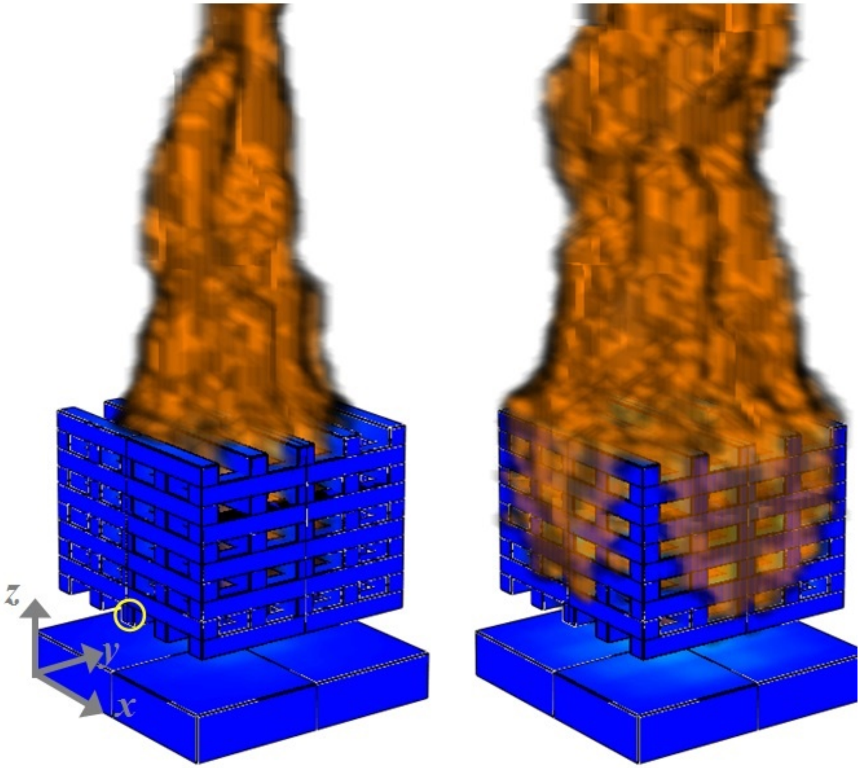
Gpyro: A Three Dimensional Generalized Pyrolysis Model

Measurement and Computation of Fire Phenomena IAFSS Workshop

June 11, 2017



Chris Lautenberger
lautenberger@reaxengineering.com
510-629-4930 x801

Reax Engineering Inc.
1921 University Avenue
Berkeley, CA 94704

Gpyro

- Open source pyrolysis model
  - http://reaxengineering.com/trac/gpyro
- Solves 0D/1D/2D/3D conservation equations inside pyrolyzing solid for
  - Gas and solid mass, species, and energy
  - Gas momentum (Darcy's law)

- Philosophy: user specifies desired level of complexity
  - Reaction mechanism
  - Anisotropic thermal and transport properties
  - Physics
  - Geometry & boundary conditions

Some Background Publications

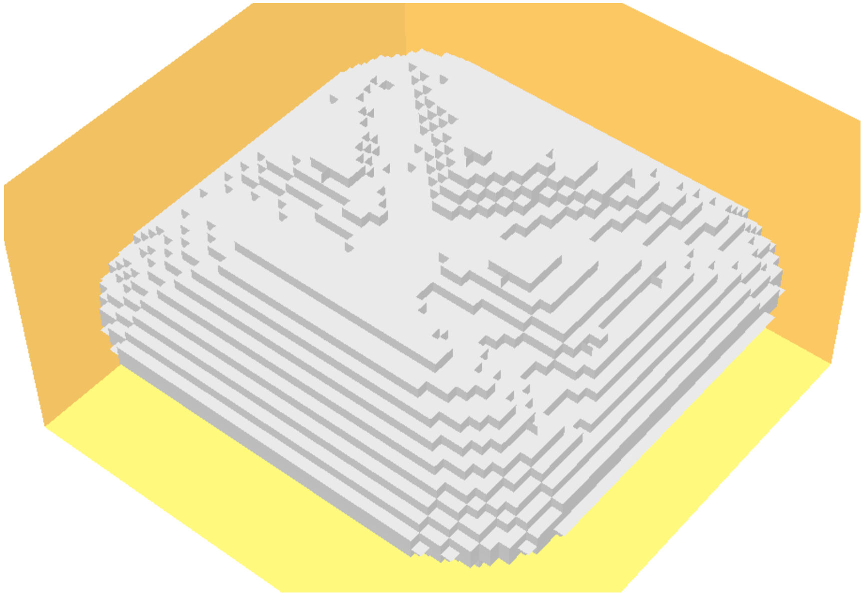
- Lautenberger, C. & Fernandez-Pello, A.C., "Generalized Pyrolysis Model for Combustible Solids," *Fire Safety Journal* **44** 819-839 (2009).
- Lautenberger, C. & Fernandez-Pello, A.C., "A Model for the Oxidative Pyrolysis of Wood," *Combustion and Flame* **156** 1503-1513 (2009).
- Dodd, A.B., Lautenberger, C., & Fernandez-Pello, A.C., "Computational Modeling of Smolder Combustion and Spontaneous Transition to Flaming," *Combustion and Flame* **159** 448–461 (2012).
- Lautenberger, C., "Gpyro3D: A Three Dimensional Generalized Pyrolysis Model," *Fire Safety Science* **11**: 193-207 (2014).

