INDIAN INSTITUTE OF TECHNOLOGY KANPUR

PROJECT TITLE:

Micromechanical Modeling of AS4/3501-6 Composites

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Submitted by:

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INTRODUCTION:

This project investigates the effective mechanical and thermal properties of AS4 carbon fibre reinforced 3501-6 epoxy matrix composites through four distinct micromechanical modeling approaches. The study compares predictions of elastic moduli (E_1, E_2, G_{12}), Poisson's ratio (ν_{12}), and coefficients of thermal expansion (α_1, α_2) across the full range of fibre volume fractions (Vf = 0-100%).

MATERIAL PROPERTIES:

The composite system consists of:

AS4 Carbon Fiber Properties:

- Longitudinal modulus, E1=225GPa
- Transverse modulus, E2=15 GPa
- In-plane shear modulus, G12=15 GPa
- Major Poisson's ratio, ν12==0.2
- Longitudinal CTE, $\alpha 1=-0.5\times10-6/\circ C$
- Transverse CTE, $\alpha 2=15\times10-6/\circ C$

3501-6 Epoxy Matrix Properties:

- Young's modulus, Em=4.2 GPa
- Poisson's ratio, vm=0.340.34
- Shear modulus, Gm=1.57 GPa
- CTE, $\alpha m=45\times10-6/\circ C$

This project analyzes AS4 carbon fiber/3501-6 epoxy composites using four methods:

1. Strength of Materials Approach
   • Rule of mixtures (longitudinal)
   • Inverse rule (transverse)
2. Standard Mechanics Approach
   • Stiffness tensor transformation
3. Hill's Concentration Method
   • Voigt-Reuss-Hill averaging
4. CCA Model
   • Concentric cylinder elasticity solution

April 10, 2025

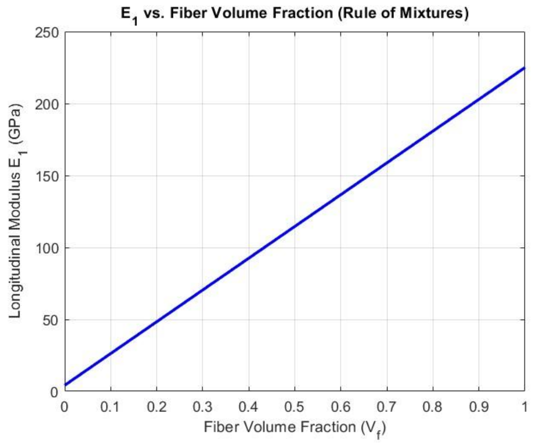
1. Strength of Materials Approach

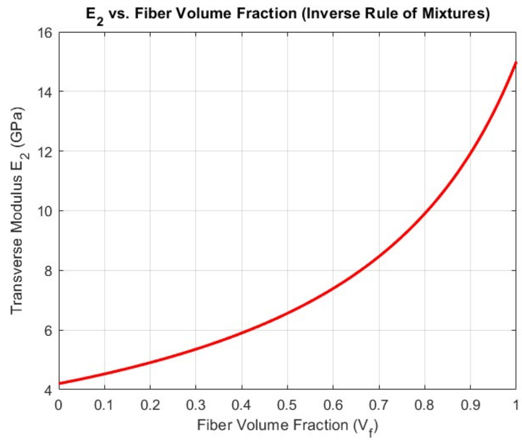
```matlab
clc; clear; close all;

% Fiber (AS4 Carbon)
Ef = 225;       % Longitudinal modulus (GPa)
Ef2 = 15;       % Transverse modulus (GPa)
Gf = 15;        % Shear modulus (GPa)
vf = 0.2;       % Poisson's ratio
alpha_f1 = -0.5e-6; % Longitudinal CTE (1/ C )
alpha_f2 = 15e-6;   % Transverse CTE (1/ C )

% Matrix (3501-6 Epoxy)
Em = 4.2;       % Isotropic modulus (GPa)
vm = 0.34;      % Poisson's ratio
Gm = Em/(2*(1+vm)); % Shear modulus (GPa)
alpha_m = 45e-6; % CTE (1/ C )

% Vary fiber volume fraction from 0 to 1
Vf_range = linspace(0, 1, 100);
results = zeros(length(Vf_range), 6);

for i = 1:length(Vf_range)
    Vf = Vf_range(i);
    Vm = 1 - Vf;

    % 1. Mechanical Properties
    E1 = Vf*Ef + Vm*Em;                         % Longitudinal modulus
    E2 = 1/(Vf/Ef2 + Vm/Em);                    % Transverse modulus
    G12 = 1/(Vf/Gf + Vm/Gm);                    % Shear modulus
    nu12 = Vf*vf + Vm*vm;                       % Poisson's ratio

    % 2. Thermal Expansion (Schapery Model)
    alpha1 = (Vf*Ef*alpha_f1 + Vm*Em*alpha_m)/E1;
    alpha2 = (1 + vf)*Vf*alpha_f2 + (1 + vm)*Vm*alpha_m - nu12*alpha1;

    % Store results
    results(i,:) = [E1, E2, G12, nu12, alpha1*1e6, alpha2*1e6];
end

% Plot E1 vs. Vf
figure(1);
plot(Vf_range, results(:,1), 'b-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Longitudinal Modulus E_1 (GPa)');
title('E_1 vs. Fiber Volume Fraction (Rule of Mixtures)');
grid on;

% Plot E2 vs. Vf
figure(2);
plot(Vf_range, results(:,2), 'r-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Transverse Modulus E_2 (GPa)');
title('E_2 vs. Fiber Volume Fraction (Inverse Rule of Mixtures)');
grid on;
```

