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A Multi-dimensional Interface Heat Transfer Model for Objects Subjected to Ambient Air Solid Propellant Fires

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Outline

- Why are off-design (ambient air) propellant fires of interest?
- Why is a deposition model needed?
- Formulation of finite element based deposition model
- Model verification studies
- Comparison with experiment
- Conclusions
- Future plans

Ambient Air Propellant Fires: Areas of Concern and Potential Scenarios

- Space probe launch safety
  - In a launch mishap, burning propellant lands in vicinity of the radioisotopic fuels used on spacecraft, leading to potential dispersion of hazardous material.
- Nuclear or conventional weapon safety
  - Many weapons systems are carried by solid propellant missiles. An accident in which the rocket case was breached and propellant began burning could expose the munition to the severe propellant fire environment.
- Missile storage safety
  - Fire starts in tactical missile storage area; burning propellant impinges on other devices leading to ignition and/or explosion.
- Hostile action effects
  - Residual propellant from a missile strike ignites adjacent energetic materials or other combustibles in shipboard compartments such as in the USS Stark incident.

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Why do we need a deposition model?

- Solid propellant fires differ from “traditional” fires in a number of ways (higher temperatures, self contained oxygen source, minimal soot, etc.).
- One of the most important differences, is the presence of aluminum particles in propellants. This leads to significant effects on heat transfer:
  - Particles affect the thermal radiation characteristics within and outside of the plume
  - Particles stick to objects which are submerged within the flow, affecting the heat transfer to the objects
    1. Solidification of hot molten droplets on the surface of the object imparts a large amount of energy transfer to the object.
    2. Over time, the deposit forms an insulating barrier which may protect the object from the fire.
    3. The objects surface properties (e.g. emissivity) may change, influencing radiant heat exchange with the fire.

- Without modification, the finite element modeling approach we have traditionally used for thermal analysis of objects in fires cannot handle the effects of deposition.

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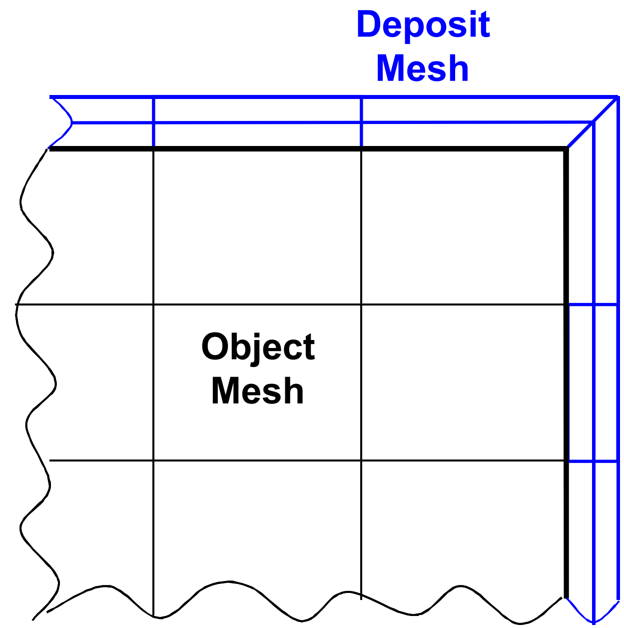
Multi-Dimensional Deposition Model

- Attach thin mesh layer to outside of object (one or more elements across thickness)
  - done only once, at time of mesh generation
  - thin layer thicknesses (~0.1 mm thick) are ok, (allows it to closely follow contours of object)
- Material properties of deposit layer vary over time to represent growing deposit
  - density
  - thermal conductivity (non-isotropic, varies in perpendicular and lateral directions)
  - volumetric energy source term (used to represent energy content of hot, deposited material)
- Improvements over our prior 1-D model (presented at JANNAF, 2005):
  - considers lateral conduction
  - more robust numerically
  - more computationally efficient (no stiff ODE solver required)
  - easier to add additional boundary conditions (convection, radiation)

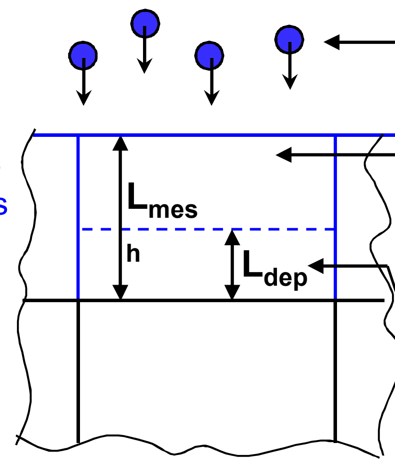


Density Formulation

(Vary density to account for growing deposit)

Blue: Deposit region (dashed lines represent true deposit thickness, solid lines are mesh thickness)

Black: Object mesh



Mass flux of particles, $\dot{m}$, adheres to object and forms a deposit of density, ρ_{mat}.

Density within finite element model (within L_{mesh}) is adjusted so that accumulated mass is conserved:

$$\rho(t) = \rho_0 + \frac{1}{L_{mesh}} \int_0^t \dot{m} dt'$$

Equivalent true deposit thickness, L_{dep}, can be calculated at every point in time:

$$L_{dep} = \frac{\rho}{\rho_{mat}} L_{mesh}$$

Definitions

- $\dot{m}$ – mass flux of deposited material (per unit area)
- ρ_{mat} – actual material density of deposit material
- ρ – deposit density used in model
- ρ_0 – initial deposit density used in model (very small, non-zero value)
- L_{dep} – deposit actual thickness (if density were ρ_{mat})
- L_{mesh} – thickness of mesh layer representing deposit

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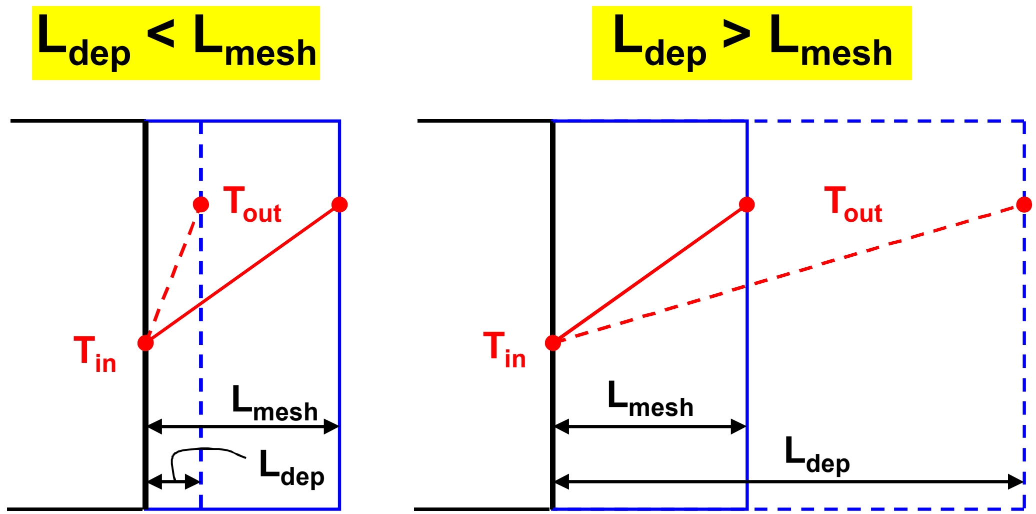
Effective Thermal Conductivity