Gpyro Development History

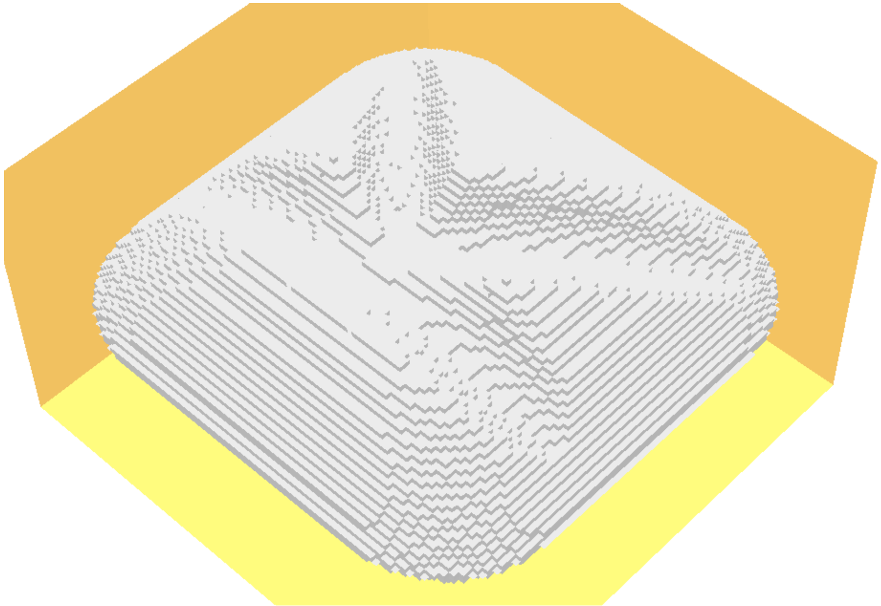
- 2004-2007: Initial development under NASA GSRP; basic 0D/1D formulation + GA optimization
- 2008-2010: Continued development (NSF); Extension to 2D, improved pressure solver & transport
- 2011: Initial 3D solver development (DOE)
- 2011-current: Generalized 3D formulation, IC's, BC's. FDS coupling, parallelization, improved solvers
- 2015-current: Coupling to ABAQUS for predicting stress development during manufacturing of polymer infiltration and pyrolysis based ceramic matrix composites

Complex Geometry

- Geometry specified as rectilinear obstructions
  - Charcoal briquette example



1.0 mm resolution



0.5 mm resolution

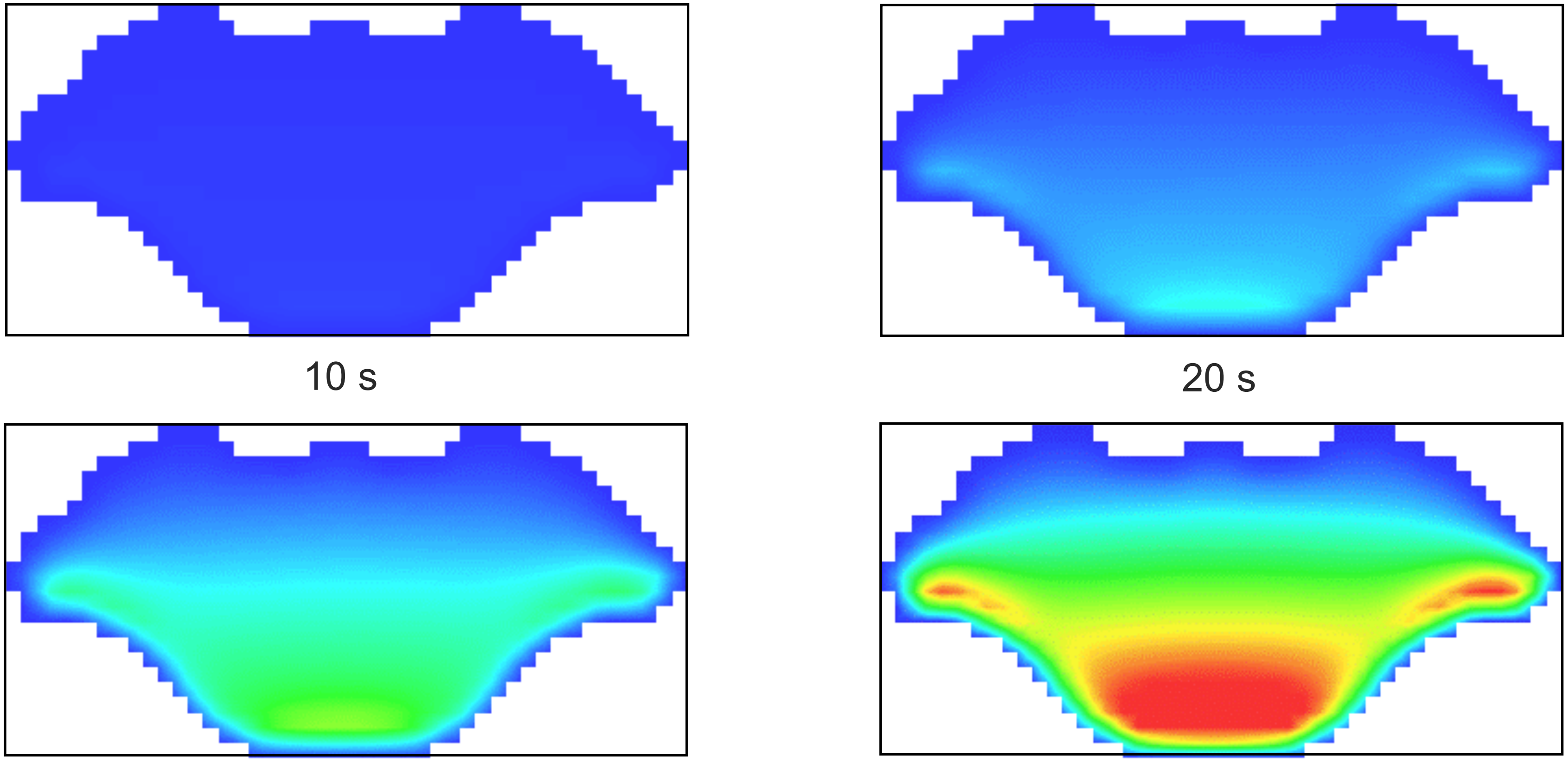
Complex Geometry

- PyroSim GUI used to import 3D geometries in .stl (Stereolithography) format and write obstructions in fortran namelist group format for parsing by Gpyro:

```
&OBST XB= -0.074, -0.072, -0.064, -0.062, 0.010, 0.014 /
&OBST XB= -0.074, -0.072, -0.062, -0.060, 0.010, 0.014 /
&OBST XB= -0.074, -0.072, -0.060, -0.058, 0.010, 0.014 /
&OBST XB= -0.074, -0.072, -0.058, -0.056, 0.008, 0.016 /
```

