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# Simulation numérique des procédés d'élaboration des composites

## Elaboration des CMO

Prepared by ESI Group Composites Manufacturing CoE (Mérignac):

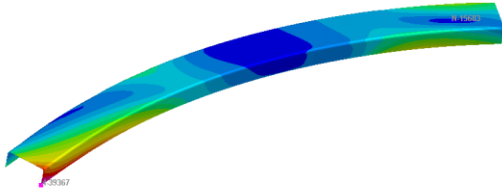
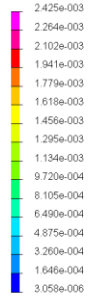
- Laurent Dufort
- **Yann Duplessis Kergomard** (Presenter)
- **Cyril Dedieu** (Presenter)
- Arnaud Dereims
- Mustapha Ziane
- Marta Perez Miguel

# ESI's PAM-COMPOSITES

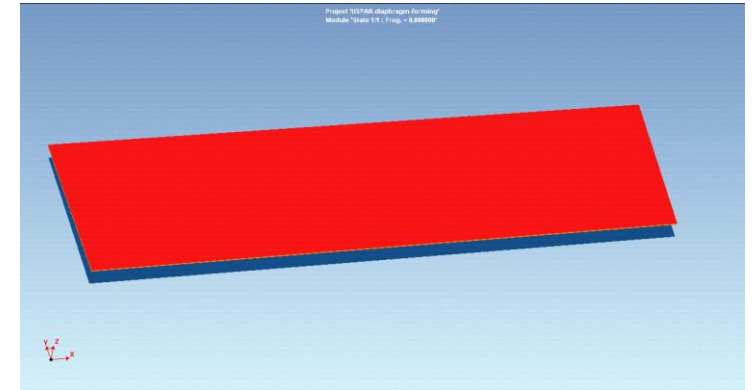
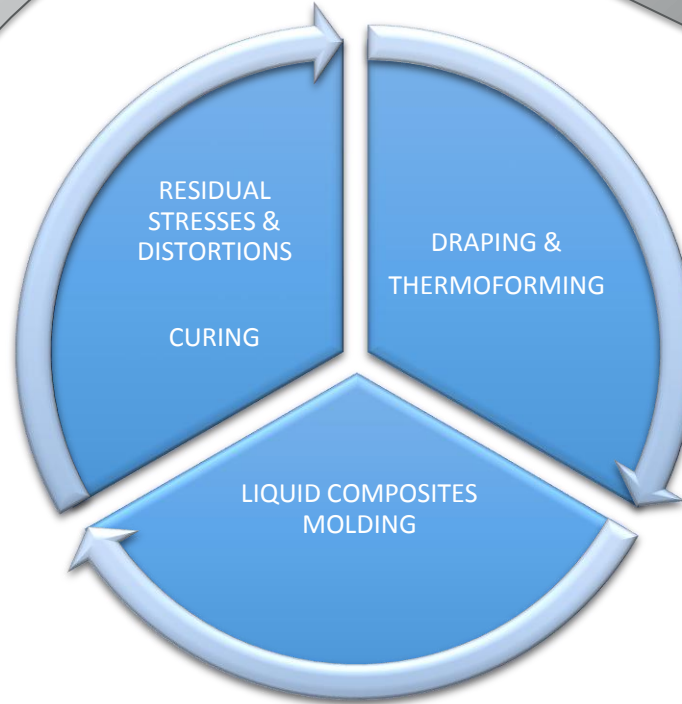
Compensated mold



U\_spar\_INFUSION\_Distortion\_STEP2  
 NODE : Displacement NORM  
 Min = 3.05709e-006 at Node 1593  
 Max = 0.0024256 at Node 3037

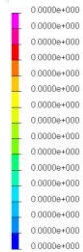


1 / 18000.000000



Temperature history  
 Degree of cure history

INFUSION\_U\_spar\_INFUSION\_HeatedFilling\_RESULT.ans  
 NODE : FILLING\_FACTOR  
 Min = 0 at Node 2025  
 Max = 0 at Node 2025



1 / 0.000000

Fiber direction  
 Thickness variation





# DRAPING & THERMOFORMING

## What for ?

**Dry & pre-impregnated reinforcements can be draped over moulds that have complex shapes**

- Preforming of dry textiles (woven fabrics, NCF, UD, mats, tapes...)
- Draping of thermoset prepregs (woven fabrics, NCF, UD, mats, tapes...)
- Thermoforming of organosheets (woven fabrics, NCF, UD, mats, tapes...)

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# DRAPING & THERMOFORMING

## Some issues



Examples of some defects related to dry textiles preforming (before LCM processes)

Defects	First Layer	Counter-Layer
In-plane Buckling (IB)		
Structure Decomposition (SD)		
Compaction & Stretch (C&S)		
Intra-ply Slip (IPS)		
Openings & Voids (VO)		



Poor part quality



Need to know the **fibre content** and **fibre orientation**, that strongly influence the **permeability** field

Examples of some defects related to dry textiles preforming (before **LCM processes**)



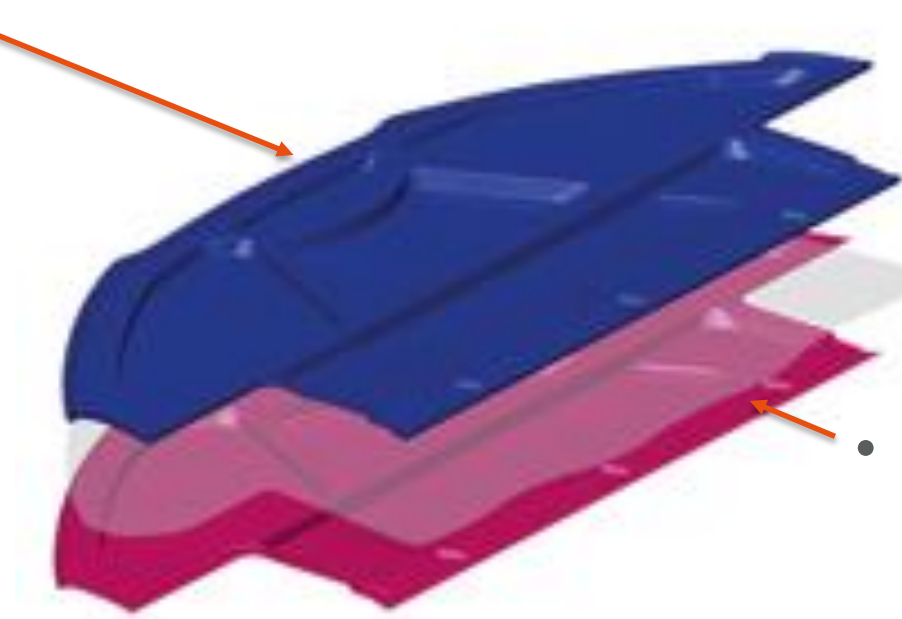


# DRAPING & THERMOFORMING

## Need a simulation tool

- **Process parameters**

- Tooling kinematics
- Pressure cycle
- Temperature cycle
- Clamping definition
- Ply definition
- ...



- **Composite material**

- Material law
- Stacking sequences
- Initial flat pattern

- **Contact & friction**

- Ply to ply
- Tool to ply

## To evaluate

### Defects

- Wrinkles
- Bridging

### Quantities of interest

- Pressure on the mold

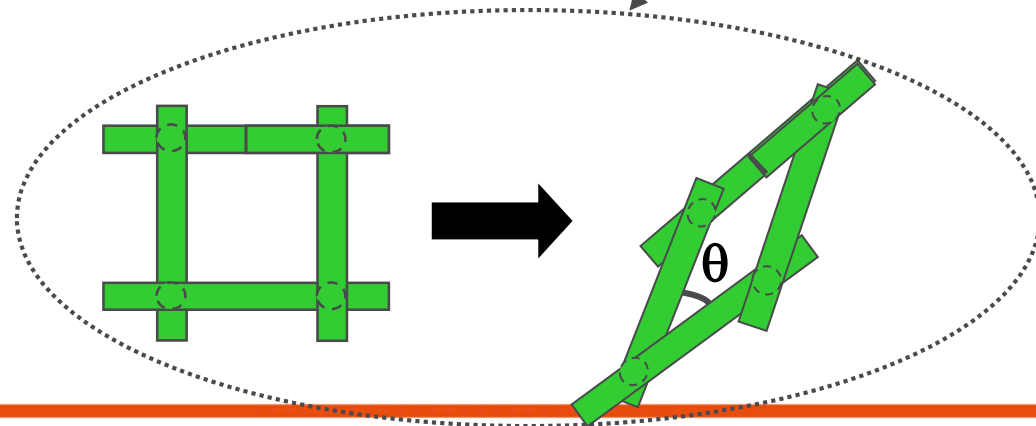
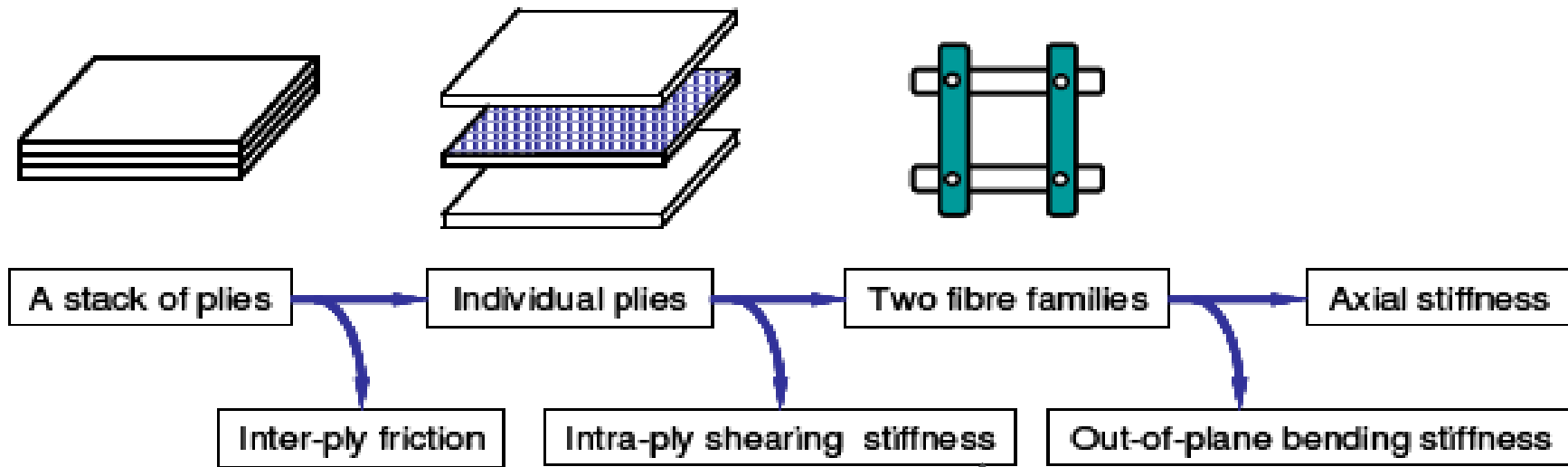
- Fibers orientation
- Fiber content
- Thickness distribution

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# DRAPING & THERMOFORMING

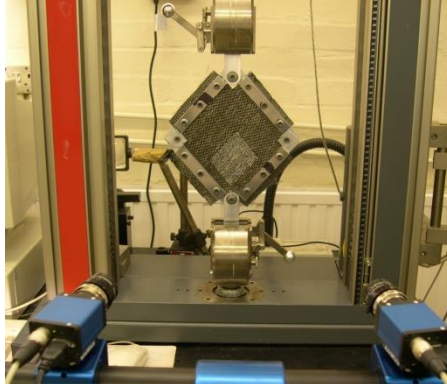
## Composite material behaviour

# Fabric Deformation Mechanisms



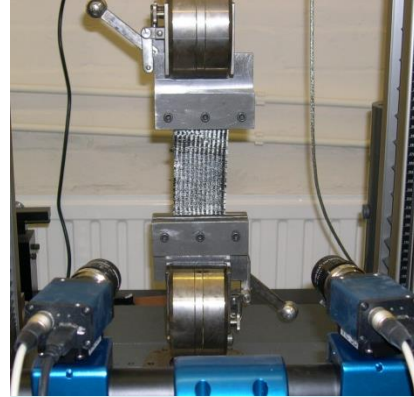
# Material characterisation

Picture frame test



- Shear stiffness
- Interlocking angle

Tensile test



- $E$  fibre
- $E$  stitch

Friction test



- Friction law

Each fabric = one material model

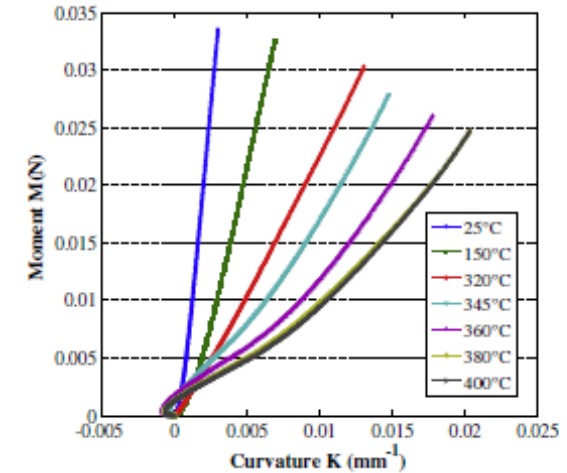
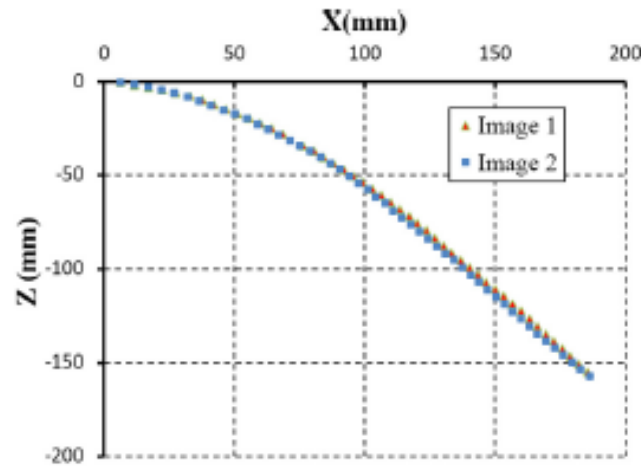
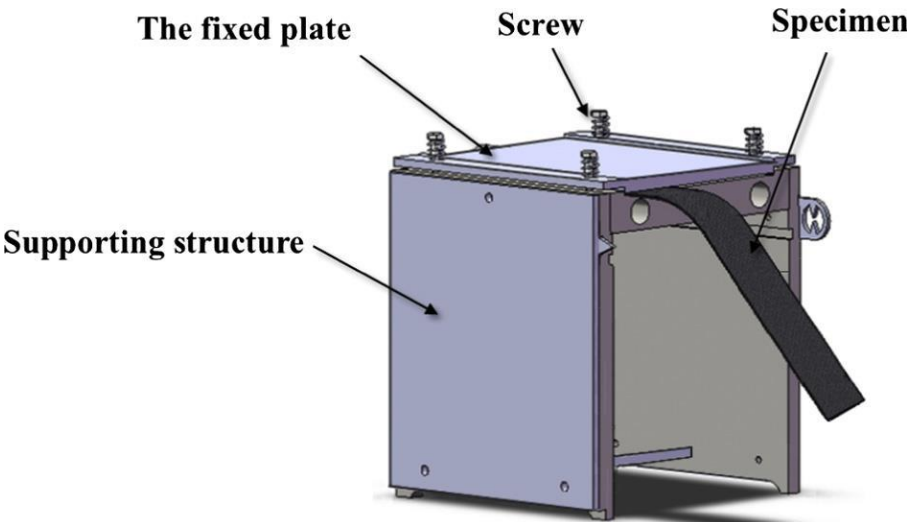
- Characterisation tests are **modelled** to fit **experimental data** in the material model

# Material characterisation

- **Bending, can be temperature dependent**

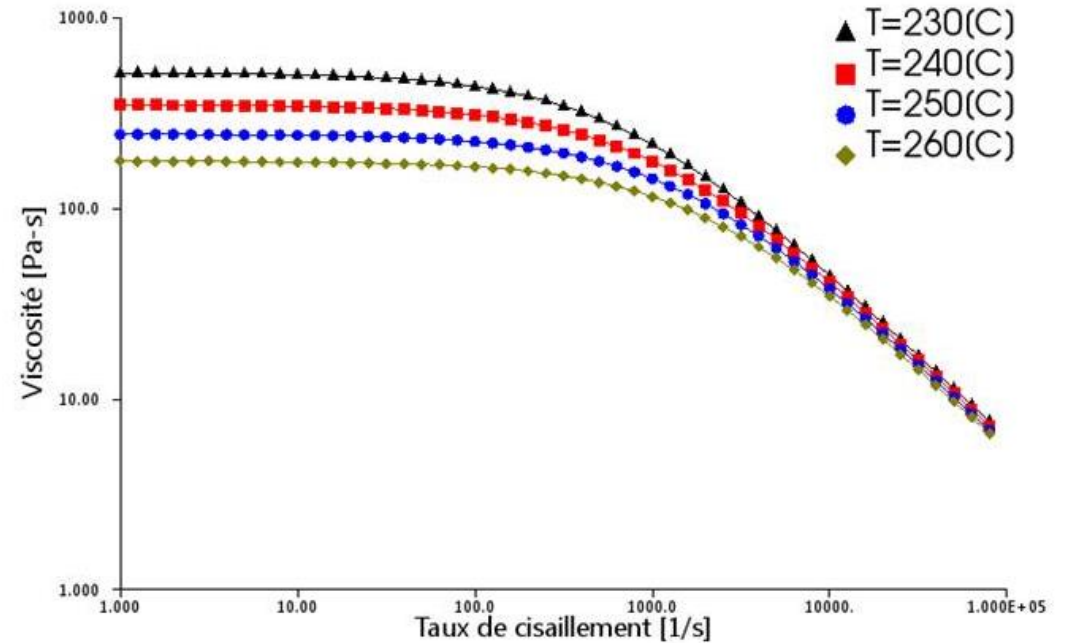
- Cantilever test

- 2 fiber direction
- 2 face position (positive and negative curvature)
- 2 possibilities to use results:
  - Measure deflection and recover it with simulation
  - Use optical measurement that captures the deflection shape and discretize it with many points. Analytical tool is used to compute bending moment/stiffness and curvature on all these points for a direct input in PAM-FORM



# Material characterisation

- **Viscous friction, can be temperature dependent**
  - Dynamic viscosity (Pa.s) of resin for prepregs, or binder for dry fabrics
    - Rheometer equipment is used
    - Viscosity for thermoset prepregs and binder
    - Viscosity =  $f(\text{shear rate})$  for thermoplastic prepregs



# Material characterisation

- Friction test, can be temperature dependent

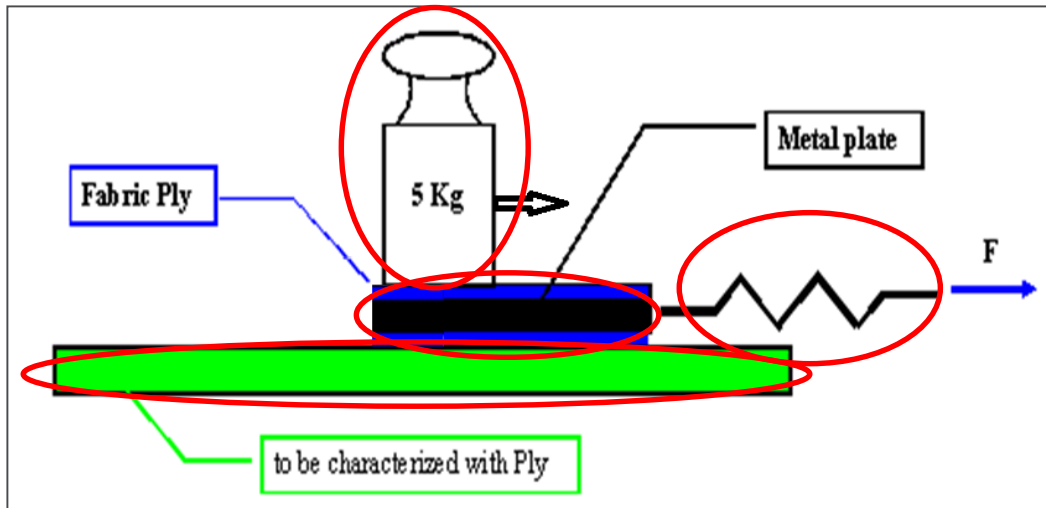


Figure 10 : Friction test trial

## Balance spring

- ❖ Placed horizontally
- ❖ Manually extended until the plate begins to move.

