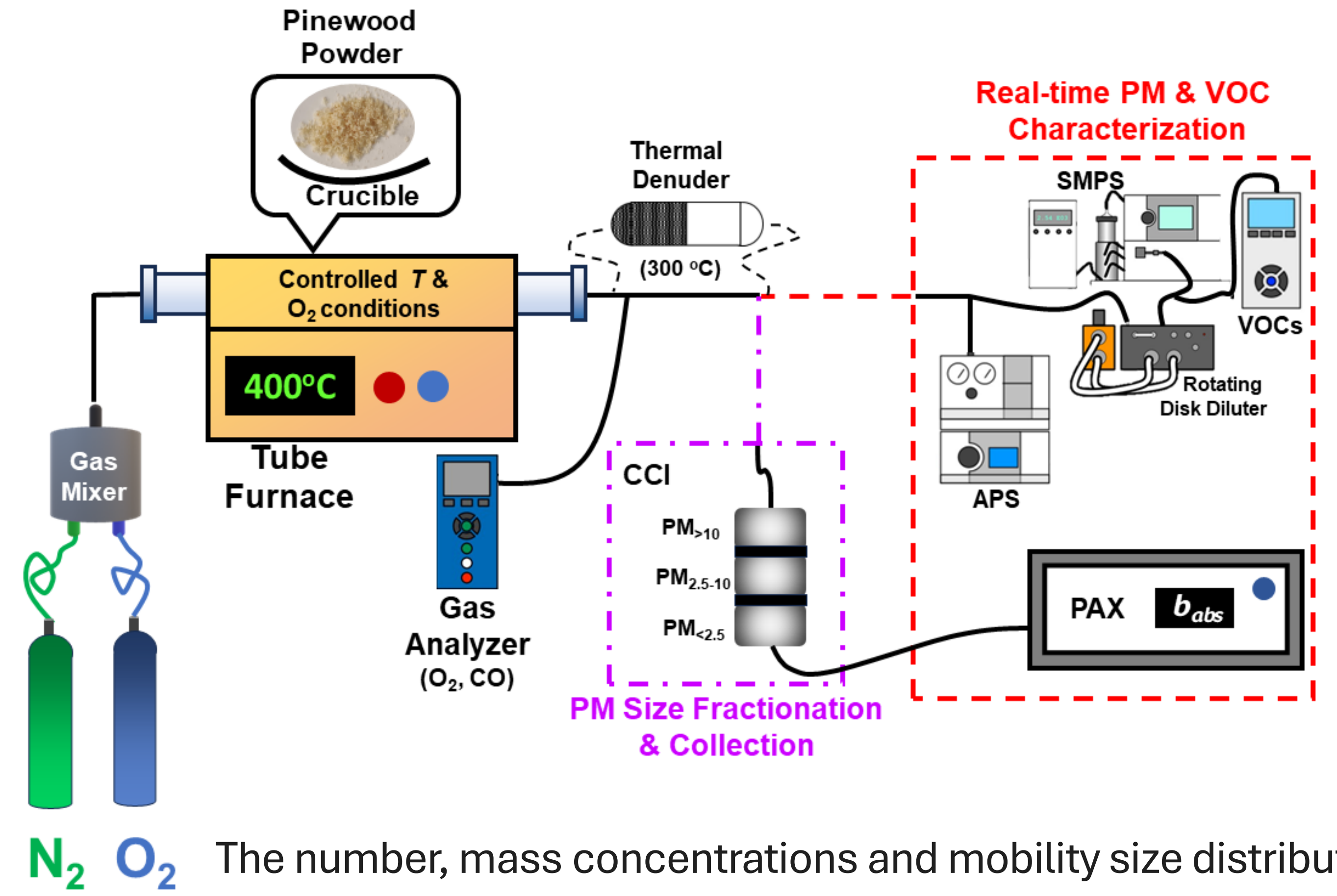

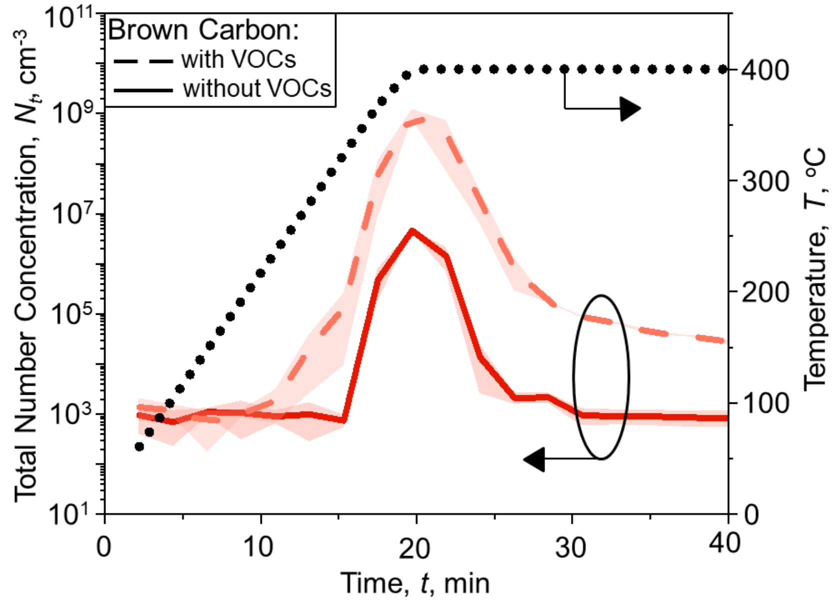

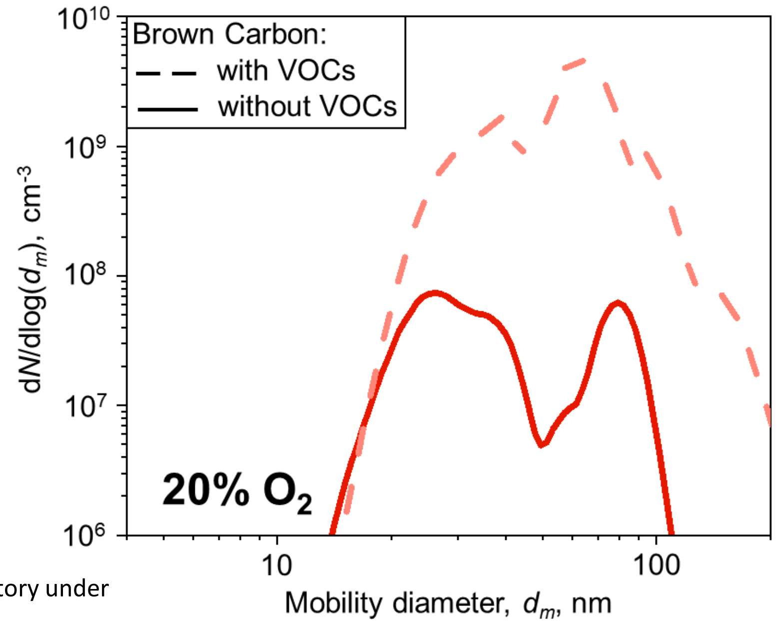

The number, mass concentrations and mobility size distributions of Brown Carbon particles with and without condensed VOCs are measured for [O2] = 0–20 vol%.

Moularas, C.; Demokritou, P.; Kelesidis, G.A. Proc Combust Inst (2024) 40, doi.org/10.1016/j.proci.2024.105513.

