

Multiscale Thermal Conductivity Modeling of 3D Woven Composite Thermal Protection System Materials

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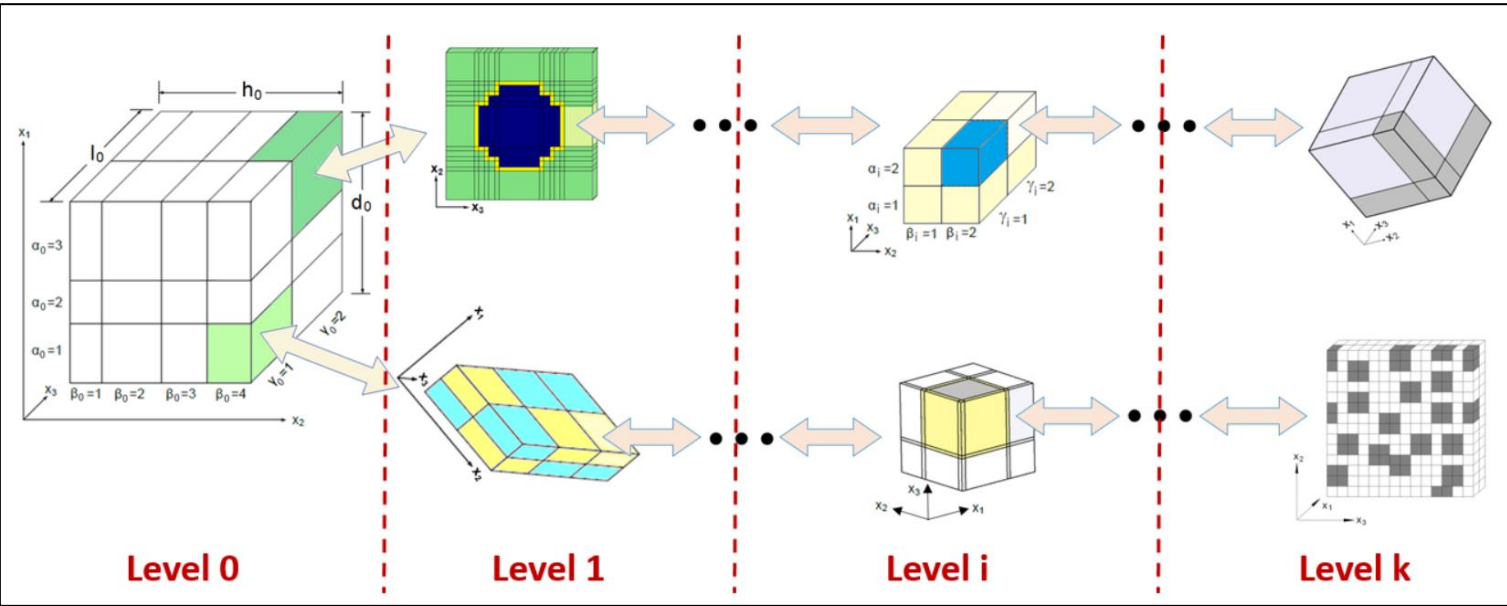
Overview

1. Multiscale Recursive Micromechanics (MsRM) for thermal conductivity
2. Multiscale model of 3D woven TPS composite
3. Results
 - Microscale
 - Mesoscale
 - Macroscale
 - Macroscale sensitivity analysis



Multiscale Recursive Micromechanics (MsRM)

Implemented in the NASA Multiscale Analysis Tool (NASMAT) software



Temperature gradient

$$\left[\frac{\partial T}{\partial x_j} \right]_i^{(\alpha_i)} = -\mathbf{X}_i^{(\alpha_i)}$$

Heat flux

$$\mathbf{q}_i^{(\alpha_i)} = \boldsymbol{\kappa}_i^{(\alpha_i)} \mathbf{X}_i^{(\alpha_i)}$$

Concentration equation
(HFGMC*)

$$\mathbf{X}_i^{(\alpha_i)} = \mathbf{A}_i^{(\alpha_i)} \bar{\mathbf{X}}_i$$

Homogenization

$$\boldsymbol{\kappa}_0^* = \sum_{\alpha_0} v_{\alpha_0} \left\{ \left(\mathbf{T}_2^1 \right)^{-1} \sum_{\alpha_1} v_{\alpha_1} \left[\left(\mathbf{T}_2^2 \right)^{-1} \sum_{\alpha_2} v_{\alpha_2} \boldsymbol{\kappa}_2^{(\alpha_2)} \mathbf{A}_2^{(\alpha_2)} \right]^{(\alpha_1)} \mathbf{A}_1^{(\alpha_1)} \right\}^{(\alpha_0)} \mathbf{A}_0^{(\alpha_0)}$$

Localization

$$\left\{ \left[\mathbf{X}_2^{(\alpha_2)} \right]^{(\alpha_1)} \right\}^{(\alpha_0)} = \left\{ \left[\mathbf{A}_2^{(\alpha_2)} \right]^{(\alpha_1)} \right\}^{(\alpha_0)} \left\{ \left[\mathbf{T}_1^2 \right]^{(\alpha_1)} \right\}^{(\alpha_0)} \left\{ \mathbf{A}_1^{(\alpha_1)} \right\}^{(\alpha_0)} \left\{ \mathbf{T}_1^1 \right\}^{(\alpha_0)} \mathbf{A}_0^{(\alpha_0)} \bar{\mathbf{X}}_0$$

*Bednarczyk, B.A., Aboudi, J., and Arnold, S.M. (2017) "Micromechanics of Composite Materials Governed by Vector Constitutive Laws" *IJSS*, 110-111, 137-151.

