IAFSS Working Group on Measurement and Computation of Fire Phenomena (MaCFP)
Condensed Phase Phenomena Subgroup

June 11, 2017
Organizing Committee:
Morgan Bruns (NIST, USA)
Thomas Rogaume (U. Poitiers, France)
Stanislav Stoliarov (U. Maryland, USA)

Overview

- Computational predictions of fire phenomena can improve fire safety
- Fire phenomena can be characterized as
  - Gas phase (yesterday)
  - Condensed phase (today)
- Ultimately, gas + condensed phases should be coupled
- There are many challenges to condensed phase measurement and computation
- Collaborative and systematic verification and validation presents a promising path forward
- A framework for accomplishing this is presented

Fire Safety through Modeling
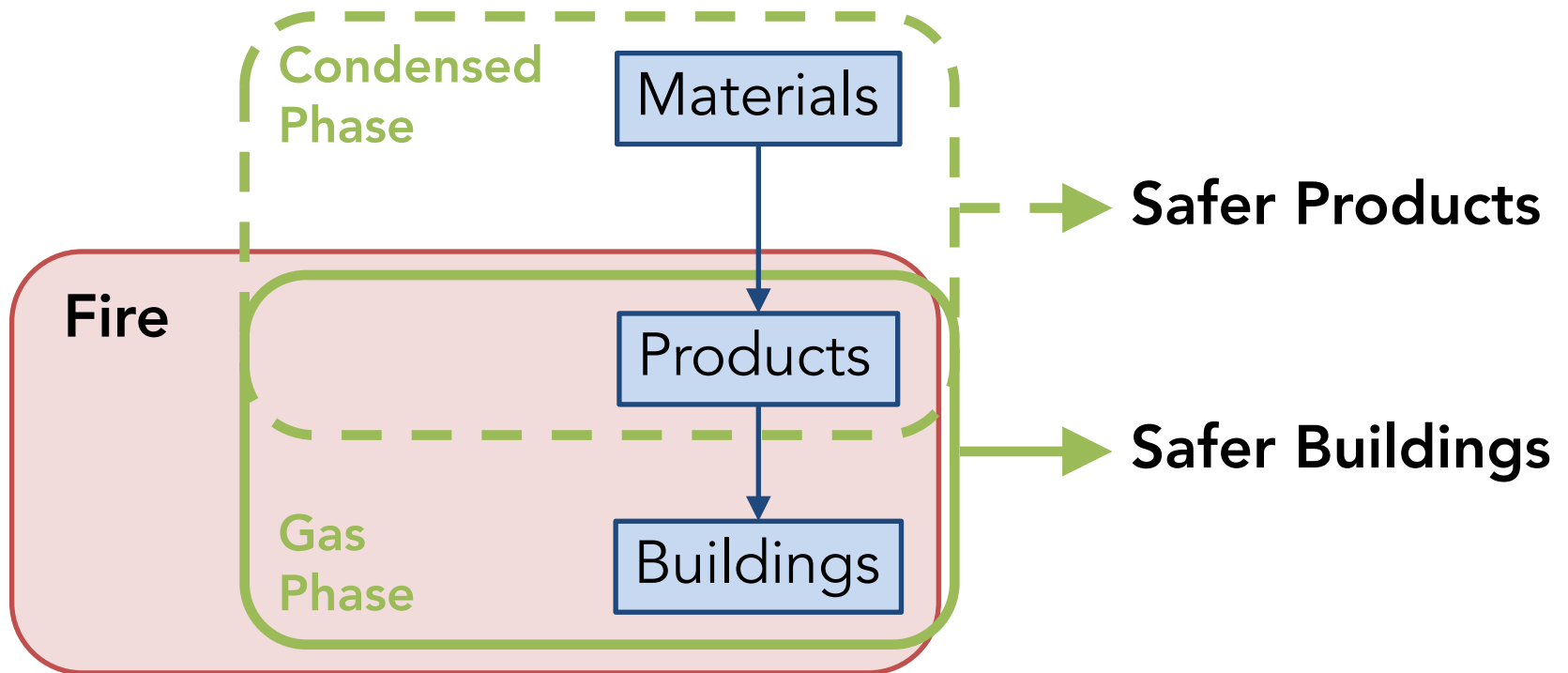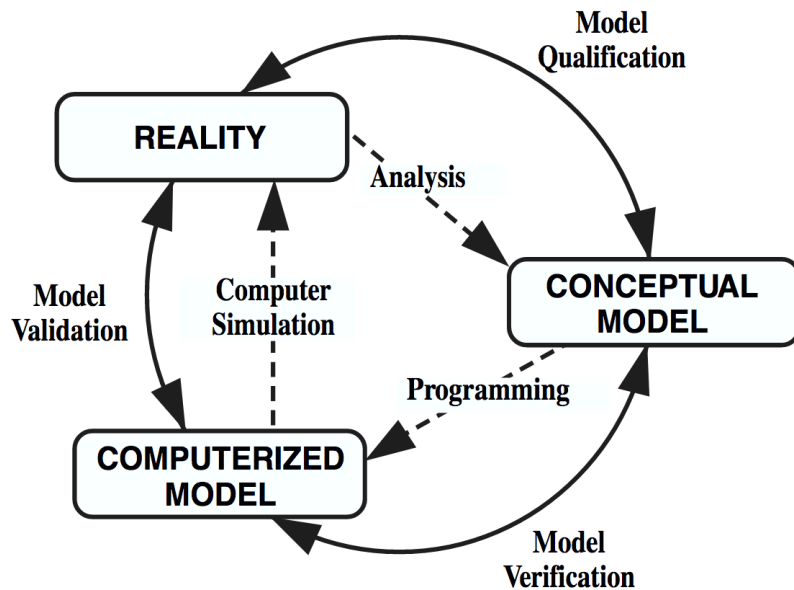
Condensed Phase Challenges