Postprocessing

- NIST Smokeview for post-processing/visualization



10 s

20 s

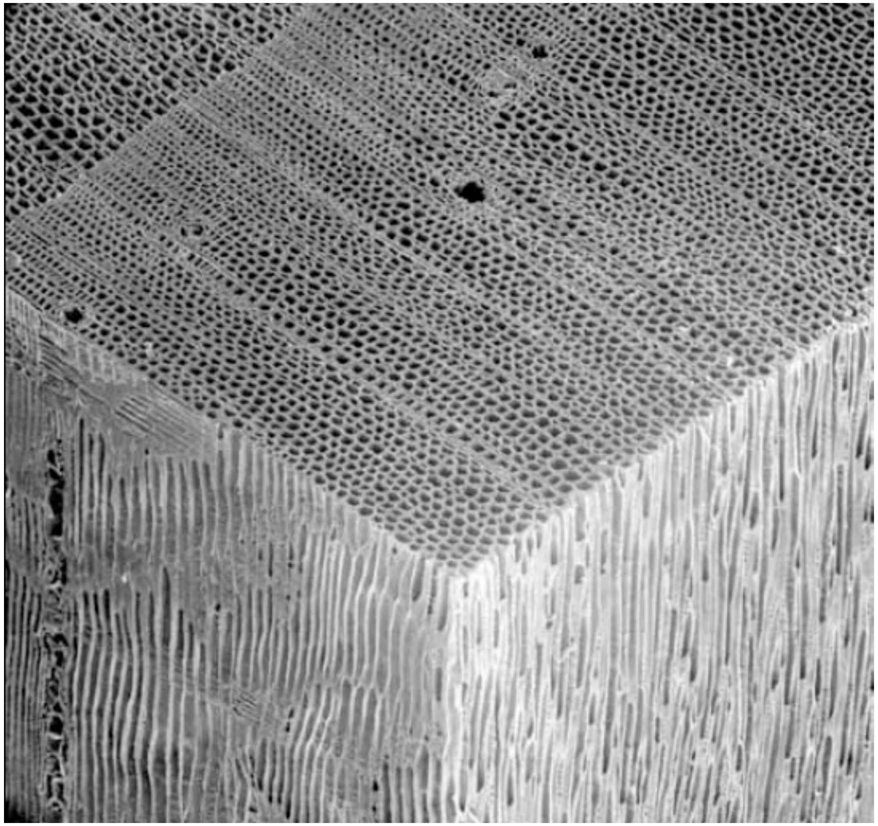
30 s

40 s

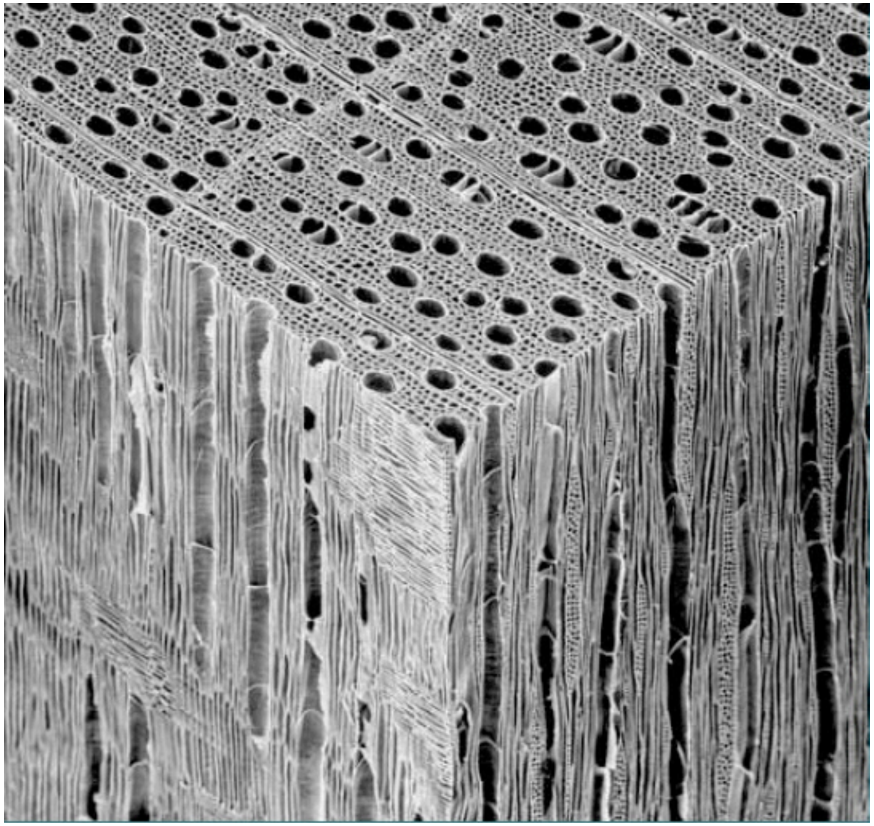
Pressure evolution in heated particle

Anisotropic Microstructure

- Gpyro's 3D formulation developed with anisotropic materials in mind



White spruce (softwood)



Red maple (hardwood)

Thermal & Transport Properties

- Anisotropic permeability and thermal conductivity
- User can specify for each solid species *i*:
  - $k_{x,i}(T)$, $k_{y,i}(T)$, $k_{z,i}(T)$
  - $K_{x,i}$, $K_{y,i}$, $K_{z,i}$ (no T dependency)
- Temperature variations in k, ρ, and c modeled as:

$$\phi(T) = \phi_0 \left(\frac{T}{T_r} \right)^{n_\phi}$$

- Weighted properties used in conservation equations:

$$\overline{k_x} = \sum X_i k_{x,i}$$

Kinetics & Reactions

- Reaction stoichiometry is general and user-specifiable
- Solid-phase pyrolysis reactions convert one solid phase species to another (e.g., wood to char) and generate one or more gaseous species (tar, gas, etc.)
- Gases in pore space can react
  - Homogeneously with other gaseous species
  - Heterogeneously with condensed phase species

Condensed-Phase Kinetic Models

- Currently 9 different kinetic models implemented:

Kinetic models - ^{m} f( ):

