SAND2014-4822C

Advances in Modeling LII from Carbonaceous Particles

Model development approach

Solve energy- and mass-balance equations

- Constrain calculations with as many known mechanisms as possible
- Constrain calculations with known parameters from non-LII data (if possible)

Compare results to LII measurements

- Use data from carefully controlled experiments
- Measure relevant parameters, e.g., ambient temperature, particle size
- Identify important discrepancies

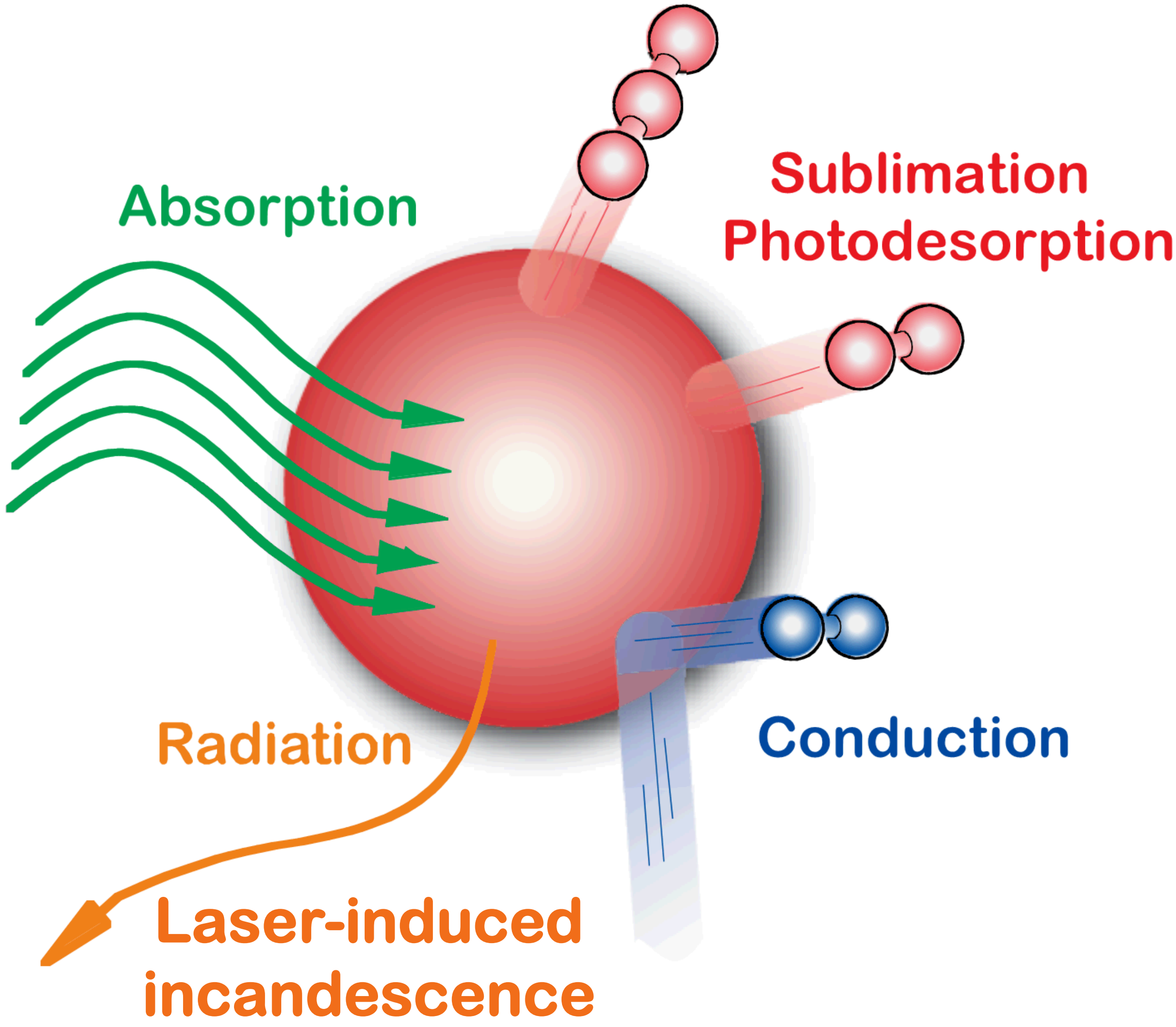
Improve model and repeat

- Target mechanisms likely responsible for discrepancies
- Broaden range of data for comparisons