(Vary conductivity to account for growing deposit)

conduction normal to surface

(conduction area is same, gradient varies)

$$\lambda_{eff,\perp} = \lambda_{mat} \frac{L_{mesh}}{L_{dep}}$$



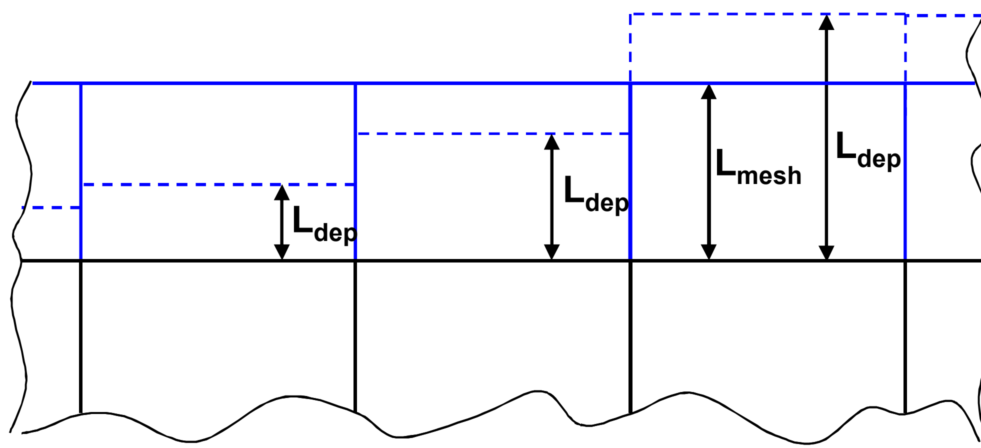
Blue Deposit Mesh

Black Object Mesh

conduction transverse to surface

(gradient is same, conduction area varies)

$$\lambda_{eff,||} = \lambda_{mat} \frac{L_{dep}}{L_{mesh}}$$



Blue Deposit Mesh

Black Object Mesh

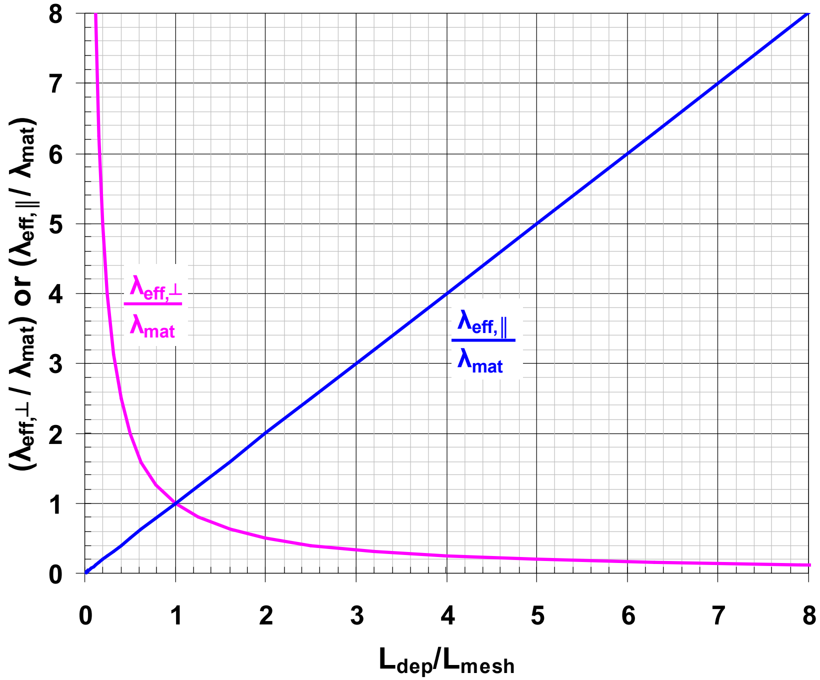
(dashed lines represent true deposit thickness, solid lines are mesh)

Effective Thermal Conductivity

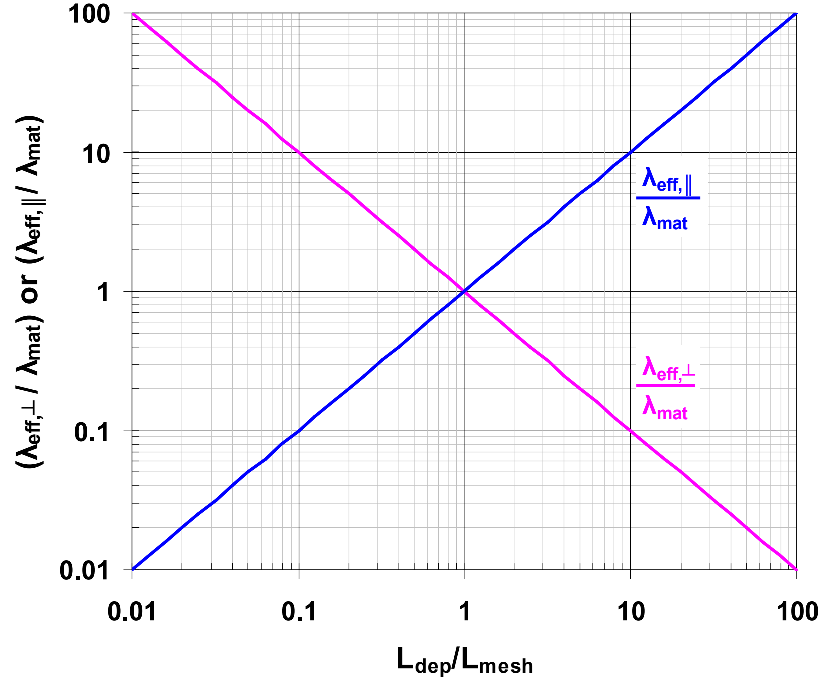
(Equations from previous slide)

Effective Thermal Conductivity in Perpendicular (⊥) and Lateral (‖) Directions as a function of Deposit Thickness

Linear Scale



Log Scale



- **With increasing deposit thickness:**
  - **Perpendicular direction effective conductivity decreases**
  - **Lateral direction effective conductivity increases**

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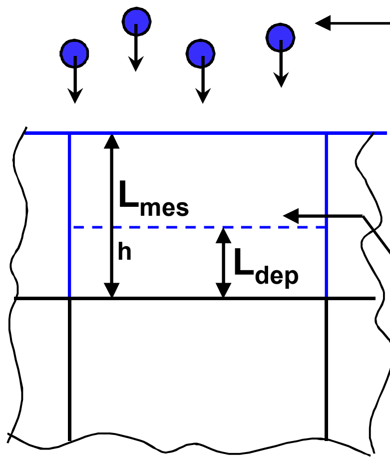
Energy Source Term