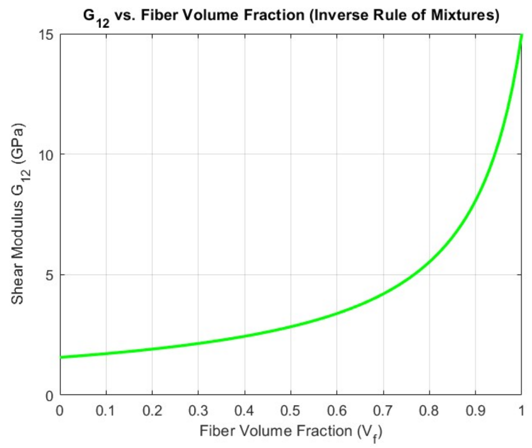
```

% Plot G12 vs. Vf
figure(3);
plot(Vf_range, results(:,3), 'g-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Shear Modulus G_{12} (GPa)');
title('G_{12} vs. Fiber Volume Fraction (Inverse Rule of Mixtures)');
grid on;

% Plot  12  vs. Vf
figure(4);
plot(Vf_range, results(:,4), 'm-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Poisson''s Ratio \nu_{12}');
title('\nu_{12} vs. Fiber Volume Fraction (Rule of Mixtures)');
grid on;

% Plot  1  vs. Vf
figure(5);
plot(Vf_range, results(:,5), 'k-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Longitudinal CTE \alpha_1 (10^{-6}/ C )');
title('\alpha_1 vs. Fiber Volume Fraction (Schapery Model)');
grid on;

% Plot  2  vs. Vf
figure(6);
plot(Vf_range, results(:,6), 'c-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Transverse CTE \alpha_2 (10^{-6}/ C )');
title('\alpha_2 vs. Fiber Volume Fraction (Schapery Model)');
grid on;
```

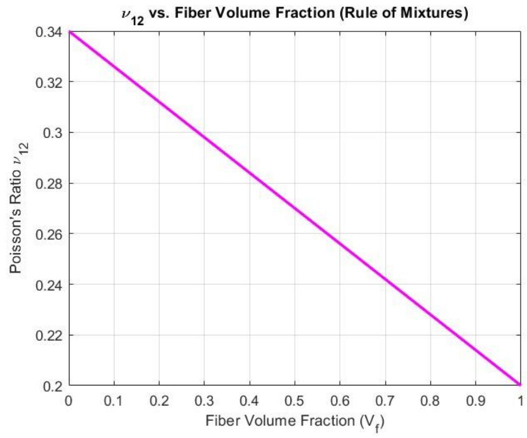
Listing 1: Strength of Materials MATLAB Code

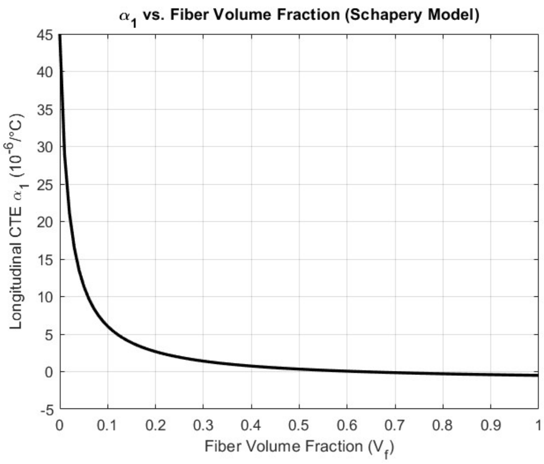
Graphical Result for Strength of Materials Approach:

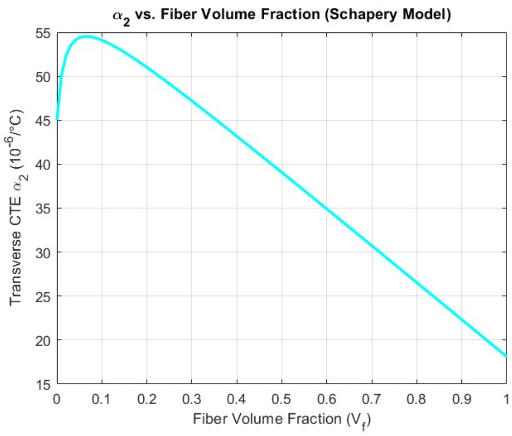












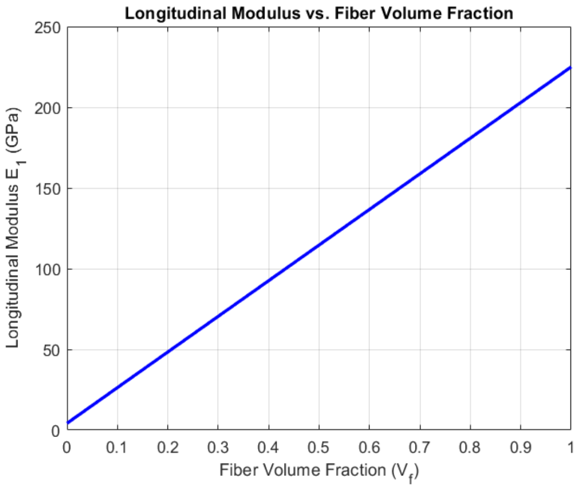
2. Standard Mechanics Approach

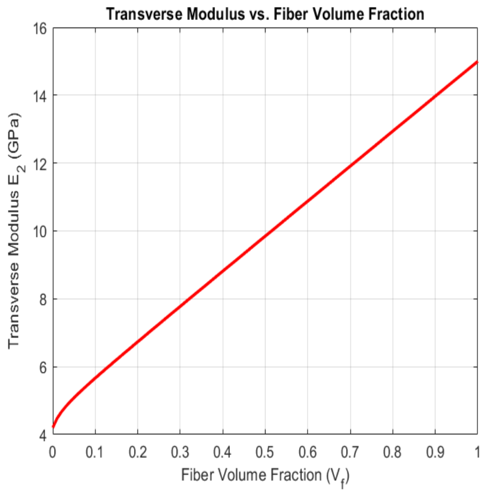
```
clc; clear; close all;

% Fiber properties (AS4 Carbon)
Ef1 = 225;      % Longitudinal modulus (GPa)
Ef2 = 15;       % Transverse modulus (GPa)
Gf12 = 15;      % Shear modulus (GPa)
vf12 = 0.2;     % Poisson's ratio
alpha_f1 = -0.5e-6; % Longitudinal CTE (1/ C )
alpha_f2 = 15e-6;   % Transverse CTE (1/ C )

% Matrix properties (3501-6 Epoxy)
Em = 4.2;       % Isotropic modulus (GPa)
vm = 0.34;      % Poisson's ratio
Gm = Em / (2*(1 + vm)); % Matrix shear modulus (GPa)
alpha_m = 45e-6; % Matrix CTE (1/ C )

% Vary volume fraction from 0 to 1
Vf_range = linspace(0, 1, 100);
results = zeros(length(Vf_range), 6); % Store E1, E2, G12, nu12, alpha1, alpha2

for i = 1:length(Vf_range)
    Vf = Vf_range(i);
    Vm = 1 - Vf;

    % Fiber stiffness matrix [Cf] (Orthotropic)
    Cf11 = Ef1 / (1 - vf12^2 * (Ef2/Ef1));
    Cf12 = vf12 * Ef2 / (1 - vf12^2 * (Ef2/Ef1));
    Cf22 = Ef2 / (1 - vf12^2 * (Ef2/Ef1));
    Cf = [Cf11, Cf12,    0;
          Cf12, Cf22,    0;
            0,    0, Gf12];

    % Matrix stiffness matrix [Cm] (Isotropic)
    Cm11 = Em / (1 - vm^2);
    Cm12 = vm * Em / (1 - vm^2);
    Cm = [Cm11, Cm12,    0;
          Cm12, Cm11,    0;
            0,    0,   Gm];

    % Effective stiffness and compliance matrices
    C_star = Vf * Cf + Vm * Cm;
    S_star = inv(C_star);         % Effective compliance

    % Mechanical properties
    E1 = 1 / S_star(1,1);
    E2 = 1 / S_star(2,2);
    G12 = 1 / S_star(3,3);
    nu12 = -S_star(1,2) / S_star(1,1);

    % Thermal expansion coefficients (Schapery's Model)
    alpha_1 = (Vf * Ef1 * alpha_f1 + Vm * Em * alpha_m) / (Vf * Ef1 + Vm * Em);
    alpha_2 = (1 + vf12)*Vf*alpha_f2 + (1 + vm)*Vm*alpha_m - nu12*alpha_1;

    % Store results
    results(i,:) = [E1, E2, G12, nu12, alpha_1*1e6, alpha_2*1e6];
end

% Plot E1 vs. Vf
figure(1);
plot(Vf_range, results(:,1), 'b-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Longitudinal Modulus E_1 (GPa)');
title('Longitudinal Modulus vs. Fiber Volume Fraction');
grid on;