$i_{\text{kinetic model}}$	f( )	**Description**
0	$(1- \ )^{n}$	Default - nth order
1	$(1/n)\ (1- \ )\ (-\ln(1- \ ))^{1-n}$	Nucleation and nucleus growing
2	$(1- \ )^{n}$	Phase boundary reaction
3	$(1/2)$	Diffusion – plane symmetry
4	$(-\ln(1- \ ))^{-1}$	Diffusion- cylindrical symmetry
5	$(3/2)\ ((1- \ )^{-1/3} - 1)^{-1}$	Diffusion – spherical symmetry
6	$(3/2)\ (1- \ )^{-1/3} \quad ^{-1}$	Diffusion – Jander’s type
7	$(1/n) \quad ^{1-n}$	Potential law
8	$(1/n)\ (1- \ )^{1-n}$	Reaction order
9	$(1- \ )^{n}\ (1 + K_{cat} \quad _{icat})$	Catalytic

Mass and Species Conservation

Solid mass	$\frac{\partial \overline{\rho}}{\partial t} = -\dot{\omega}'''_{fg}$
Gas mass	$\frac{\partial \left(\rho_g \overline{\psi} \right)}{\partial t} + \frac{\partial \dot{m}''_x}{\partial x} + \frac{\partial \dot{m}''_y}{\partial y} + \frac{\partial \dot{m}''_z}{\partial z} = \dot{\omega}'''_{fg}$
Solid species	$\frac{\partial \left(\overline{\rho} Y_i \right)}{\partial t} = \dot{\omega}'''_{fi} - \dot{\omega}'''_{di}$
Gas species	$\frac{\partial \left(\rho_g \overline{\psi} Y_j \right)}{\partial t} + \frac{\partial \left(\dot{m}''_x Y_j \right)}{\partial x} + \frac{\partial \left(\dot{m}''_y Y_j \right)}{\partial y} + \frac{\partial \left(\dot{m}''_z Y_j \right)}{\partial z} = -\frac{\partial \dot{j}''_{j,x}}{\partial x} - \frac{\partial \dot{j}''_{j,y}}{\partial y} - \frac{\partial \dot{j}''_{j,z}}{\partial z} + \dot{\omega}'''_{fj} - \dot{\omega}'''_{dj}$

Energy and Momentum Conservation

Solid energy	$\frac{\partial\left(\overline{\rho}\overline{h}\right)}{\partial t}+\frac{\partial\left(\dot{m}''_x h_g\right)}{\partial x}+\frac{\partial\left(\dot{m}''_y h_g\right)}{\partial y}+\frac{\partial\left(\dot{m}''_z h_g\right)}{\partial z}=-\frac{\partial\dot{q}''_x}{\partial x}-\frac{\partial\dot{q}''_y}{\partial y}-\frac{\partial\dot{q}''_z}{\partial z}+\dot{Q}'''_s+\sum_{i=1}^{M}\left(\dot{\omega}'''_{fi}-\dot{\omega}'''_{di}\right)h_i$
Gas energy	$T_g = T$ (can also explicitly solve gas energy)
Solid mom.	N/A (no movement/shrinkage of solid phase in 3D)
Gas mom.	Solved as pressure evolution equation derived from mass conservation, Darcy's law, and ideal gas law

Numerical Solution (Patankar)

$$a_p\phi_P = a_E\phi_E + a_W\phi_W + a_s\phi_S + a_N\phi_N + a_T\phi_T + a_B\phi_B + b_P$$

$$a_E = \frac{\left(\bar{k}_x/\bar{c}\right)_e}{\left(\delta x\right)_e}\Delta y\Delta z \qquad a_N = \frac{\left(\bar{k}_y/\bar{c}\right)_n}{\left(\delta y\right)_n}\Delta x\Delta z \qquad a_T = \frac{\left(\bar{k}_z/\bar{c}\right)_t}{\left(\delta z\right)_t}\Delta x\Delta y$$

$$a_W = \frac{\left(\bar{k}_x/\bar{c}\right)_w}{\left(\delta x\right)_w}\Delta y\Delta z \qquad a_S = \frac{\left(\bar{k}_y/\bar{c}\right)_s}{\left(\delta y\right)_s}\Delta x\Delta z \qquad a_B = \frac{\left(\bar{k}_z/\bar{c}\right)_b}{\left(\delta z\right)_b}\Delta x\Delta y$$

$$b_P = a_P^\circ h_P^\circ + \dot{S}_P'''\Delta x\Delta y\Delta z$$

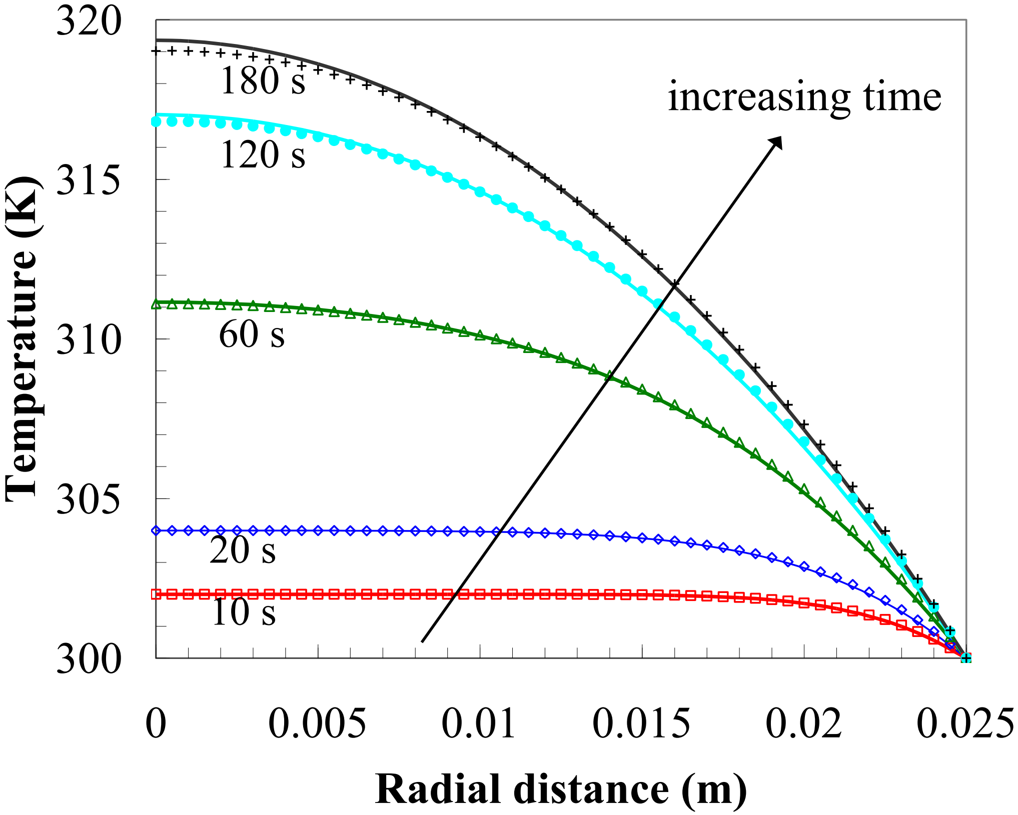
$$\dot{S}_P''' = \dot{Q}_s''' + \sum_{i=1}^{M}\left(\dot{\omega}_{fi}''' - \dot{\omega}_{di}'''\right)h_i - \frac{\partial\left(\dot{m}_x''h_g\right)}{\partial x} - \frac{\partial\left(\dot{m}_y''h_g\right)}{\partial y} - \frac{\partial\left(\dot{m}_z''h_g\right)}{\partial z}$$