## Fabric

- ❖ Wrapped around a metal plate
- ❖ Dimensions: 100mmX175mm

The static friction coefficient:  $\mu_s = \frac{F_s}{W}$

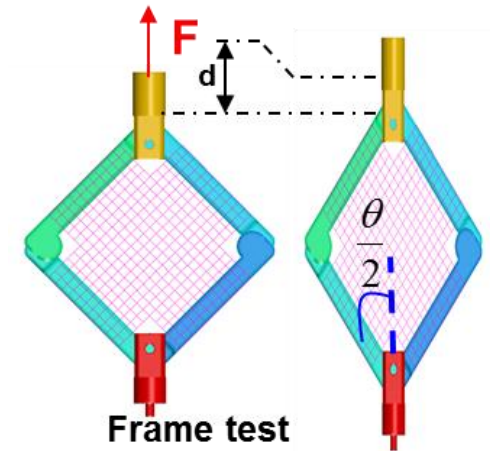
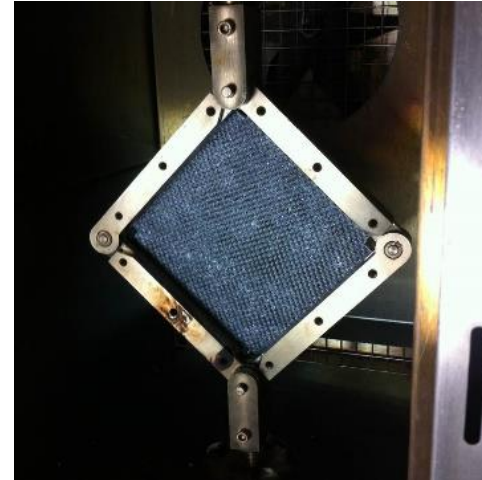
The dynamic friction coefficient:  $\mu_d = \frac{F_d}{W}$

- ❖ Placed upon the fabric

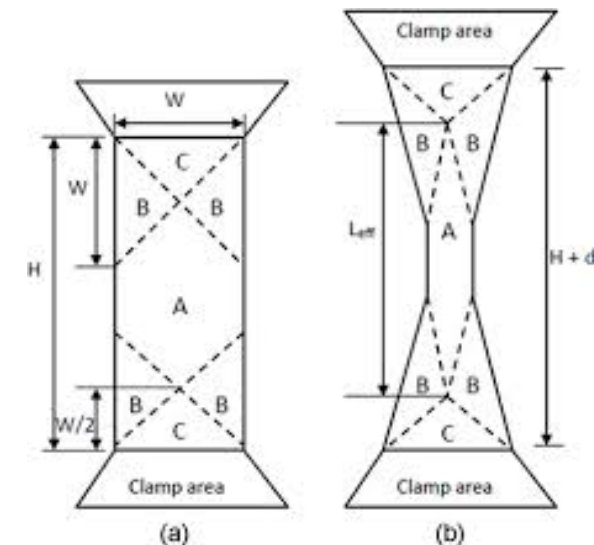
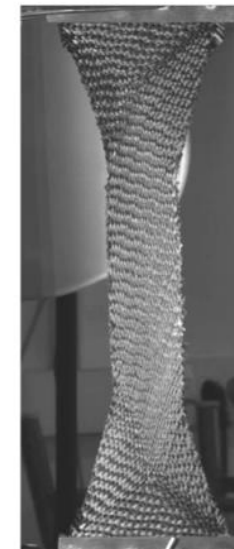
# Material characterisation

- **In-plane shear (can be temperature dependent)**

- Picture frame test
  - For NCF or woven fabric
    - NCF usually requires test for positive and negative shear since behavior is usually not symmetric due to stitching

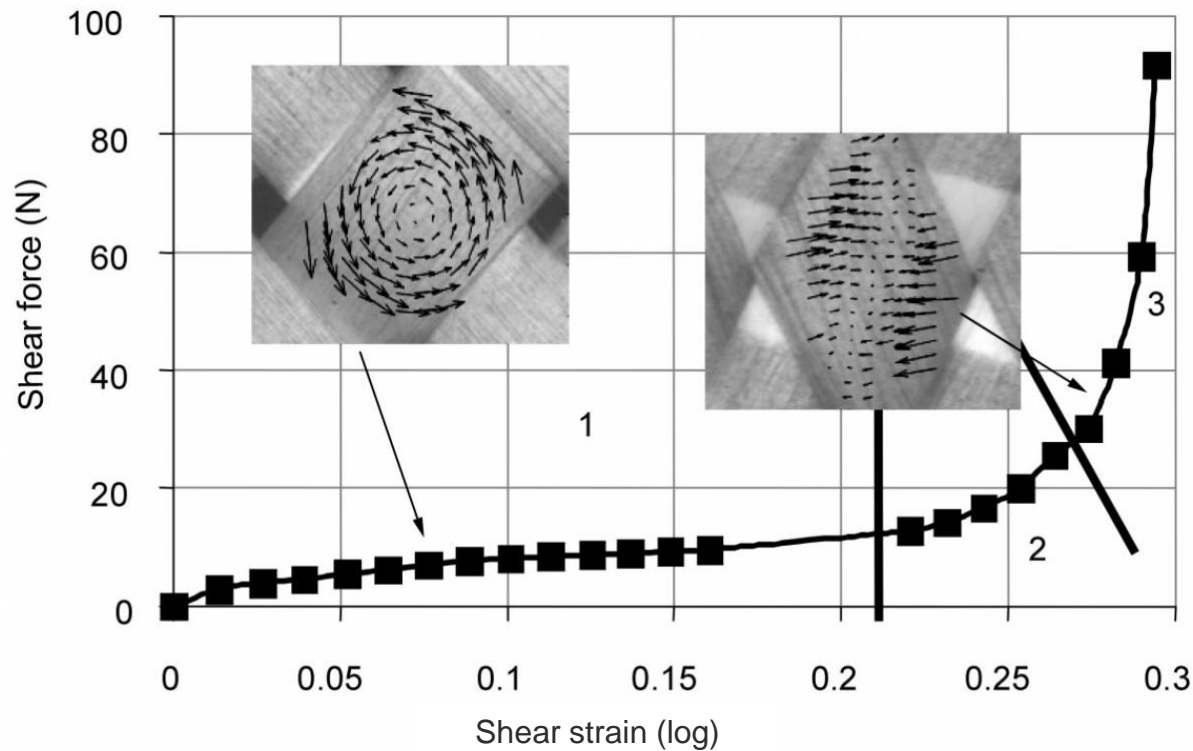


- Bias extension test
  - Coupons with ratio of 3 between length and width
  - For woven fabric





# Material characterisation



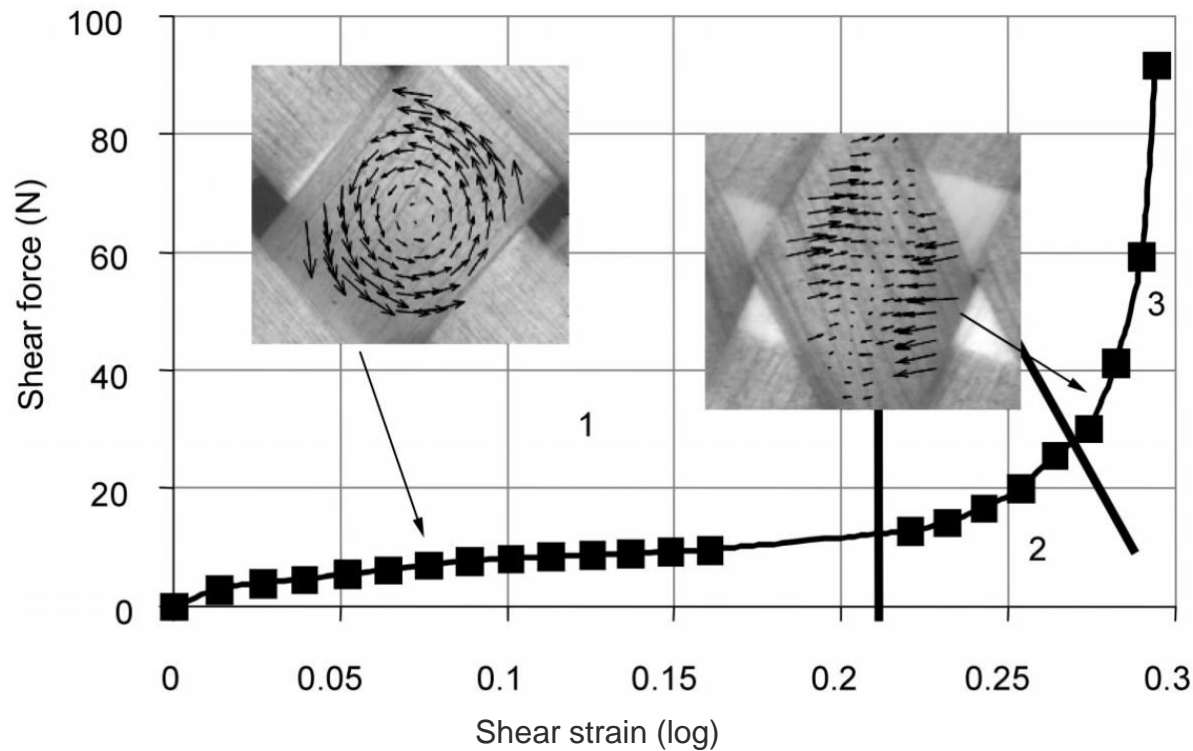
## • Picture frame test - glass plain weave

- Strain computed with image correlation
- **Zone 1** : small load - yarn submitted to rotation
- Shear-locking angle: beginning of zone 2
- The contact networks develop, partial (**Zone 2**) and total (**Zone 3**) lateral compression

3.16 Shear curve and optical analysis (Dumont, 2003). (2)

(2) *Composites forming technologies. Chapter 3: Finite element analysis of composite forming, P. Boisse.*

# Material characterisation



- **Picture frame test - glass plain weave**

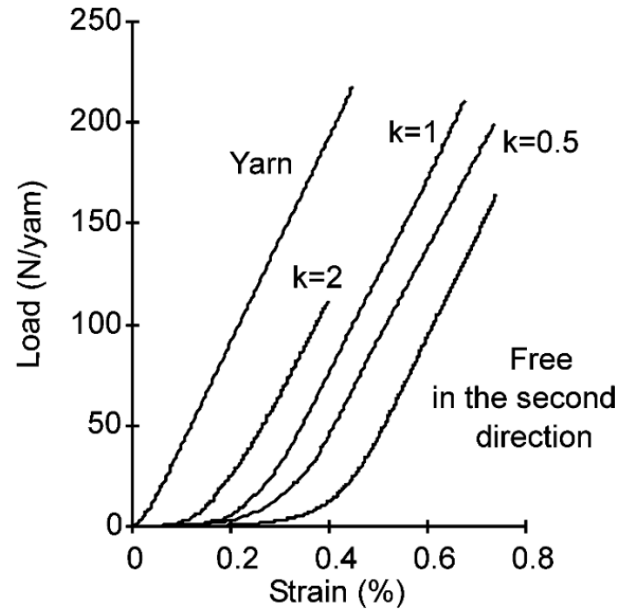
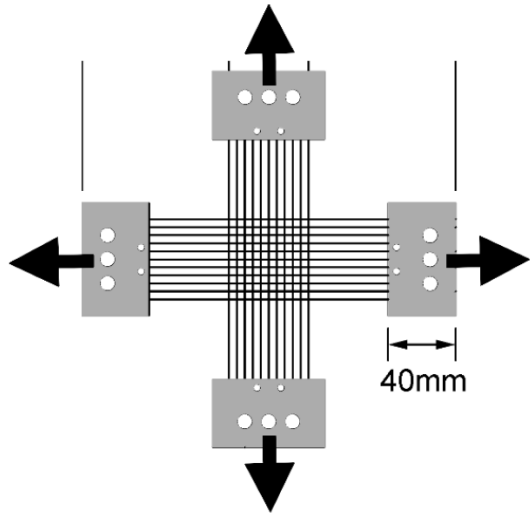
- Strain computed with image correlation
- **Zone 1** : small load - yarn submitted to rotation
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- **MULTISCALE** nature of the material

3.16 Shear curve and optical analysis (Dumont, 2003). (2)

(2) *Composites forming technologies. Chapter 3: Finite element analysis of composite forming, P. Boisse.*

# Material characterisation



- **Biaxial tensile test**

- Different strain ratio between warp and weft directions
- **Non-linear** response, **coupling** between both directions

- **MULTISCALE** nature of the material

\* 3.13 Cross shape specimen and tensile curves for different warp weft strain ratios  $k$ .

\* *Composites forming technologies. Chapter 3: Finite element analysis of composite forming, P. Boisse.*

# DRAPING & THERMOFORMING

## Models & Constitutive law\*

### Discrete methods

Mapping

Particle based methods

Truss based methods

- geometrical models, fishnet
- interacting **particles** via an energy function
- periodic arrangements of fibre bundles

### Continuous methods

Elastic

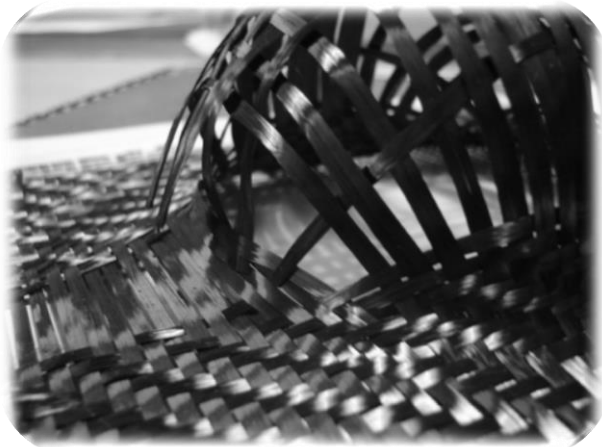
Viscous models

Both

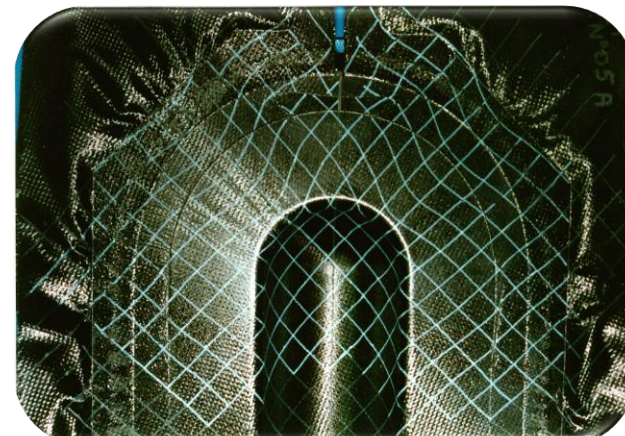
- many models in the literature, **solid**
- inextensible **fluid**

# Continuous approach

# Continuous approach



≠



# HYPOELASTIC MODEL

# Hypoelastic models

- Constitutive law (fibrous reinforcements):

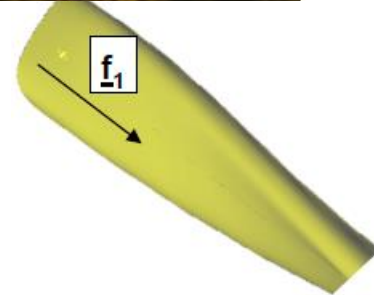
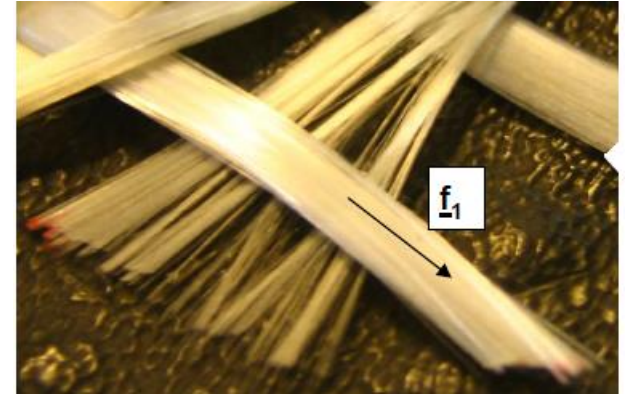
$$\sigma^\nabla = \mathbb{C} : \mathbf{D}$$