```

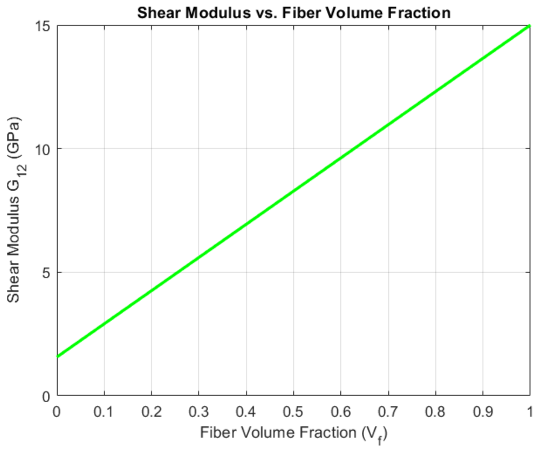
```
% Plot E2 vs. Vf
figure(2);
plot(Vf_range, results(:,2), 'r-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Transverse Modulus E_2 (GPa)');
title('Transverse Modulus vs. Fiber Volume Fraction');
grid on;

% Plot G12 vs. Vf
figure(3);
plot(Vf_range, results(:,3), 'g-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Shear Modulus G_{12} (GPa)');
title('Shear Modulus vs. Fiber Volume Fraction');
grid on;

% Plot  12  vs. Vf
figure(4);
plot(Vf_range, results(:,4), 'm-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Poisson''s Ratio \nu_{12}');
title('Poisson''s Ratio vs. Fiber Volume Fraction');
grid on;

% Plot  1  vs. Vf
figure(5);
plot(Vf_range, results(:,5), 'k-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Longitudinal CTE \alpha_1 (10^{-6}/ C )');
title('Longitudinal CTE vs. Fiber Volume Fraction');
grid on;

% Plot  2  vs. Vf
figure(6);
plot(Vf_range, results(:,6), 'c-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Transverse CTE \alpha_2 (10^{-6}/ C )');
title('Transverse CTE vs. Fiber Volume Fraction');
grid on;
```

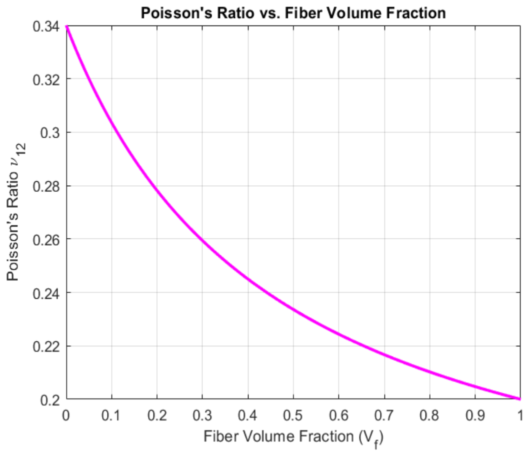
Listing 2: Standard Mechanics MATLAB Code

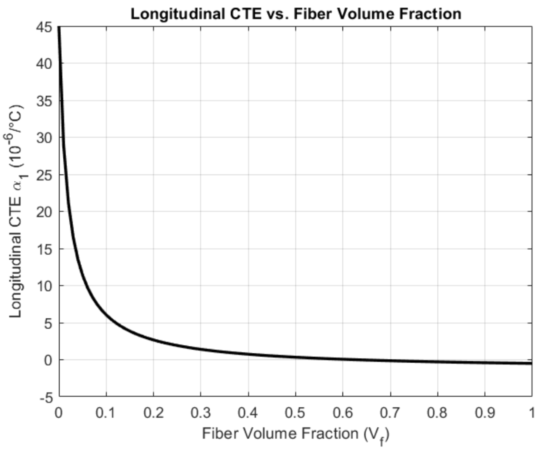
Graphical Result for Standard Mechanics Approach:

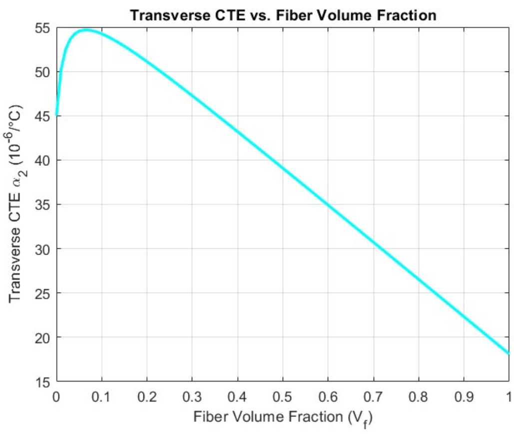












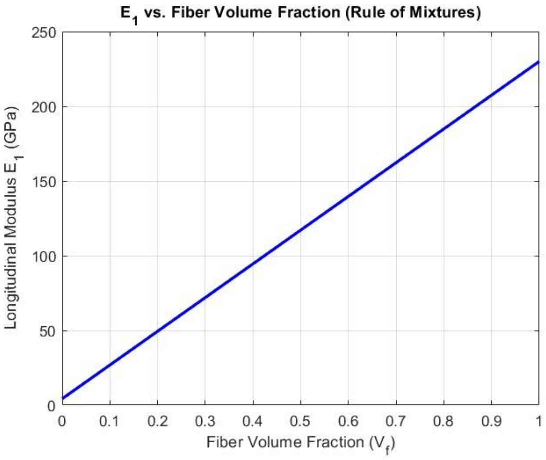
3. Hill's Concentration Factor Approach

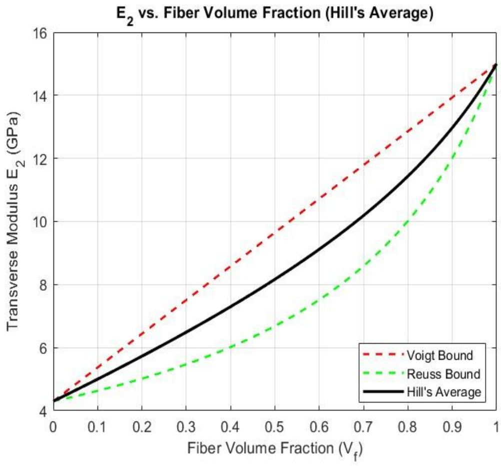
```
clc; clear; close all;
format shortg;

% Fiber (AS4 Carbon)
Ef = 230;       % Longitudinal modulus (GPa)
Ef2 = 15;       % Transverse modulus (GPa)
Gf = 30;        % Shear modulus (GPa)
vf = 0.2;       % Poisson's ratio
alpha_f1 = -0.5e-6; % Longitudinal CTE (1/ C )
alpha_f2 = 10e-6;   % Transverse CTE (1/ C )

% Matrix (3501-6 Epoxy)
Em = 4.3;       % Isotropic modulus (GPa)
Gm = 1.6;       % Shear modulus (GPa)
vm = 0.35;      % Poisson's ratio
alpha_m = 60e-6; % CTE (1/ C )

% Vary fiber volume fraction from 0 to 1
Vf_range = linspace(0, 1, 100);
results = zeros(length(Vf_range), 10); % Corrected to store 10 columns

for i = 1:length(Vf_range)
    Vf = Vf_range(i);
    Vm = 1 - Vf;

    % 1. Longitudinal Modulus (E1)
    E1 = Vf*Ef + Vm*Em;

    % 2. Transverse Modulus (E2) - Hill's Average
    E2_V = Vf*Ef2 + Vm*Em;       % Voigt bound
    E2_R = 1/(Vf/Ef2 + Vm/Em);   % Reuss bound
    E2 = (E2_V + E2_R)/2;        % Hill's average

    % 3. Shear Modulus (G12) - Hill's Average
    G_V = Vf*Gf + Vm*Gm;         % Voigt bound
    G_R = 1/(Vf/Gf + Vm/Gm);     % Reuss bound
    G12 = (G_V + G_R)/2;         % Hill's average

    % 4. Poisson's Ratio (v12)
    v12 = Vf*vf + Vm*vm;

    % 5. Thermal Expansion Coefficients
    alpha1 = (Vf*Ef*alpha_f1 + Vm*Em*alpha_m)/E1;
    alpha2 = Vf*alpha_f2 + Vm*alpha_m;

    % Store results (now 10 values)
    results(i,:) = [E1, E2_V, E2_R, E2, G_V, G_R, G12, v12, alpha1*1e6, alpha2*1e6];
end

% Plot E1 vs. Vf
figure(1);
plot(Vf_range, results(:,1), 'b-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Longitudinal Modulus E_1 (GPa)');
title('E_1 vs. Fiber Volume Fraction (Rule of Mixtures)');
grid on;

% Plot E2 vs. Vf with bounds
figure(2);
plot(Vf_range, results(:,2), 'r--', 'LineWidth', 1.5); hold on;
plot(Vf_range, results(:,3), 'g--', 'LineWidth', 1.5);
plot(Vf_range, results(:,4), 'k-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Transverse Modulus E_2 (GPa)');
title('E_2 vs. Fiber Volume Fraction (Hill''s Average)');
```

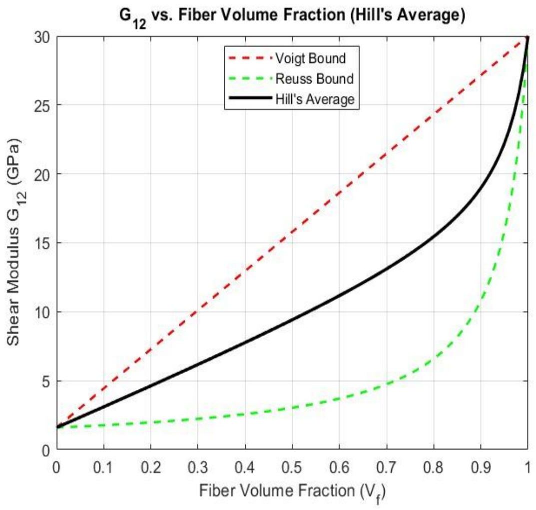
```
legend('Voigt Bound', 'Reuss Bound', 'Hill''s Average', 'Location', 'best');
grid on;

% Plot G12 vs. Vf with bounds
figure(3);
plot(Vf_range, results(:,5), 'r--', 'LineWidth', 1.5); hold on;
plot(Vf_range, results(:,6), 'g--', 'LineWidth', 1.5);
plot(Vf_range, results(:,7), 'k-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Shear Modulus G_{12} (GPa)');
title('G_{12} vs. Fiber Volume Fraction (Hill''s Average)');
legend('Voigt Bound', 'Reuss Bound', 'Hill''s Average', 'Location', 'best');
grid on;

% Plot  12  vs. Vf
figure(4);
plot(Vf_range, results(:,8), 'm-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Poisson''s Ratio \nu_{12}');
title('\nu_{12} vs. Fiber Volume Fraction (Rule of Mixtures)');
grid on;

% Plot  1  vs. Vf
figure(5);
plot(Vf_range, results(:,9), 'k-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Longitudinal CTE \alpha_1 (10^{-6}/ C )');
title('\alpha_1 vs. Fiber Volume Fraction');
grid on;

% Plot  2  vs. Vf
figure(6);
plot(Vf_range, results(:,10), 'c-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Transverse CTE \alpha_2 (10^{-6}/ C )');
title('\alpha_2 vs. Fiber Volume Fraction (Rule of Mixtures)');
grid on;
```