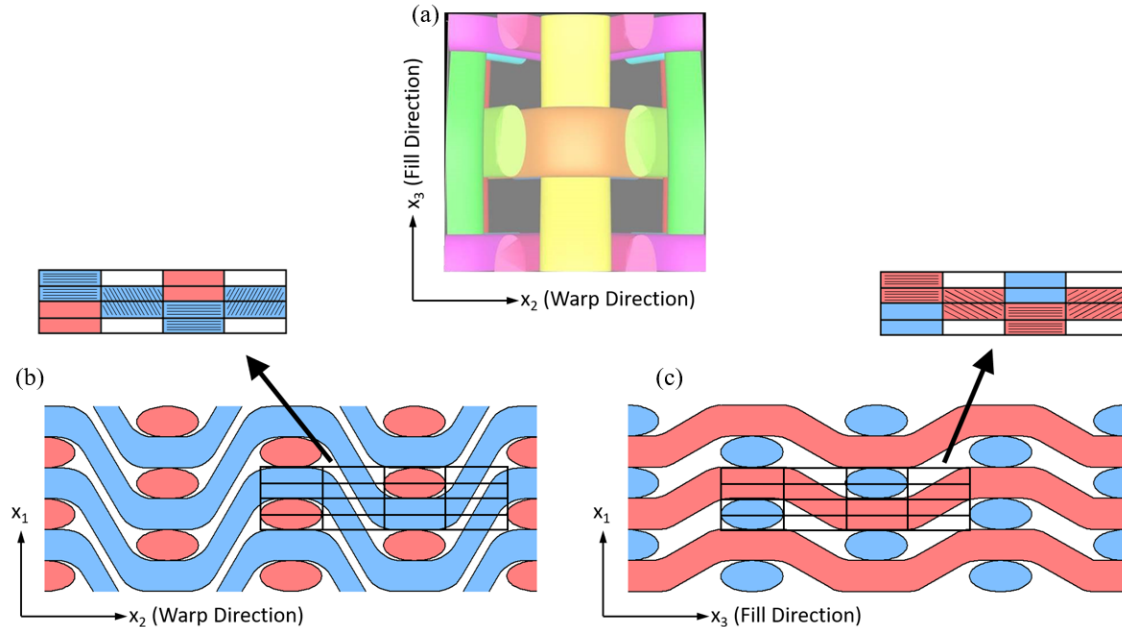


3D Medium Density Carbon Phenolic (3MDCP)

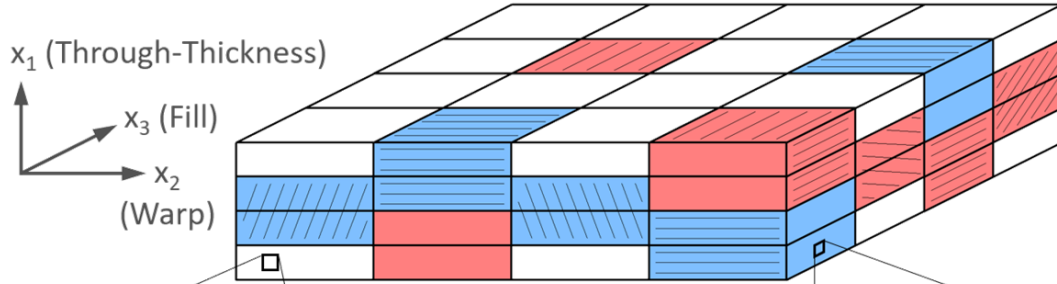
High-Fidelity Generalized Method of Cells (HFGMC)
model of 3MDCP woven microstructure



Image from: Fahy, W.P., Chang, A., Wu, H., and Koo, J.H.
"Recent Developments of Ablative Thermal Protection
Systems for Atmospheric Entry", AIAA SciTech 2021, 19–
21 January, 2021.

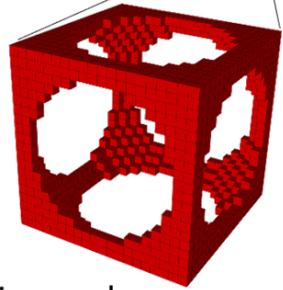


MsRM Model of 3MDCP

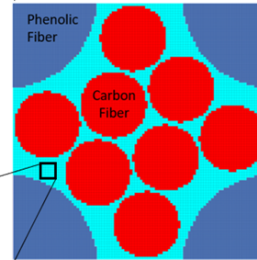


Macroscale
Woven Composite

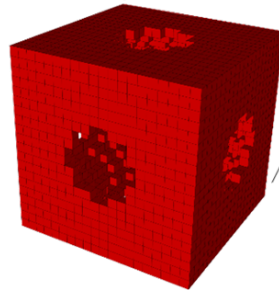
Note: Detailed microscopy and CT-scan studies underway