(Source term to account for additional energy from particles)

Blue: Deposit region (dashed lines represent true deposit thickness, solid lines are mesh thickness)

Black: Object mesh



Mass flux of particles, $\dot{m}$, having enthalpy, h_p, adheres to object.

$$h_p = \left(\delta(T_p)\Delta h_{fus} + \int_{T_{ref}}^{T_p} C dT \right)$$

Enthalpy of current deposit, h_{dep}.

$$h_{dep} = \left(\delta(T_{dep})\Delta h_{fus} + \int_{T_{ref}}^{T_{dep}} C dT \right)$$

Volumetric energy source applied within deposit elements (at mesh integration points):

$$q''' = \frac{\dot{m}}{L_{mesh}} \left(h_p - h_{dep} \right)$$

<u>Definitions</u>

$\dot{m}$ – mass flux of deposited material (per unit area)

C – material specific heat

Δh_{fus} – heat of fusion

$\delta(T)$ – Heaviside step function (δ=1 if $T>T_{melt}$; δ=0 otherwise)

T_p – temperature of incoming particles

T_{dep} – temperature of current deposit (at element integration points)

L_{mesh} – thickness of mesh layer representing deposit

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Model Verification & Validation

"Verification" Ensure that the model is implemented correctly by comparing with known solutions, test problems, etc.

"Validation" Ensure that model represents reality by comparing with well-defined experiments.

Verification was performed using a series of 4 test problems designed to show that:

1. energy is conserved (without phase change)
2. energy is conserved (with phase change)
3. thermal conductivity in perpendicular direction is correct
4. thermal conductivity in lateral direction is represented correctly

Preliminary validation was performed by comparing the model with a propellant fire test with a flat plate calorimeter (Test Matrix #10 from NASA/SNL test series).

- model inputs were obtained from experiment (where possible) or from a CFD-based flame code (this particular test was chosen based on availability of CFD analysis)
- comparison metric is calorimeter thermocouple time-temperature histories

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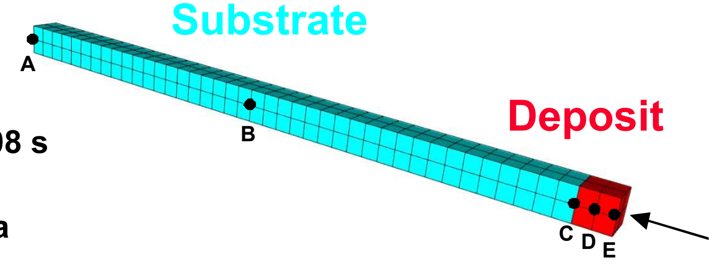
Verification Test Problem 1
(Check for Energy Conservation w/o Phase Change)

Substrate
- 2 mm thick mesh
- density = 2700 kg/m^3
- heat capacity = 900 J/kg-K
- total mass 5.4 kg per m^2 of area
- initial temperature = 300 K

Deposit
- 0.1 mm thick mesh
- heat capacity = 900 J/kg-K
- deposition rate 5 kg/m^2-s for 1.08 s then deposition turned off
- total mass: 5.4 kg per m^2 of area
- initial temperature = 2800 K

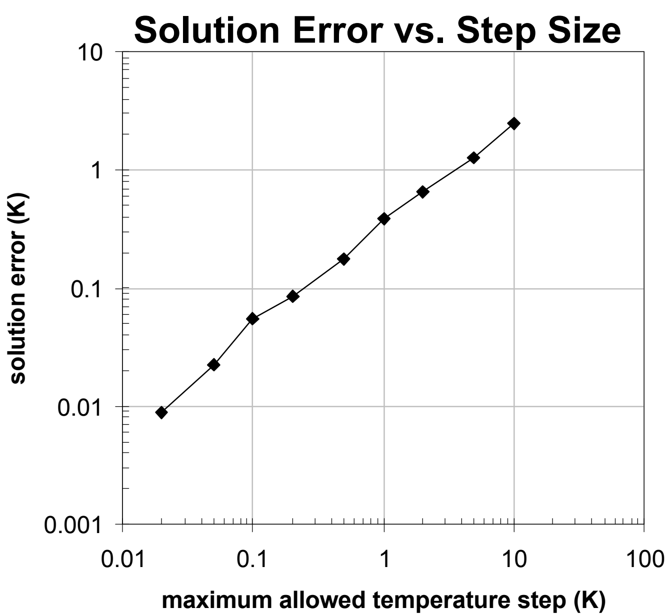


arrow indicates direction of deposition

Final (analytic) solution: T=1550 K

- Transient calculation was run to point where temperatures stopped changing
- Transient step size varied
- Checked level of agreement with analytic solution
- Result: Solution error was reduced commensurate with step size

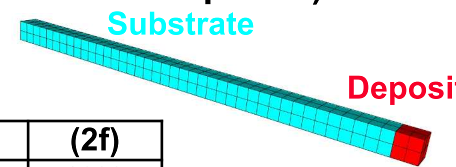
∴ Energy is conserved



Verification Test Problem 2

(Check for Energy Conservation with Phase Change)

- Same geometry as Verification Test Problem 1 (equal mass in Deposit & Substrate)
- Included phase change energy (Δh_{fus}) in Deposit and/or Substrate (6 different combinations, changed melting point). Phase change was distributed over a small ΔT (solidus-to-liquidus).
- Results compared with analytic solution for each combination
- Smallest transient step size from Problem 1 used (baseline error ~0.01K)



	Test	(1)	(2a)	(2b)	(2b-2)*	(2c)	(2d)	(2e)	(2f)
Initial State (Substrate)	T_{melt} (K)	N/A	933	933	933	1933	1933	933	2933
	$\Delta h_{fus,s}$ (kJ/kg)	N/A	400	400	400	400	400	400	400
	$T_{initial}$ (K)	300	300	300	300	300	300	300	300
	Substrate phase	N/A	solid	solid	solid	solid	solid	solid	solid
Initial State (Deposit)	T_{melt} (K)	N/A	933	1933	1933	933	1933	2933	2933
	$\Delta h_{fus,dep}$ (kJ/kg)	N/A	400	400	400	400	400	400	400
	$T_{initial}$ (K)	2800	2800	2800	2800	2800	2800	2800	2800
	phase	**N/A**	**liquid**	**liquid**	**liquid**	**liquid**	**liquid**	solid	solid
Final Equilibrium State	T_{final} [analytic] (K)	1550.00	1327.78	1550.00	1550.00	1550.00	1772.22	1327.78	1550.00
	T_{final} [model] (K)	1549.99	1328.22	1550.96	1549.97	1550.02	1772.35	1328.26	1549.99
	Error (K)	**0.01**	**0.44**	**0.96**	**0.03**	**0.02**	**0.13**	**0.48**	**0.01**
	Substrate phase	N/A	**liquid**	**liquid**	**liquid**	solid	solid	**liquid**	solid
	Deposit phase	N/A	**liquid**	solid	solid	**liquid**	solid	solid	solid

* with 50 K solidus-to-liquidus range; other cases had 3 K range.