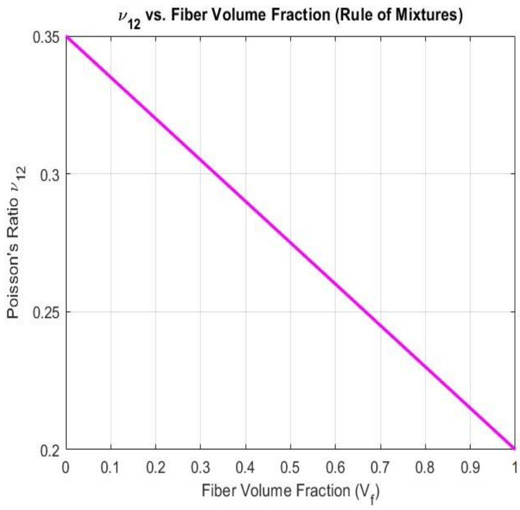
Listing 3: Hill's Method MATLAB Code

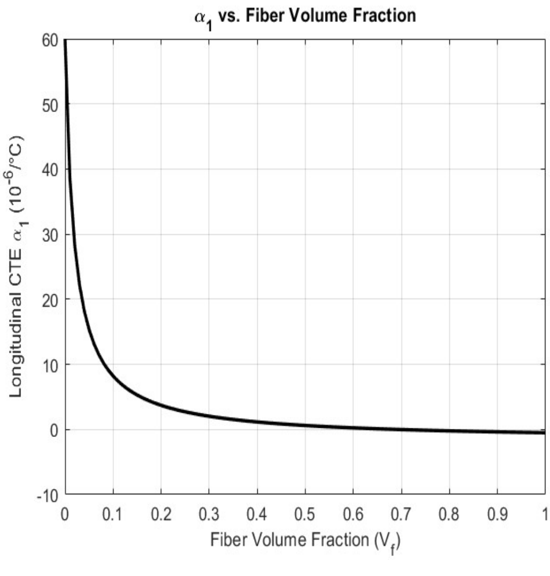
Graphical Result for Hill's Concentration Factor Approach:

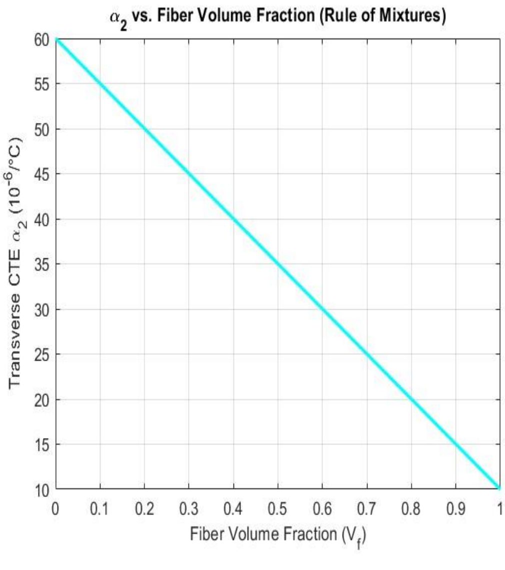












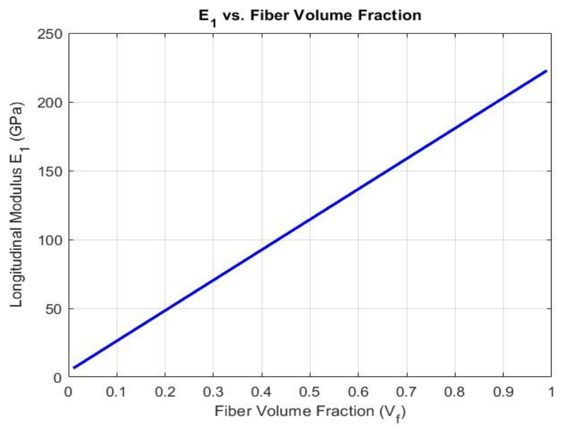
4. Concentric Cylinder Assemblage (CCA) Approach