Microscale
Inter-tow Porous Phenolic Resin



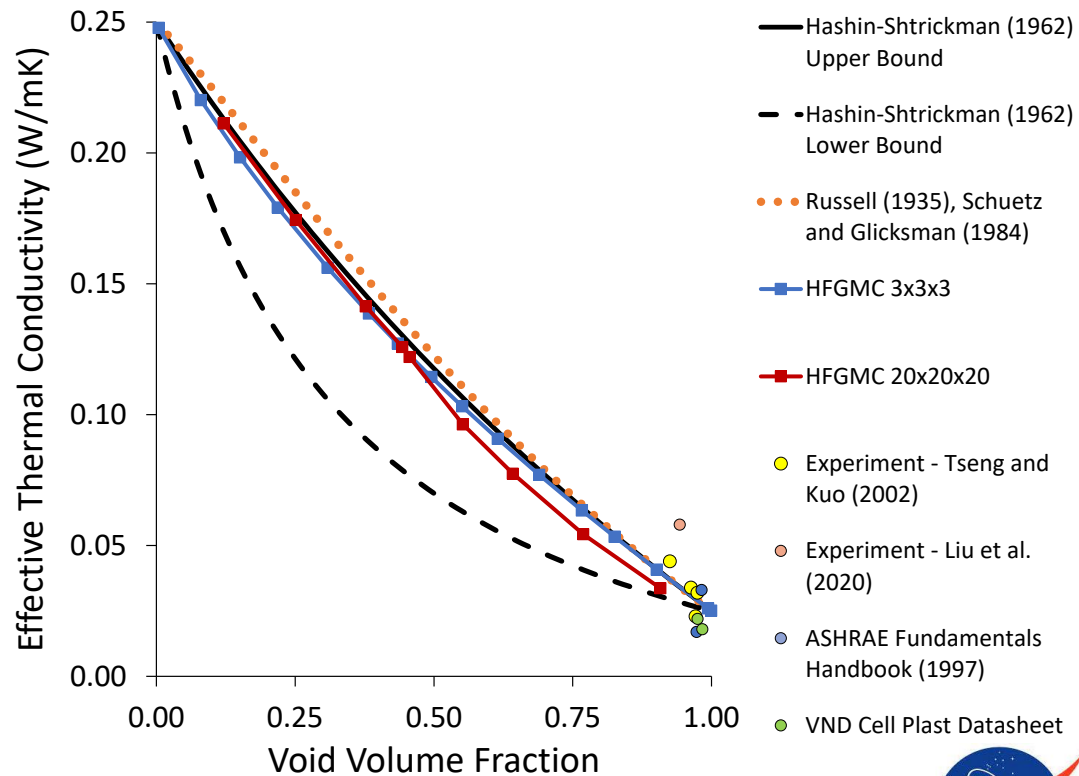
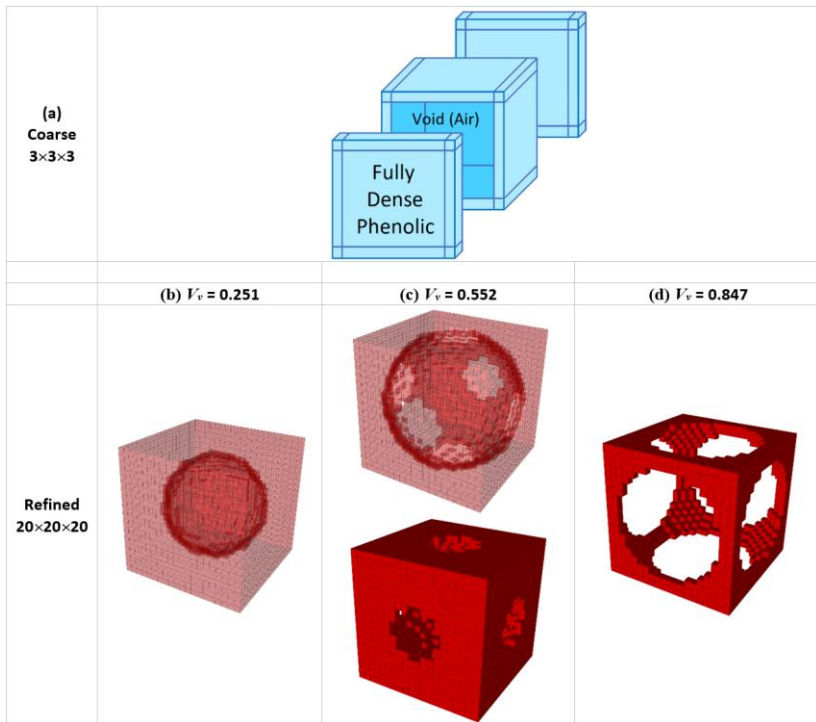
Mesoscale
Blended Tow



