



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

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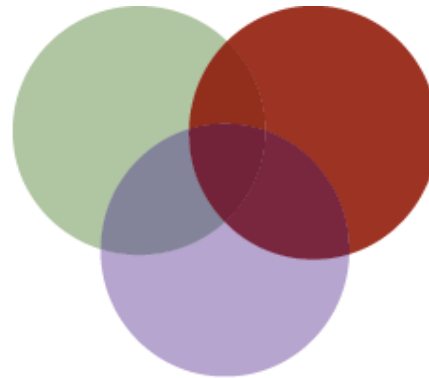
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COMSOL Conference 2009, Milano, 14-16th October



## Institute of Polymer Materials and Plastics Engineering

Renewable  
Resource Materials



Composite  
Technologies

Melt Processing

Our guiding theme:  
From the basic material  
to the final structure



## Motivation

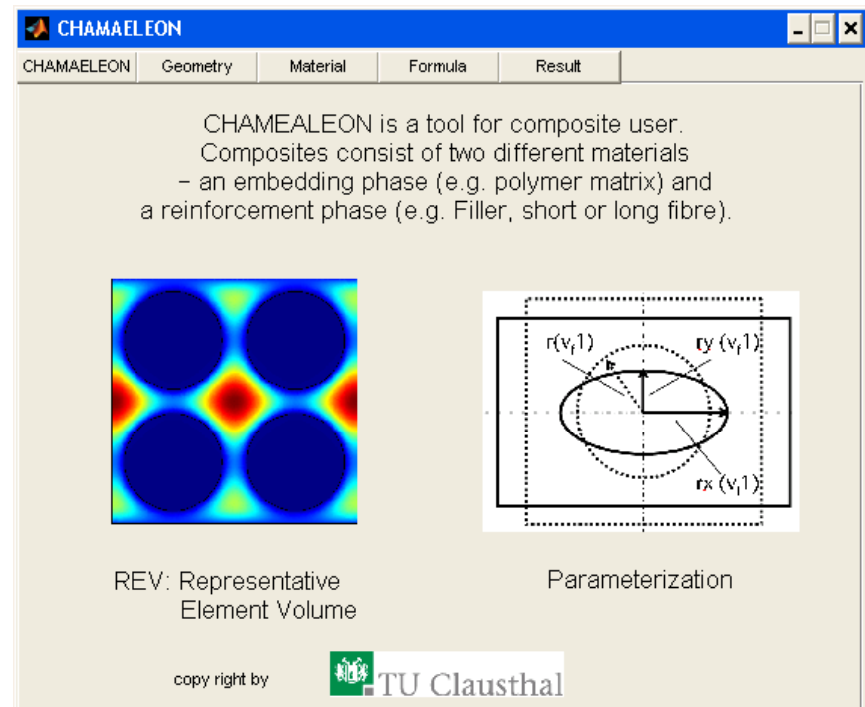
- Composite material as an important material for the industry
- Complexity of the geometry
- Development of fast, reliable, cost optimized manufacturing
- Reduction of the research development time



Manufacturing process simulation (MPS)

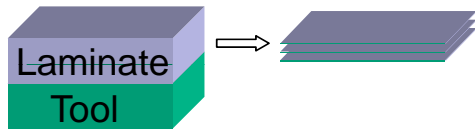
## CHAMAELEON: Description

- Combination of COMSOL and Matlab features
  - GUI from Matlab
  - Solving a field problem in COMSOL
  