- Error increases when either the Substrate or Deposit had a phase change (worst case was both); this is caused by "stepping over" part of the phase change energy. This can be mitigated by increasing the temperature range for phase change (cf. cases 2b and 2b-2) or reducing step size.
- Error caused by phase change in Deposit was similar to that caused by phase change in Substrate. (cf. cases 2a, 2e with 2d)

∴ Energy conservation in deposition model with phase change is similar to energy conservation in baseline finite element materials with phase change.

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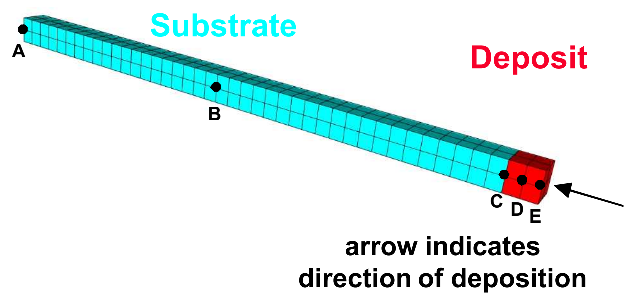
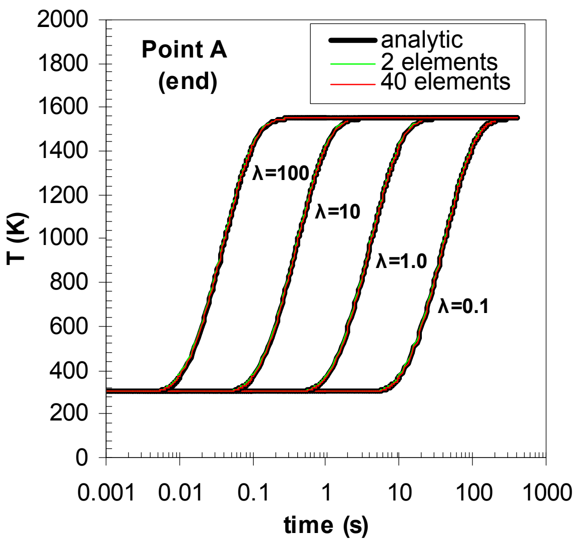
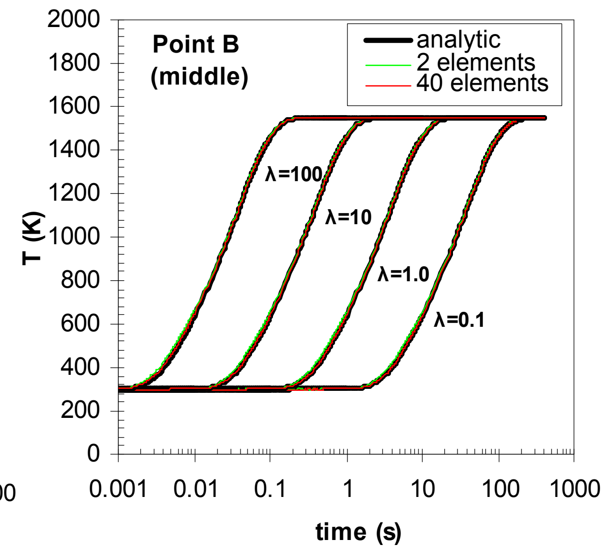
Verification Test Problem 3

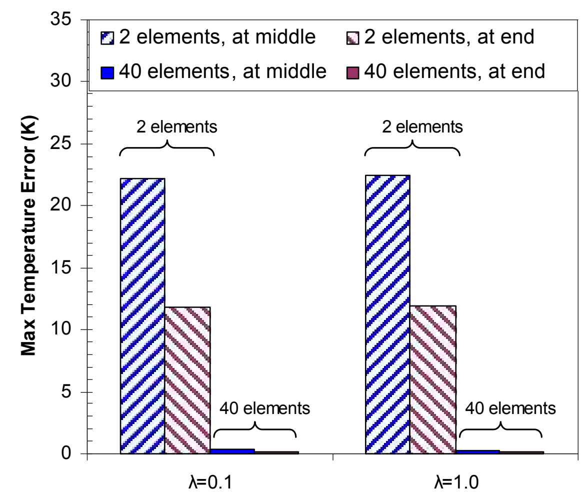
(Check Perpendicular Direction Thermal Conductivity)

- Same geometry as Verification Test Problem 1
- 2 elements or 40 elements across deposit thickness
- Material deposited at a high rate (10,000 x faster than Problem 1) so that all Deposit energy content is there prior to appreciable heat conduction into Substrate.
- This represents a conduction problem with suddenly applied temperature BC (an analytic solution exists for comparison.)
- Thermal conductivity varied over several orders of magnitude