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Progress in Modeling 1/2

Laminar Smoke Point (LSP) soot modelling for fires

LSP is a <u>simplified soot model</u>:

- incorporates the main soot processes (nucleation, growth and oxidation)
- remains <u>computationally fast</u>
- <u>accounts for fuel effects</u>, using ethylene as a basis for initial calibration and linking it to the LSP height of the fuel

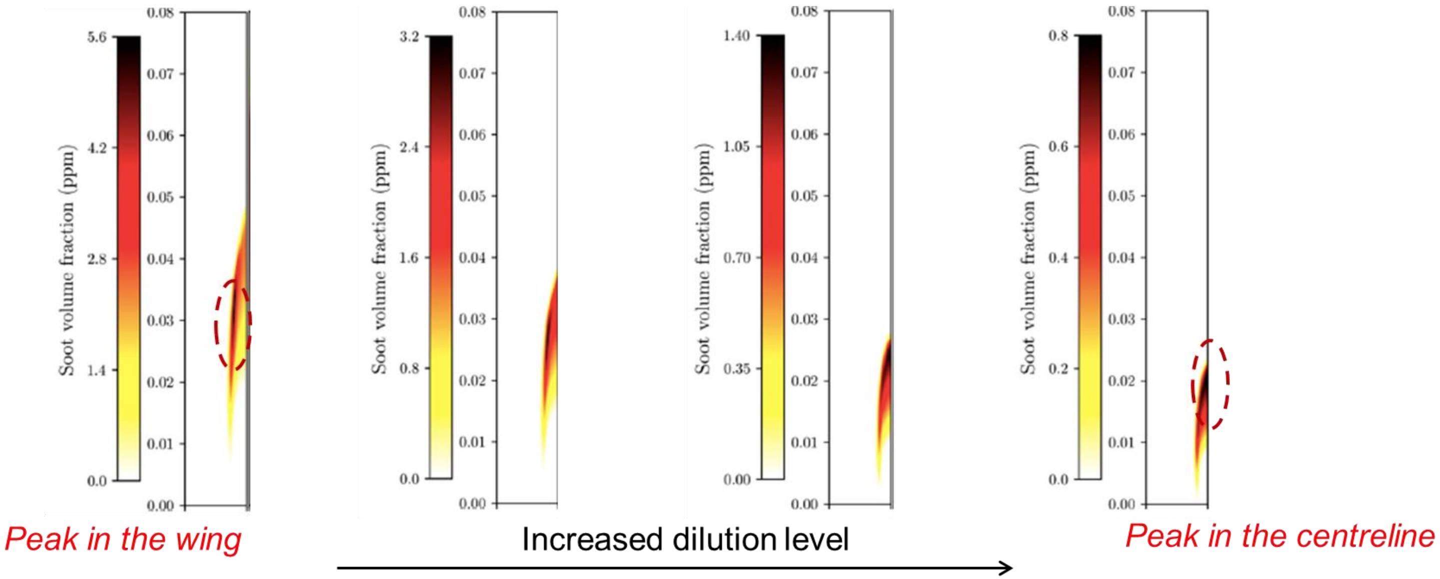
Validated over 16 laminar flames:

different fuels, different nitrogen dilution levels,
effect of reduced gravity

Perspectives

- Further model developments, e.g., polydispersity of soot particles
- Further validation: e.g., solid fuels (biomass)
- Future applications: enclosure fires, wildland fires, etc.

<u>Validation</u>: 'migration' of the peak soot volume fraction from the wings to the centreline with increasing N_2 dilution levels (based on experimental data of *Smooke et al.* (1999 – 2005)