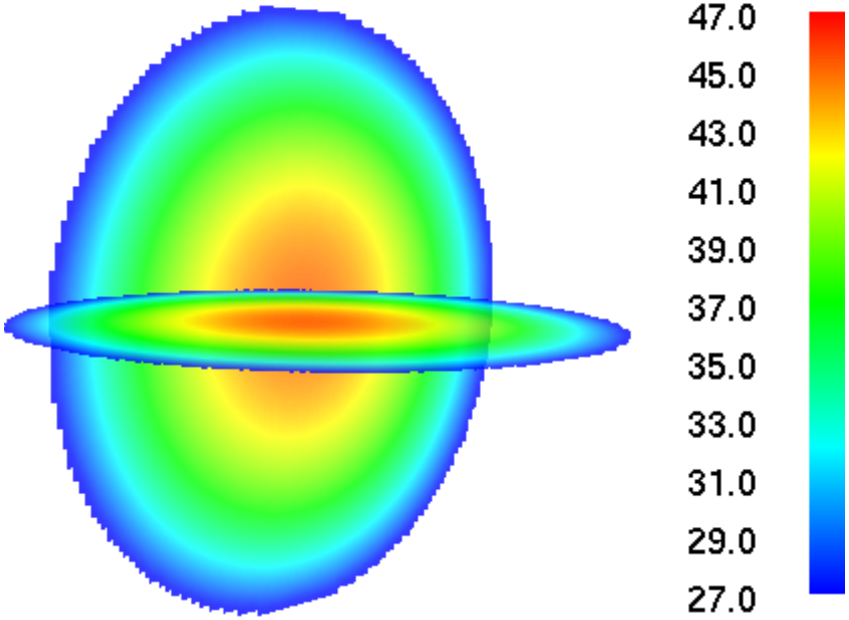
$$a_p = a_E + a_W + a_S + a_N + a_T + a_B + a_P^\circ \qquad a_P^\circ = \bar{\rho}_P^\circ\frac{\Delta x\Delta y\Delta z}{\Delta t}$$

Numerical Solution Methodology

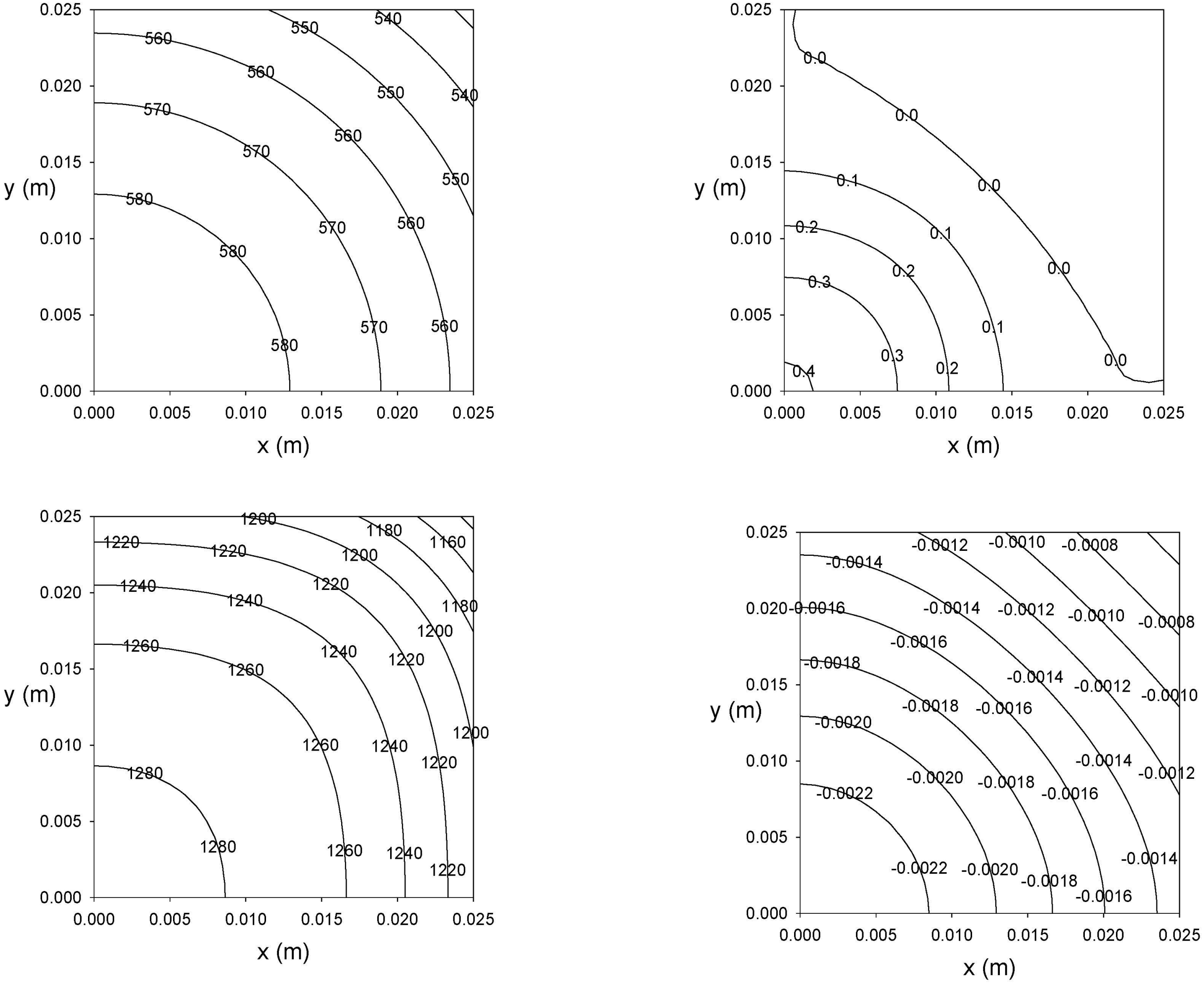
- Fully implicit formulation
  - Multiple iterations per timestep
- Relaxation to prevent solution divergence
- Special treatment of reaction source terms to ensure non-negative mass fractions
- Line by line TDMA solver
  - TDMA in one direction, Gauss Seidel iteration in other 2
  - TDMA direction alternated between iterations
- Convergence determined from user-specified residuals