Share model with community

- Improve interface and distribute
- Get feedback and improve model

The LII model: Version 3



The LII model: Version 3

Absorption, Radiation, Signal

- Depend on temperature, wavelength, soot maturity

Sublimation, Super-sublimation (photoexcitation)

- Include Kelvin effect
- Remove C_1, C_2, and C_3

Conduction

- Thermal accommodation coefficient depends on surface temperature, maturity
- Surface area depends on morphology
- Knudsen regime most of the time, otherwise, McCoy and Cha

Oxidation

- Influences surface maturity

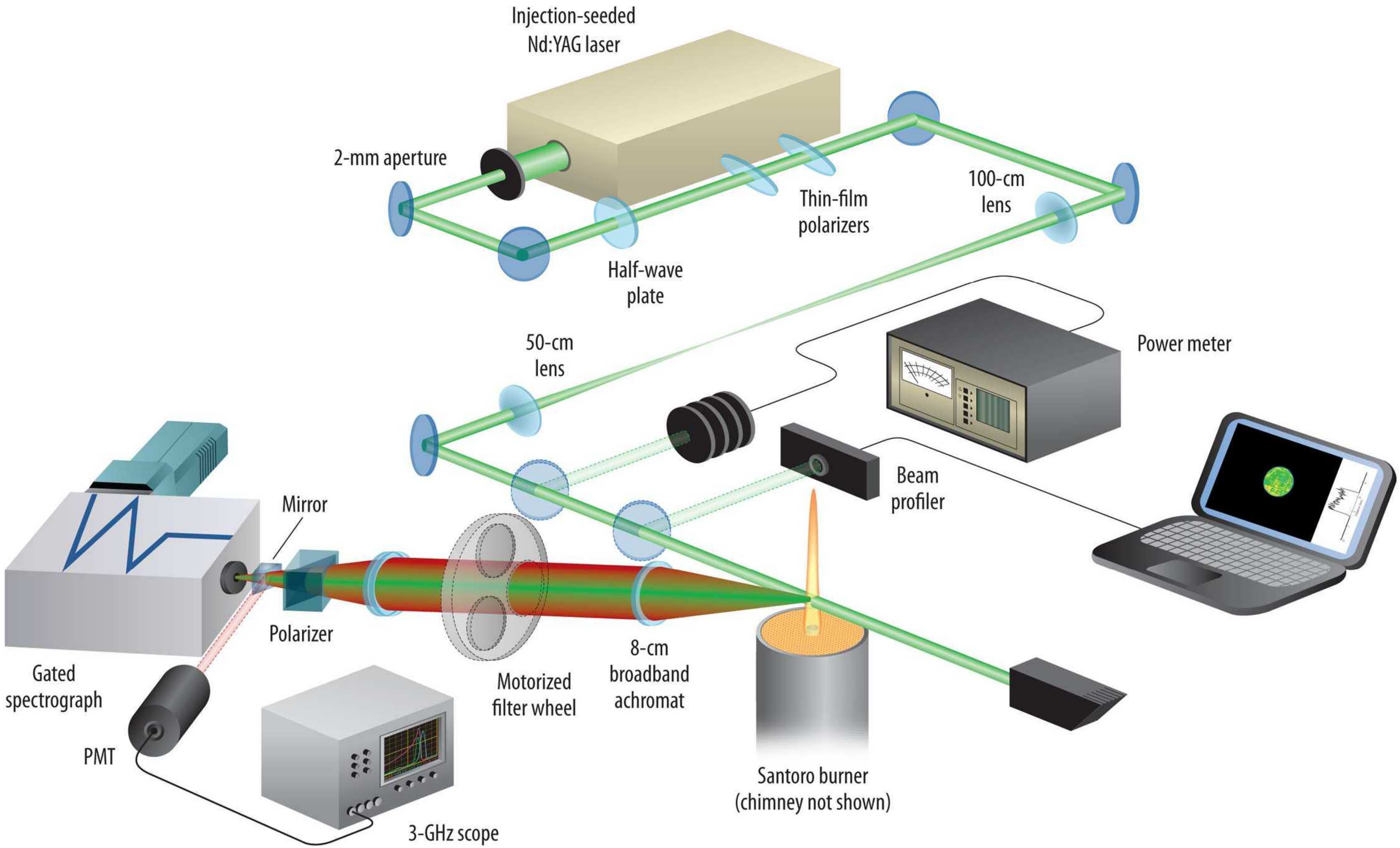
Annealing

- Surface annealing is separable from bulk annealing

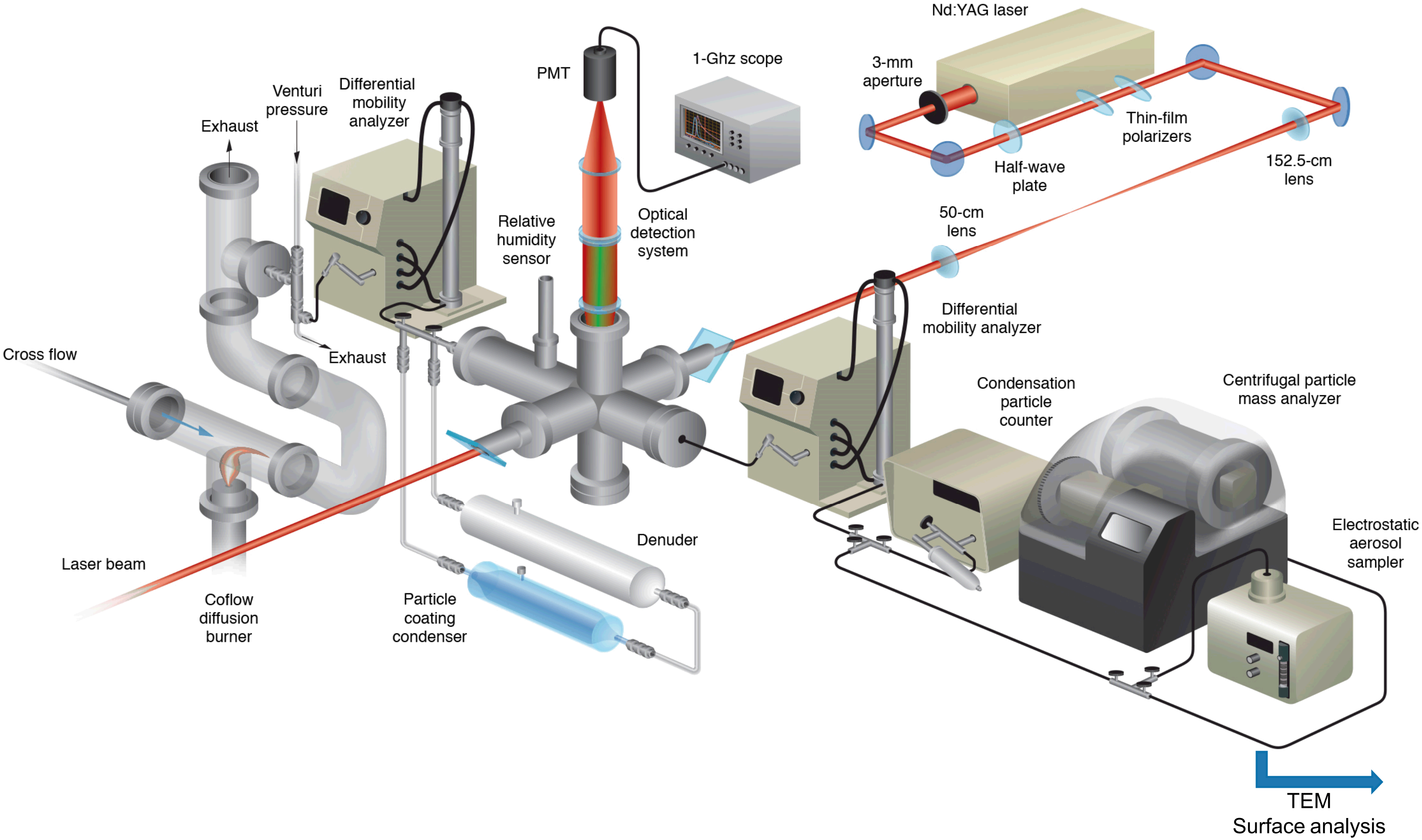
Other

- Thermionic emission
- Volatile coatings

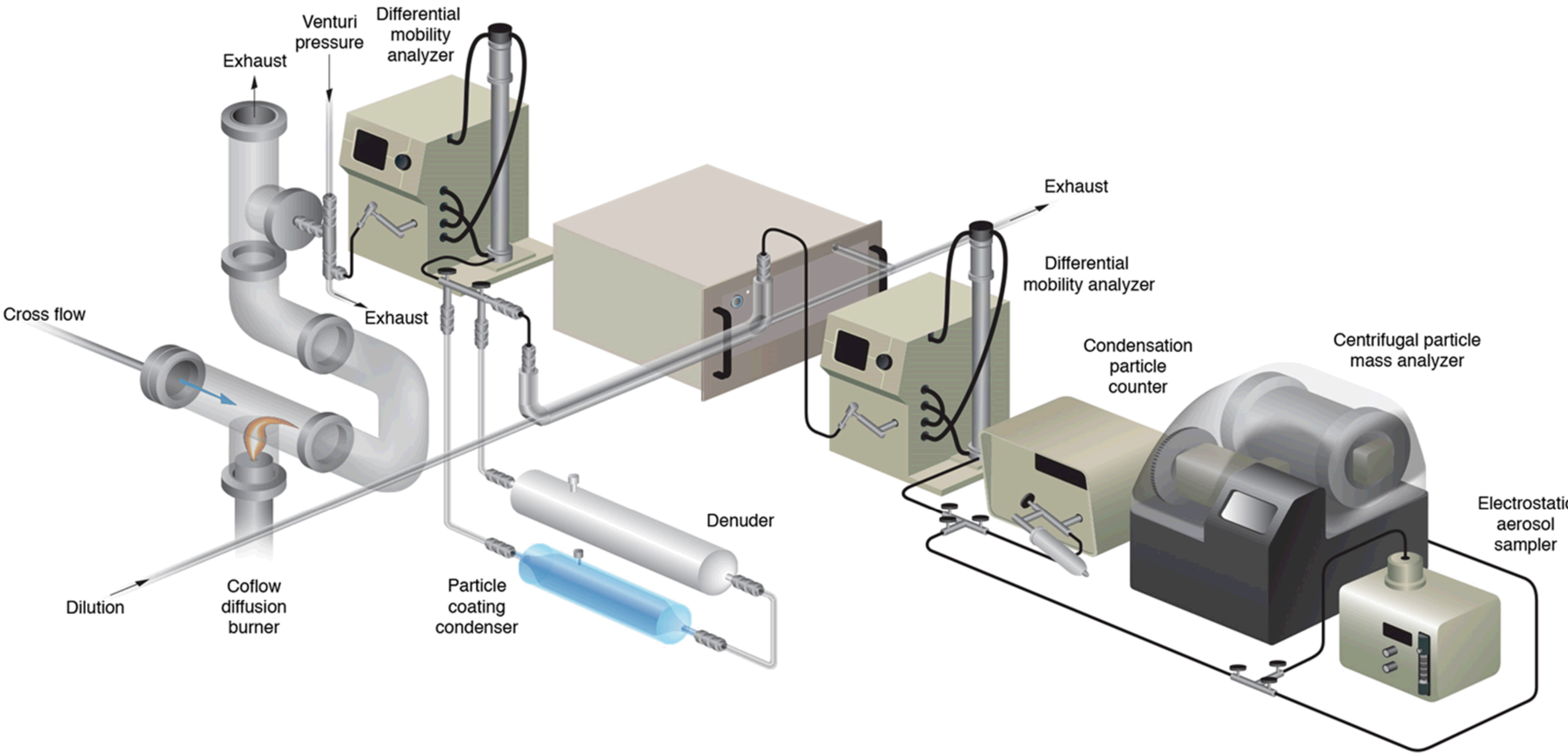
Validation data: Flame LII and Temperature