$\mathbf{D}$  : strain rate tensor

$\sigma^\nabla$ : objective stress rate tensor

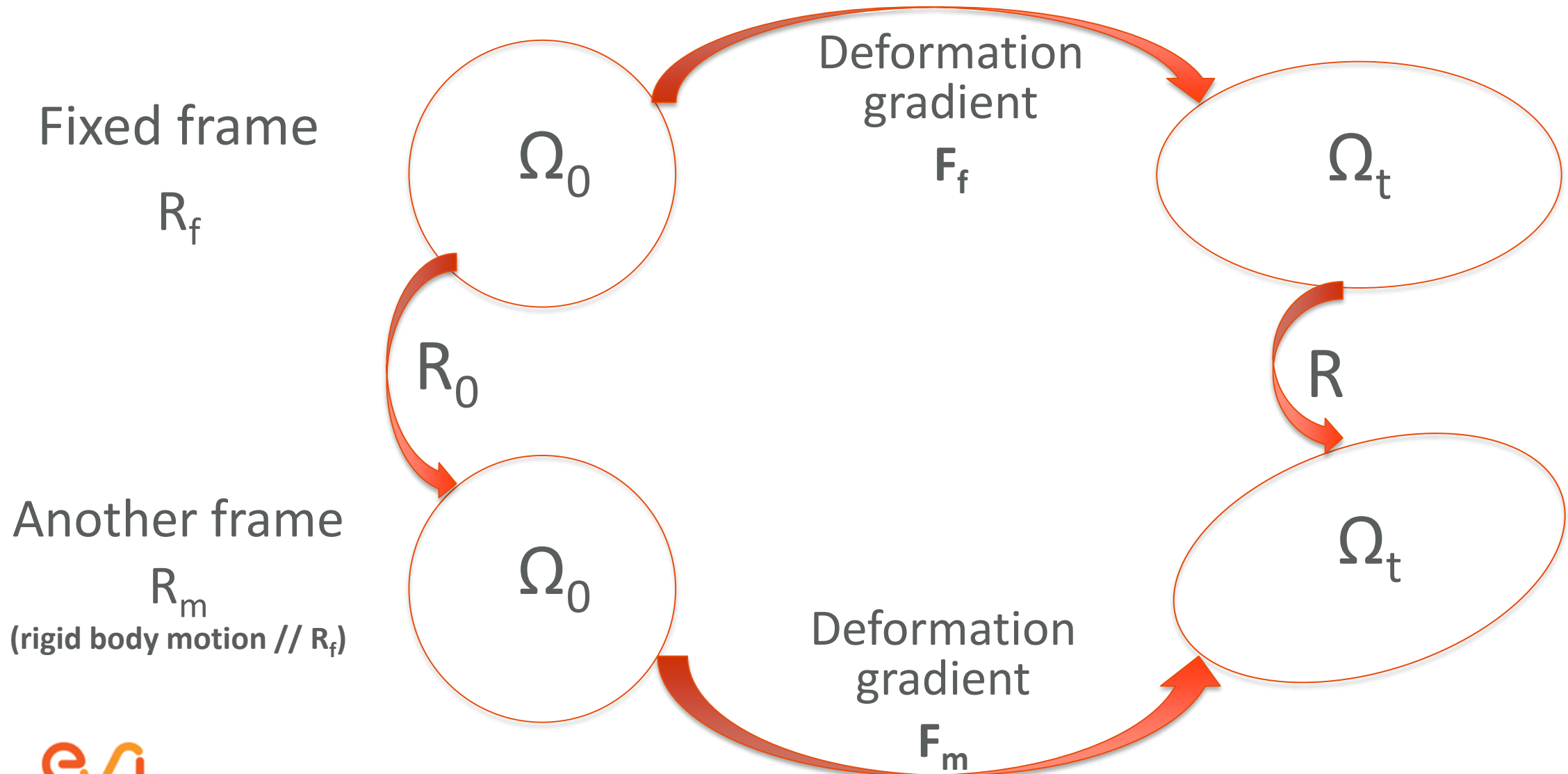
- ✓ Objectivity

- Frame invariance principle: the stress rate should not depend on the frame definition !
- A rigid body motion should not imply a stress rate

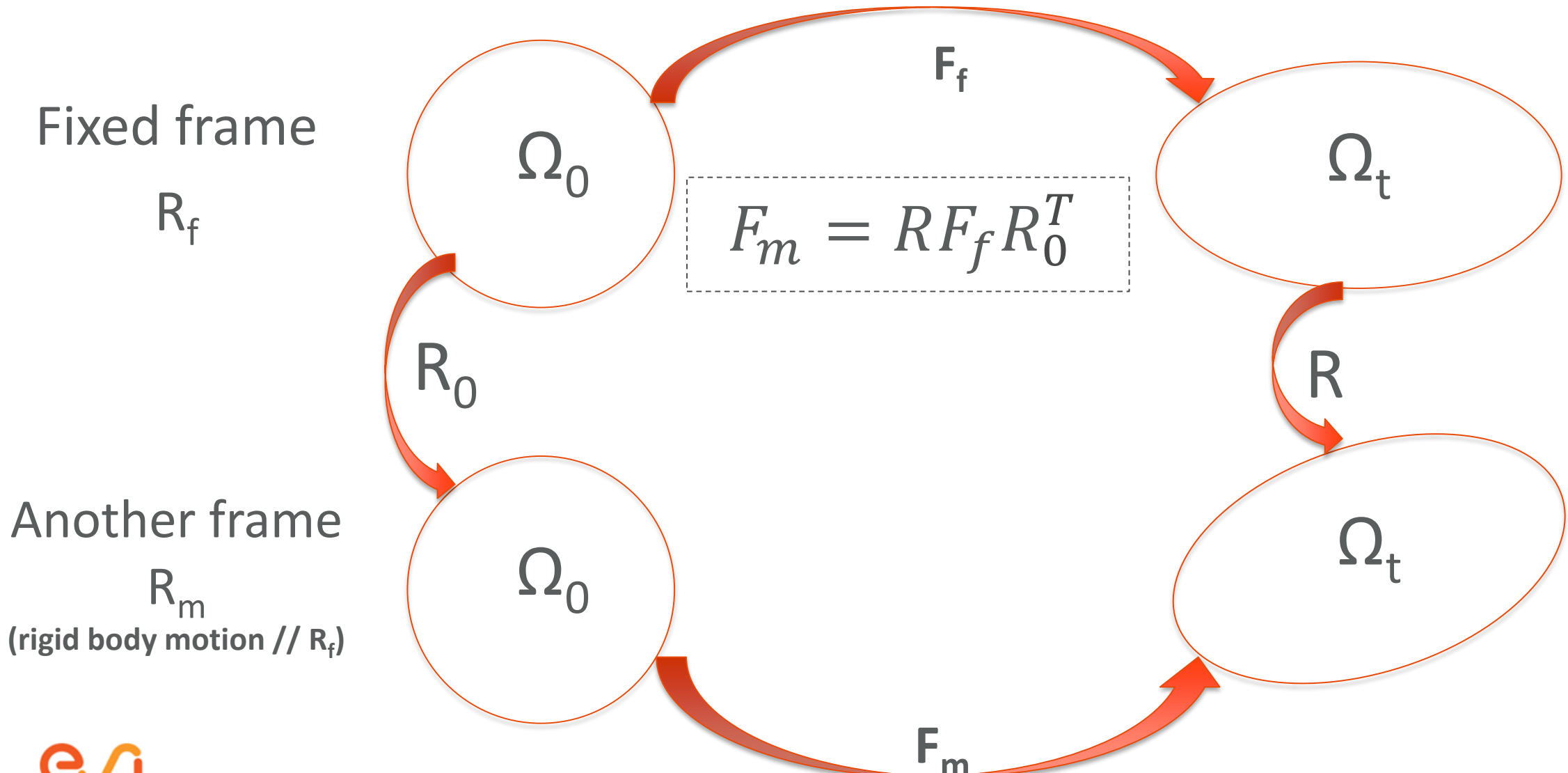




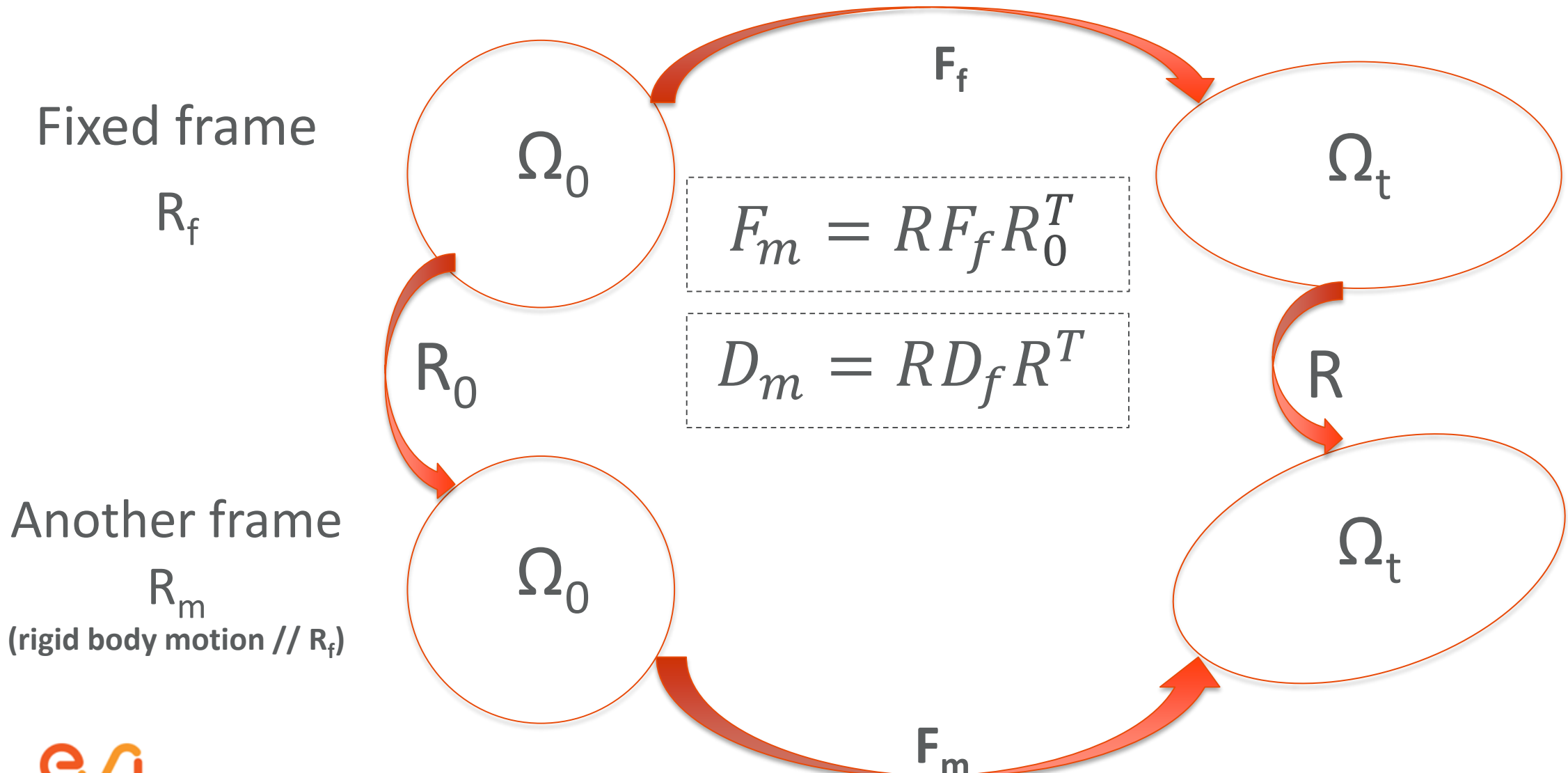
# Hypoelastic models



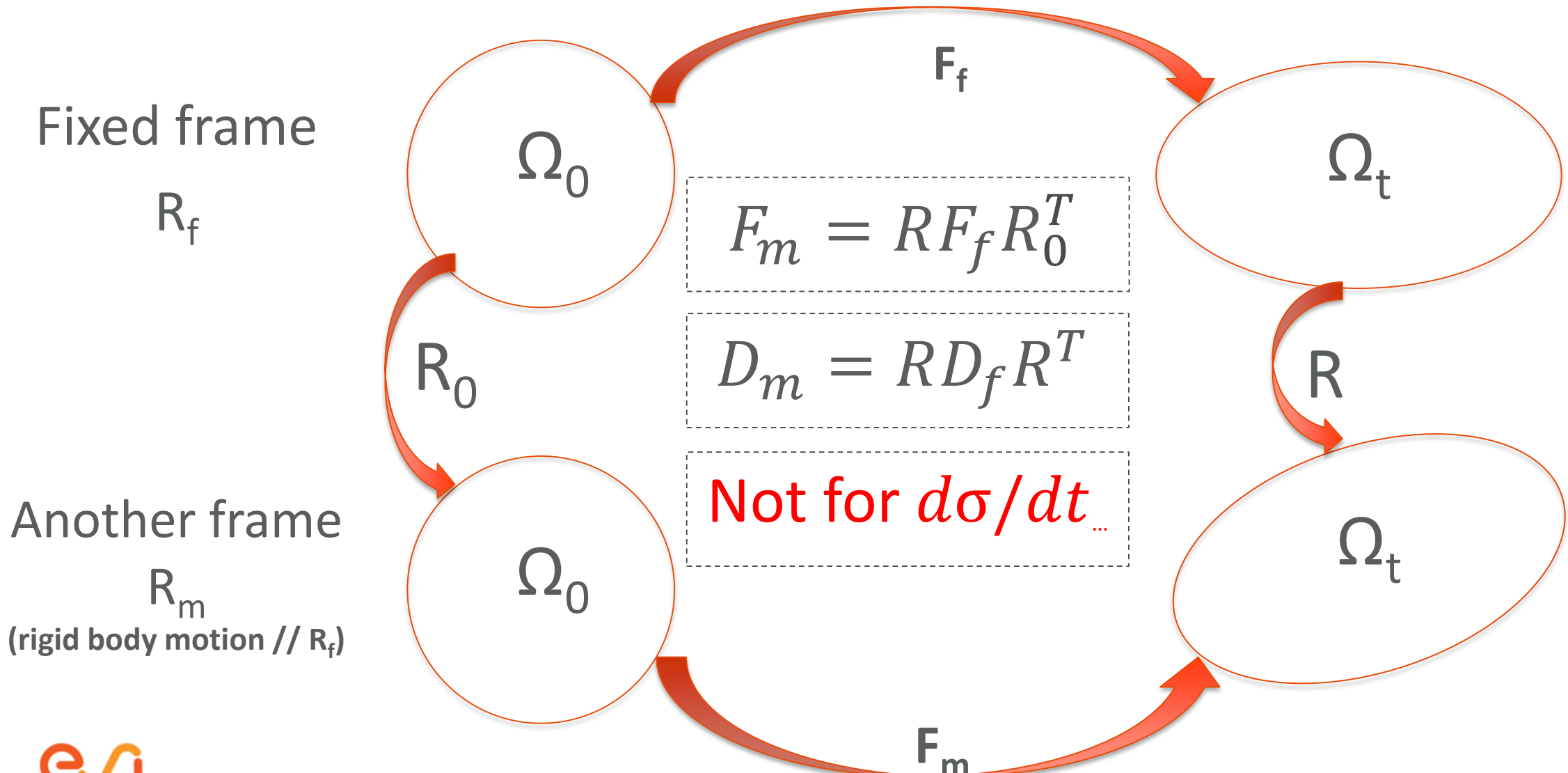
# Hypoelastic models



# Hypoelastic models



# Hypoelastic models



# Hypoelastic models

Classic objective derivatives (Jaumann, Green-Naghdi, ...)

$$\sigma^{\nabla} = \dot{\sigma} + \sigma \cdot \Omega - \Omega \cdot \sigma$$

With:  $\Omega = \dot{Q} \cdot Q^T$  (rigid body rotation)

$Q$ : corotational frame rotation (rigid body rotation)

$\dot{Q}$ : rotation rate

## Consequences

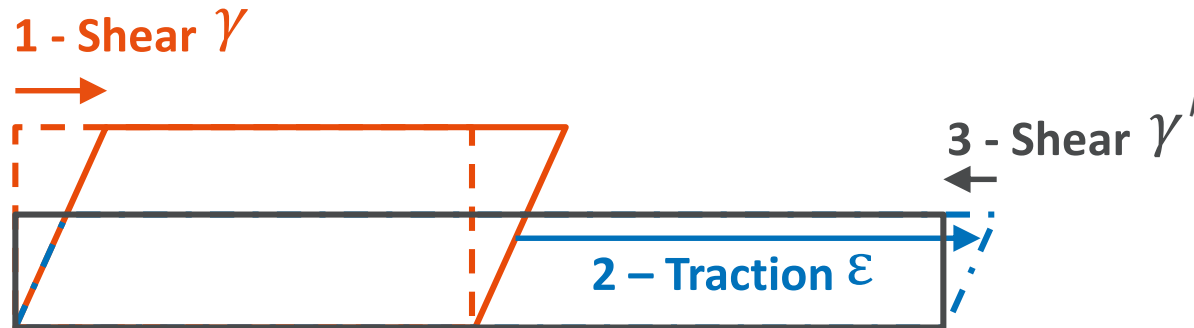
- ❖ Orthotropic axes updated by the rotation  $Q$
- ❖ But  $Q$  is not exactly the local material rotation, the orthotropic axes are not aligned with the fibre direction
- ❖ When shear deformation is important the orthotropic axes are far from being aligned with the fibre direction
- ❖ This is why non-orthogonal model have been developed\*

# Hypoelastic models

- Constitutive law (fibrous reinforcements):

$$\sigma^{\nabla} = \mathbb{C} : \mathbf{D}$$

Why **hypoelastic** ?