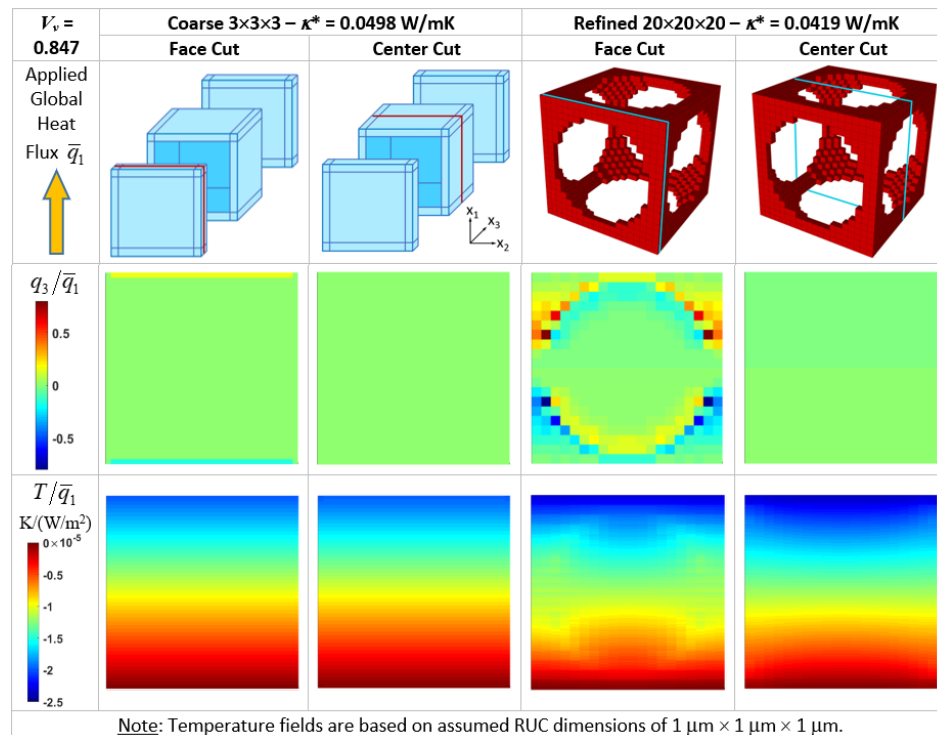
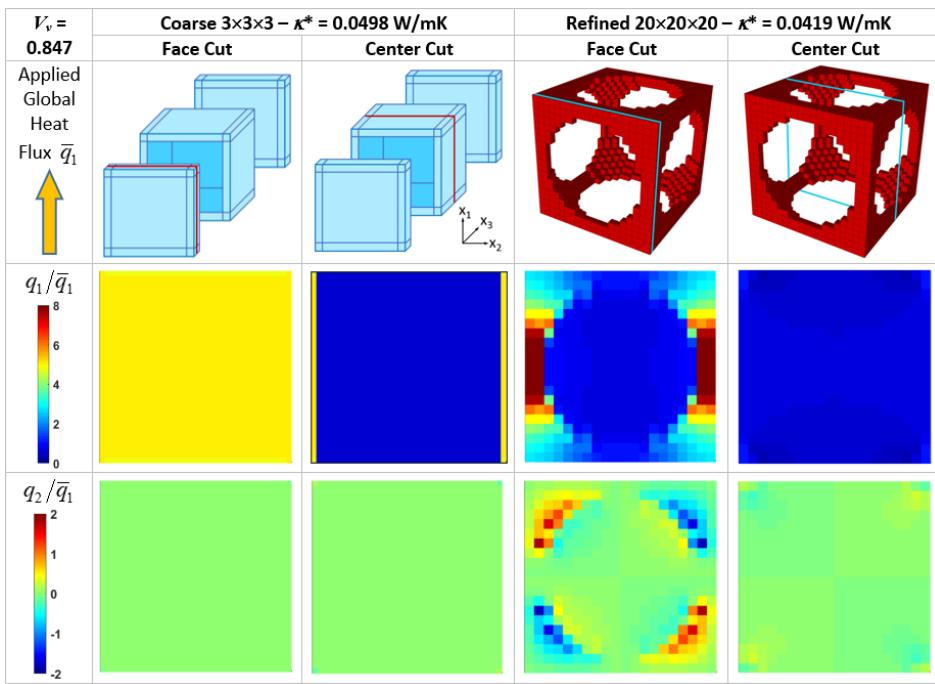
Microscale
Intra-tow Porous Phenolic Resin

	κ_{Axial} (W/mK)	$\kappa_{\text{Transverse}}$ (W/mK)
AS4 Carbon Fiber	6.83	0.5
Phenolic Fiber	0.25	0.25
Phenolic Matrix	0.25	0.25
Air inside voids	0.025	0.025

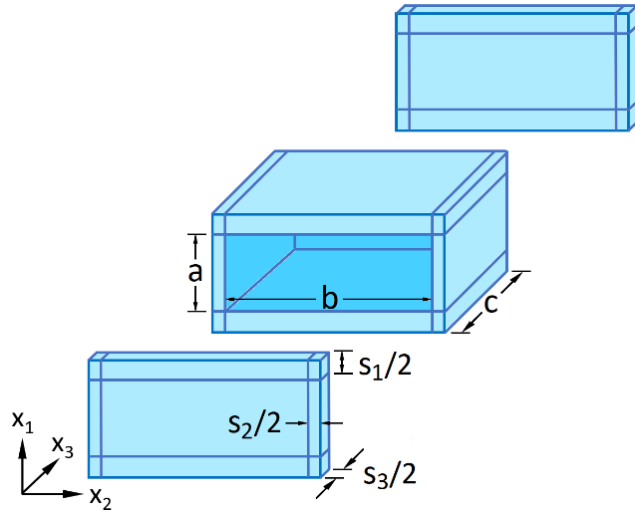
Microscale Effective Conductivity Predictions