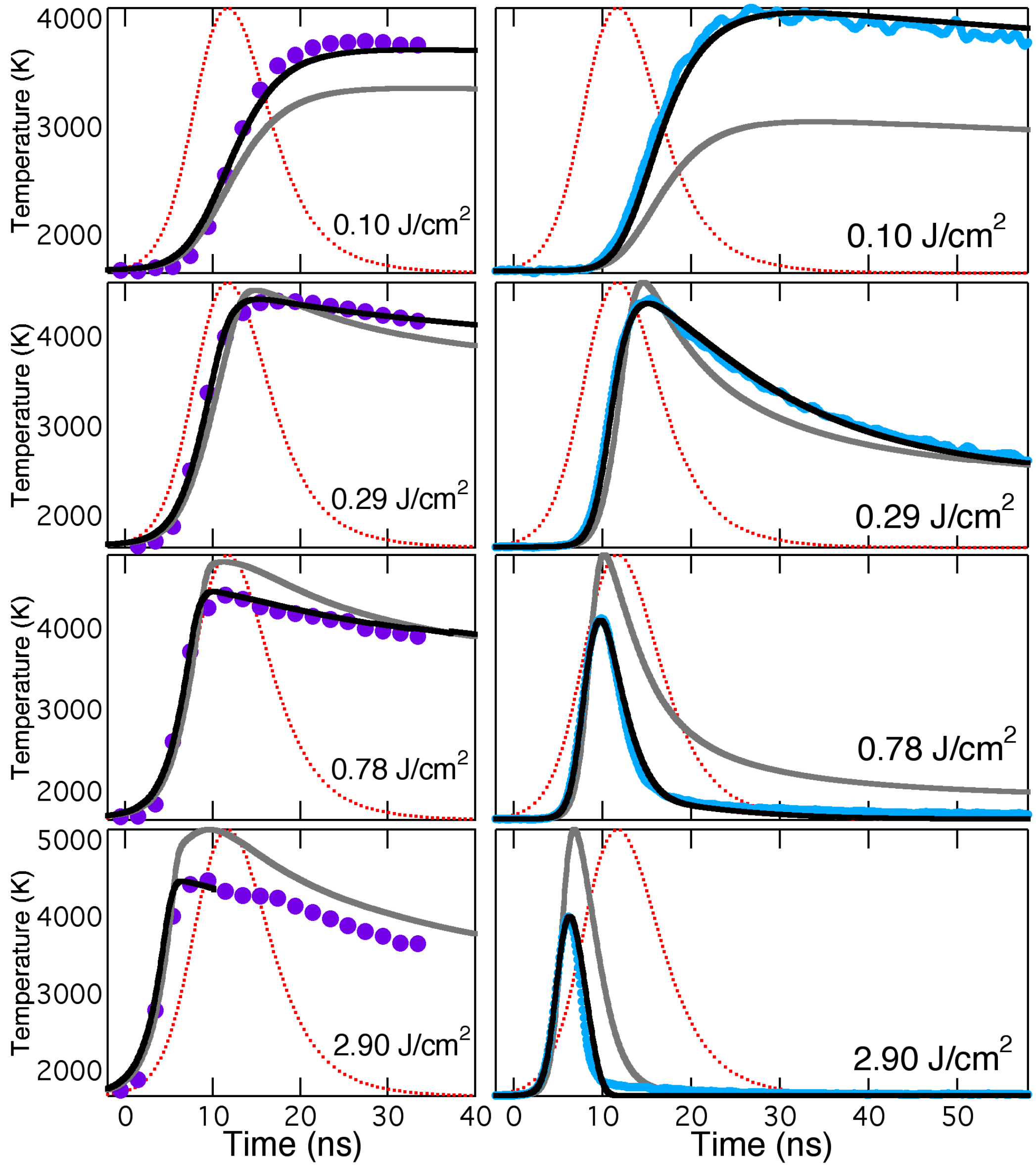
Validation data: Low temperature, coatings