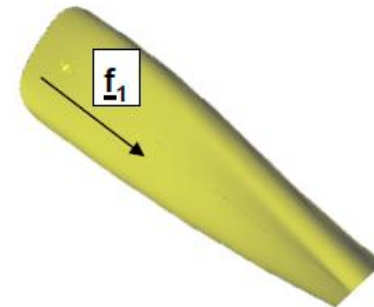
- Constitutive law (fibrous reinforcements):

$$\sigma^{\nabla} = \mathbb{C} : \mathbf{D}$$

Why **hypoelastic** ?

It can be shown that the stress state depends on the **loading path** (1)

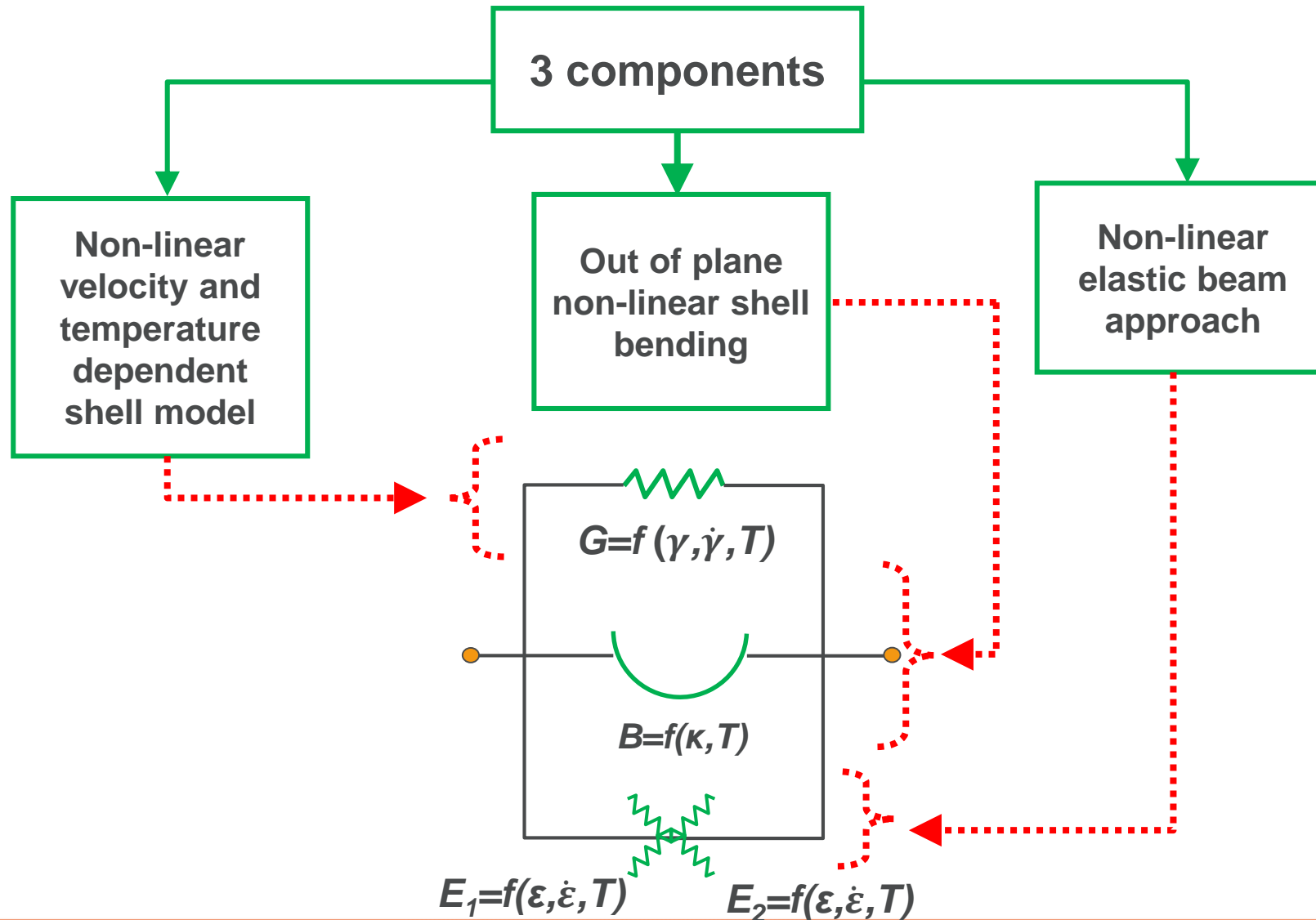
- The initial configuration can be recovered **without** or **with** stresses
- The stresses can be cancelled without recovering the initial configuration



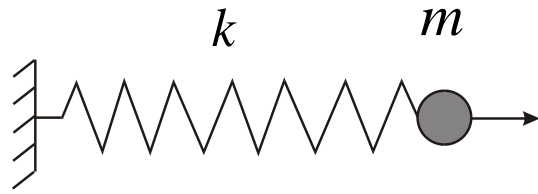
It can be shown that the stress state depends on the **loading path** (1)

- The initial configuration can be recovered **without** or **with** stresses
- The stresses can be cancelled without recovering the initial configuration

# Approche continue

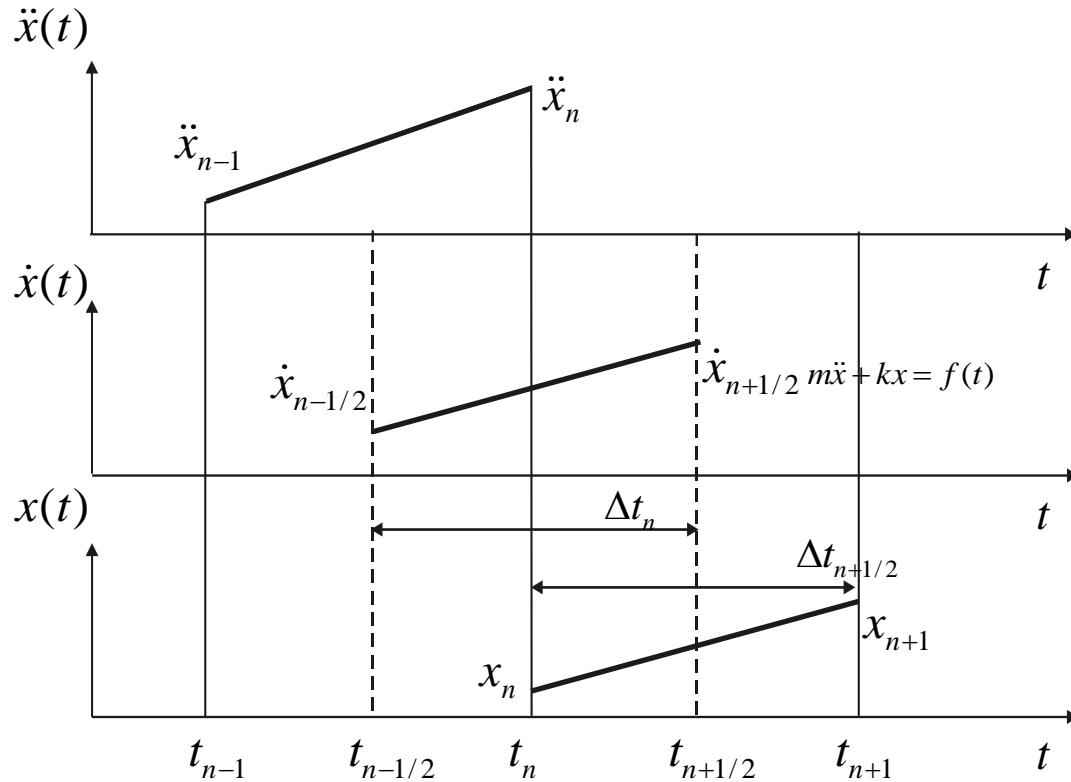


# The explicit integration scheme



$x$ : displacement

$$m\ddot{x}_n + kx_n = f_n(t)$$



$$(1) \quad \ddot{x}_n = m^{-1}(f_n - kx_n)$$

$$(2) \quad \dot{x}_{n+1/2} = \dot{x}_{n-1/2} + \Delta t_n \ddot{x}_n$$

$$(3) \quad x_{n+1} = x_n + \Delta t_{n+1/2} \dot{x}_{n+1/2}$$



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# DRAPING & THERMOFORMING

## Simulations Examples

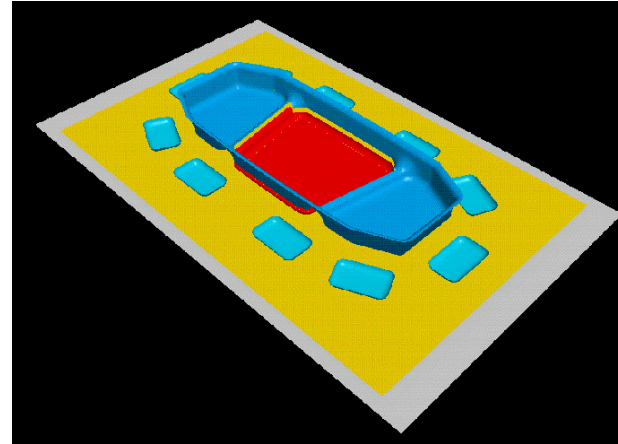
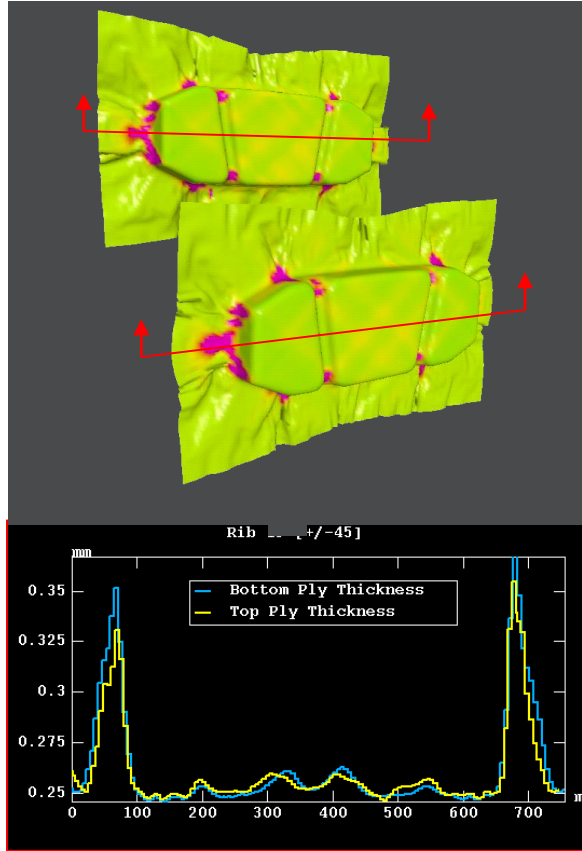
# ESI PAM-COMPOSITES



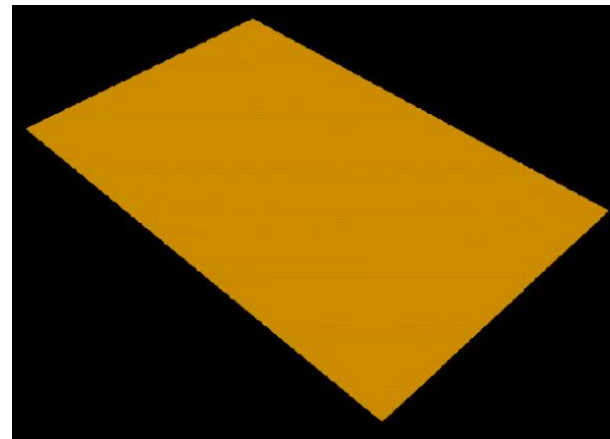
# AIRBUS

## Thermoplastic forming application: Wing box thermoforming

Thickness per ply

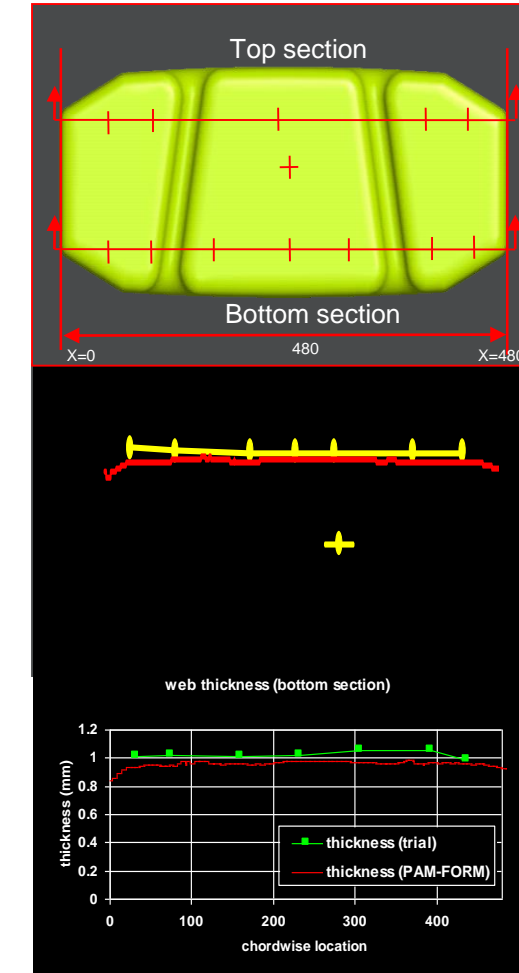


Process animation

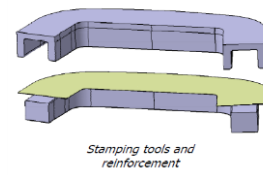


Laminate thickness

Ultrasonic measurement versus simulation

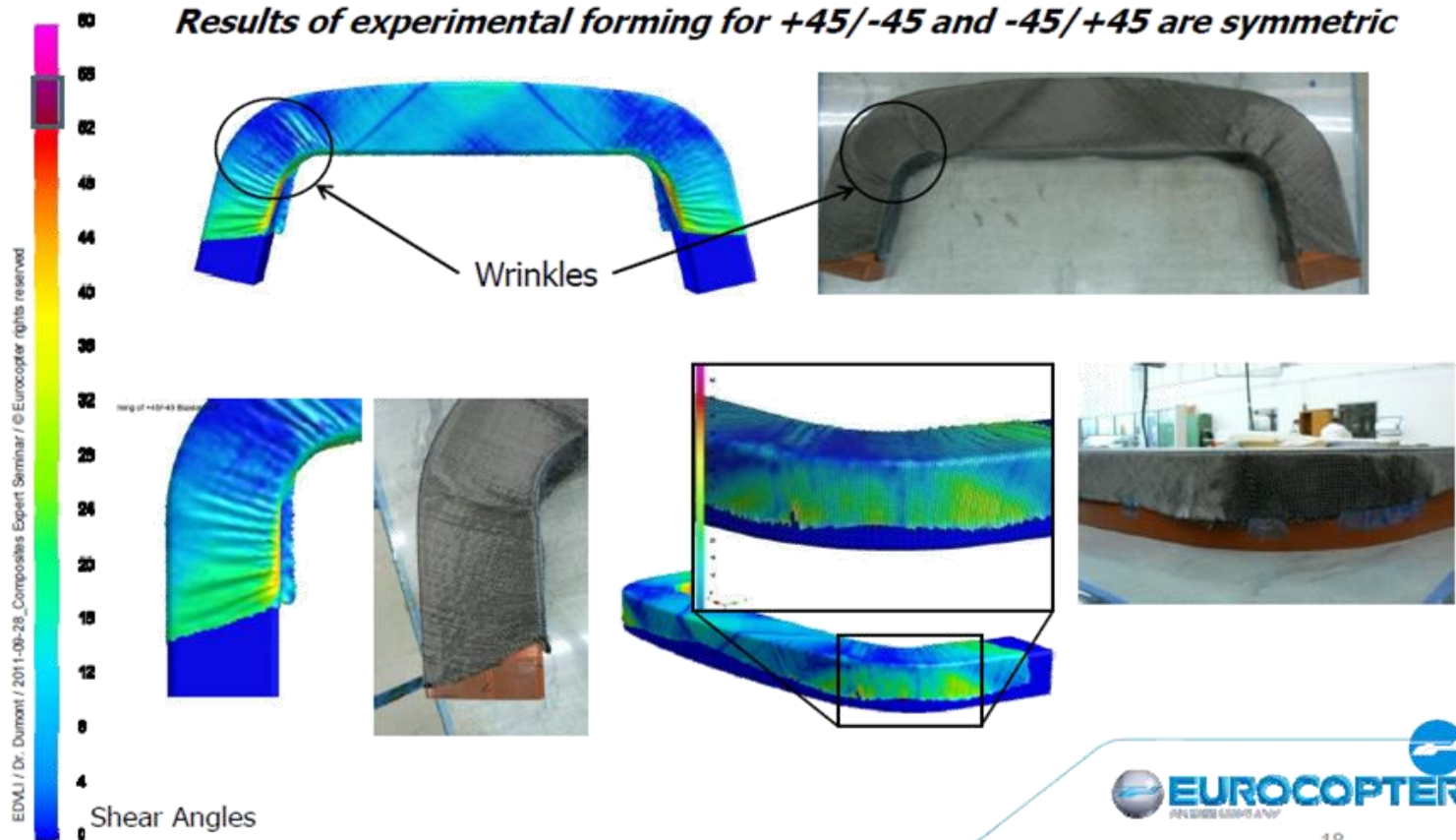


# ESI PAM-COMPOSITES



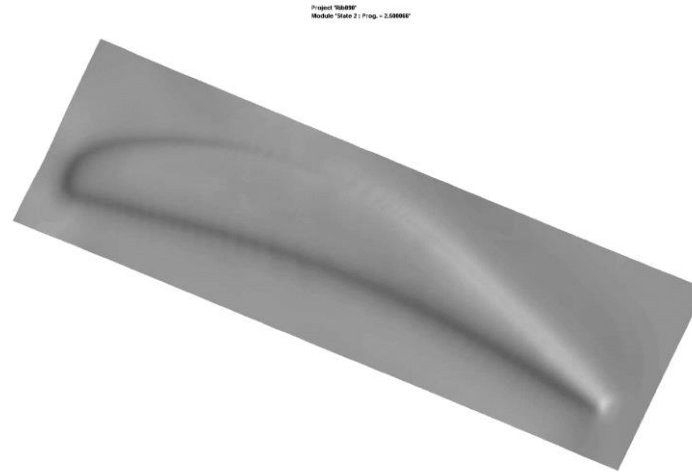
## Preforming application: Fabric shearing and wrinkle prediction