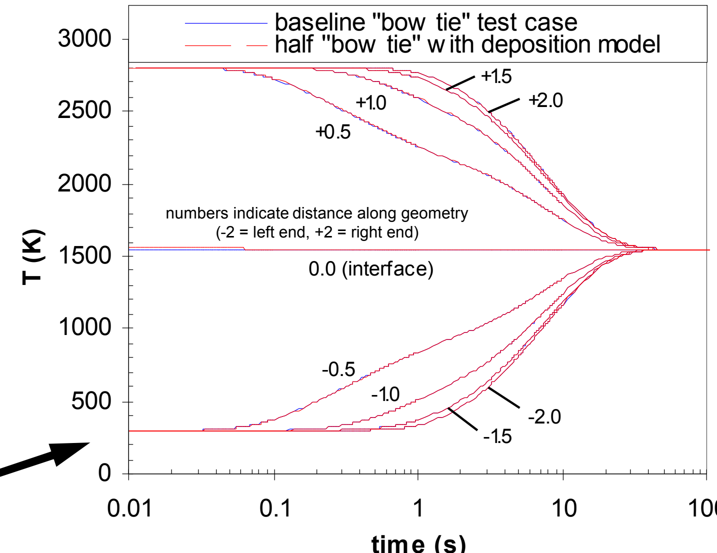


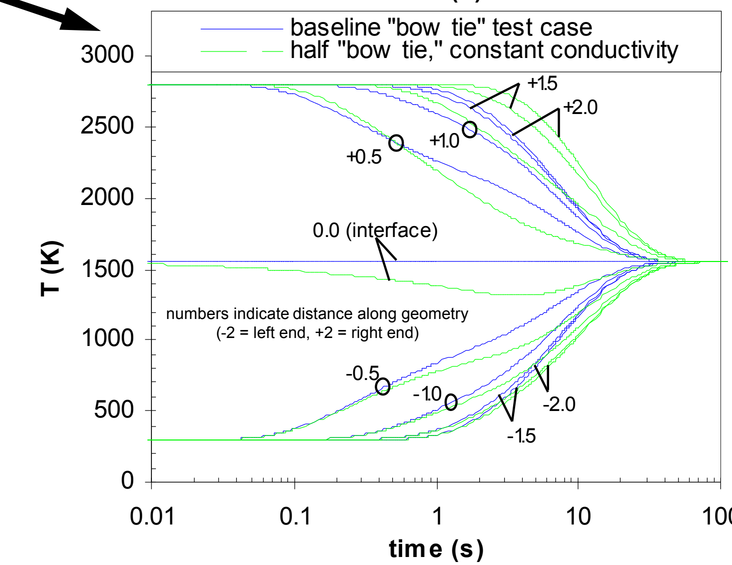
∴ Analytic solution reproduced, indicating that the perpendicular direction thermal conductivity formulation is implemented correctly in deposit model.

Verification Test Problem 4

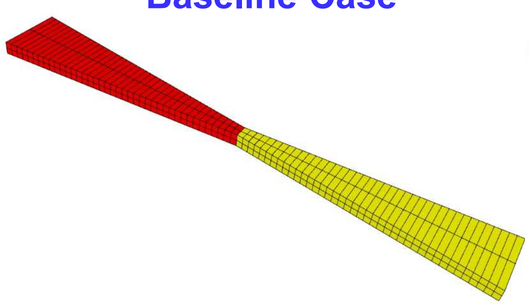
(Check Lateral Direction Thermal Conductivity)

- **Symmetric "bow tie" geometry used as baseline case**
  - **left & right halves had same properties**
  - **left side initially at 300 K, right side at 2800K**
  - **temporal response at various locations tracked**
- **Asymmetric geometry used as deposit test case**
  - **left side: baseline at 300 K**
  - **right side: deposition model (2800 K), deposited very quickly**
  - **deposit oriented crossways to the geometry such that lateral direction heat transfer is along length of object**
  - **deposit is non-uniform, linearly varying along length**
  - **temporal response at various locations tracked**
- **Deposition model results track baseline results very well.**
- **Constant conductivity case does not track baseline well.**

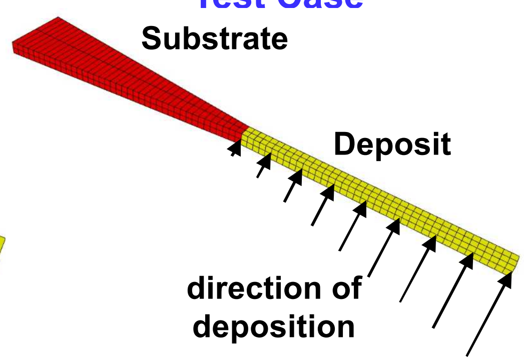




Baseline Case



Test Case

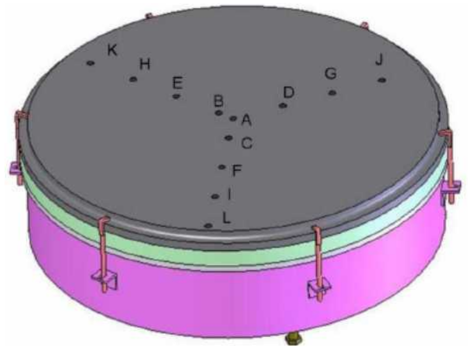


∴ Lateral direction thermal conductivity formulation is implemented correctly in deposition model.

Validation Test Problem

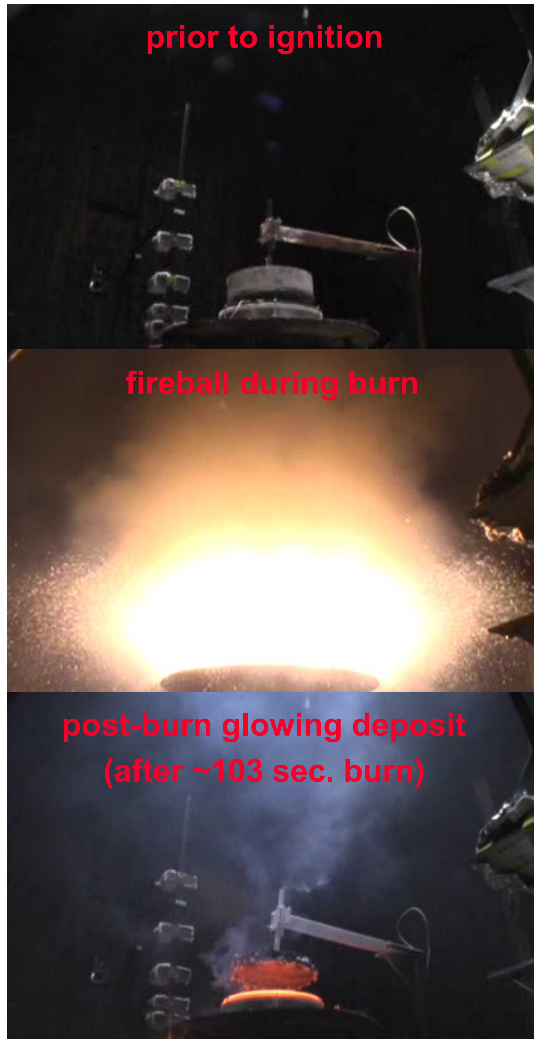
(Experimental Data—NASA-SNL Test Series, Matrix #10)

Graphite Flat Plate Calorimeter (design showing TC locations)

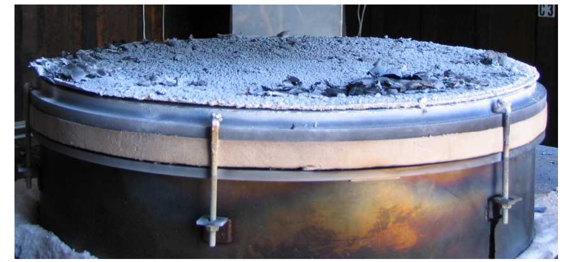


Downward-facing Propellant Charge Held Above Calorimeter

Images pulled from video (same scale on all)

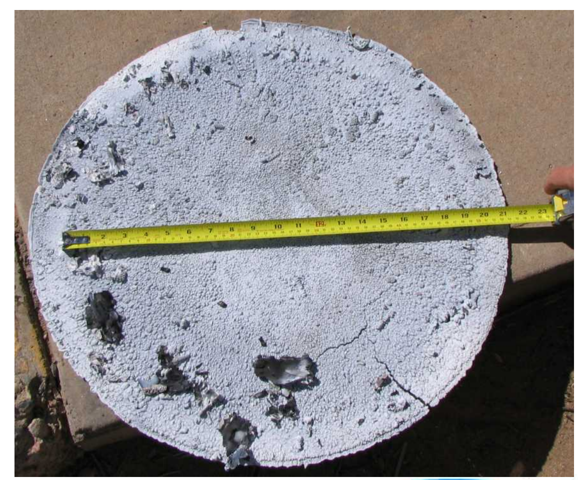


Post-test Calorimeter with Deposit



Deposit Removed from Plate:

- 3.038 kg.
- approx. 50/50 mix of Al/Al_2O_3
- fairly uniform thickness



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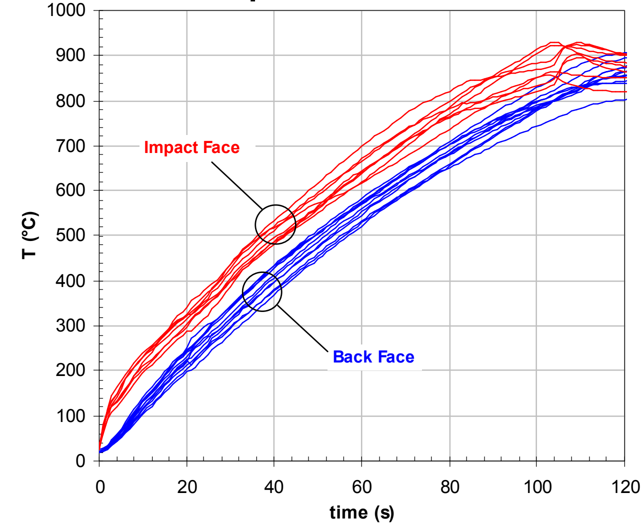
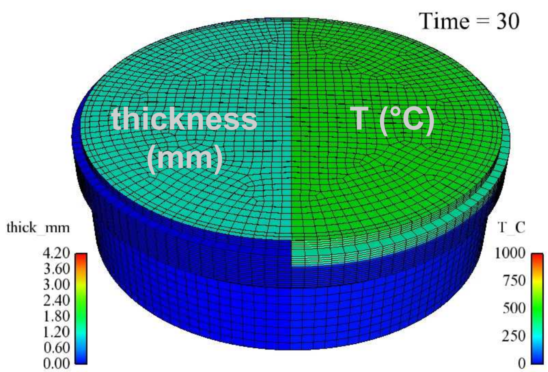
Validation Test Problem

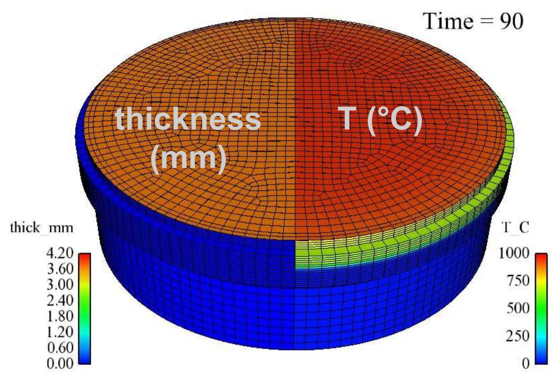
(Experimental Data—NASA-SNL Test Series, Matrix #10)

- Model inputs taken from experiment when possible (some of these were measured post test at room temperature):
  - burn time (103 s)
  - deposit weight (3.038 kg, distributed nearly uniformly)
  - mass flux (0.11 kg/m^2-s from deposit weight, area, burn time)
  - impacting droplet temperature (2400 K)
  - composition (approx. 50% Al, 50% Al_2O_3, measured post test)
  - deposit density (1720 kg/m^3 at room temperature)
  - thermal diffusivity (0.55 cm^2/s at room temperature
  - thermal conductivity (10 W/m-K at room temperature, from diffusivity)
- Other inputs recommended from VULCAN fire simulations:
  - incident radiant heat flux (500 kW/m^2)
  - convection coefficient (40 W/m^2-K)
  - convection temperature (2950 K)
  - deposit emissivity (0.5)

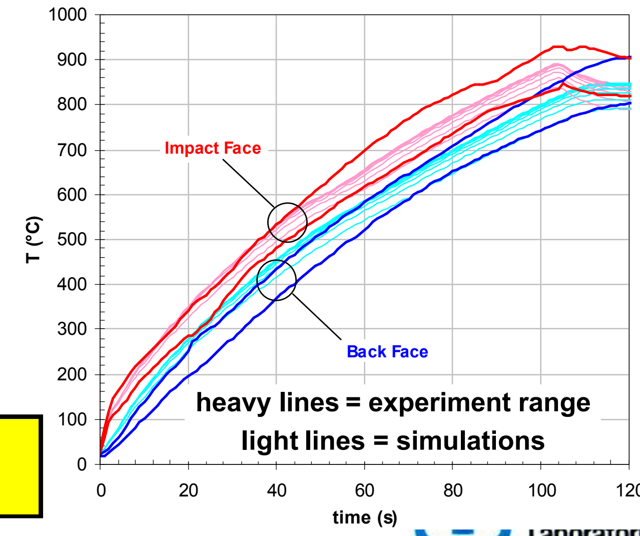
Experimental Data







Experiment & Simulations



∴ With parameters fixed by available data, reasonable agreement of simulation with experimental temperatures was achieved.

Conclusions

- A new model for deposit behavior has been developed and implemented.
- Improvement over previous work:
  - allows for multi-dimensional (behavior)
  - allows for easier integration of radiation & convection boundary conditions
  - more numerically robust
- The model uses time-varying
  - density,
  - non-isotropic thermal conductivity, and
  - volumetric heat sources

  to represent growing deposit layer.
- A suite of model verification test problems demonstrated that energy was conserved and correct thermal conduction behavior was achieved.
- Model compared reasonably with experimental measurements using measured and predicted parameters.

Current and Future Plans

- Code Coupling
  - We are actively working on coupling this model directly to a CFD flame code (Sierra Mechanics—Fuego). This will allow time-and-spatially varying deposit characteristics (rate, temperature, composition,) to be included more easily, as well as provide feedback to the flame.
- Additional Physics
  - We have begun investigating chemical / physical phenomena associated with the deposit and substrate materials. These may include:
    - intermetallic or thermite type reactions between deposit and substrate,
    - dissolution or alloying of deposit and substrate,
    - continued combustion of deposited material (vaporization of aluminum, heterogeneous surface combustion, or re-entrainment of aluminum droplets).
  - We would like to develop the capability to represent these phenomena within the finite element framework.

Acknowledgements

We appreciate the efforts of:

- Vern Nicolette for the VULCAN simulations used as some of the boundary conditions in model validation.
- Experimental team (NASA, SNL, Ktech, En'Urga, FOILS, NMSU, U. Alabama) for the data used for comparison.

This work was funded by SNL under Campaign Six and Verification & Validation programs.

Questions?