Verification – "Cartesian Sphere" with Internal Heat Generation





Verification – Heat Conduction in 3D Parallelepiped



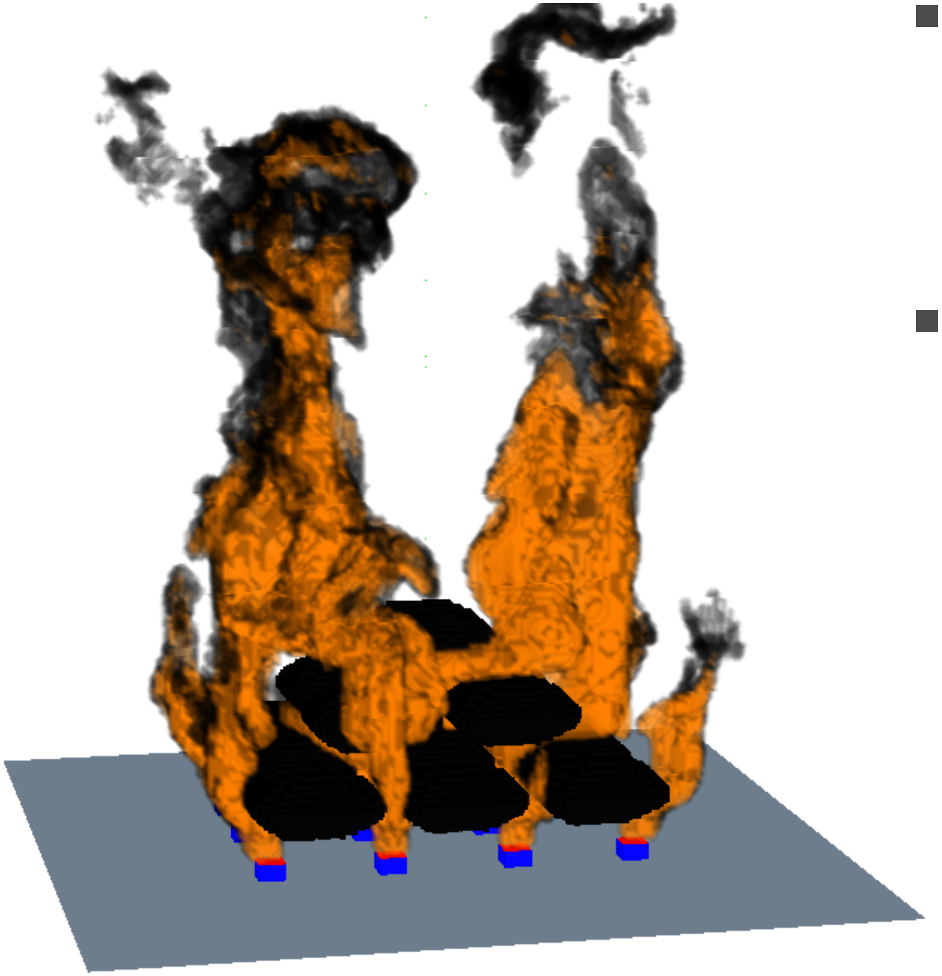
$t = 60$ s

$t = 1200$ s

Solution

% Error

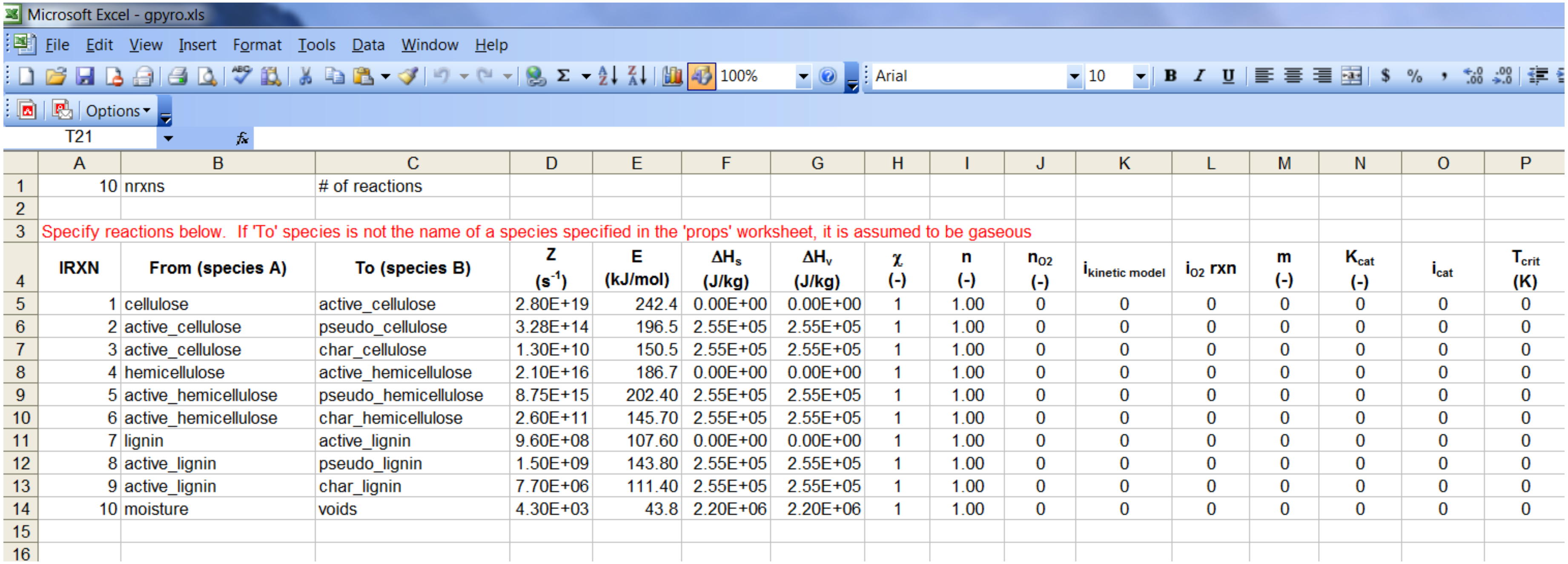
Gpyro Coupling to FDS



- Fully coupled to Fire Dynamics Simulator
- Limitations
  - Geometry is static – no shrinkage
  - Objects can't "burn away"

Input Deck

- Excel-based "front end" with VB macros
- Miller and Beland reaction mechanism example:



10 nrxns # of reactions

Specify reactions below. If 'To' species is not the name of a species specified in the 'props' worksheet, it is assumed to be gaseous

IRXN	From (species A)	To (species B)	Z (s^{-1})	E (kJ/mol)	ΔH_s (J/kg)	ΔH_v (J/kg)	χ (-)	n (-)	n_{O2} (-)	$i_{kinetic\ model}$	i_{O2} rxn	m (-)	K_{cat} (-)	i_{cat}	T_{crit} (K)
1	cellulose	active_cellulose	2.80E+19	242.4	0.00E+00	0.00E+00	1	1.00	0	0	0	0	0	0	0
2	active_cellulose	pseudo_cellulose	3.28E+14	196.5	2.55E+05	2.55E+05	1	1.00	0	0	0	0	0	0	0
3	active_cellulose	char_cellulose	1.30E+10	150.5	2.55E+05	2.55E+05	1	1.00	0	0	0	0	0	0	0
4	hemicellulose	active_hemicellulose	2.10E+16	186.7	0.00E+00	0.00E+00	1	1.00	0	0	0	0	0	0	0
