A Consistent Environment for the Numerical Prediction of the Properties of Composite Materials

J. Schumacher
G. Ziegmann (Institute of Polymer Materials and Plastics Engineering)
P. Fideu (CTC GmbH Stade), A. Herrmann (Faserinstitut Bremen e.V.)

COMSOL Conference 2009, Milano, 14-16th October
Our guiding theme: From the basic material to the final structure
Motivation

- Composite material as an important material for the industry
- Complexity of the geometry
- Development of fast, reliable, cost optimized manufacturing
- Reduction of the research development time

Manufacturing process simulation (MPS)
CHAMAELEON: Description

- Combination of COMSOL and Matlab features
  - GUI from Matlab
  - Solving a field problem in COMSOL

- Flexibility
  - Multiscale modeling
  - Parameterization

- Numerical homogenization

J. Schumacher
Institute of Polymer Materials and Plastics Engineering

A Consistent Environment for the Numerical Prediction of the Properties of Composite Materials
Geometry: Multiscale Modeling

- **Macro Level**

- **Micro/meso Level**

REV: Representative Elementary Volume
Geometry: Parameterization

A Consistent Environment for the Numerical Prediction of the Properties of Composite Materials
Material properties

- Packing density

Hexagonal

\[ \varphi_{\text{max}} = 0.91 \]

Quadrangular

\[ \varphi_{\text{max}} = 0.79 \]
Formula

- Environment for physical problems
- Interface between COMSOL and Matlab

**KamalSourour:**

\[ \alpha_I = (k^\alpha \alpha^m) \cdot (1 - \alpha)^n \]

with \( k = A \cdot \exp(-E/(R \cdot T)) \) [Arrhenius]

\( R = 8.315 \text{ J/molK} \)

Description:
Curing reaction of resin depending on the fibre content and the material properties

**Reaction kinetics:**

- \( A = 127500 \) [1/s]
- \( E = 63400 \) [J/mol]
- \( m = 0.9 \) [-]
- \( n = 2.1 \) [-]
- \( h = 550000 \) [J/kg]

**Solver time:**

\( 1:10:60*100 \) (start:inc:end) [s]
Formula for thermal properties

- **Rule of Mixture**
  - Density:
    \[ \rho_l = v_f \cdot \rho_f + (1 - v_f) \cdot \rho_m \]
  - Thermal conductivity:
    \[ \lambda_l = v_f \cdot \lambda_f + (1 - v_f) \cdot \lambda_m, \quad \lambda_l = \frac{\lambda_f \cdot \lambda_m}{v_f \cdot \lambda_m + v_m \cdot \lambda_f} \]
  - Heat Capacity:
    \[ c_{pl} = \frac{v_f \cdot \rho_f \cdot c_{pf} + (1 - v_f) \cdot \rho_m \cdot c_{pm}}{v_f \cdot \rho_f + (1 - v_f) \cdot \rho_m} \]

- **Curing kinetics**
  \[ \frac{d\alpha}{dt} = (k \cdot \alpha^n) (1 - \alpha)^n \]

with

\[ k = A \cdot \exp\left(\frac{-E}{RT}\right) \]

Kamal Sourour

Arrhenius

J. Schumacher
Institute of Polymer Materials and Plastics Engineering
Use of COMSOL

- Equation
  - Heat transfer by Conduction:
    \[ \rho C_p \frac{dT}{dt} - \nabla \cdot (k \nabla T) = Q \]
  - PDE general mode for implementation of the KamalSourour equation
    \[ e \frac{\partial^2 u}{\partial t^2} + d \frac{\partial u}{\partial t} + \nabla \cdot \Gamma = F \]

  with

  \[ e = 0, \quad d = 1, \quad \Gamma = 0 \quad \text{and} \quad F = (k \cdot \alpha^m)(1 - \alpha)^n \]
Results

- Numerical homogenization
  - Analytical
    \[ \lambda_l = \nu_f \lambda_f + (1 - \nu_f) \lambda_m, \]
  - Numerical:
    Thermal conductivity from the heat flux equation:
    \[ \dot{q} = -\lambda \cdot \text{grad}T \]
    Implementation in COMSOL:
    Subdomain Integration:
    \[ \lambda \approx -\text{flux} / \text{grad}T \]
Results

- Influence of exothermic reaction

![Temperature vs. Time Graph]

Temperature peak due to the exothermic reaction
Conclusion and outlook

- CHAMAELEON especially designed for user with interest in:
  - Fast investigation of the influence on global laminate properties
  - Optimization of the process parameter

- Principle of CHAMAELEON extensible to other physical area such as:
  - moisture behaviour,
  - electrical or mechanical properties

- Intention of 3D illustrations considering the growing complexity of the geometry
Thank you for your attention!

Institute of Polymer Materials and Plastics Engineering

Agricolastraße 6
D-38678 Clausthal-Zellerfeld
Tel. +49 (0) 53 23 / 72 – 20 80
Fax +49 (0) 53 23 / 72 – 23 24
http://www.puk.tu-clausthal.de

josefine.schumacher@tu-clausthal.de