- Complex chemistry
- Multiscale
- Multiphase
- State dependent properties
- Varied mechanical behavior
- Moving boundaries
- Coupling to gas phase
- etc…

Ohlemiller and Shields, 2008

Model development limited by lack systematic verification and validation

Model Verification and Validation

Schlesinger et al., 1979

"**Verification**: …determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model."

"**Validation**: …determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model."
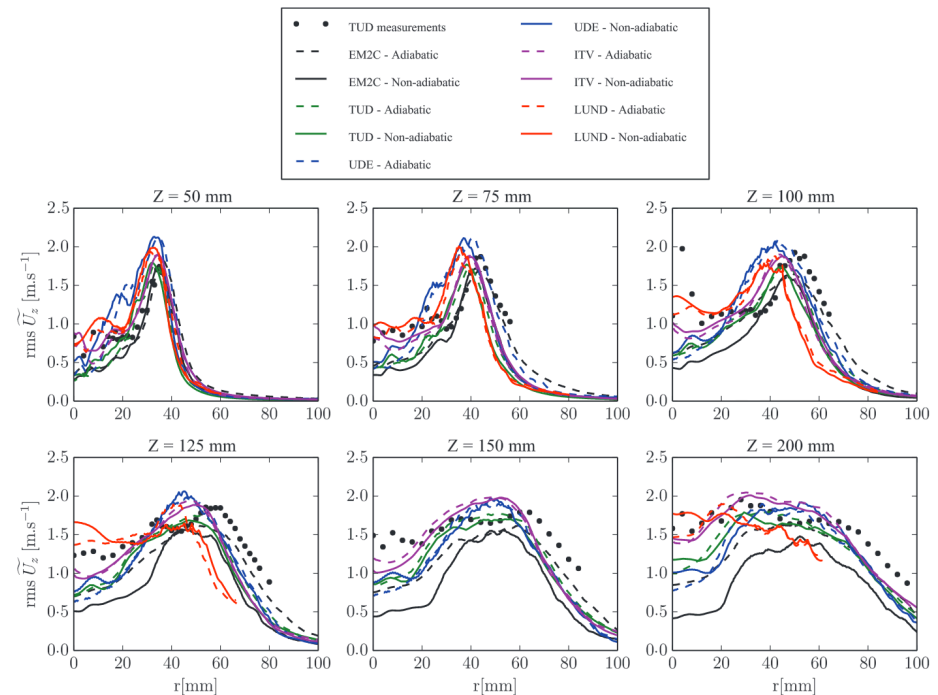
AIAA, 1998