Microscale Local Fields



Oblate Void Shape

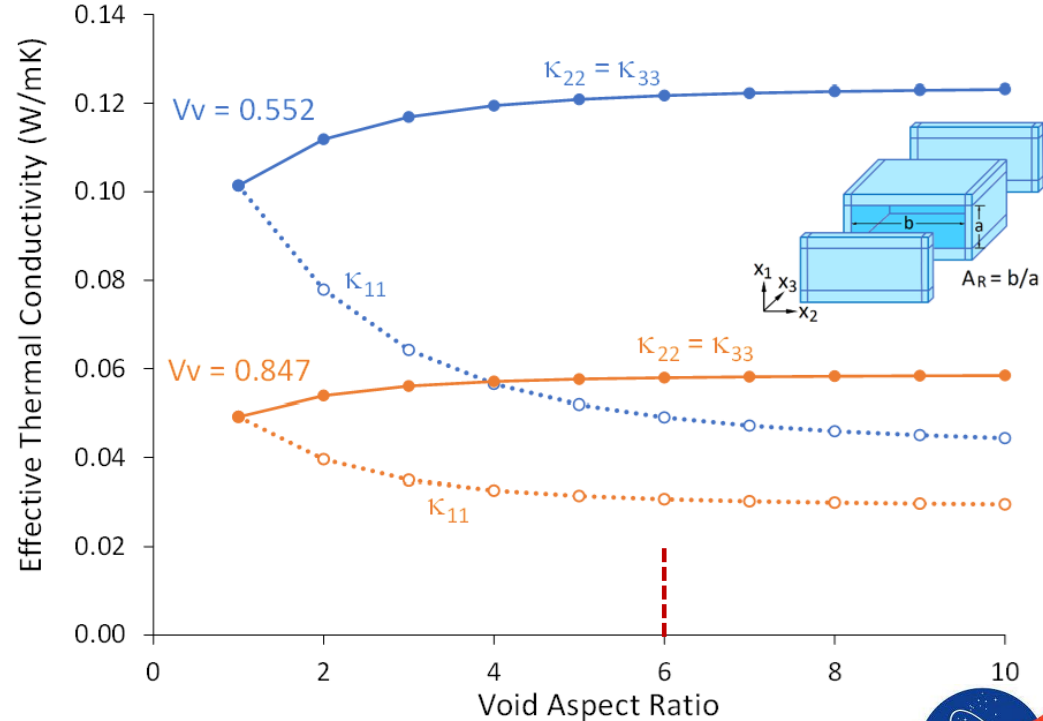


$$A_R^2 a^3 - V_v (1 - A_R^2) a - V_v A_R = 0$$

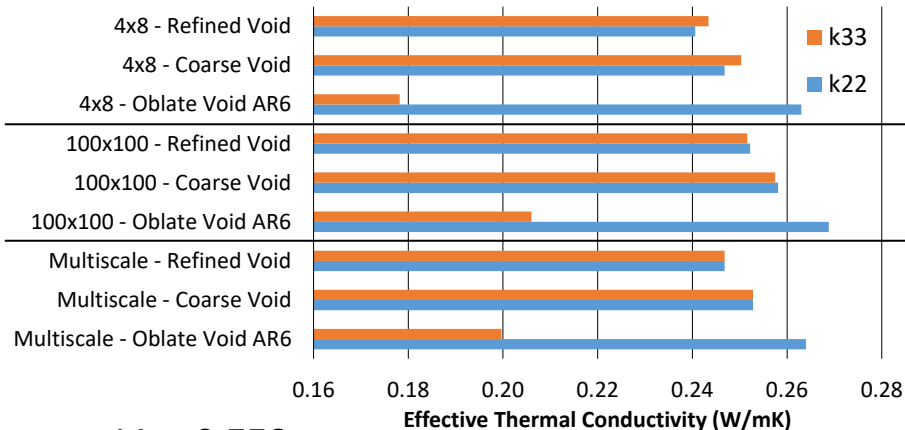
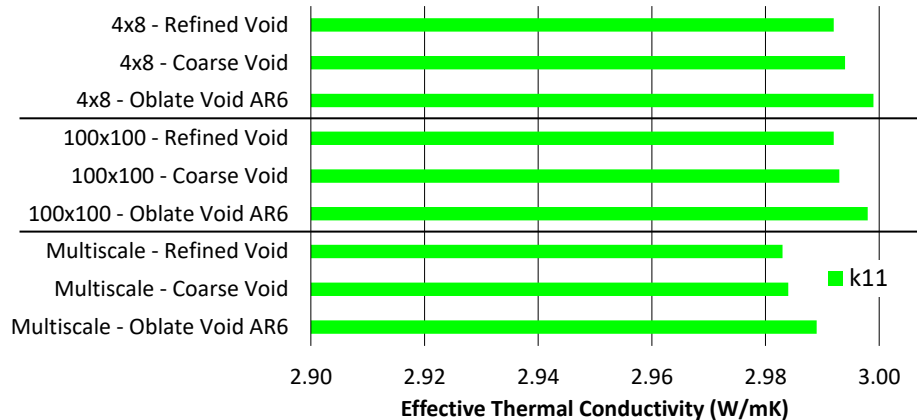
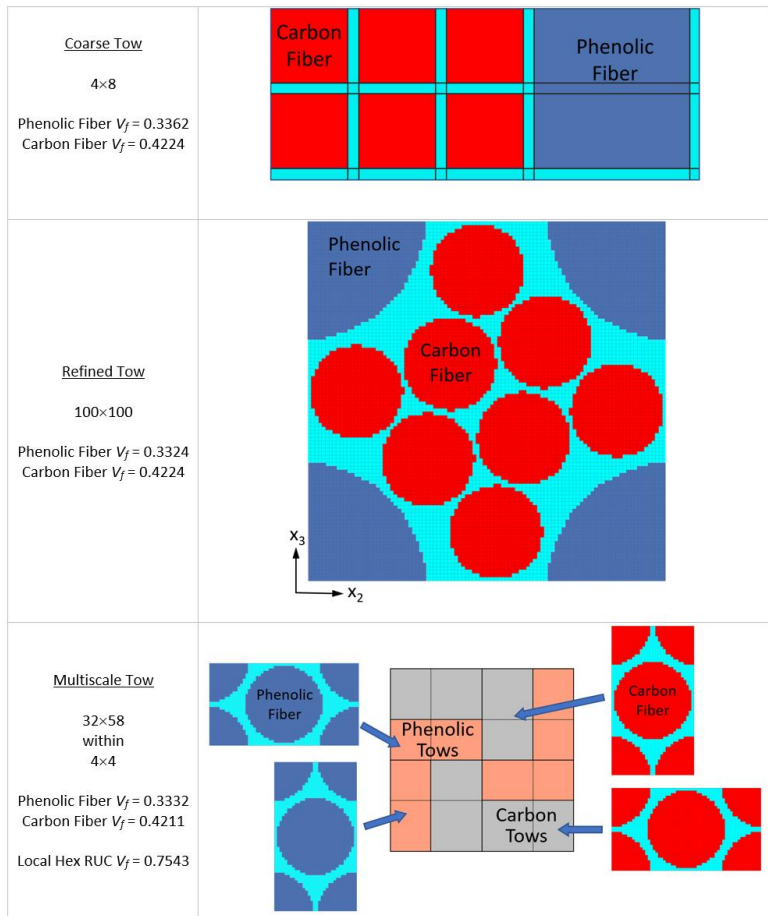
$$A_R = \frac{b}{a} \quad s_1 = A_R (1 - b) \quad \frac{s_1}{s_2} = A_R$$