- Flexibility
  - Multiscale modeling
  
  - Parameterization
  
- Numerical homogenization

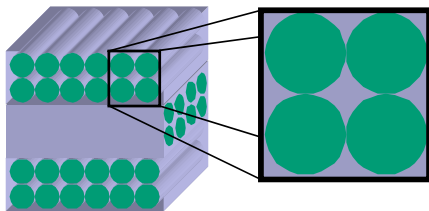


# Geometry: Multiscale Modeling

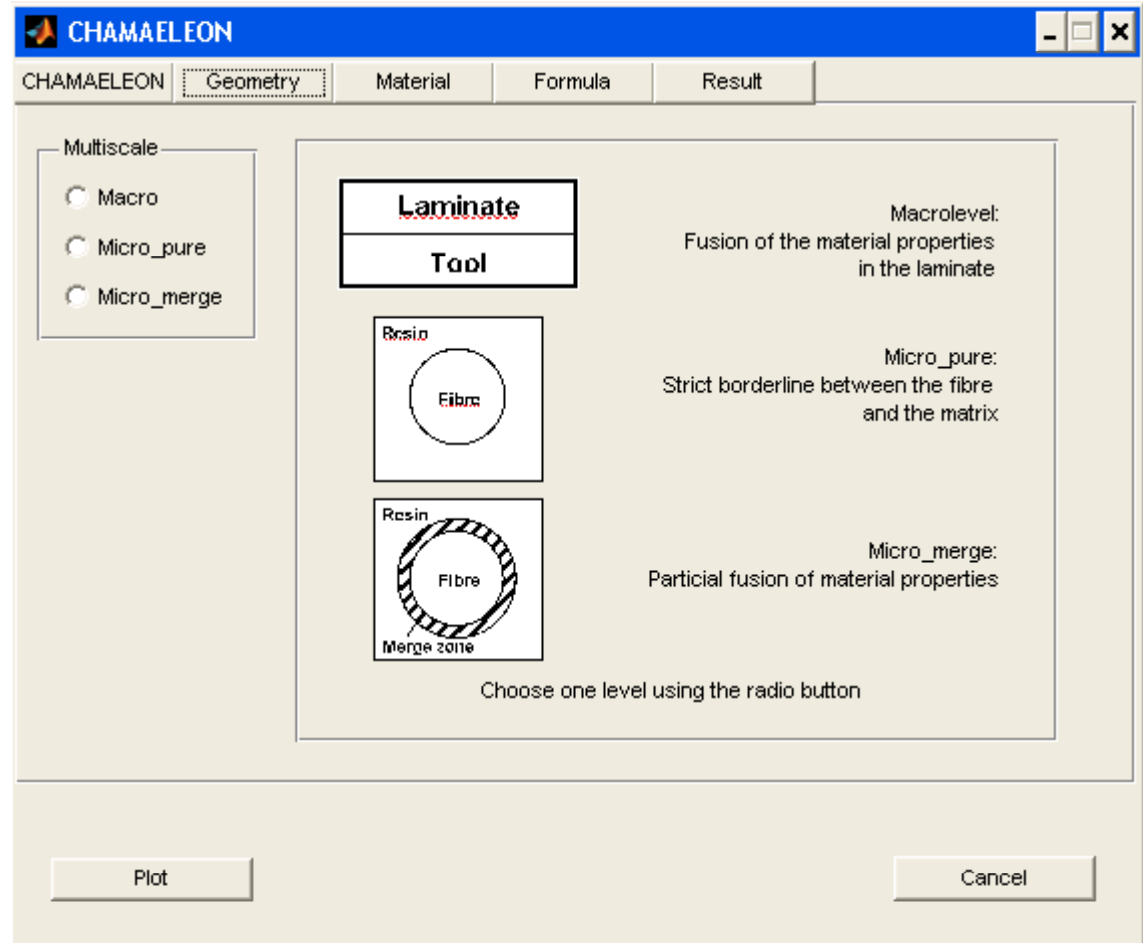
## Macro Level



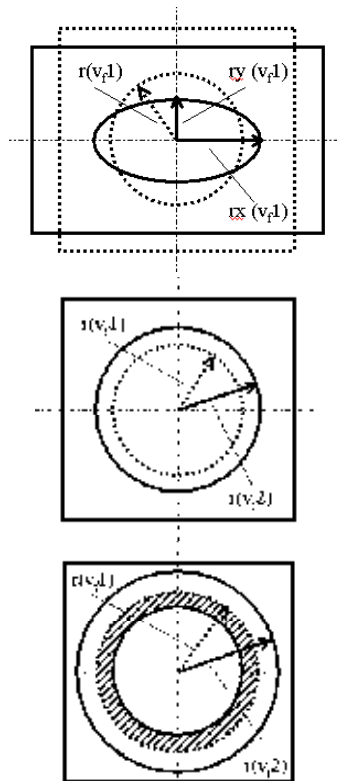
## Micro/meso Level



REV:  
Representative  
Elementary  
Volume



## Geometry: Parameterization



CHAMAELEON
\_ □ ×

CHAMAELEON | Geometry | Material | Formula | Result

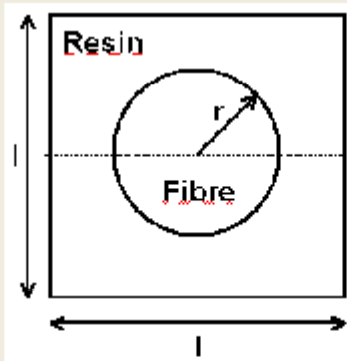
Multiscale

Macro

Micro\_pure

Micro\_merge

Micro\_pure



Microscale function describes a combination of a single fibre robe embedded in a resin cell