Validation data: Long-pulse/CW LII

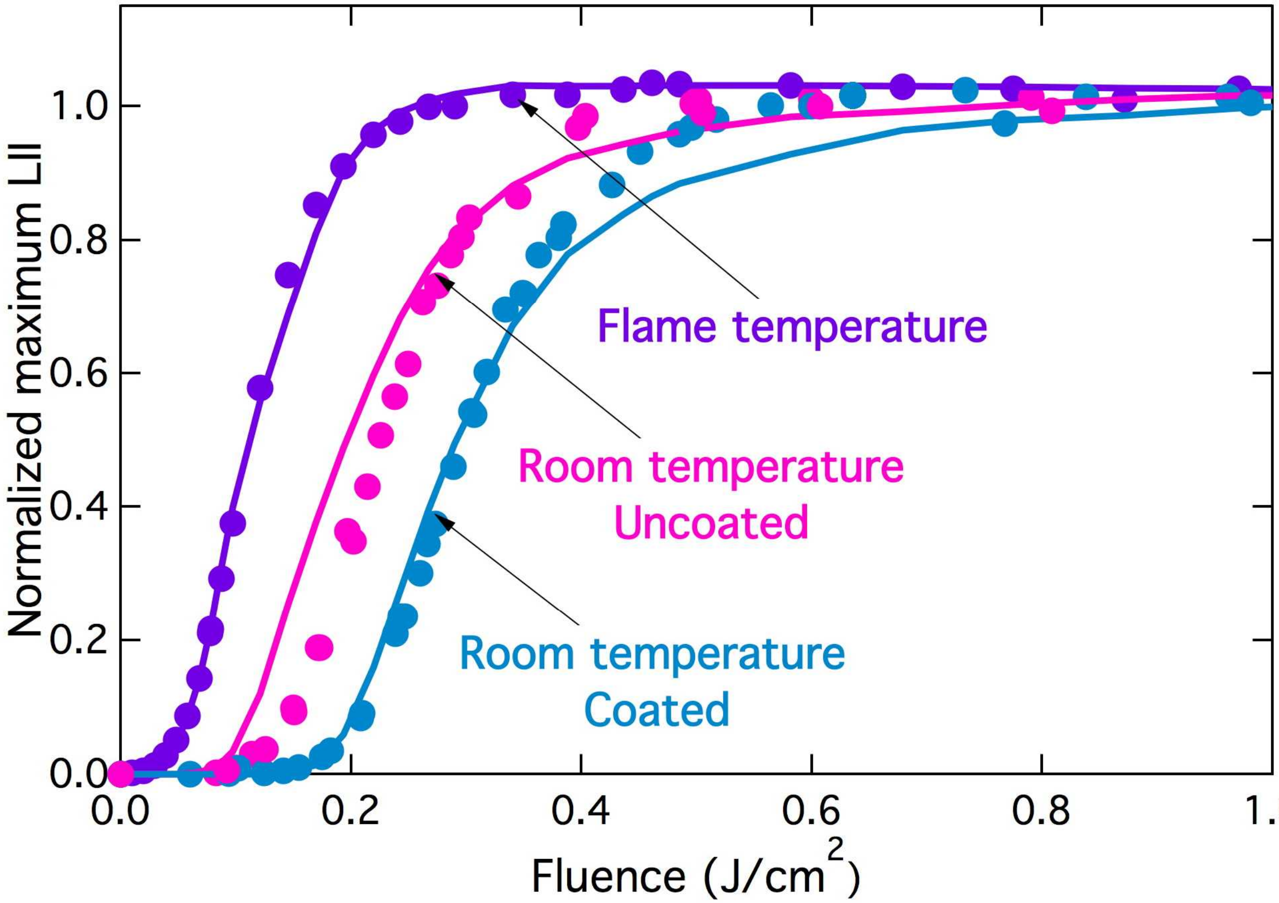


Laser-Induced Incandescence (LII)



Model Advances – Effects of Coatings

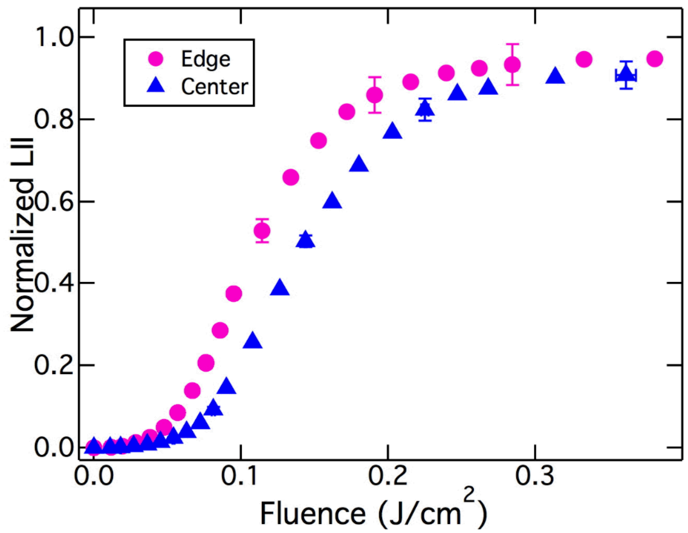
- Assuming 78% Oleic acid by mass

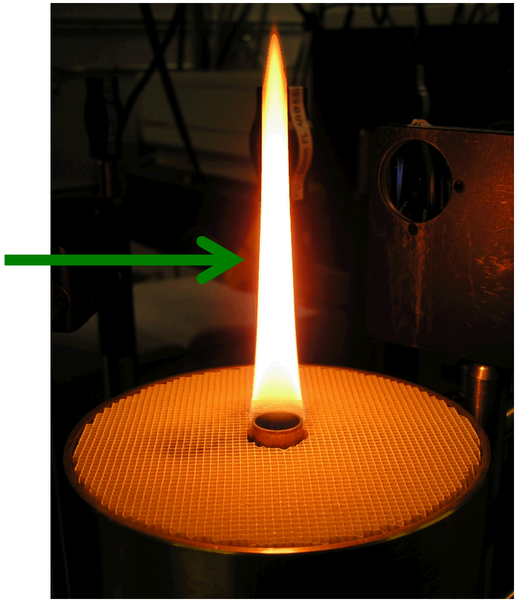


Effects of particle maturity on LII signal

Santoro co-flow diffusion flame

Peak LII with 1064-nm laser





- Potential reasons for fluence shift
  - Higher σ_{abs} for edge soot
  - Coating on center soot
  - Lower temperature in center