8

Effect of oblate void aspect ratio

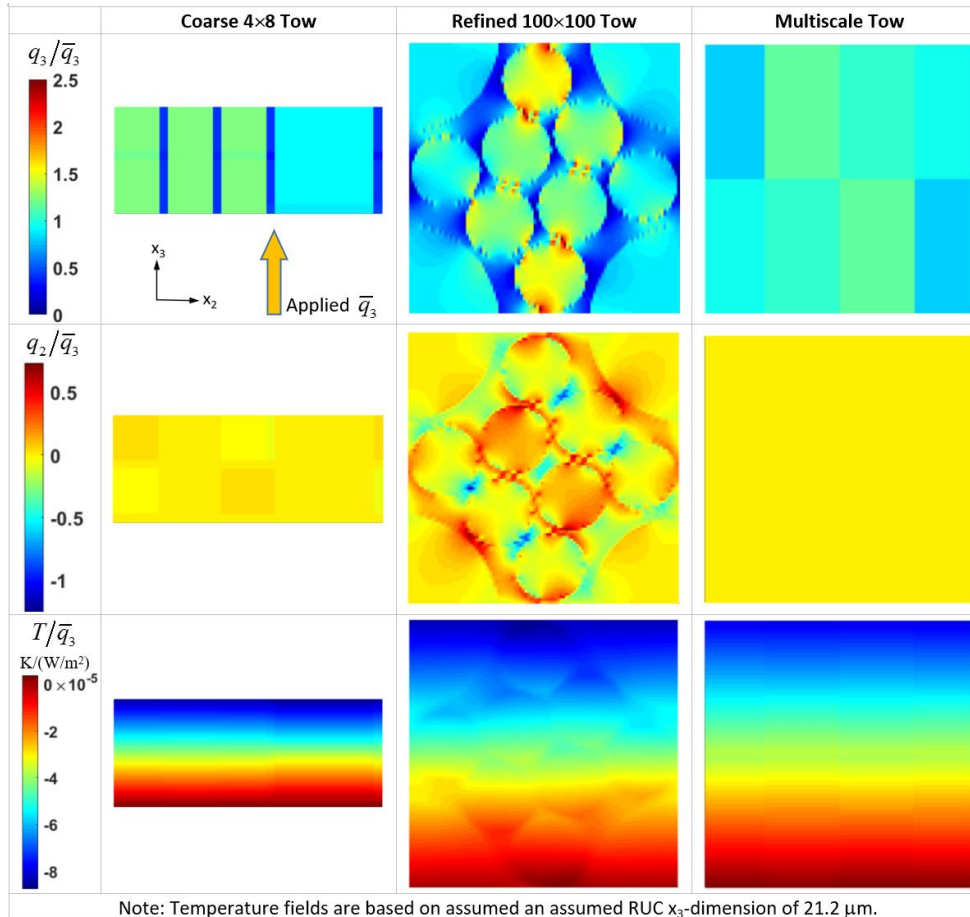


Mesoscale (Blended Tow) Effective Thermal Conductivities



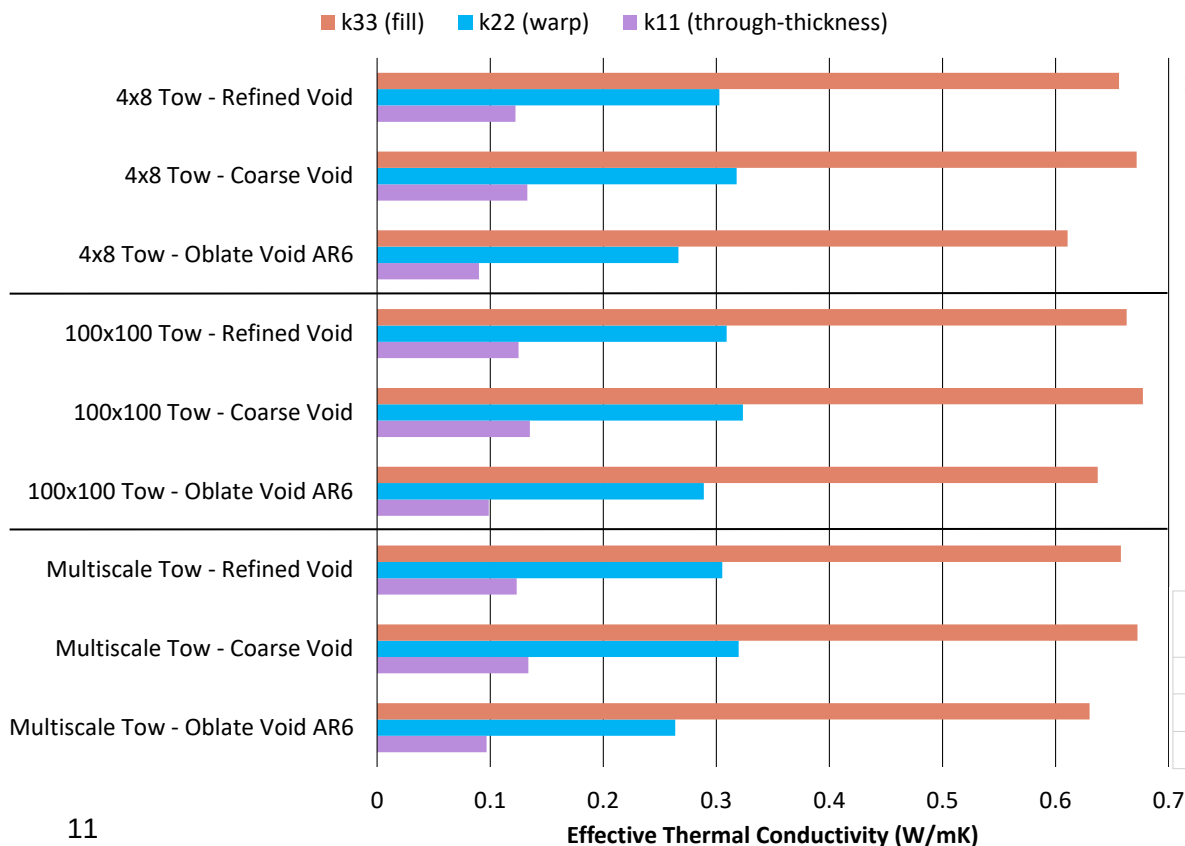
Intra-tow $V_v = 0.552$

Mesoscale (Blended Tow) Local Thermal Fields

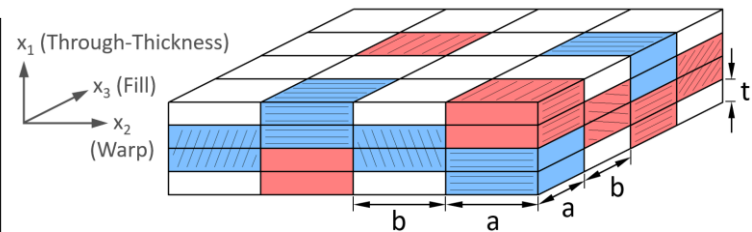


	κ_{Axial} (W/mK)	$\kappa_{\text{Transverse}}$ (W/mK)
AS4 Carbon Fiber	6.83	0.5
Phenolic Fiber	0.25	0.25
Phenolic Matrix	0.25	0.25
Air inside voids	0.025	0.025

Macroscale (3MDCP) Effective Thermal Conductivities



Inter-tow $V_v = 0.847$ Intra-tow $V_v = 0.552$



Geometric Parameters