Both the area of the RVE ( $l^2$ ) and the fibre volume content ( $\phi$ ) are changeable depending on the packing density

phi

rx  [mm]

ry  [mm]

Packing density

Hexagonal

Quadratic

Dimension

2D

3D

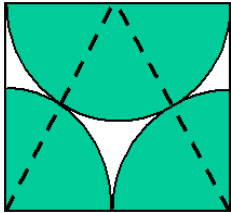
Plot

Cancel

## Material properties

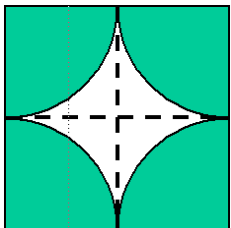
- Packing density

### Hexagonal



$$\varphi_{\text{max}} = 0.91$$

### Quadratic



$$\varphi_{\text{max}} = 0.79$$

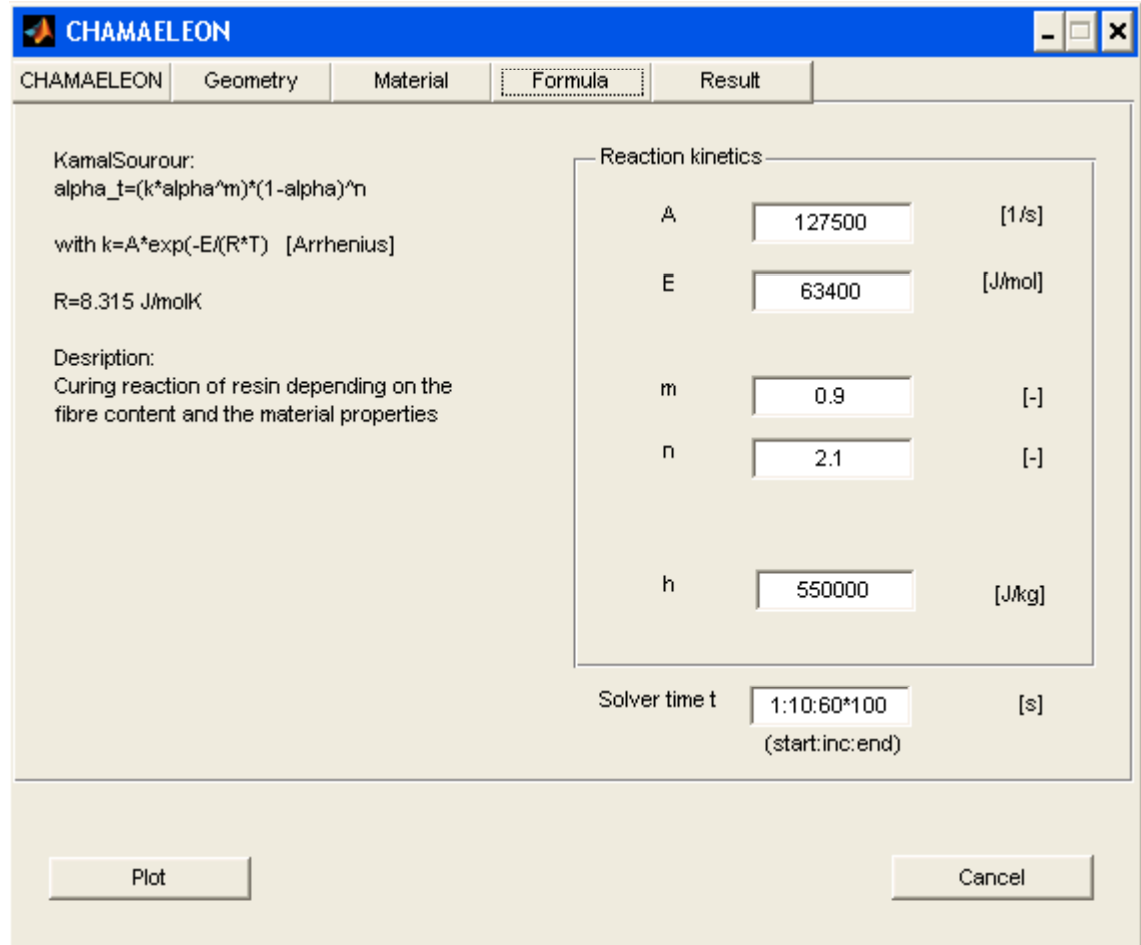
CHAMAELEON

CHAMAELEON   Geometry   **Material**   Formula   Result

Fibre			Matrix		
rho	<input type="text" value="1790"/>	[kg/m <sup>3</sup> ]	rho	<input type="text" value="1260"/>	[kg/m <sup>3</sup> ]
cp	<input type="text" value="712"/>	[J/kgK]	cp	<input type="text" value="1260"/>	[J/kgK]
k	<input type="text" value="26"/>	[W/mK]	k	<input type="text" value="0.167"/>	[W/mK]

## Formula

- Environment for physical problems
- Interface between COMSOL and Matlab



**CHAMAELEON**

CHAMAELEON    Geometry    Material    **Formula**    Result

KamalSourour:  
 $\alpha_t = (k \cdot \alpha^m) \cdot (1 - \alpha)^n$   