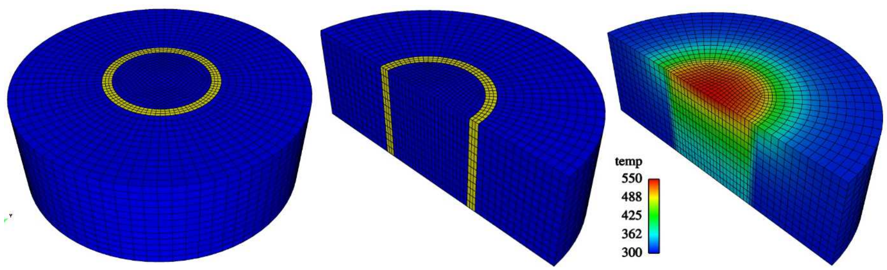
Backup Slides

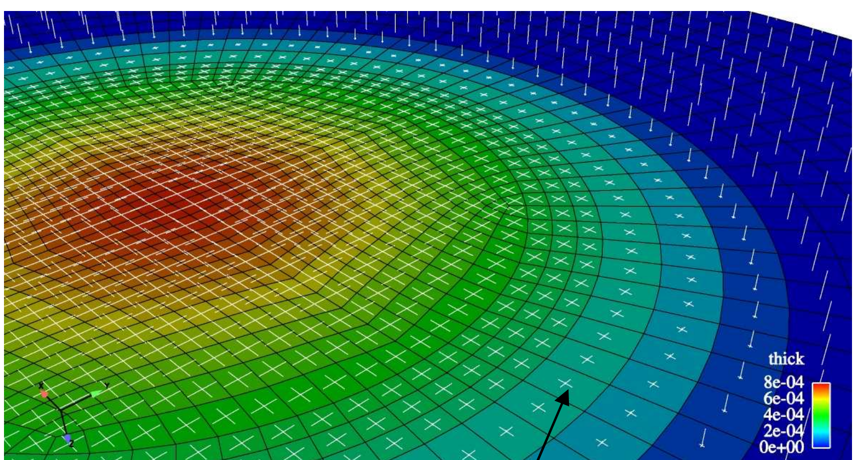
Multi-Dimensional Deposition Model

(Demonstration of Flat Geometry)

Button Calorimeter

(Gaussian distribution of deposit)

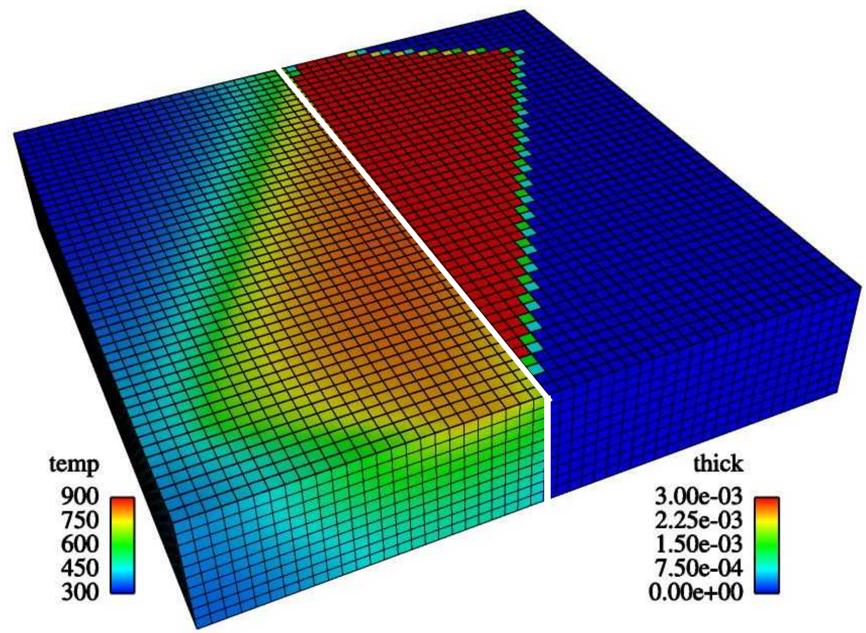




white lines proportional to thermal conductivity in various directions

Flat Plate

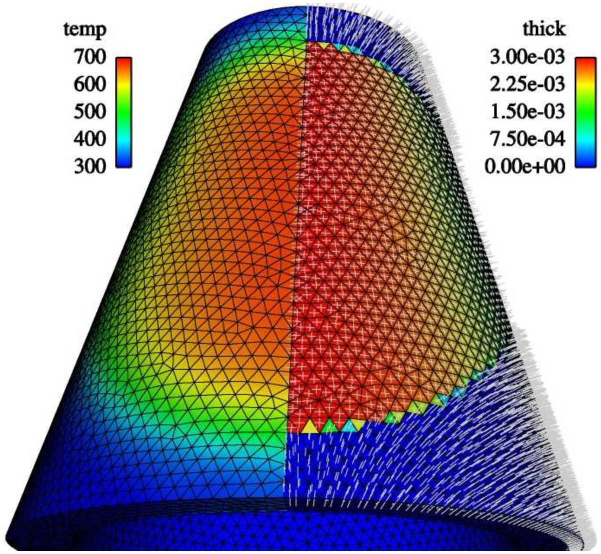
(partially exposed to deposit)

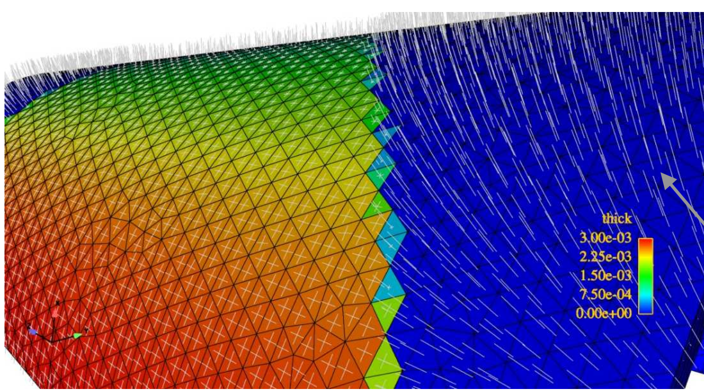


Multi-Dimensional Deposition Model

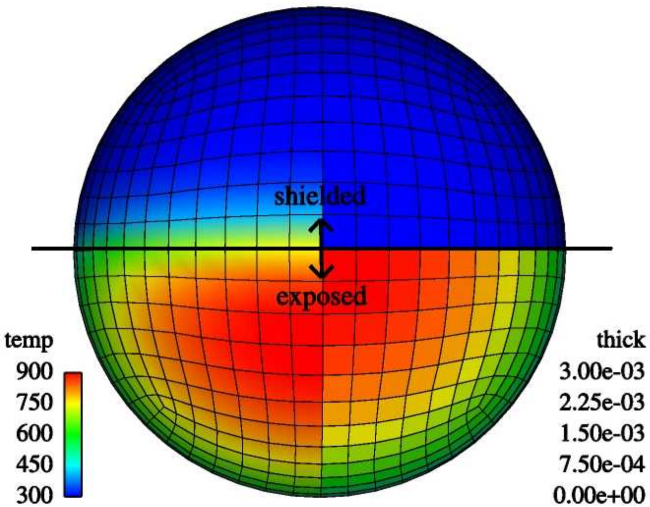
(Demonstration of Conical & Spherical Geometries)