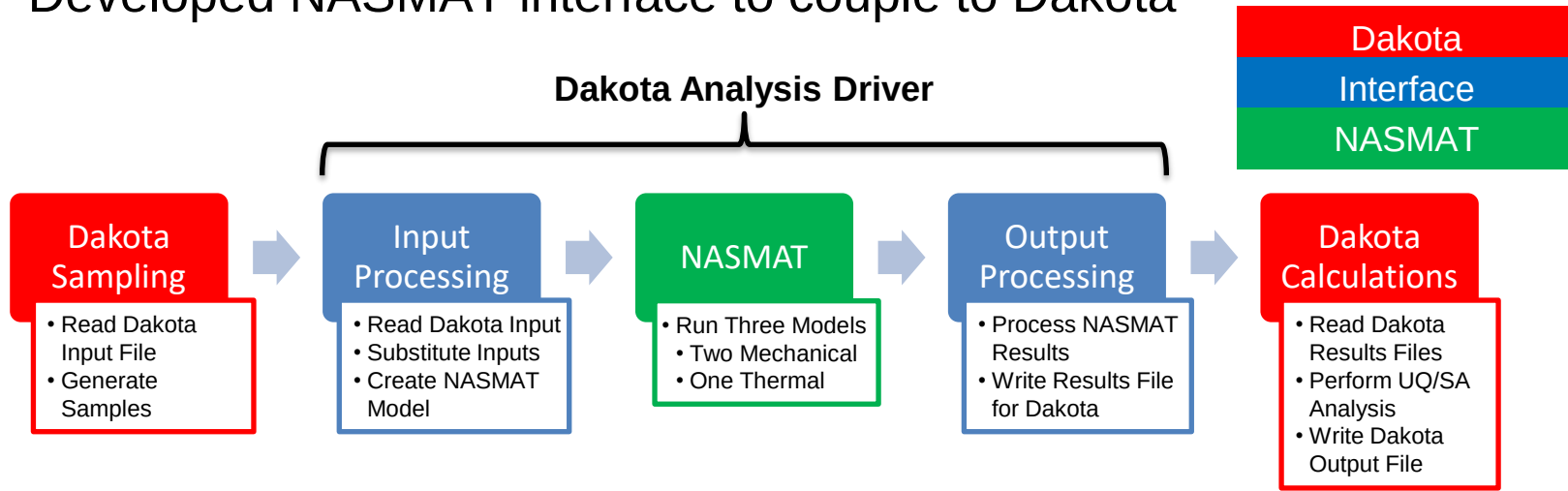
a (mm)	b (mm)	t (mm)	Fill Angle (°)	Warp Angle (°)
1.41	1.13	0.177	17.4	46.8

Overall Constituent Volume Fractions

	Phenolic Fiber	Carbon Fiber	Fully Dense Phenolic Matrix	Void
4x8 Tows	0.1869	0.2349	0.1281	0.4501
100x100 Tows	0.1858	0.2349	0.1290	0.4513
Multiscale Tows	0.1852	0.2341	0.1291	0.4515

Sensitivity Analysis through Dakota Coupling

- Dakota - open-source software from Sandia National Laboratories
 - Uncertainty Quantification (UQ)
 - Sensitivity Analysis (SA)
 - Optimization
 - Parameter Estimation
- Developed NASMAT interface to couple to Dakota