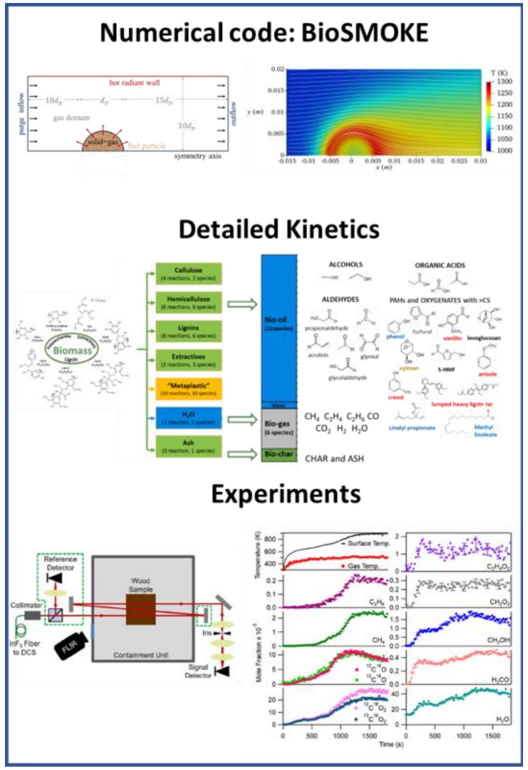


Shahrooz Motaghian & Tarek Beji (2024) A laminar smoke point-based soot model considering surface growth and soot reactions, *Combustion Theory and Modelling*, 28:2, 172-197, DOI: 10.1080/13647830.2023.2267526

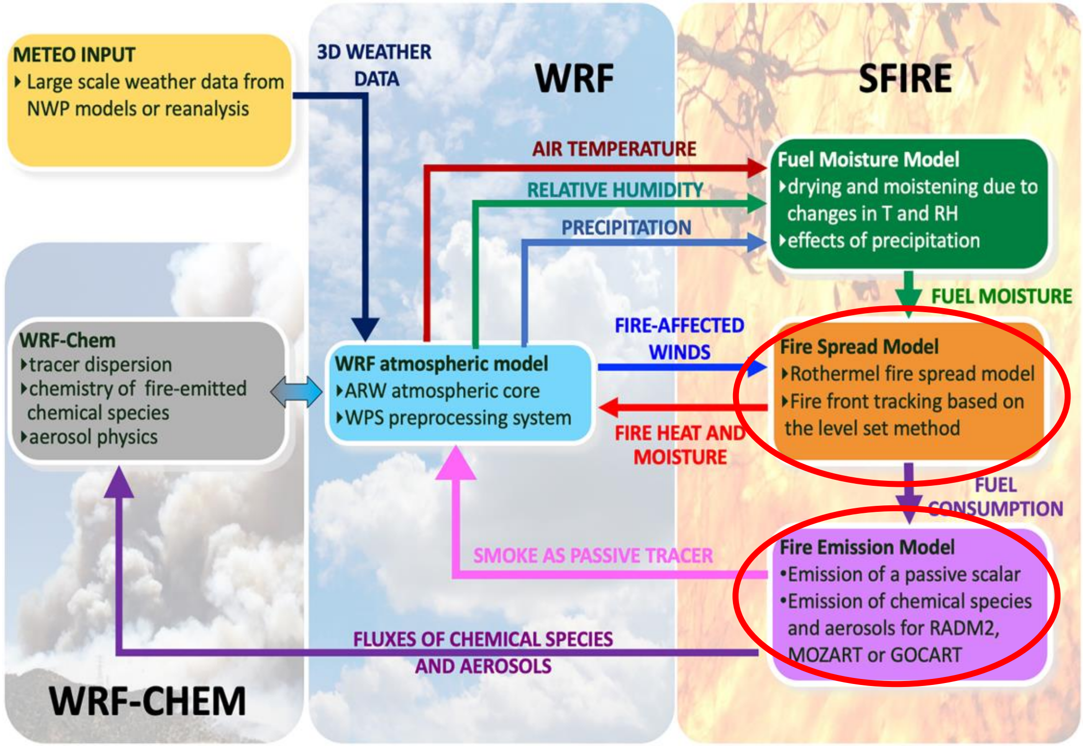
Progress in Modeling 2/2

WiPP: Monday, July 22
1P104

Integration of WRF-SFIRE-CHEM with BioSMOKE data as input



New algorithm



Input of WRF-SFIRE-CHEM	Current inputs	Future inputs
Fuel burning rates	Burnup model (Albini et al., 1995)	Multilayer model involving new parametrized fuel consumption that includes pyrolysis and smoldering
Emission factors	Static emission factors empirically estimated in flaming conditions	Dynamic profiles including smoldering emissions

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Thank you for the attention!
Questions?