Validation Pyramid
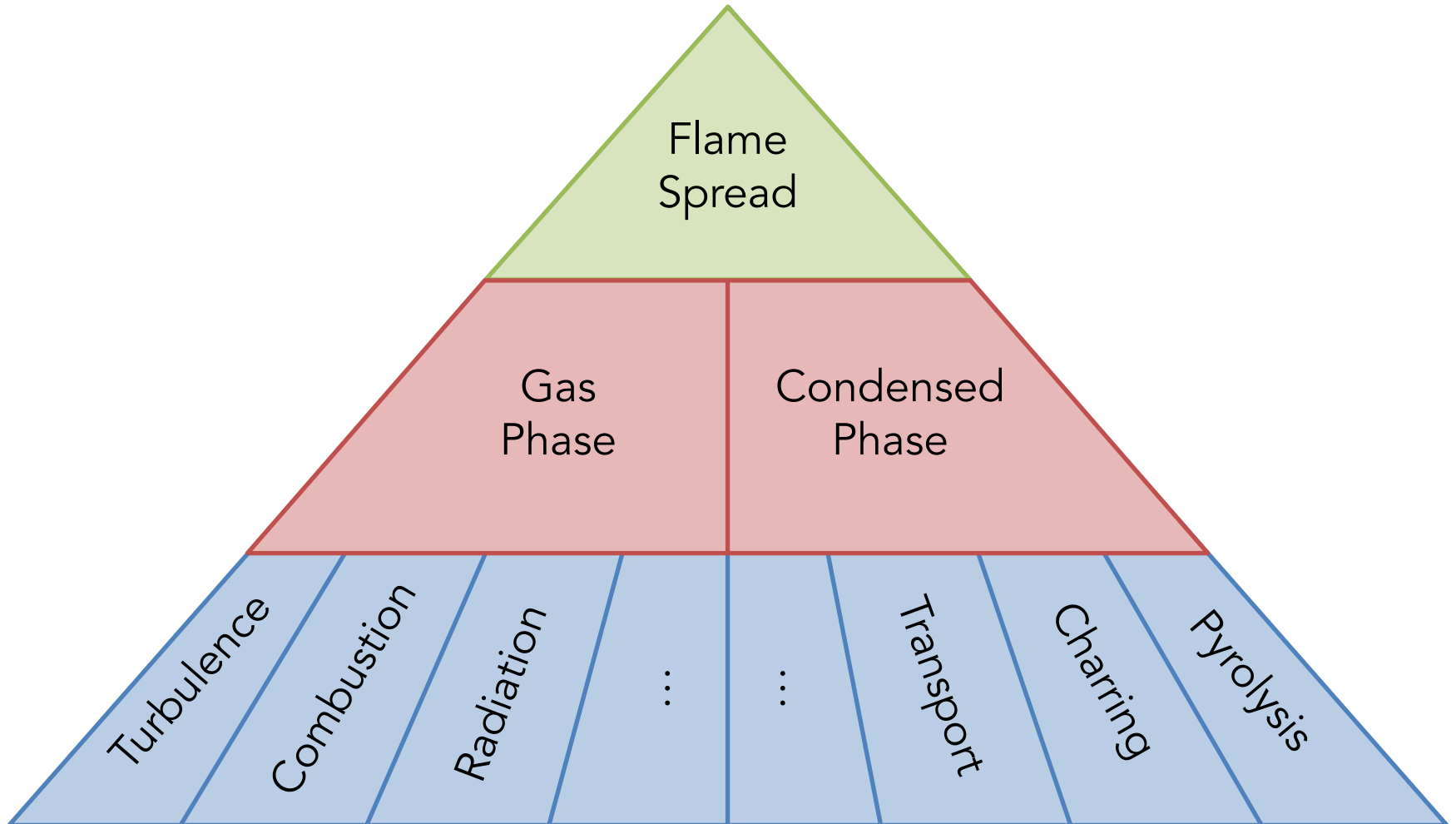
Sandia TNF Workshop

"International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames"

"…an open and ongoing international collaboration among experimental and computational researchers in turbulent combustion."