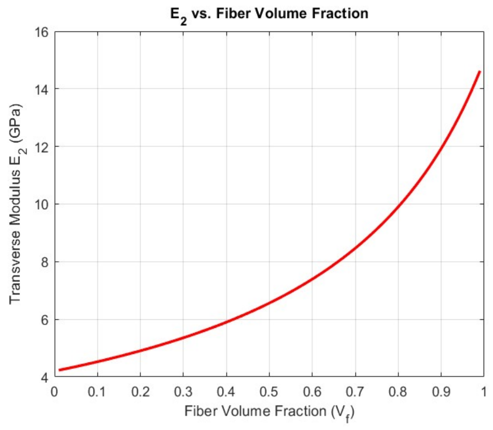
```
clc; clear; close all;

% Fiber properties (AS4 Carbon)
Ef1 = 225;        % Longitudinal modulus (GPa)
Ef2 = 15;         % Transverse modulus (GPa)
Gf12 = 15;        % In-plane shear modulus (GPa)
Gf23 = 7;         % Transverse shear modulus (GPa)
vf12 = 0.2;       % Major Poisson's ratio
alpha_f1 = -0.5e-6; % Longitudinal CTE (1/ C )
alpha_f2 = 15e-6;   % Transverse CTE (1/ C )

% Matrix properties (3501-6 Epoxy)
Em = 4.2;         % Isotropic modulus (GPa)
vm = 0.34;        % Poisson's ratio
Gm = Em/(2*(1+vm)); % Matrix shear modulus (GPa)
alpha_m = 45e-6; % Matrix CTE (1/ C )

% Vary fiber volume fraction from 0 to 1
Vf_range = linspace(0.01, 0.99, 100);
results = zeros(length(Vf_range), 8);

%% Calculations
for i = 1:length(Vf_range)
    Vf = Vf_range(i);
    Vm = 1 - Vf;

    % 1. Longitudinal Modulus (Rule of Mixtures)
    E1 = Vf*Ef1 + Vm*Em;

    % 2. Transverse Modulus (Inverse Rule of Mixtures)
    E2 = 1/(Vf/Ef2 + Vm/Em);

    % 3. In-plane Shear Modulus (Inverse Rule of Mixtures)
    G12 = 1/(Vf/Gf12 + Vm/Gm);

    % 4. Transverse Shear Modulus (CCA Model - Simplified)
    G23 = Gm*(Gf23 + Gm + Vf*(Gf23 - Gm))/(Gf23 + Gm - Vf*(Gf23 - Gm));

    % 5. Major Poisson's Ratio (Rule of Mixtures)
    nu12 = Vf*vf12 + Vm*vm;

    % 6. Thermal Expansion Coefficients (Schapery's Model)
    alpha1 = (Vf*Ef1*alpha_f1 + Vm*Em*alpha_m)/(Vf*Ef1 + Vm*Em);
    alpha2 = (1 + vf12)*Vf*alpha_f2 + (1 + vm)*Vm*alpha_m - nu12*alpha1;

    % Store results
    results(i,:) = [E1, E2, G12, G23, nu12, alpha1*1e6, alpha2*1e6, Vf];
end

% 1. Longitudinal Modulus E1
figure(1);
plot(results(:,8), results(:,1), 'b-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Longitudinal Modulus E_1 (GPa)');
title('E_1 vs. Fiber Volume Fraction');
grid on;

% 2. Transverse Modulus E2
figure(2);
plot(results(:,8), results(:,2), 'r-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Transverse Modulus E_2 (GPa)');
title('E_2 vs. Fiber Volume Fraction');
grid on;

```

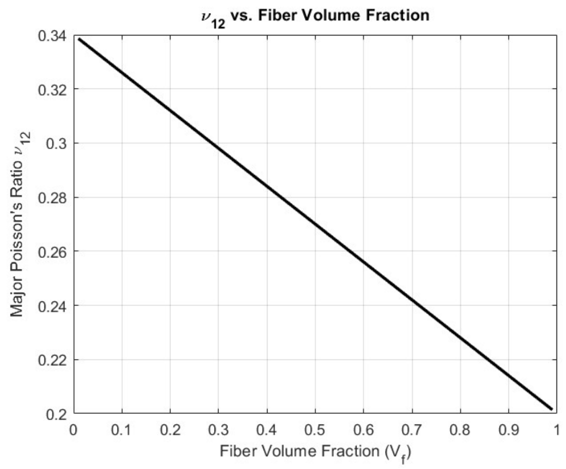
```
% 3. In-plane Shear Modulus G12
figure(3);
plot(results(:,8), results(:,3), 'g-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('In-plane Shear Modulus G_{12} (GPa)');
title('G_{12} vs. Fiber Volume Fraction');
grid on;

% 4. Transverse Shear Modulus G23
figure(4);
plot(results(:,8), results(:,4), 'm-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Transverse Shear Modulus G_{23} (GPa)');
title('G_{23} vs. Fiber Volume Fraction');
grid on;

% 5. Major Poisson's Ratio nu12
figure(5);
plot(results(:,8), results(:,5), 'k-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Major Poisson''s Ratio \nu_{12}');
title('\nu_{12} vs. Fiber Volume Fraction');
grid on;

% 6. Longitudinal CTE alpha1
figure(6);
plot(results(:,8), results(:,6), 'c-', 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Longitudinal CTE \alpha_1 (10^{-6}/ C )');
title('\alpha_1 vs. Fiber Volume Fraction');
grid on;

% 7. Transverse CTE alpha2
figure(7);
plot(results(:,8), results(:,7), 'color', [0.5 0 0.5], 'LineWidth', 2);
xlabel('Fiber Volume Fraction (V_f)');
ylabel('Transverse CTE \alpha_2 (10^{-6}/ C )');
title('\alpha_2 vs. Fiber Volume Fraction');
grid on;
```