 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	<input type="text" value="127500"/>	[1/s]
E	<input type="text" value="63400"/>	[J/mol]
m	<input type="text" value="0.9"/>	[-]
n	<input type="text" value="2.1"/>	[-]
h	<input type="text" value="550000"/>	[J/kg]

Solver time t  [s]  
 (start:inc:end)



## Formula for thermal properties

### ■ Rule of Mixture

- Density:

$$\rho_l = v_f * \rho_f + (1 - v_f) * \rho_m$$

- Thermal conductivity:

$$\lambda_l = v_f * \lambda_f + (1 - v_f) * \lambda_m, \quad \lambda_t = \frac{\lambda_{fl} \lambda_m}{v_f \lambda_m + v_m \lambda_{ft}}$$

- Heat Capacity:

$$c_{pl} = \frac{v_f * \rho_f * c_{pf} + (1 - v_f) * \rho_m * c_{pm}}{v_f * \rho_f + (1 - v_f) * \rho_m}$$

### ■ Curing kinetics

$$\frac{d\alpha}{dt} = (k \cdot \alpha^m)(1 - \alpha)^n$$

KamalSourour

with

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

Arrhenius

## 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

$$\lambda_l = v_f * \lambda_f + (1 - v_f) * \lambda_m,$$

- Numerical:

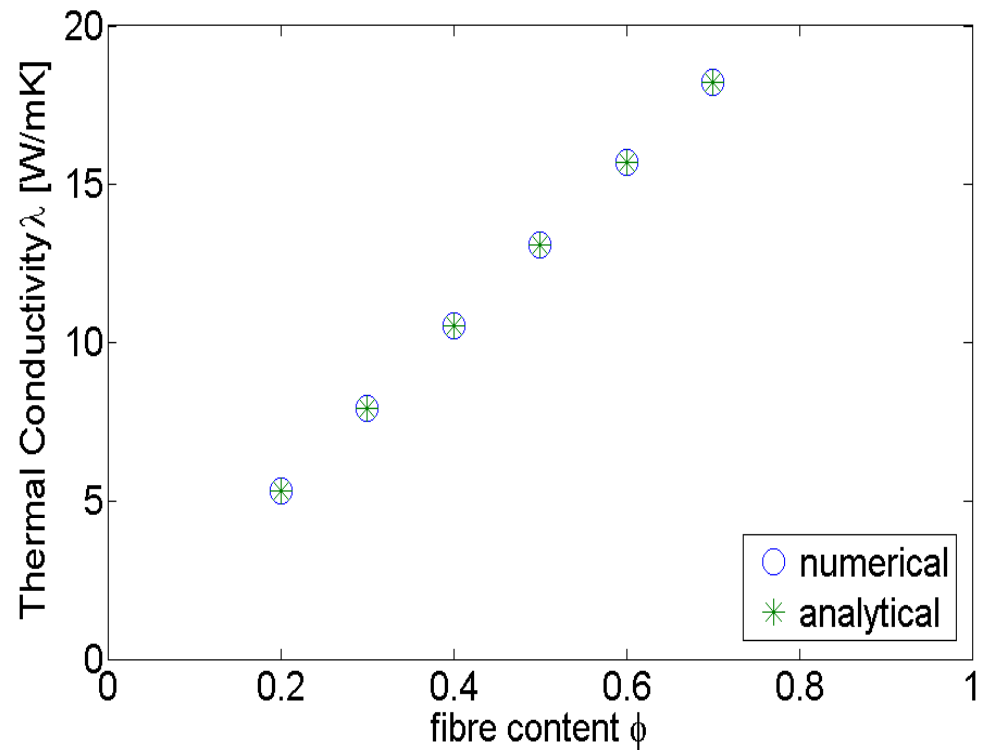
Thermal conductivity from the heat flux equation:

$$\dot{q} = -\lambda \cdot gradT$$

Implementation in COMSOL:

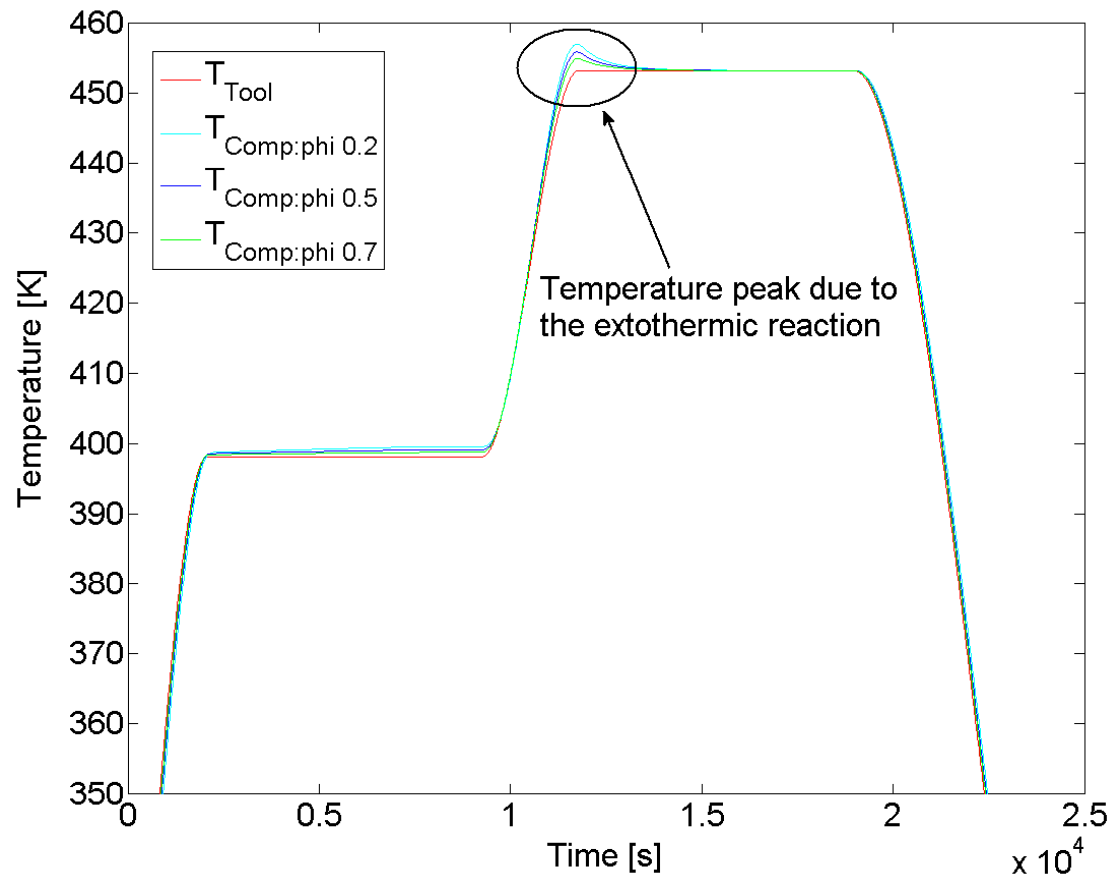
Subdomain Integration:

➡  $\lambda \approx -flux / gradT$



## Results

- Influence of 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!

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