Objectives:
1) Share data
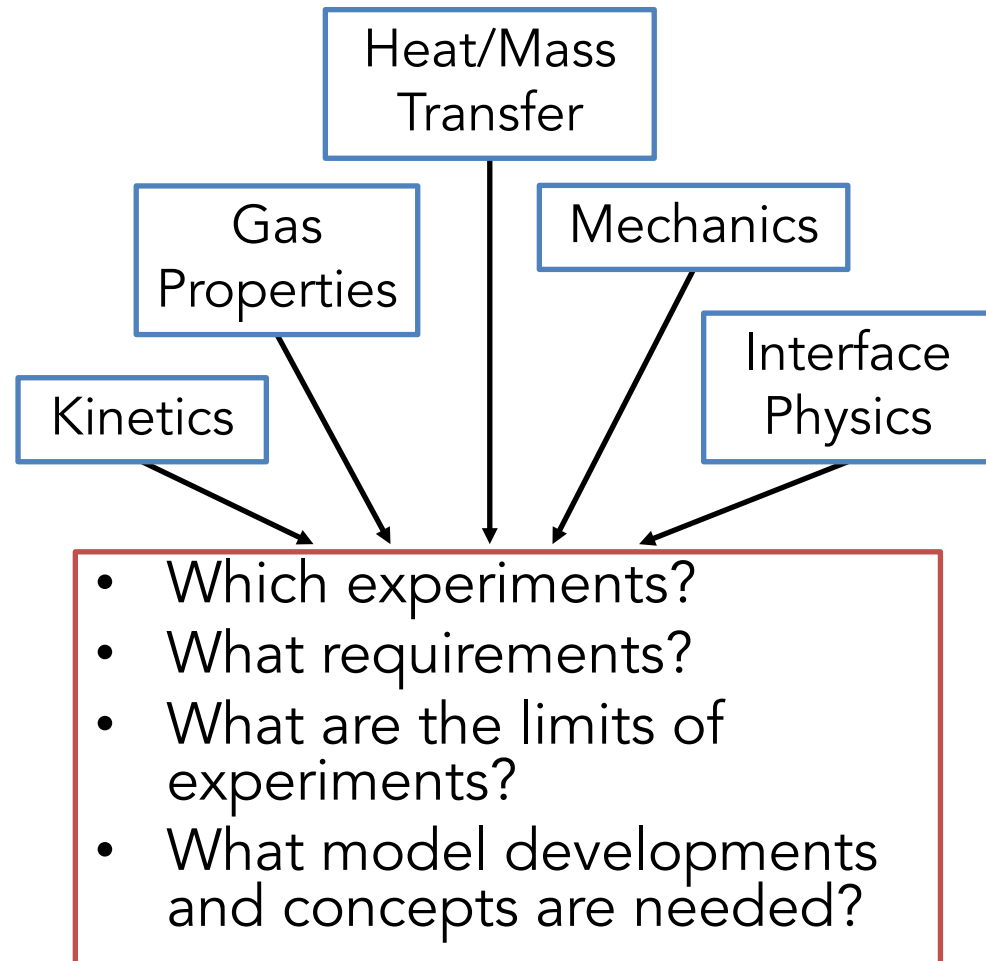2) Enable model-data comparisons
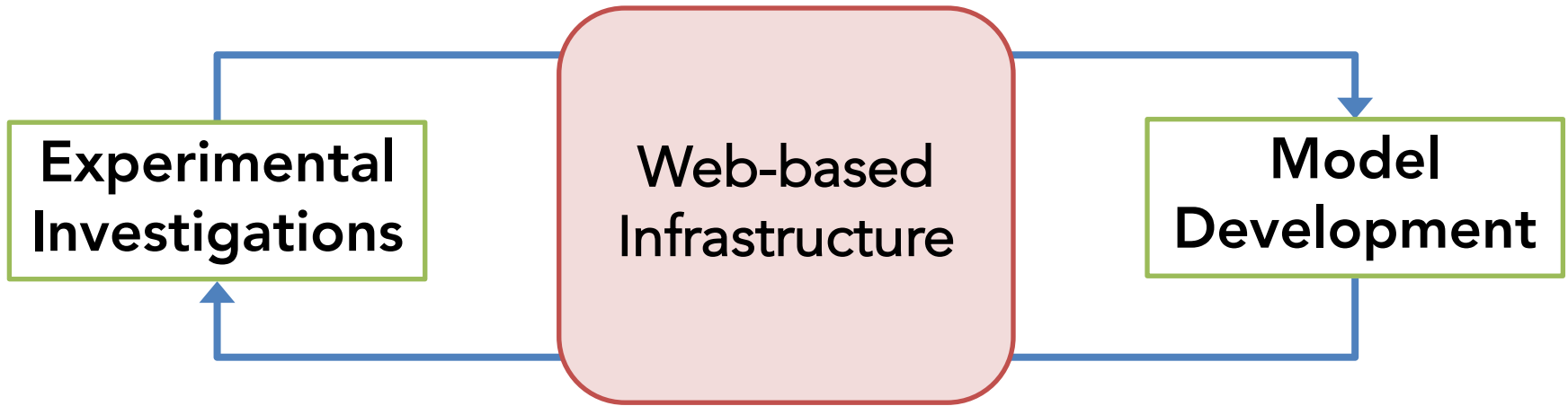3) Direct future research