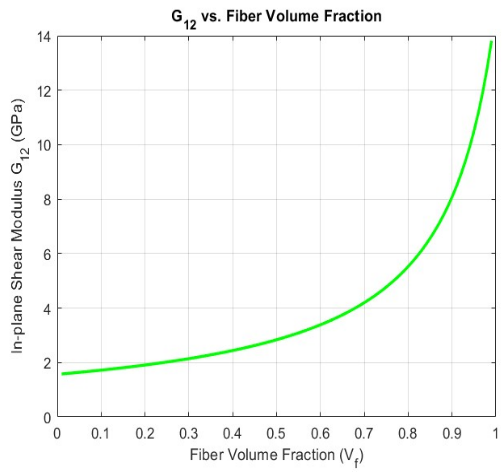
Listing 4: CCA Method MATLAB Code

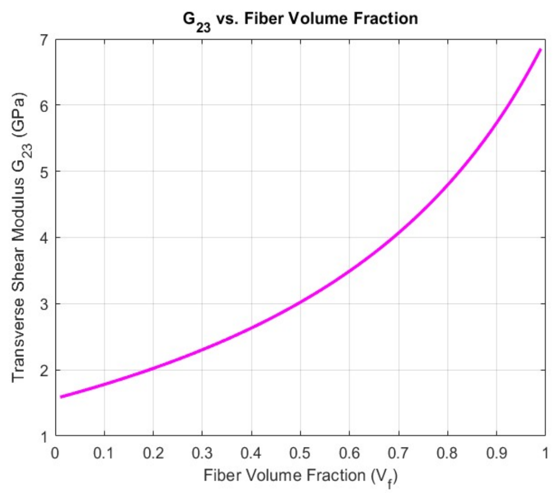
Graphical Result for Concentric Cylinder Assemblage (CCA) Approach:

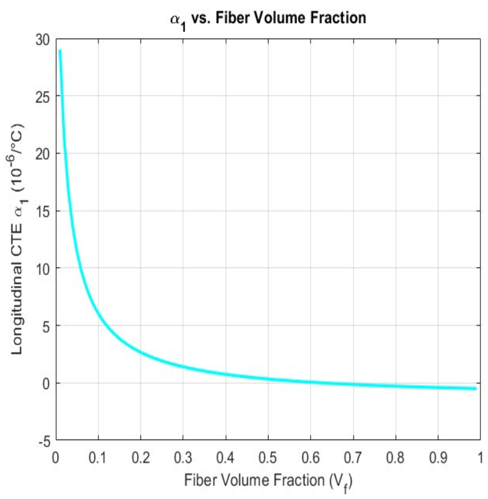


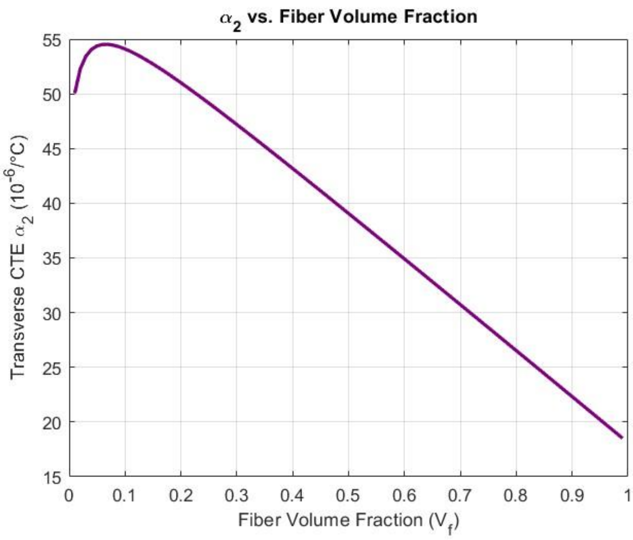












α_2 vs. Fiber Volume Fraction
Transverse CTE α_2 (10^{-6}/°C)
55
50
45
40
35
30
25
20
15
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Fiber Volume Fraction (V_f)

CONCLUSION:

The micromechanical modeling of AS4/3501-6 composites using four different analytical methods provided a comprehensive comparison of their predictive capabilities. Each model demonstrated varying levels of accuracy and applicability depending on the property being evaluated:

- The Strength of Materials approach, while simple and easy to implement, was found to be best suited for predicting the longitudinal modulus but showed significant limitations in estimating transverse and shear behavior.
- The Standard Mechanics approach improved upon these estimates by accounting for stiffness tensors and anisotropic effects, offering more accurate predictions for both moduli and Poisson's ratio.
- Hill's Method provided balanced results by averaging the Voigt and Reuss bounds, making it particularly useful for estimating transverse modulus and shear modulus with moderate computational effort.
- The Concentric Cylinder Assemblage (CCA) model, being the most physically representative, yielded the most accurate and realistic values, especially for transverse and shear moduli, as well as thermal expansion coefficients, thanks to its ability to model the interaction between fiber and matrix in a cylindrical geometry.

The graphical results further confirmed that the CCA model consistently approximates the mechanical response closer to expected behavior compared to the other methods, particularly in the transverse and thermal domains. For high-fidelity simulations or design-critical applications, the CCA model is therefore recommended, whereas simpler methods may suffice for preliminary design estimates.