Sensitivity Analysis Input Variables

Geometry Parameters

Quantity	Variable	Mean	CV
Tow Width (mm)	W_TOW	1.41224	0.1
Matrix Width (mm)	W_MAT	1.12776	0.1
Tow Height (mm)	TOW_H	0.35306	0.1
AS4 Tow Fiber Vol. Fr.	VF_CF	0.754	0.1
Phenolic Fiber Vol. Fr.	VF_P	0.754	0.1
Inter-tow porosity	INTER_V	0.847	0.1
Intra-tow porosity	INTRA_V	0.552	0.1

Material Properties

Quantity	Variable	Mean	CV
AS4 Axial κ (W/m*K)	K11_CF	6.83	0.1
AS4 Transverse κ (W/m*K)	K22_CF	0.5	0.1
Phenolic κ (W/m*K)	K_P	0.25	0.1
Void κ (W/mm*K)	K_V	0.000025	0.1

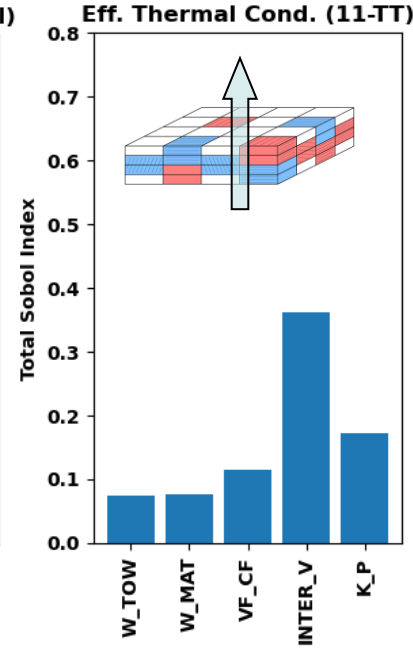
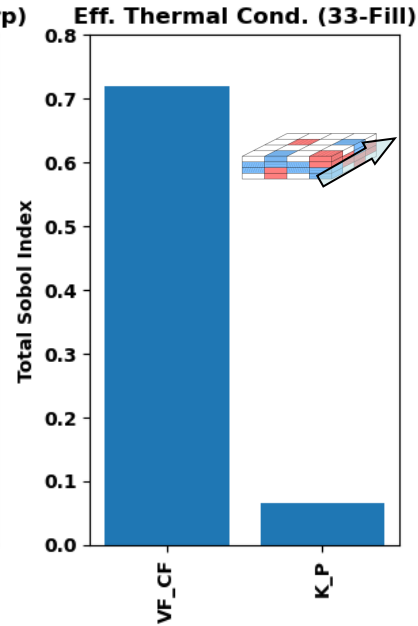
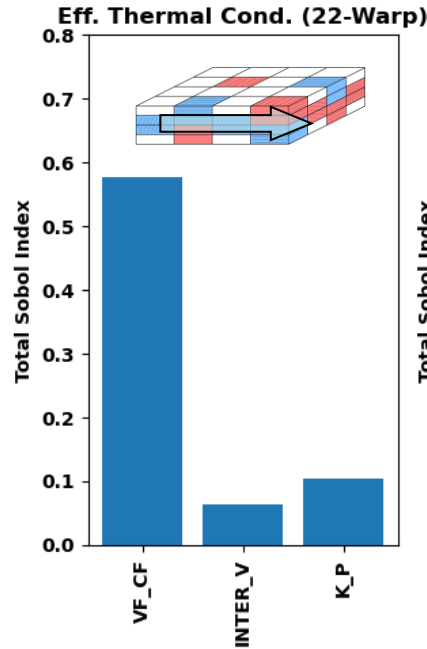
- 780 samples generated using Latin Hypercube Sampling (more likely needed)
- Variance-based decomposition (Sobol method) used to determine importance of inputs
- First and Total Sobol indices computed
- Total Sobol indices from all contributions sum to one
- Higher the index, more significant the input parameter
- Values less than 0.05 not shown



Sensitivity Analysis Results

- Warp/Fill directions consistent, Carbon fiber volume fraction dominant
- Results different for through-thickness direction (likely due to less CFs aligned in that direction)
- *MsRM efficiency is critical here*

Tow Width (mm)	W_TOW
Matrix Width (mm)	W_MAT
Tow Height (mm)	TOW_H
AS4 Tow Fiber Vol. Fr.	VF_CF
Phenolic Fiber Vol. Fr.	VF_P
Inter-tow porosity	INTER_V
Intra-tow porosity	INTRA_V



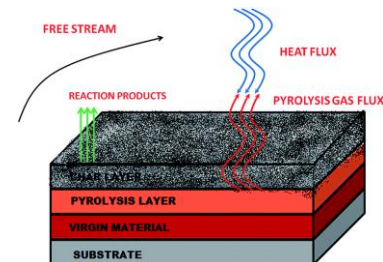
AS4 Axial K (W/m*K)	K11_CF
AS4 Transverse K (W/m*K)	K22_CF
Phenolic K (W/m*K)	K_P
Void K (W/mm*K)	K_V



Major Points

- Multiscale Recursive Micromechanics (MsRM)
 - Version for effective thermal conductivity using HFGMC theory
- Very effective for predictions for 3MDCP (3D woven TPS)
 - Effect of microstructure for void, blended tow, woven composite
 - Sensitivity studies
- Future work:
 1. Coupling with mechanical problem damage progression
 2. Ablation physics
 3. Design/optimize *the* material – ICME

microscopy and test results forthcoming



Badhe & Balasubramanian
(2014) RSC Advances