5	active_hemicellulose	pseudo_hemicellulose	8.75E+15	202.40	2.55E+05	2.55E+05	1	1.00	0	0	0	0	0	0	0
6	active_hemicellulose	char_hemicellulose	2.60E+11	145.70	2.55E+05	2.55E+05	1	1.00	0	0	0	0	0	0	0
7	lignin	active_lignin	9.60E+08	107.60	0.00E+00	0.00E+00	1	1.00	0	0	0	0	0	0	0
8	active_lignin	pseudo_lignin	1.50E+09	143.80	2.55E+05	2.55E+05	1	1.00	0	0	0	0	0	0	0
9	active_lignin	char_lignin	7.70E+06	111.40	2.55E+05	2.55E+05	1	1.00	0	0	0	0	0	0	0
10	moisture	voids	4.30E+03	43.8	2.20E+06	2.20E+06	1	1.00	0	0	0	0	0	0	0

Input File Structure

- Fortran namelist-group based inputs

```
&GPYRO_RXNS
NRXNS       = 10,
CFROM(1)    = 'cellulose',
CTO(1)      = 'active_cellulose',
Z(1)        = 2.8E+19,
E(1)        = 242.4 …
```

- Can be generated with Excel-based front end or edited manually with a text editor

Outputs

- Three primary types of output
  - Point dumps: Write specific quantity at particular x,y,z location to .csv file as function of time
  - Profile dumps: Dumps a quantity in one the profile direction, *e.g.* $T(z)$ at fixed x,y as function of time
  - Slice dumps: Dump quantity in a plane to binary file format that can be post-processed in NIST’s Smokeview

- Can also dump integrated quantities
  - Total mass, total mass loss, instantaneous mass loss rate, etc.