Fiorina et al., 2015

MaCFP—Condensed Phase Phenomena Subgroup

"The purpose of the Condensed Phase Phenomena subgroup is to facilitate data sharing among researchers in order to improve predictions of thermal decomposition and pyrolysis in fire."

http://www.iafss.org/macfp-condensed-phase-phenomena/

Heat/Mass Transfer

Gas Properties

Mechanics

Kinetics

Interface Physics

- Which experiments?
- What requirements?
- What are the limits of experiments?
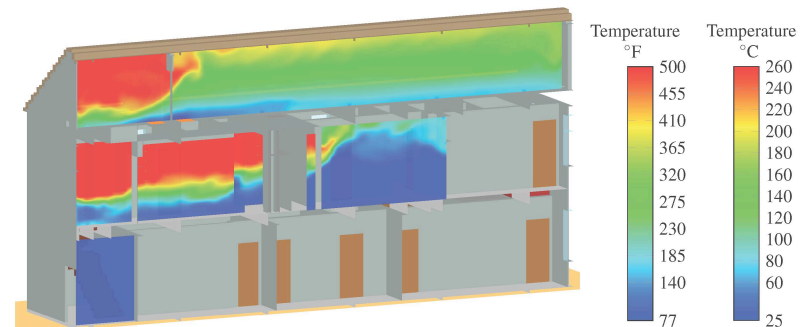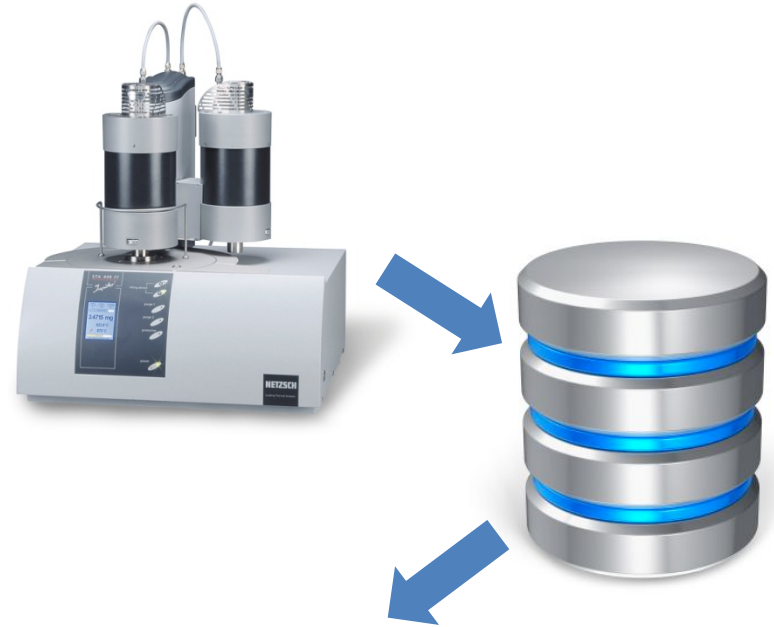- What model developments and concepts are needed?
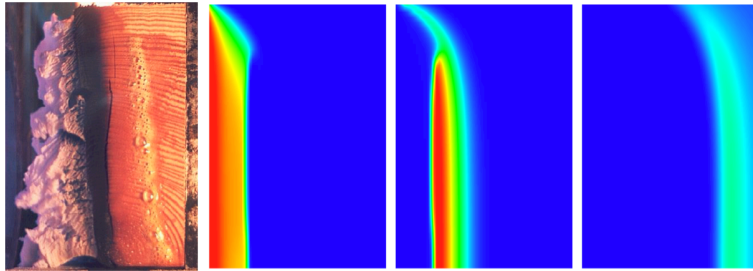
Proposed Framework