Forming – Results of  $\pm 45$  NCF: Sh. angles

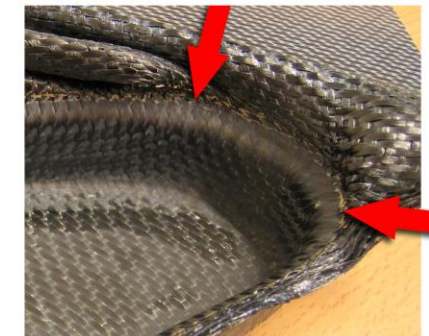
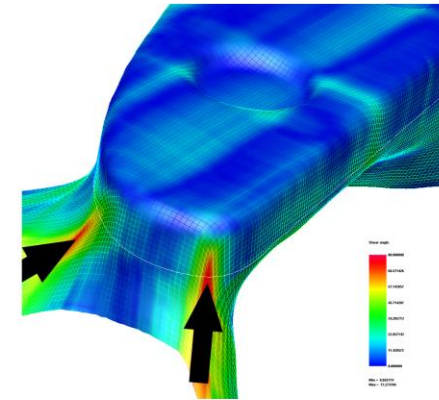
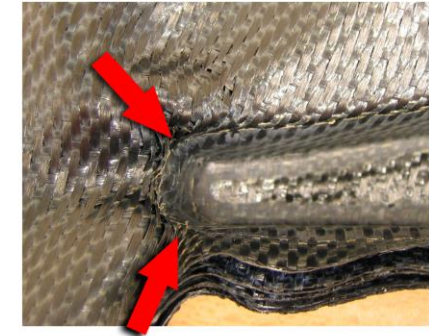
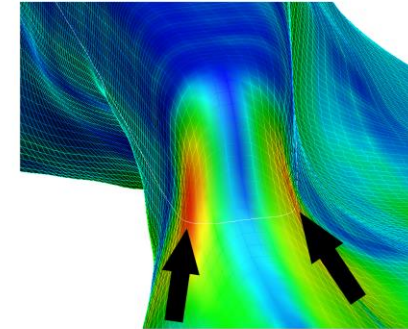


# ESI PAM-COMPOSITES

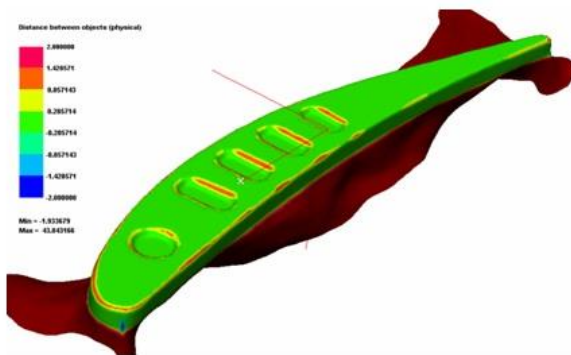
## Thermoplastic forming application: Flap rib Rubber Pad Forming



Rubber pad forming simulation

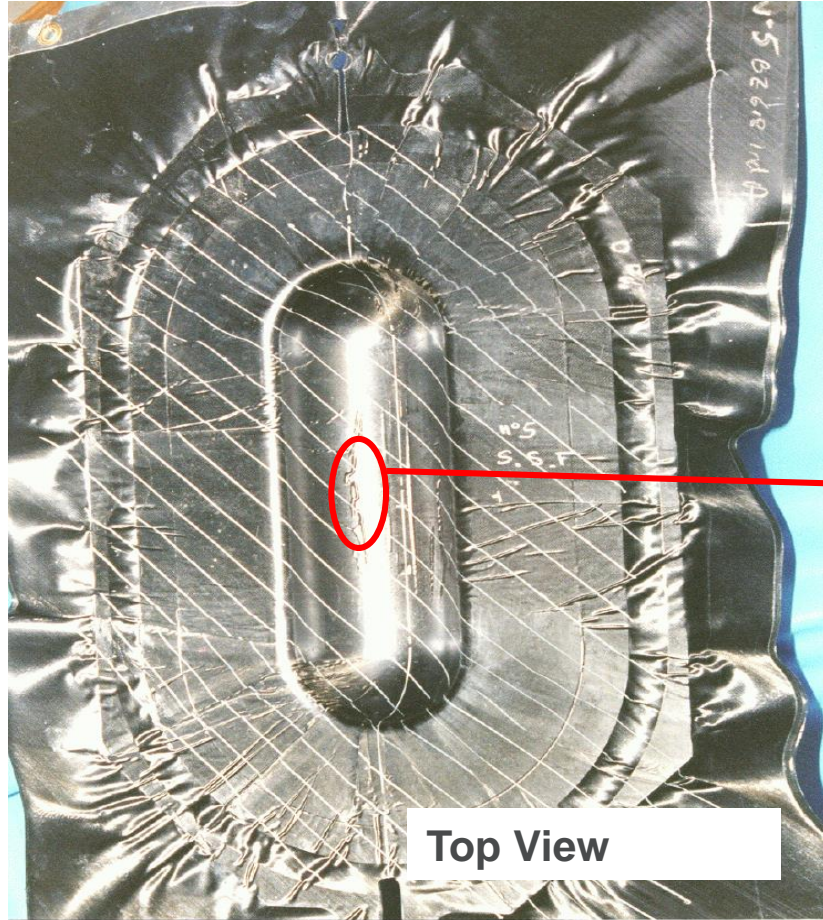


Fabric shearing

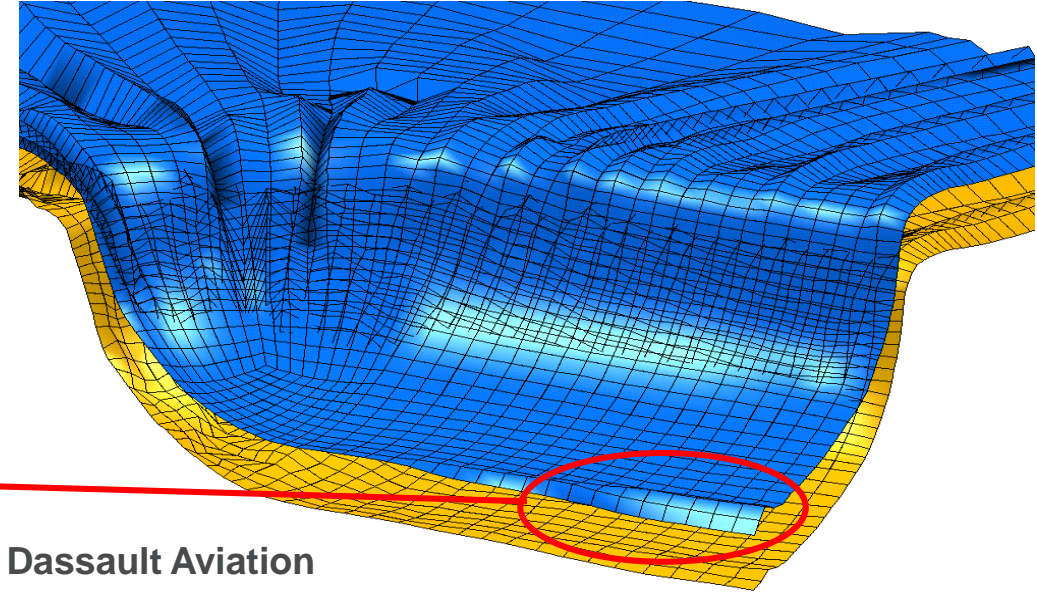


Bridging effect

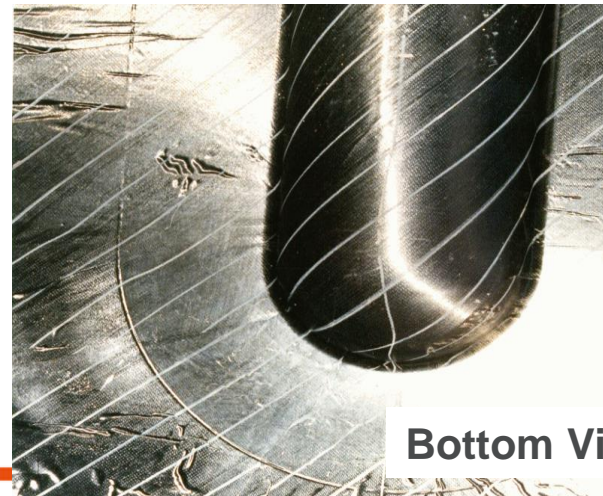
# UD Thermoforming



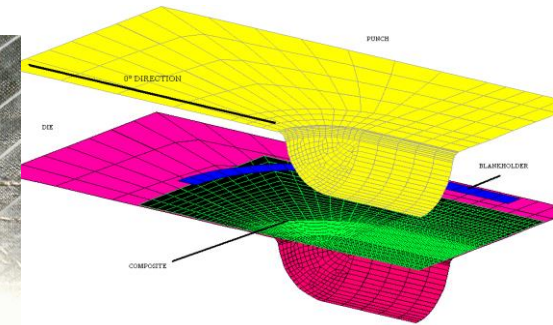
Top View



Dassault Aviation



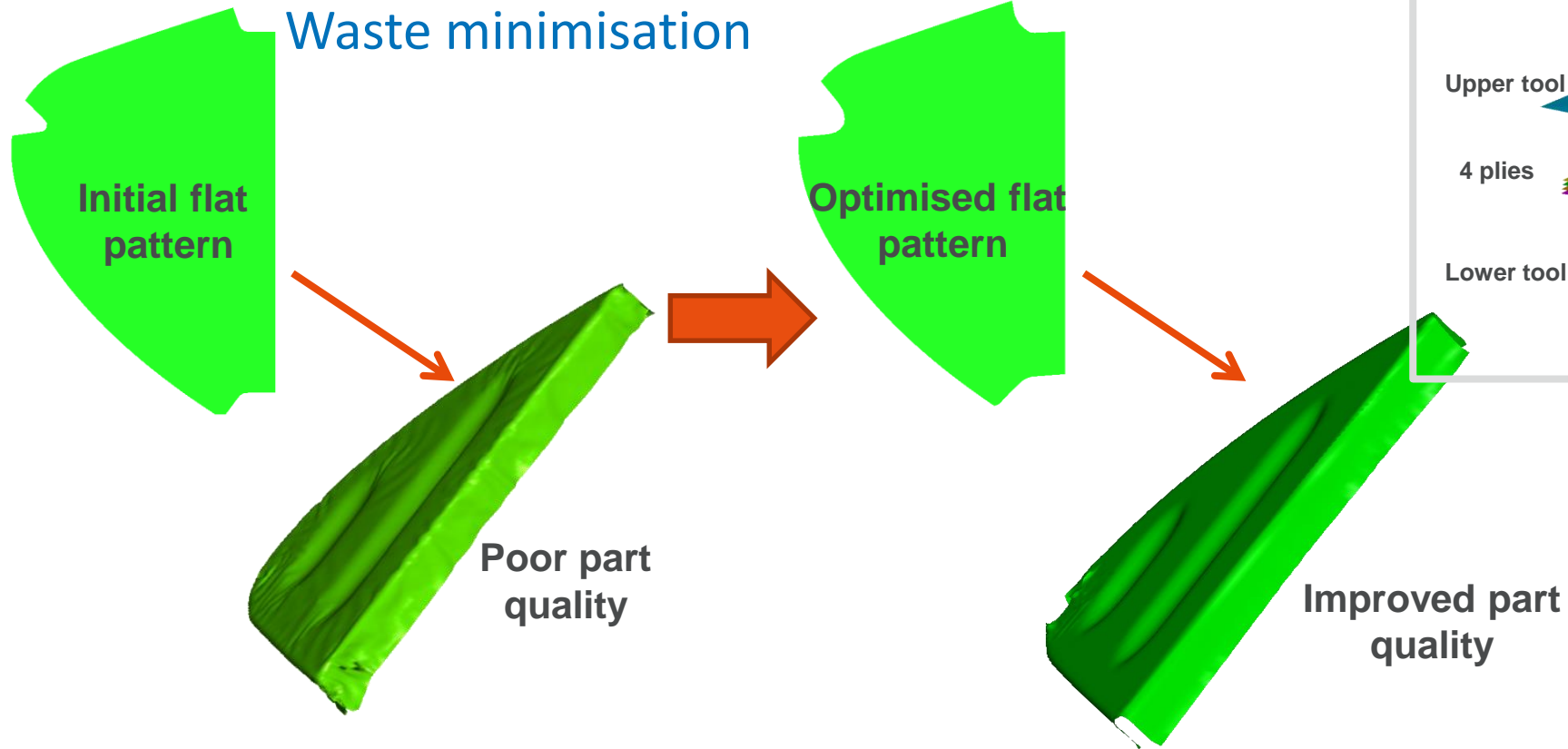
Bottom View



# ESI PAM-COMPOSITES

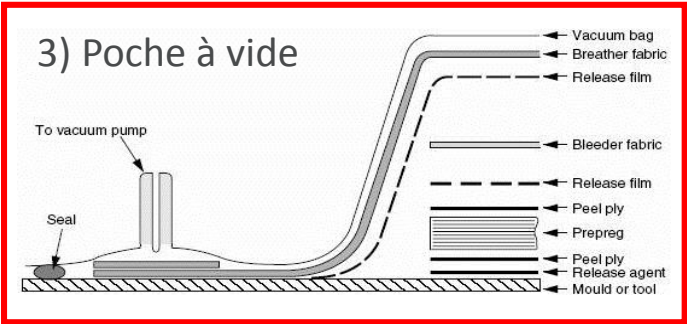
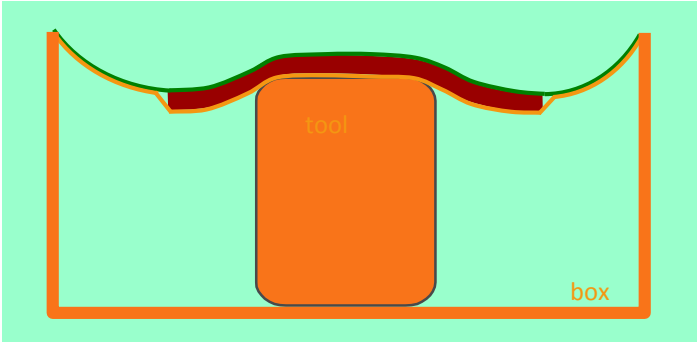
**AIRBUS**

Thermoplastic forming application: **Flat pattern optimization**



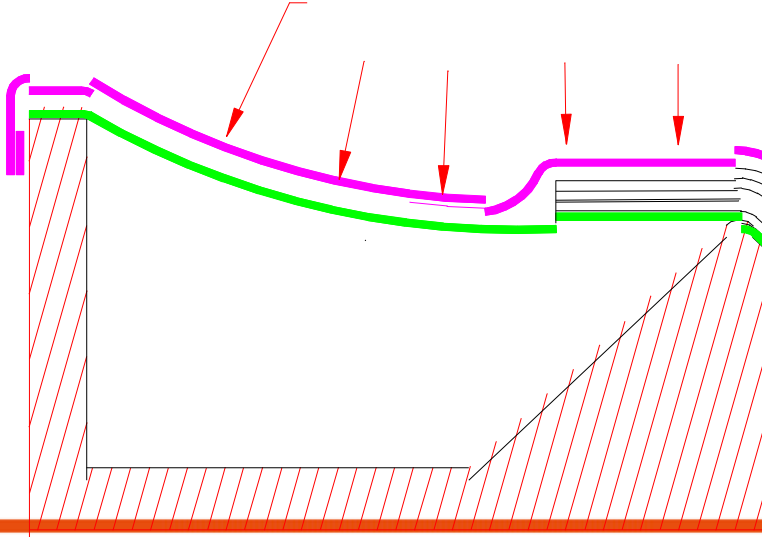
Flat pattern optimization  
4 plies / thermoplastic matrix

# Double diaphragm forming



Avant formage

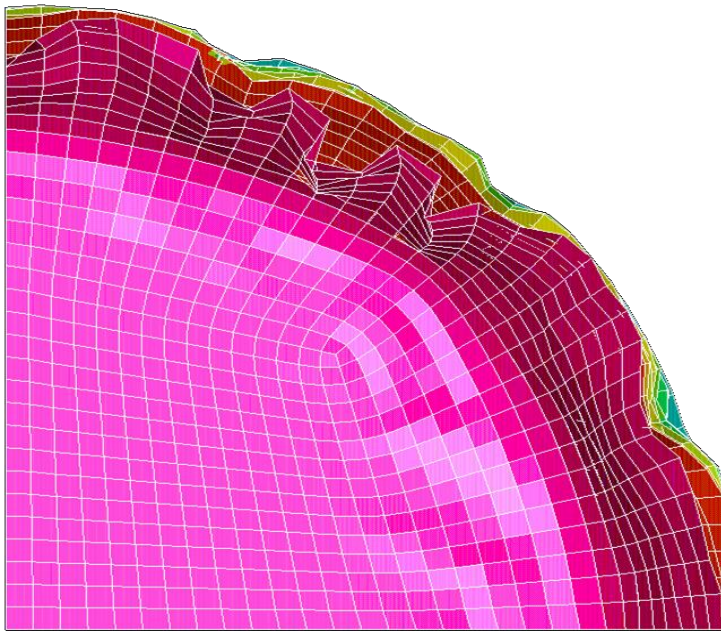
Chauffage pour assouplir la matrice



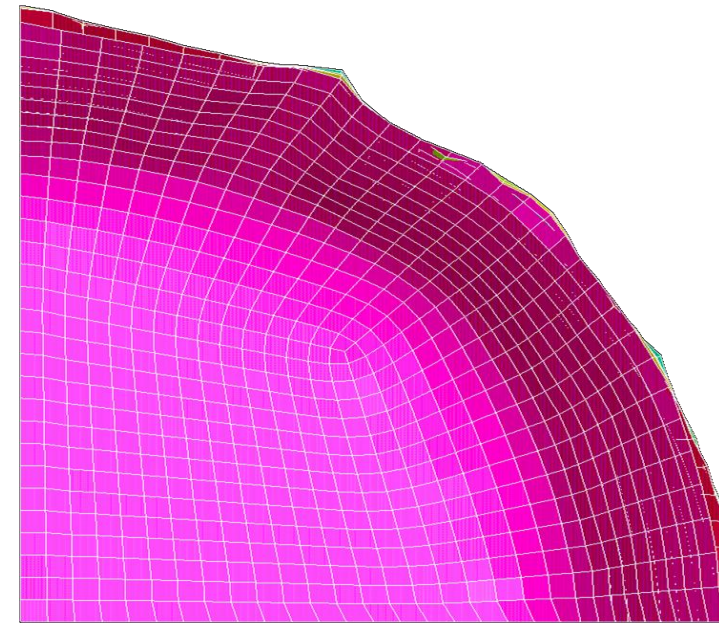
# Example of what the results can tell us