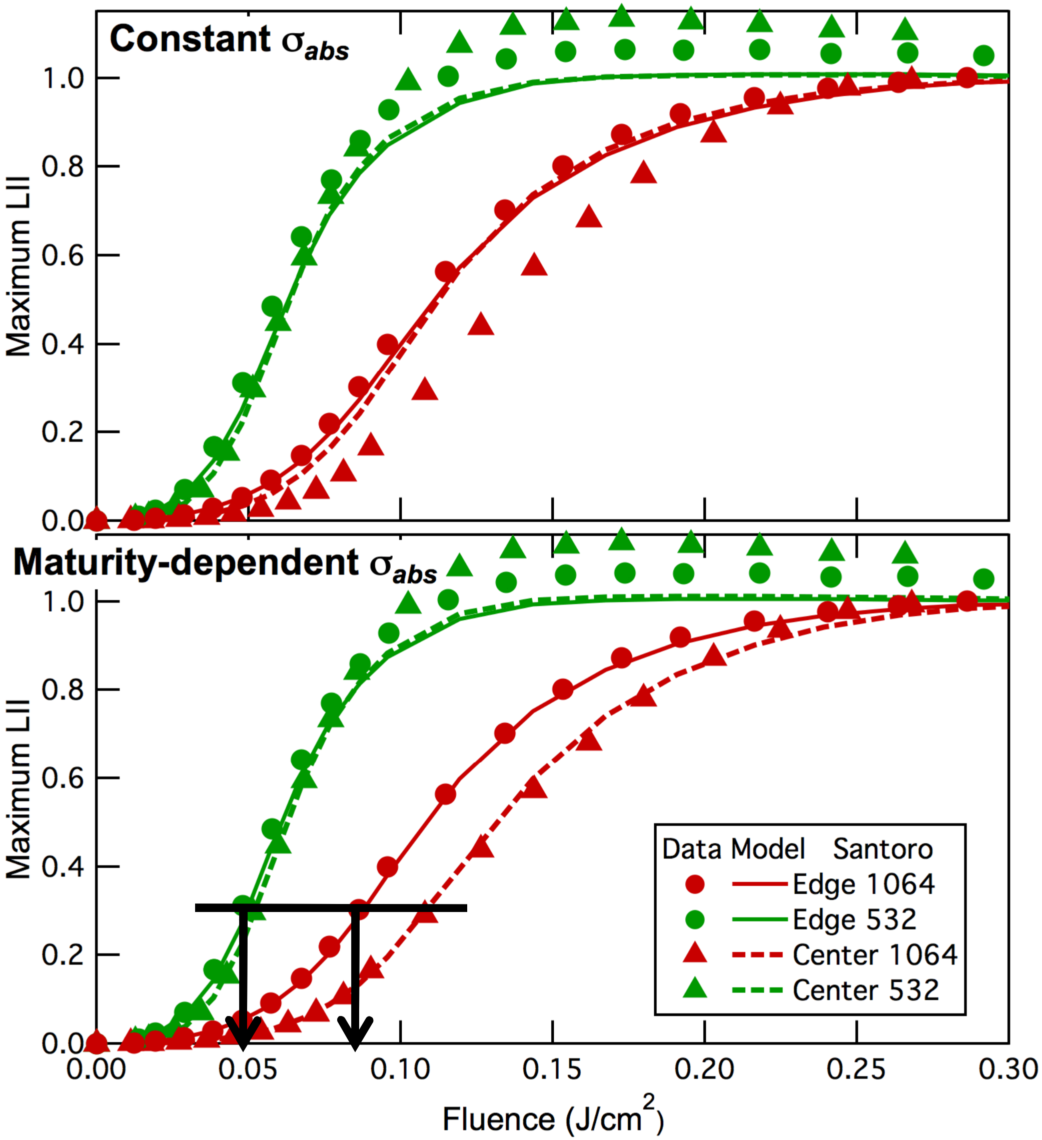
López-Yglesias, Schrader, Michelsen, *J. Aerosol Sci.*, **75**, 43-64, 2014.

Effects of particle maturity on LII signal

As soot maturity increases, σ_{abs} increases, but

$$\frac{\sigma_{abs}(532)}{\sigma_{abs}(1064)}$$ decreases.