1. Experimental Data
2. Numerical Models
3. Parameter Sets + Comparisons
4. Discussion Forum

1. Experimental Data
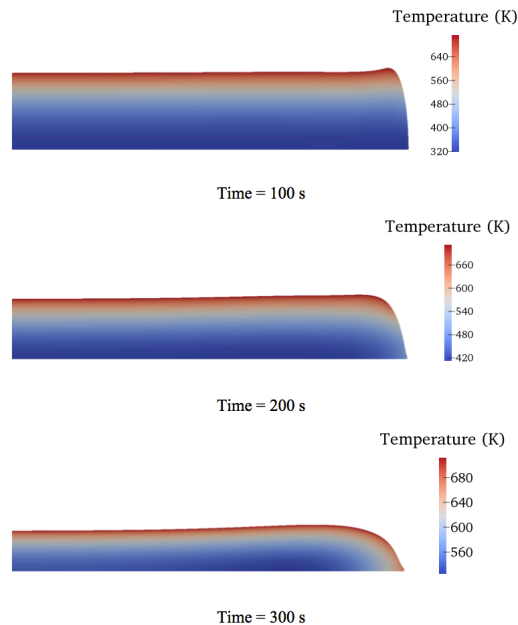
- Examples
  - TGA
  - DSC
  - Slab gasification
- Focus on condensed phase prohibits flaming
- Requirements
  - Standard formatting
  - Review committee
  - Peer-reviewed?

2. Numerical Models

Lautenberger, 2014

Bruns, 2015

- Examples
  - Gpyro
  - ThermaKin
  - FDS Solid Model

- Requirements
  - Open source
  - Available documentation
  - Minimum physics: pyrolysis + heat transfer

3. Parameter Sets + Comparisons

- Examples
  - Various publications
  - FDS Validation Guide
- Requirements
  - Complete specification of model parameters
  - Specified link between data and parameters
- Goodness of fit
  - Plots
  - Sum of square errors
  - Alternatives?
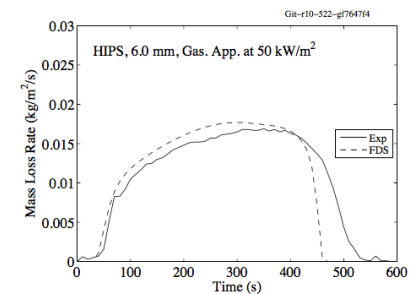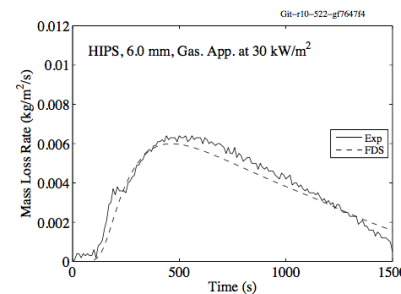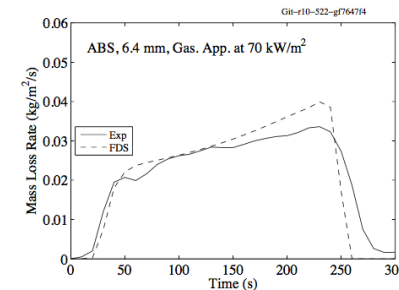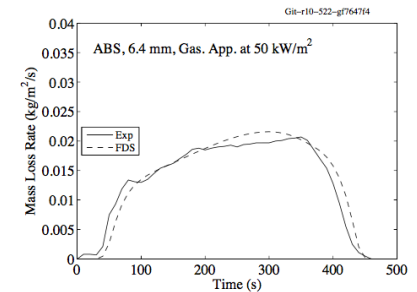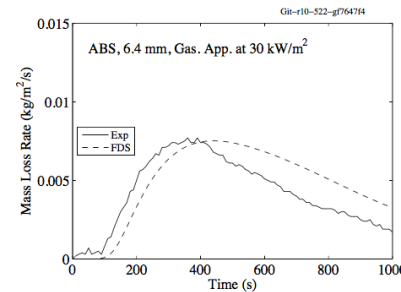
FDS Validation Guide—UMD Polymers