## Comparison between two forming strategies

Use of one single diaphragm  
=> **wrinkles**



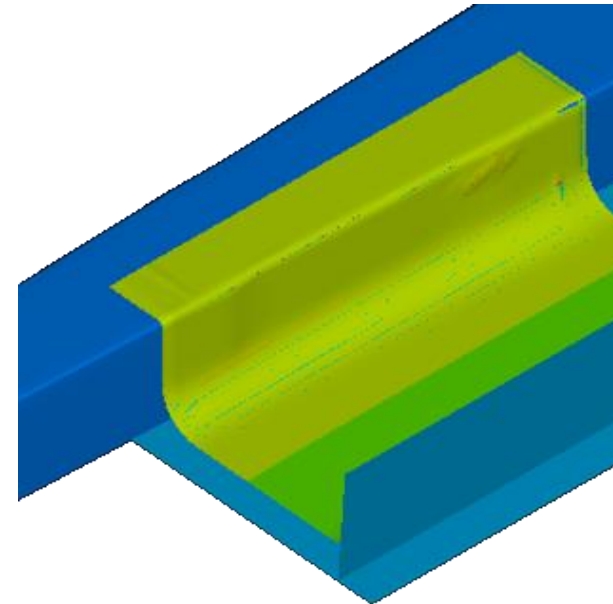
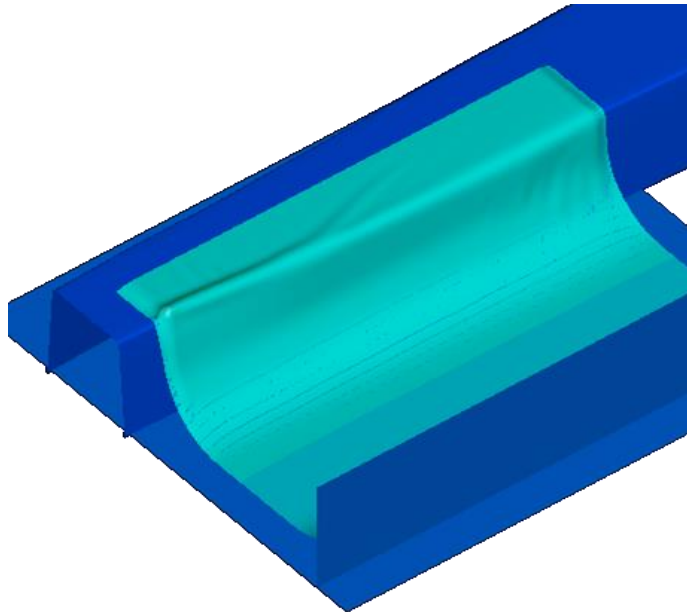
Use of two diaphragms  
=> **No wrinkle**





# Forming of a composite stringer

## Double diaphragm forming

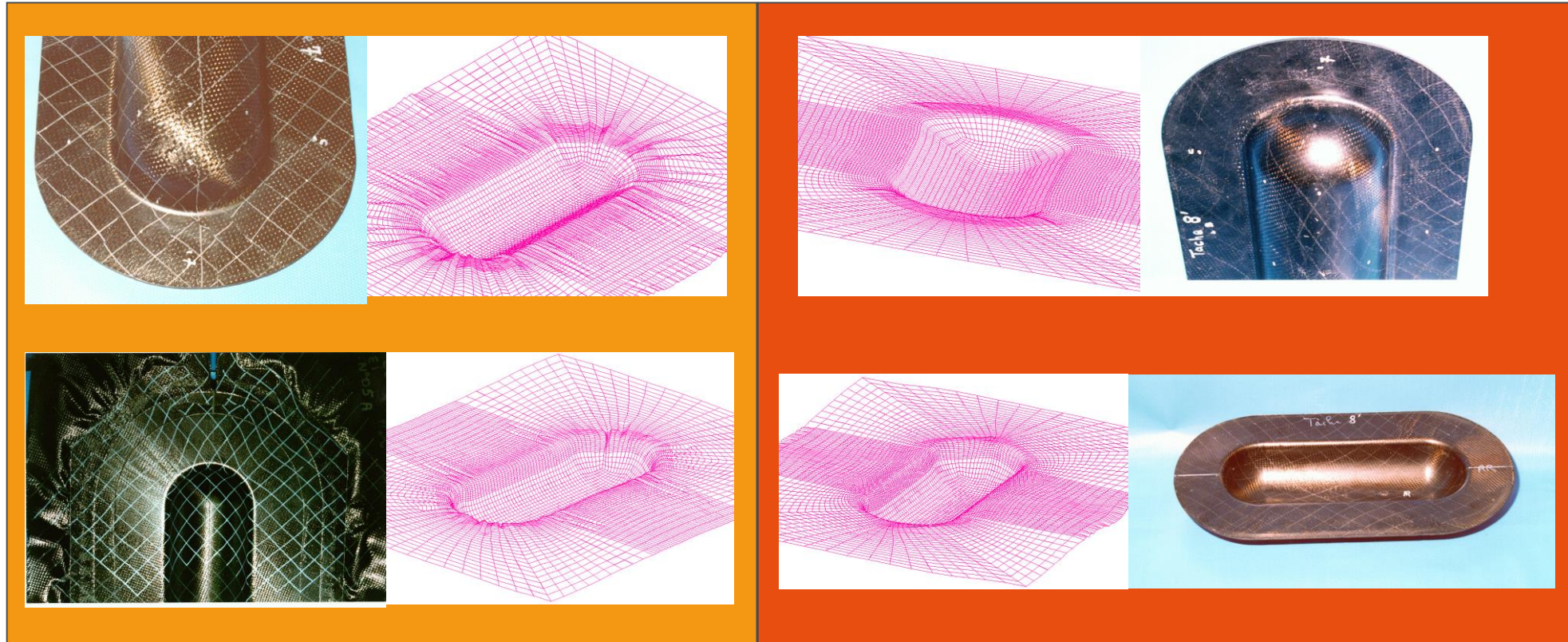


- The number of plies has an influence on the laminate deformation

# Woven Fabrics Thermoforming

## — Punch velocity selection

Dassault Aviation



**PUNCH VELOCITY=40.mm/s**

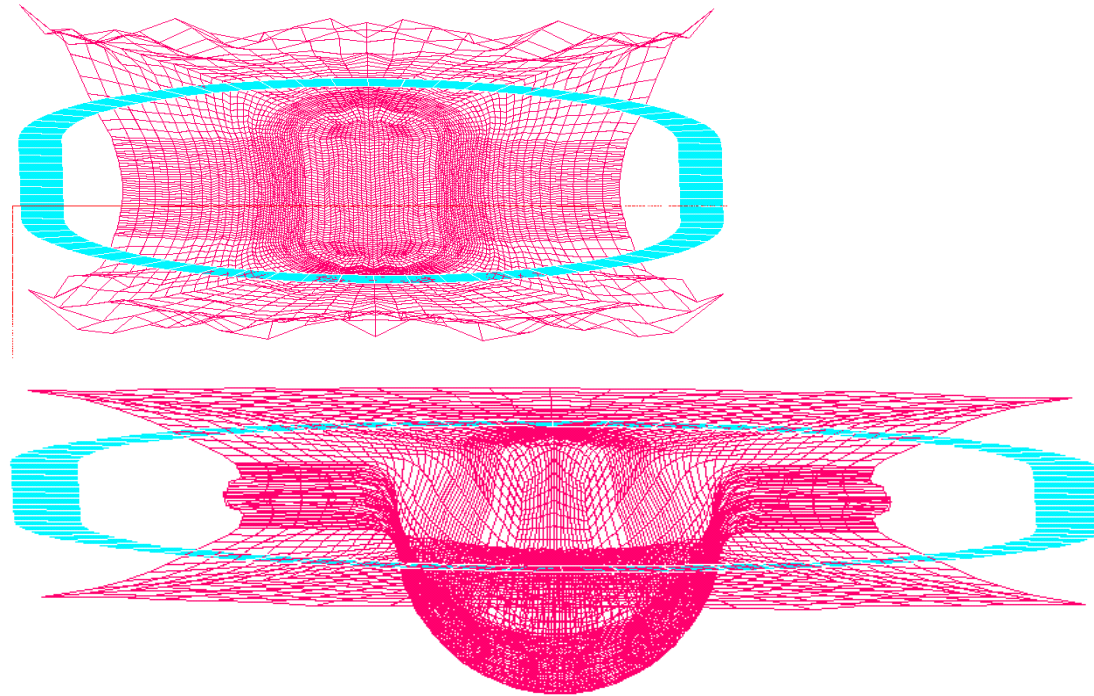
**PUNCH VELOCITY= 5.mm/s**

*(PEI-CETEX; 8 plies)*

# Simulation

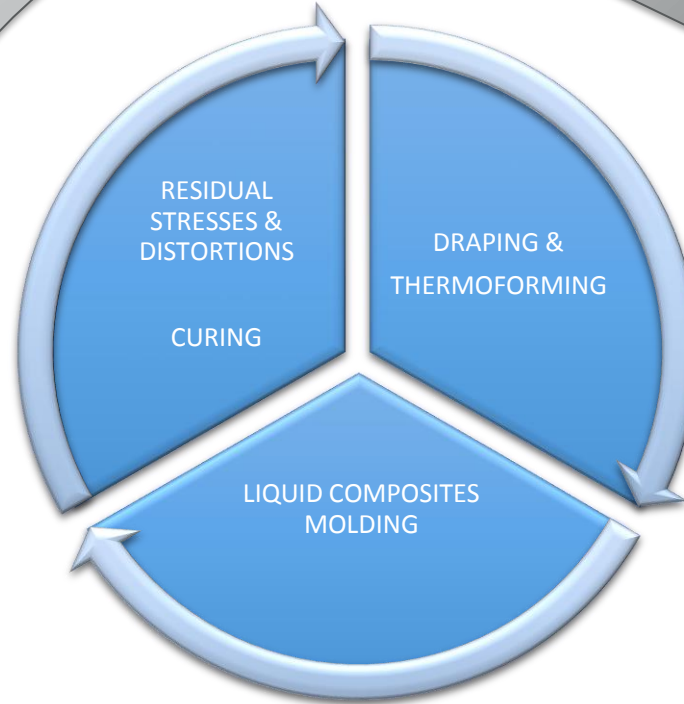
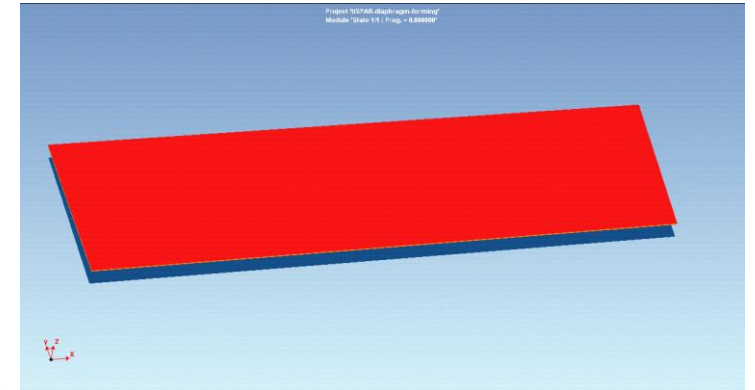
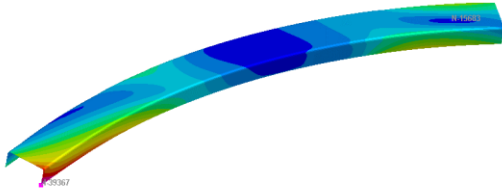
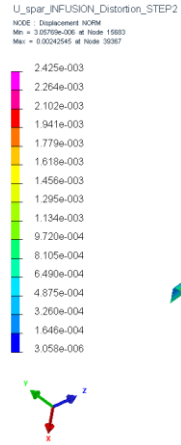
## Woven Fabrics Thermoforming

- Clamping system definition
- Laminate definition

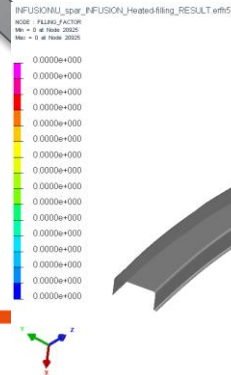


# ESI's PAM-COMPOSITES

Compensated mold



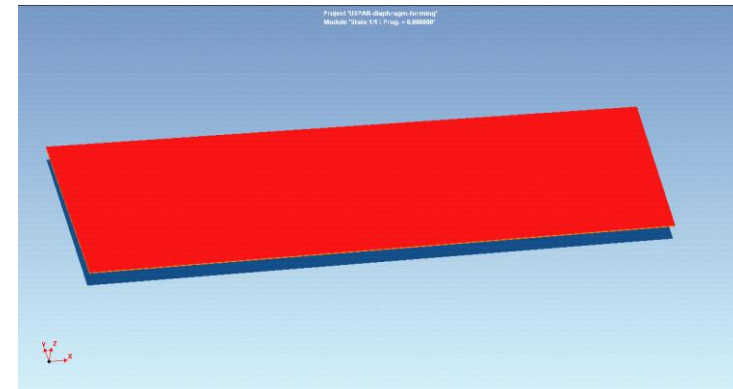
Temperature history  
 Degree of cure history



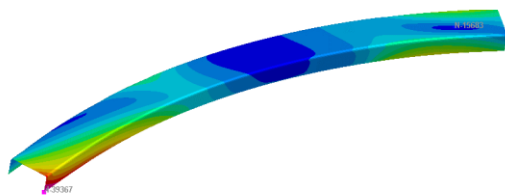
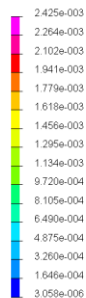
Fiber direction  
 Thickness variation

# ESI's PAM-COMPOSITES

Compensated mold

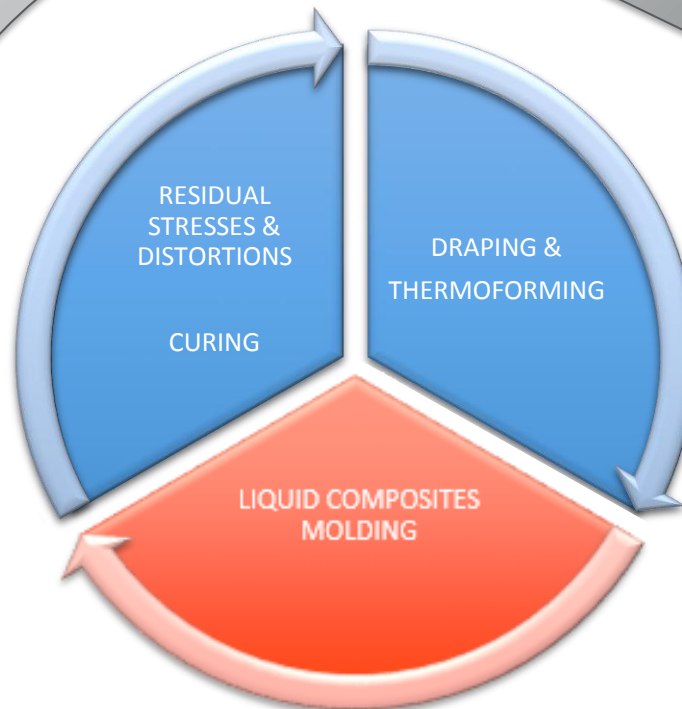


U\_spar\_INFUSION\_Distortion\_STEP2  
 NODE : Displacement NORM  
 Min = 3.05709e-006 at Node 15993  
 Max = 0.0024256 at Node 30367



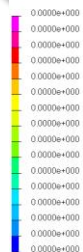
esi | PAM-COMPOSITES

1 / 18000.000000



Temperature history  
 Degree of cure history

INFUSION\_U\_spar\_INFUSION\_HeatedFilling\_RESULT.ans  
 NODE : FILLING\_FACTOR  
 Min = 0 at Node 20025  
 Max = 0 at Node 20025



1 / 0.000000

Fiber direction  
 Thickness variation

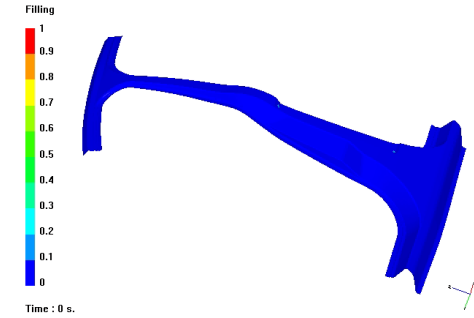
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# Liquid Composite Moulding

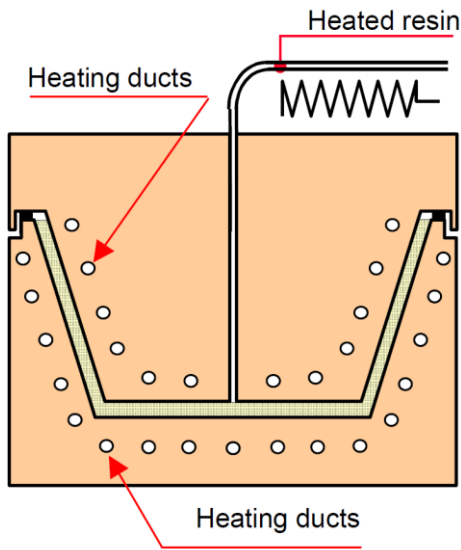
## What for ?

# Liquid Composite Moulding

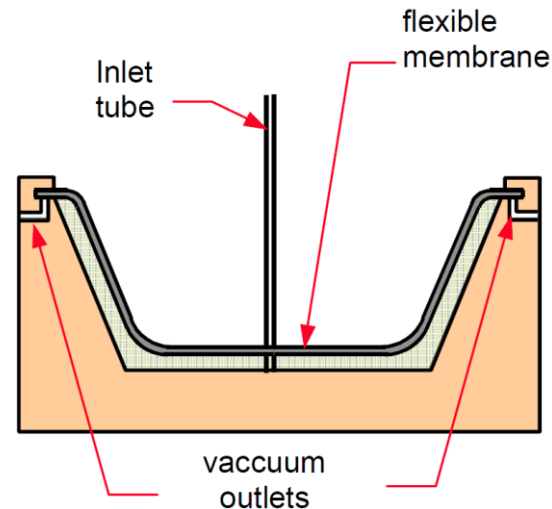
What for ?