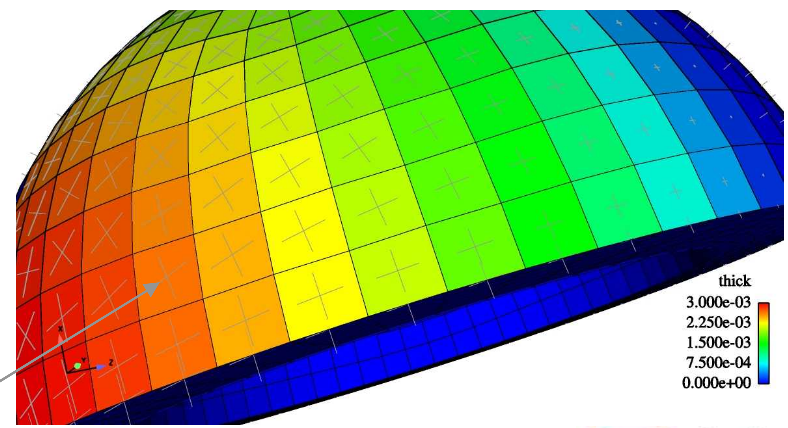
Conical Geometry
(with tetrahedral elements)





Spherical Geometry
(partially shielded)





lines proportional to thermal conductivity in various directions

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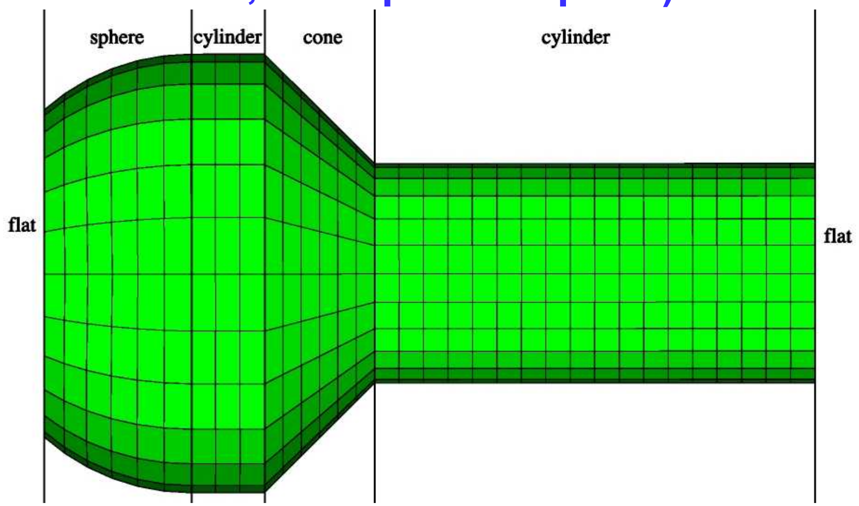
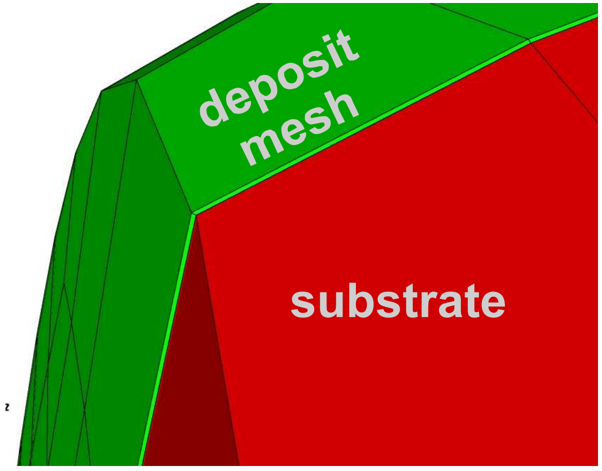
Multi-Dimensional Deposition Model

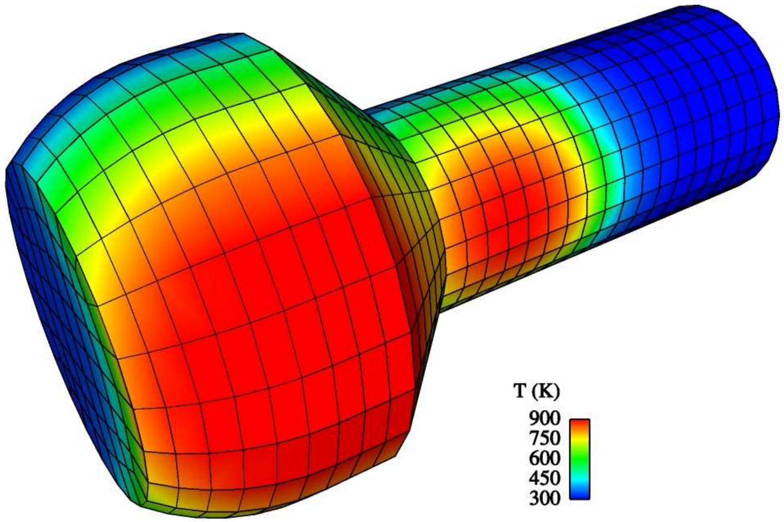
(Demonstration of Various Geometries)

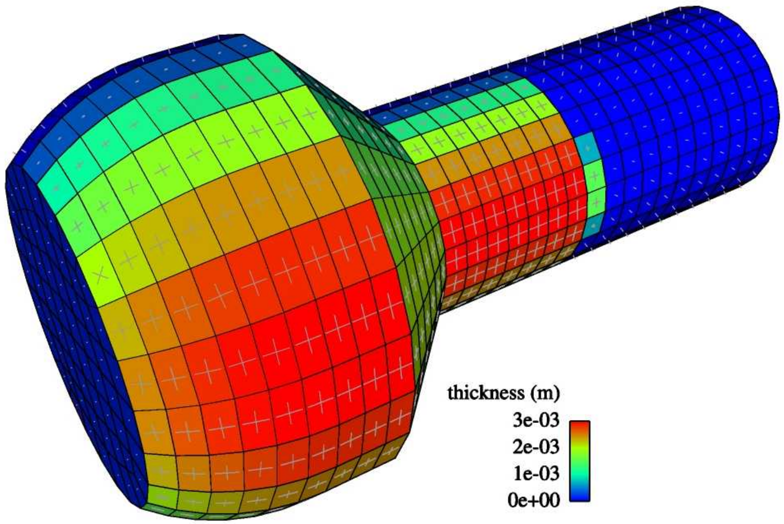
Composite Geometry

(made of flat, cylindrical, conical, and spherical parts)









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