4. Discussion Forum

- Topics
  - Needed experiments
  - Necessary model developments
  - Numerical challenges
- Possible tools
  - Google Groups
  - Others?

FDS and Smokeview Discussions Shared publicly
62 of many topics ☆ G+1

Welcome to the Discussion Group site for FDS and Smokeview.
This is the primary discussion forum for FDS and Smokeview related topics.

The FDS and Smokeview homepage is https://pages.nist.gov/fds-smv
For bug reports or feature requests go to https://github.com/firemodels/fds/issues

NOTE: To post to the forum you will need to have an account with Google. To setup an account click here. You can use any email address for a Google account.

Before you post for the first time, please read this advice for posting to the group:
https://github.com/firemodels/fds/wiki/Effective-Posting

IMPORTANT:
Policies for the Discussion Group have been posted. Please read them at the following URL:
https://github.com/firemodels/fds/wiki/FDS-SMV-Group-Policies

Running multiple MPI jobs under Windows
By Kevin - 3 posts - 72 views 📢

Summer School on Fire Dynamics Modelling
By Lukas A. - 3 posts - 91 views 🏁

Problem with the modelisation of fireball using FDS 6
By brad_fds6 - 11 posts - 33 views

Tunnel fire - boundary conditions
By Giordana - 1 post - 10 views

Problem concerning Multi-Mesh slice output files (.sf)
By Ilyas_Ogx - 3 posts - 27 views

Regarding application of Heat flux on the obstruction
By Ijaz Fazil Syed Ahmed Kabir - 5 posts - 11 views

Adiabatic Condition Verification
By jmmunita - 8 posts - 18 views

Temperature gradient - initial condition in solids
By Danny Hopkin - 3 posts - 19 views

INSIDE WALL TEMPERATURE
By majid @gmail.com - 12 posts - 39 views

FDS/Smokeview Google Group

Will require regular community participation or else it won't be used!

Agenda

Sunday, June 11

8:00 – 8:15 am	Welcome and overview of "Condensed Phase Phenomena Subgroup" (M. Bruns, T. Rogaume, S. Stoliarov)
8:15 – 8:35 am	Kinetics and thermodynamics of condensed phase decomposition (I. Leventon)
8:35 – 8:55 am	Ignition from the condensed phase (A. Brown)
8:55 – 9:15 am	Physics and chemistry of the gas-condensed phase interface (F. Richard)
9:15 – 9:45 am	Open discussion
9:45 – 10:05 am	*Coffee break*
10:05 – 10:25 am	Heat and mass transfer in the condensed phase (S. Hostikka)
10:25 – 10:45 am	Coupling of condensed and gas phase models (Y. Wang)
10:45 – 11:05 am	Inverse modeling and model complexity in computational pyrolysis: applications to PMMA and wood in fire conditions (G. Rein)
11:05 – 11:25 am	Applications of generalized pyrolysis models (C. Lautenberger)
11:25 – 11:55 am	Open Discussion
11:55 am – 12:25 pm	Next steps and plan for next workshop
12:25 – 13:25 pm	*Lunch* (provided)

Discussion Topics and Next Steps

- Discussion of proposed framework
- Identification of existing data sets
- Design, implementation, and maintenance of website
- Volunteers
- Schedule next meeting