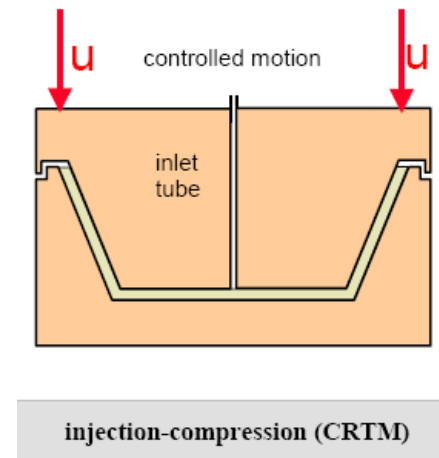
## Impregnation of dry preform with resin and curing



- RTM



- Infusion



- C-RTM

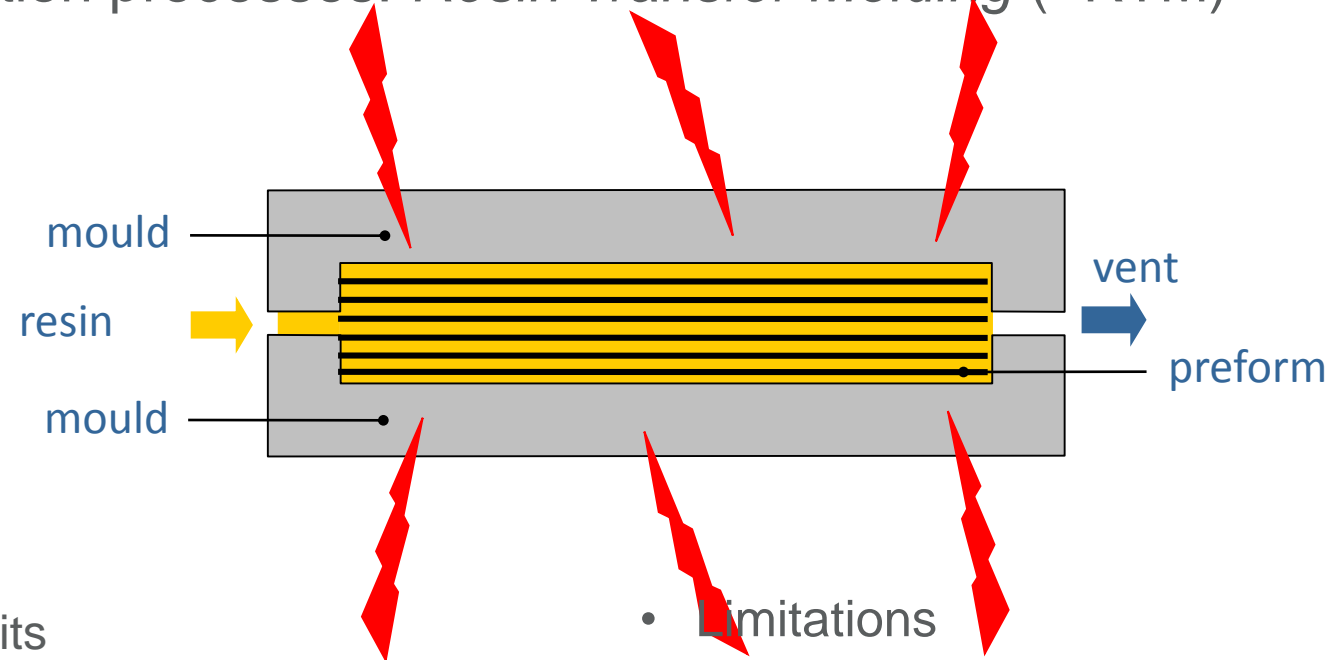
- HP-RTM
- Curing
- ...

# Liquid Composite Moulding

## What for ? Resin Transfer Moulding

LCM process (=Liquid Composite Molding)

- Injection processes: *Resin Transfer Molding* (=RTM)



- Benefits

- Low storage costs
- Good geometrical properties
- High fiber volume fraction

- Limitations

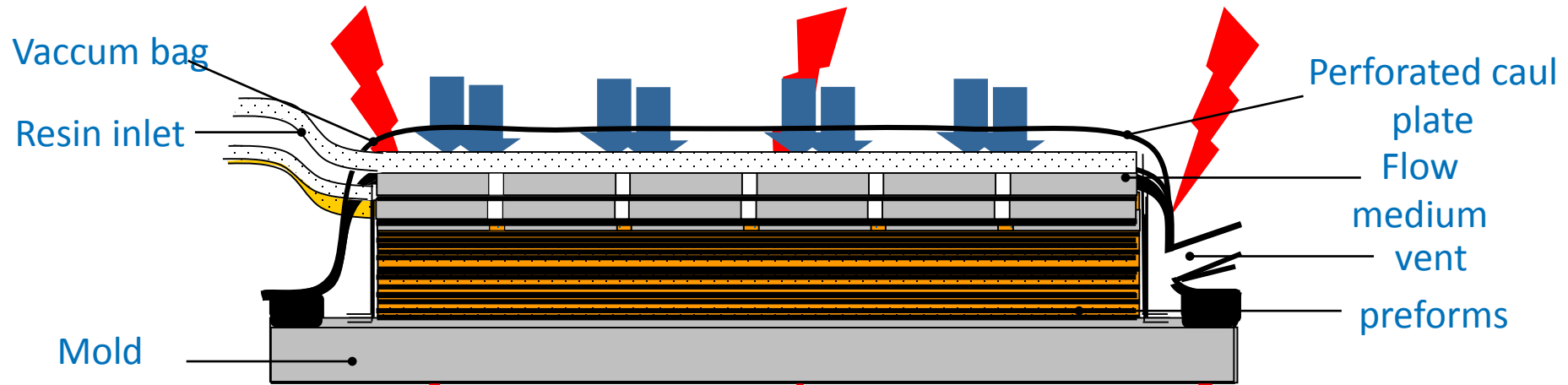
- Mould cost
- Small parts
- Impregnation difficulties for complex shapes



# Liquid Composite Moulding

## What for ? Liquid Resin Infusion

- Flexible tooling + through thickness impregnation



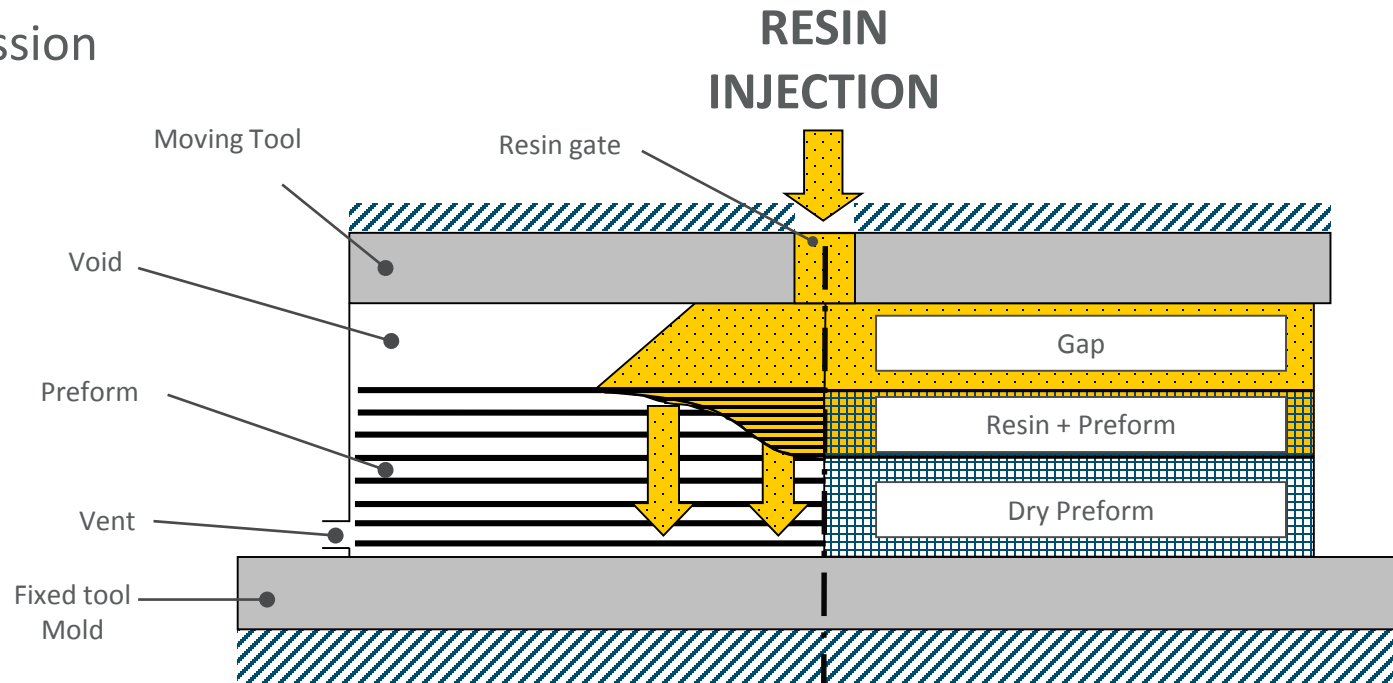
- Benefits
  - Low storage costs
  - High fiber volume fraction
  - Low mold cost
  - Big parts
  - Good impregnation

- limits
  - Bad thickness control
  - Difficult to set-up

# Liquid Composite Moulding

## What for ? Compression Resin Transfer Molding (C-RTM)

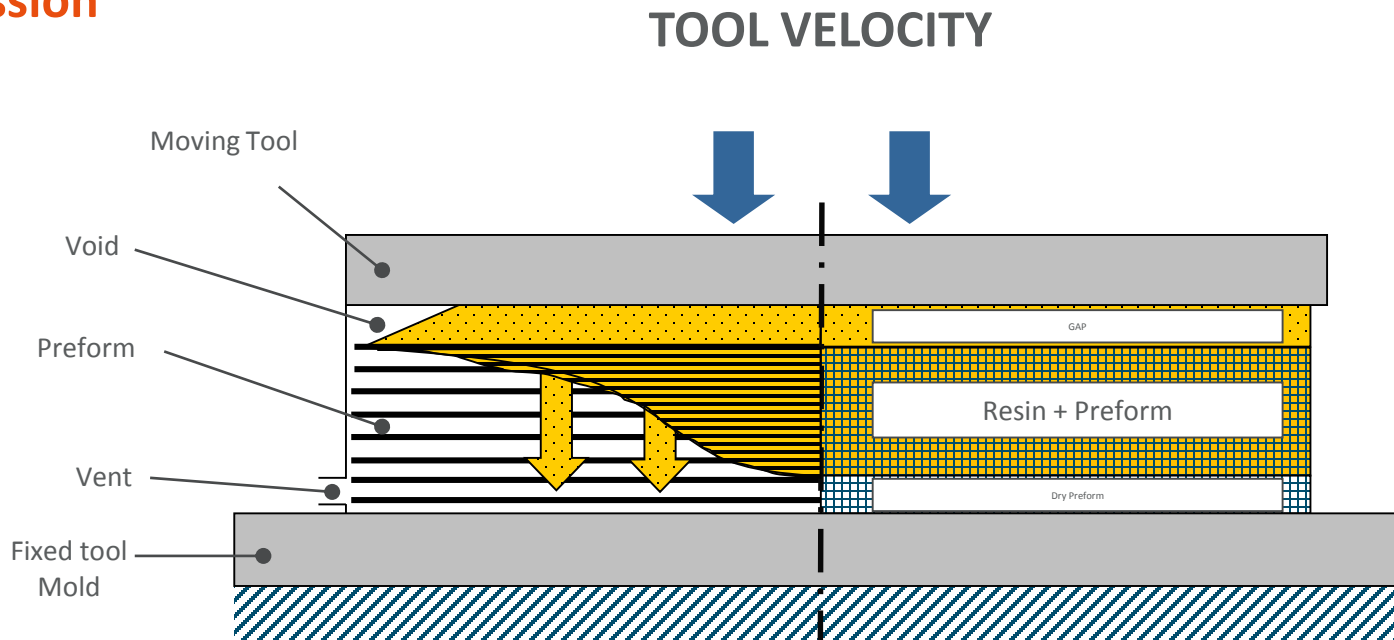
- Process is split in 2 stages
  - **Injection**
  - Compression



# Liquid Composite Moulding

## What for ? Compression Resin Transfer Molding (C-RTM)

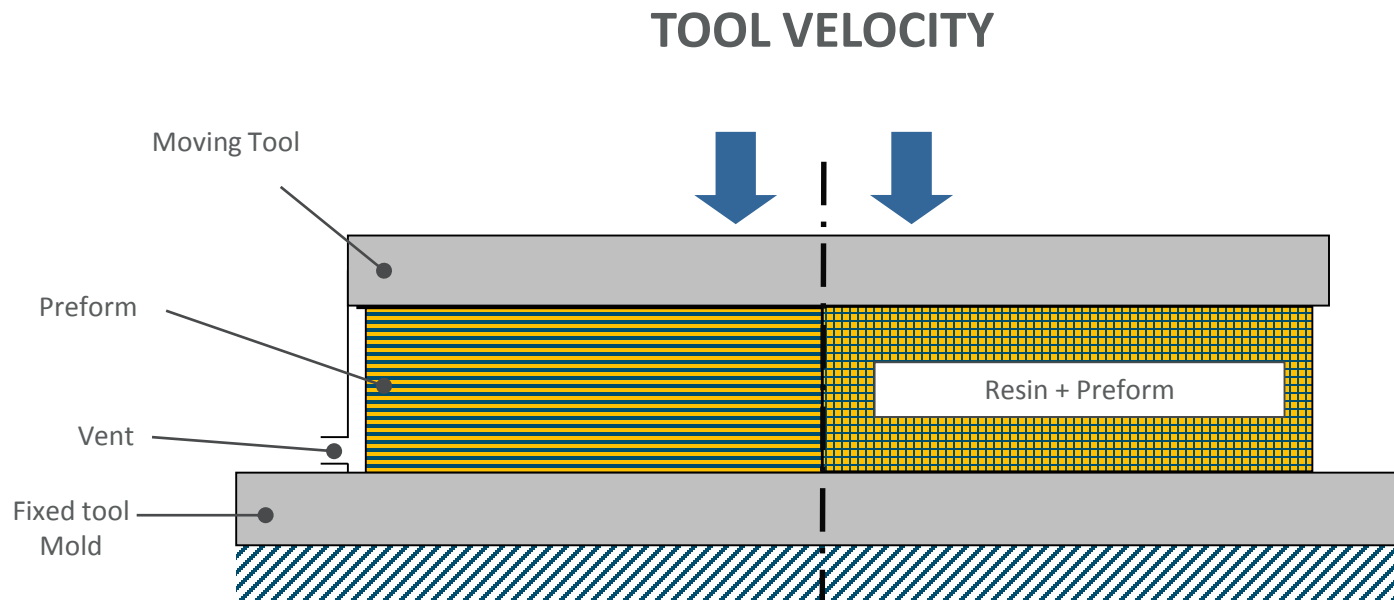
- Process is split in 2 stages
  - Injection
  - **Compression**



# Liquid Composite Moulding

## What for ? Compression Resin Transfer Molding (C-RTM)

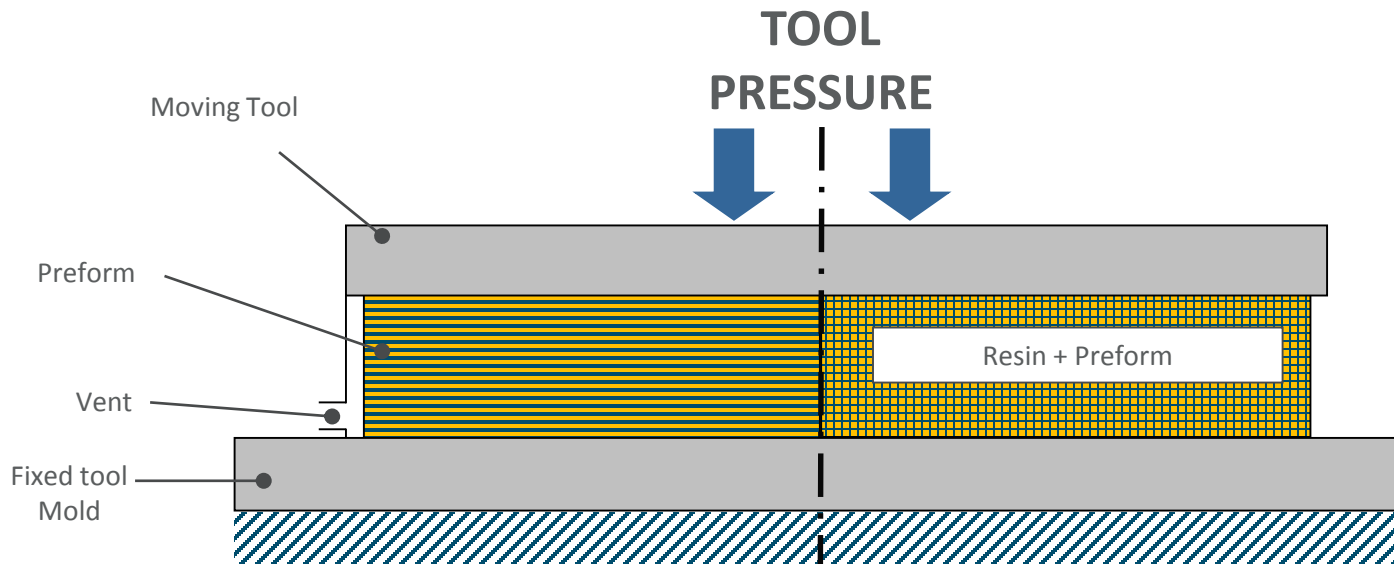
- Process is split in 2 stages
  - Injection
  - **Compression**