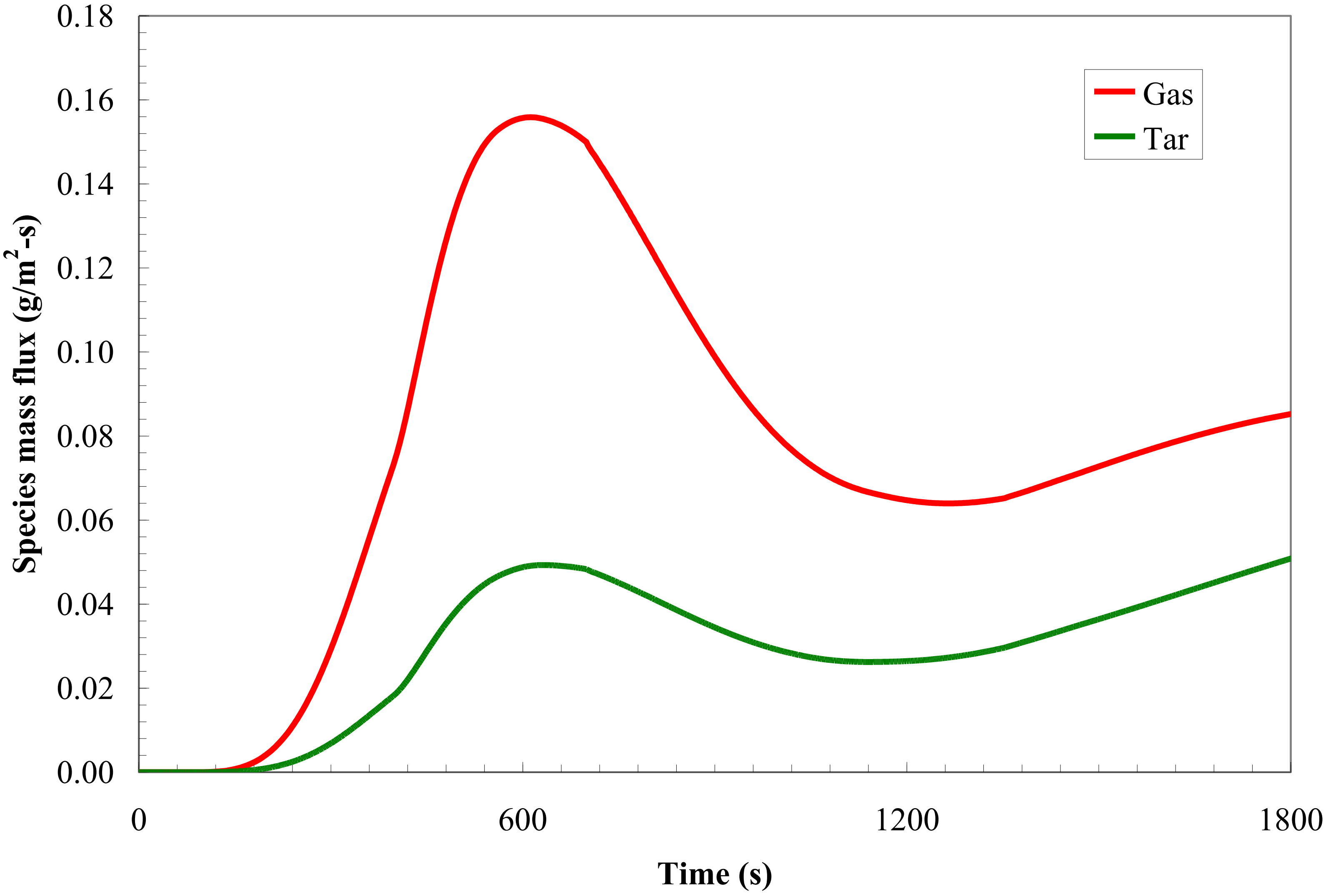
Current Limitations

- Particle shrinkage / swelling not accounted for in 2D/3D formulation (only in 1D)
- No submodel for liquid transport
- Underlying grid is Cartesian so curved surfaces have to be approximated by “stair stepping”
- FDS geometry is static
- Basic error checking in place but spurious inputs can lead to segmentation fault with no error message
- Documentation lags current code

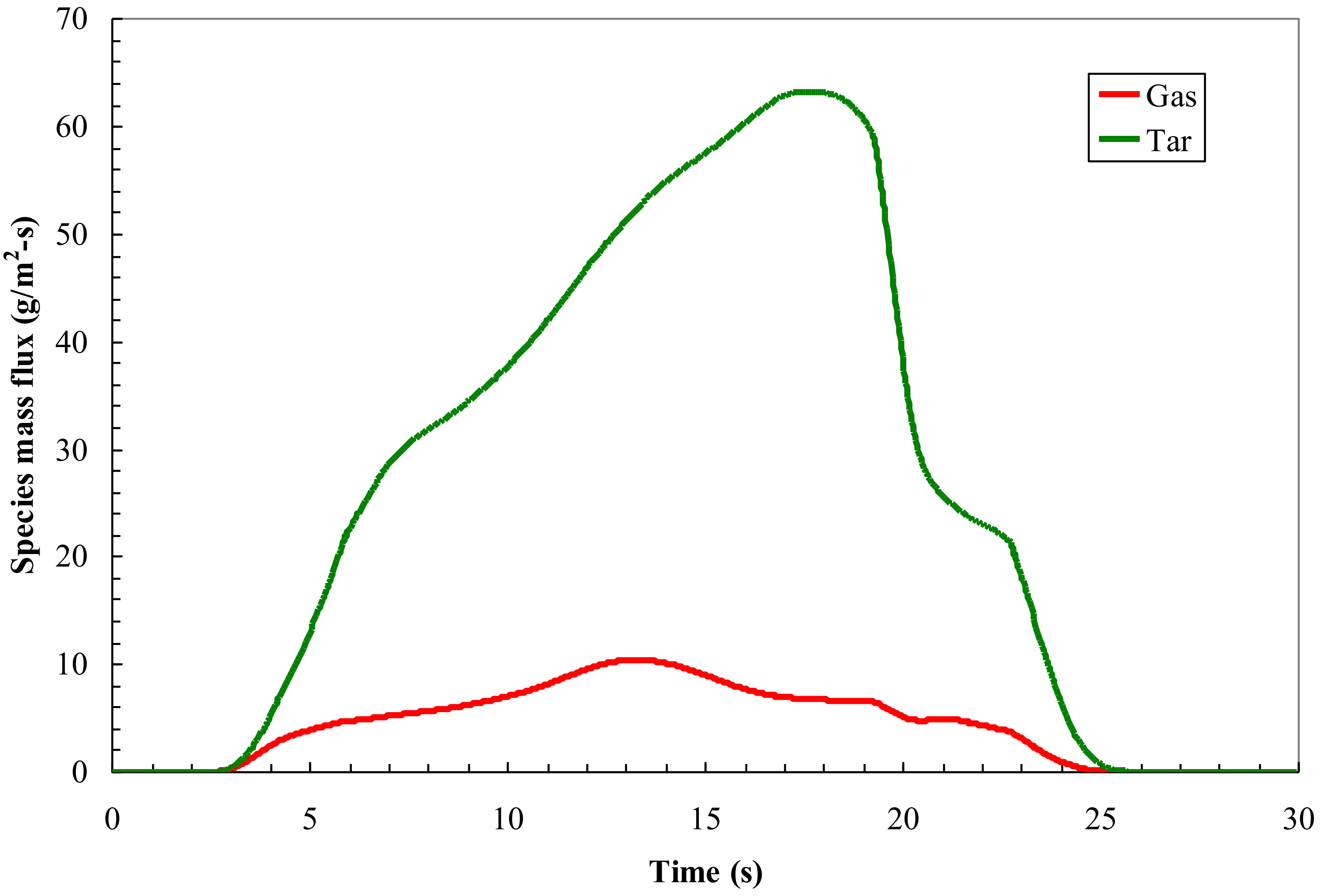
Example – 1D Wood Pyrolysis

- Representative softwood thermal properties
- 3 mm particle heated on both faces
- Miller and Beland 9-step reaction mechanism
  - Cellulose, hemicellulose, lignin
- Demonstrate cariable gas/tar yields with heating rate
  - Slow pyrolysis: 9 kW/m^2
  - “Fast” pyrolysis: 75 kW/m^2

Example – 1D Wood Pyrolysis – Slow



Example – 1D Wood Pyrolysis – “Fast”



Questions?

lautenberger@reaxengineering.com