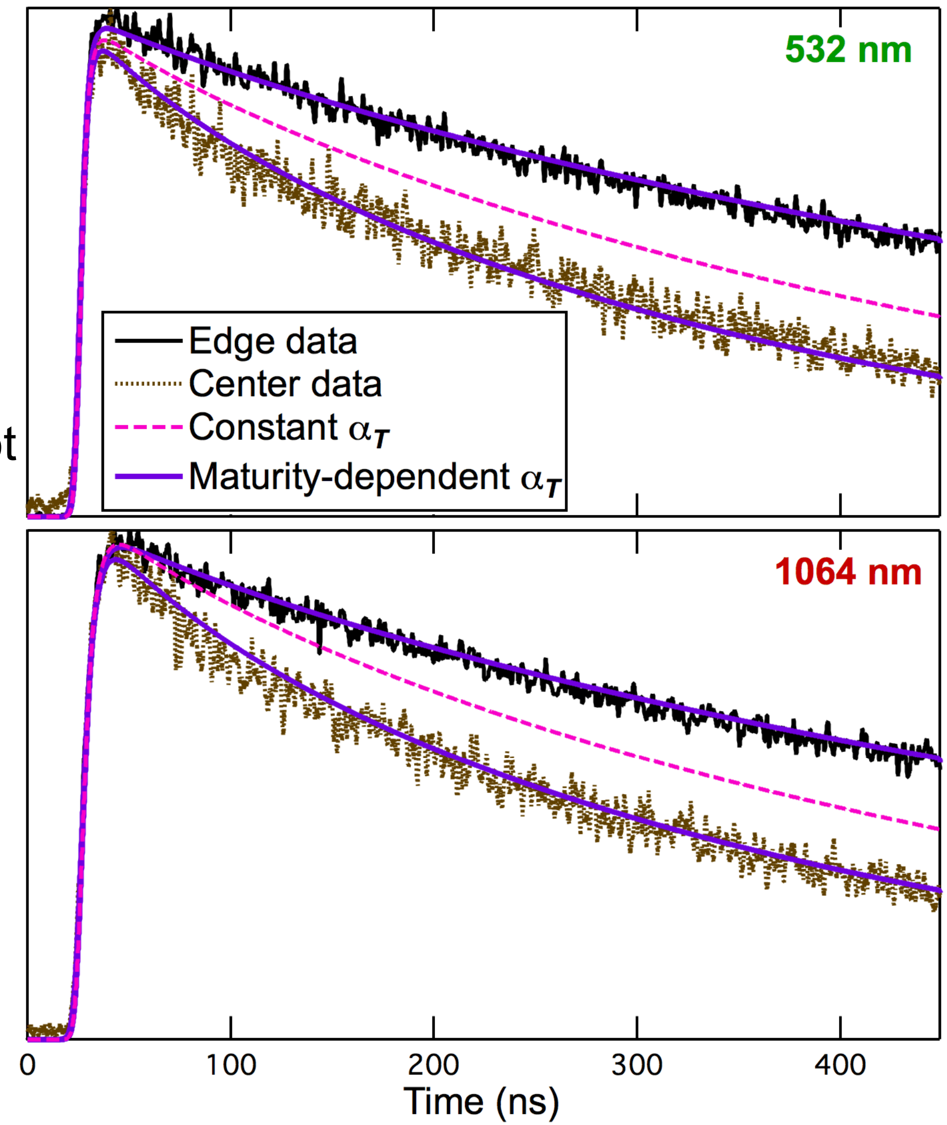
$$\frac{\sigma_{abs}(532)}{\sigma_{abs}(1064)} = \frac{F_{1064}(LII_{max})}{F_{532}(LII_{max})}$$



López-Yglesias, Schrader, Michelsen, *J. Aerosol Sci.*, **75**, 43-64, 2014.

Effects of particle maturity on LII signal

- Potential reasons for differences
  - Smaller particle size for center soot
  - Lower temperature in center
  - More compact morphology for edge soot
  - Higher α_T for center soot



As soot maturity increases, α_T decreases.

López-Yglesias, Schrader, Michelsen, *J. Aerosol Sci.*, **75**, 43-64, 2014.

Conclusions

Status of development

- Close to completion

Next steps

- Compare with other data sets, e.g., soot maturity experiments, long-pulse/CW LII
- Incorporate data from other experiments, e.g., SP-AMS

Community model

- First version written in modern Fortran using Agile development - CLiiME
- Feedback for other options
- Need beta testers