# Liquid Composite Moulding

## What for ? Compression Resin Transfer Molding (C-RTM)

- Process is split in 2 stages
  - Injection
  - **Compression**



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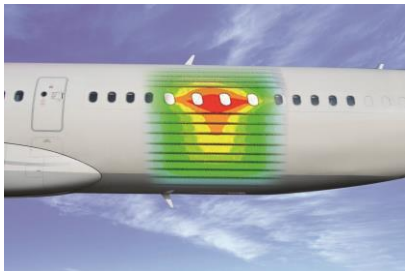
# Liquid Composite Moulding

## Industrial issues

# Liquid Composite Moulding

## Industrial issues : Aeronautic industry

- Medium to large parts
- Main constraints:
  - Part design cannot be modified easily
    - Processability of the designed part
    - Process design cost
  - Manufactured part quality (very few porosity, no distortion...)
- New constraints:
  - Manufacturing time and cost



G\_MKT\_RL\_10\_345, Courtesy of EADS Innovation Works, Infusion simulation of a fuselage panel with PAM-RTM

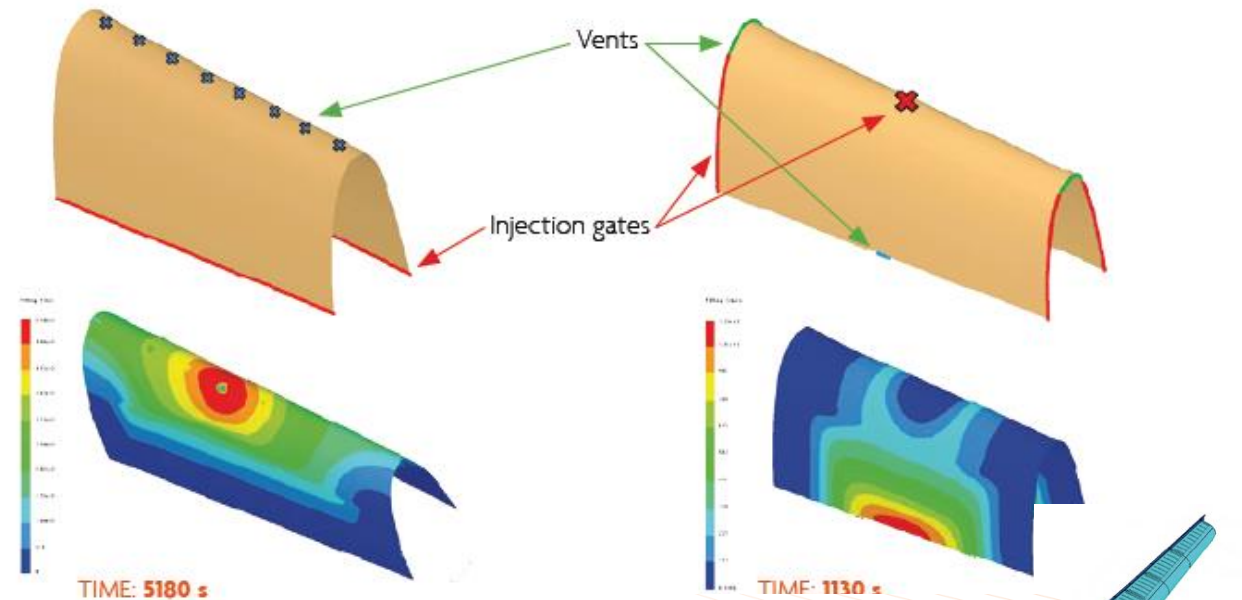


G\_MKT\_R\_L\_13\_255, Courtesy of VZLÚ

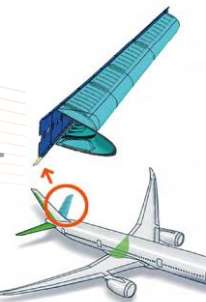
Simulation time divided by 5 thanks to simulation  
Better quality parts with less scraps (better reproducibility)

INITIAL INJECTION CONFIGURATION

OPTIMIZED INJECTION CONFIGURATION



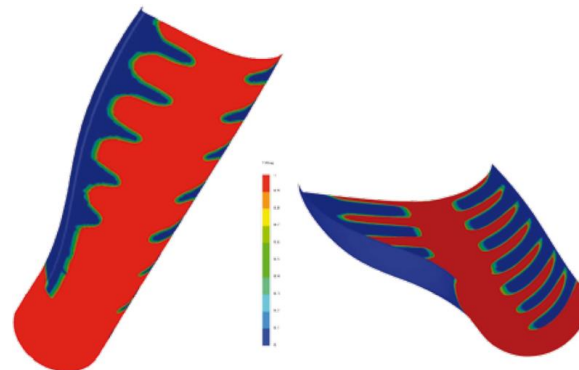
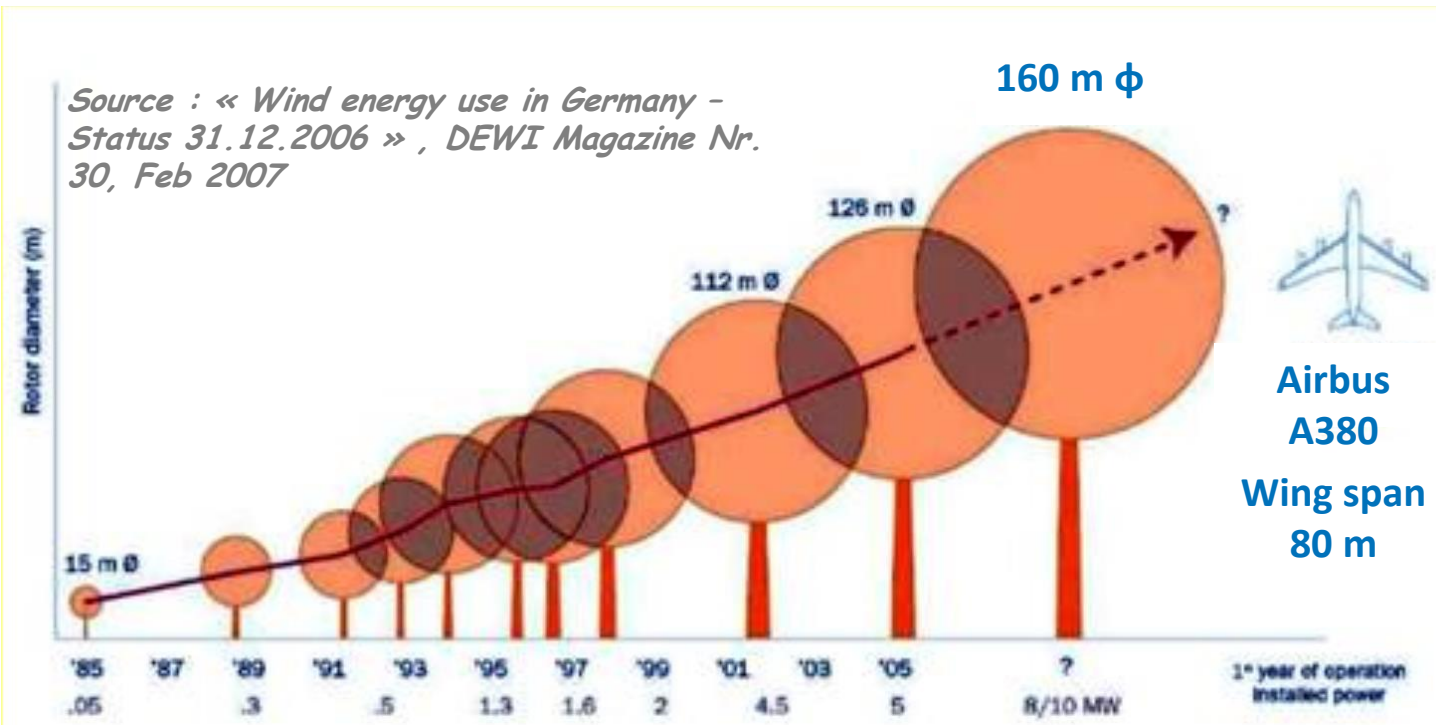
**AER**nnova



# Liquid Composite Moulding

## Industrial issues : Wind industry

- Large to very large parts
- Some region very thick (> 10 cm)
- Main constraints:
  - Size of the parts:
    - Processability of the designed part
    - Process design cost
  - Manufactured part quality for the critical structural part (spar)
  - Manufacturing and material cost



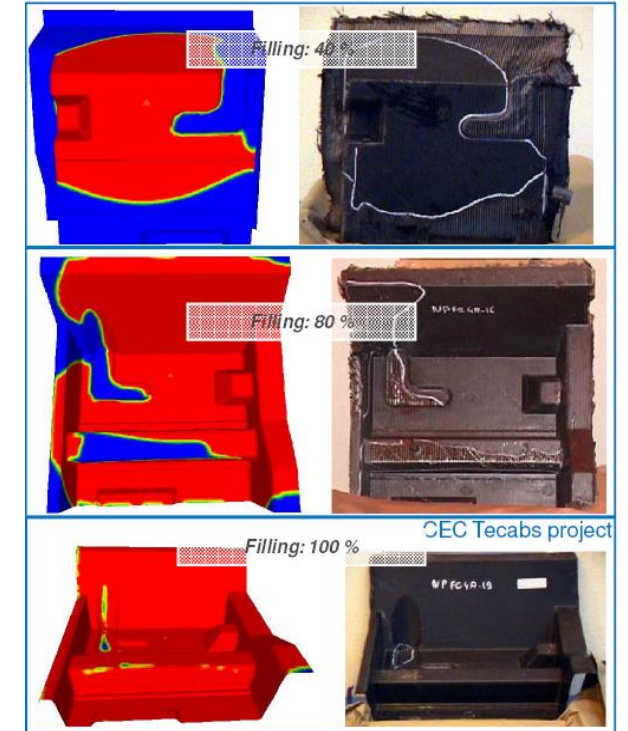
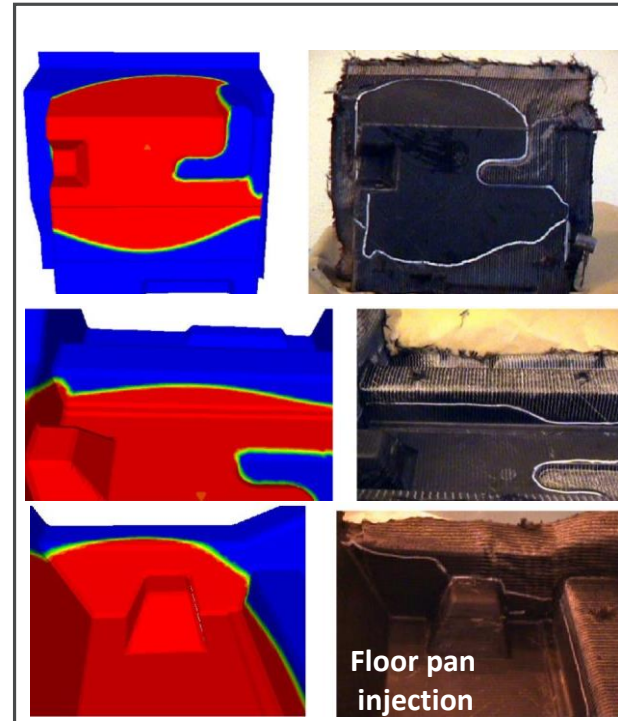
An 81.6 meter long offshore wind turbine rotor blade & Analysis of several injection strategies with PAM-RTM on the root of the rotor blade  
G.MKT.R.L14.625



# Liquid Composite Moulding

## Industrial issues : Automotive industry

- Small to medium parts
- Main constraints:
  - Material cost
  - Manufacturing **time** window (< 2-3') and **cost**
    - Processability of the designed part
    - Process design cost



RTM application: Automotive floor panel

---

# Liquid Composite Moulding

## How to simulate and Why

# Why simulate LCM process ?

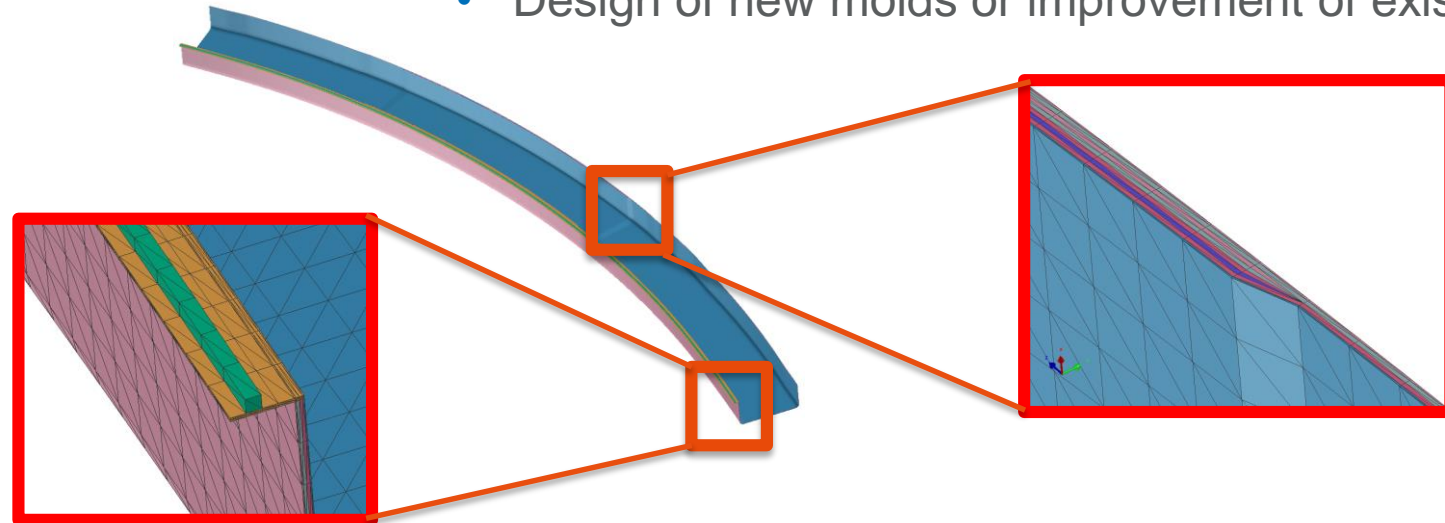
To Determine and Optimize process parameters such as:

- **Process parameters:**

- locate injection gates and vents
- Flow rates or pressure
- Vacuum
- Temperature cycle

- **Material / Design**

- Material behavior  $f(T, t)$
- Ply book
- Design of new molds or improvement of existing molds



Through prediction of:

- Air traps
- Micro porosity
- Injection time

- Temperature evolution
- Degree of cure evolution
- Pressure in the mold

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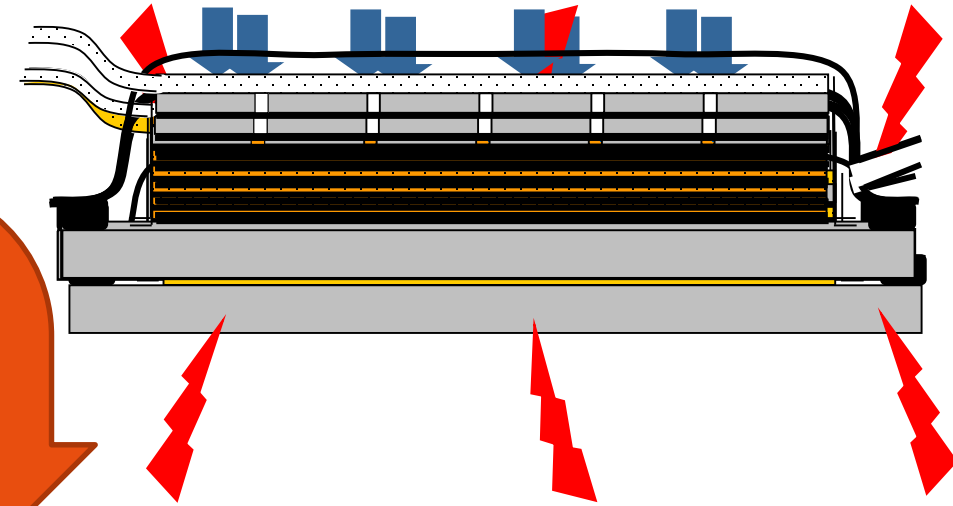
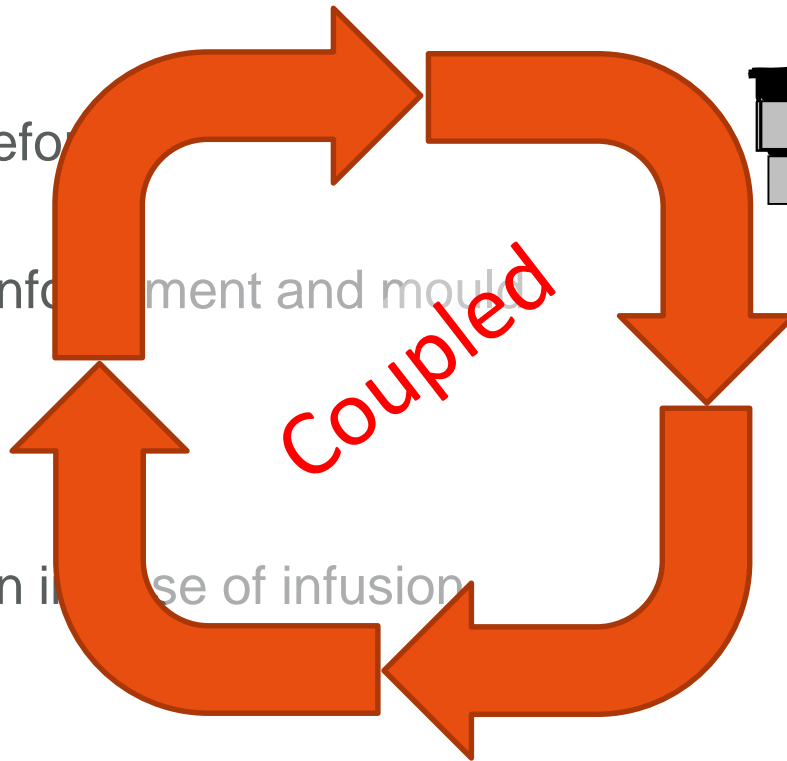
# Liquid Composite Moulding

## Physics involved

# Liquid Composite Moulding

## Physics involved: Modelling

- Four physical phenomena are modeled
  - Flow of resin inside the preform
  - Heat exchanges inside reinforcement and mould
  - Chemical reaction of resin
  - Reinforcement deformation in case of infusion



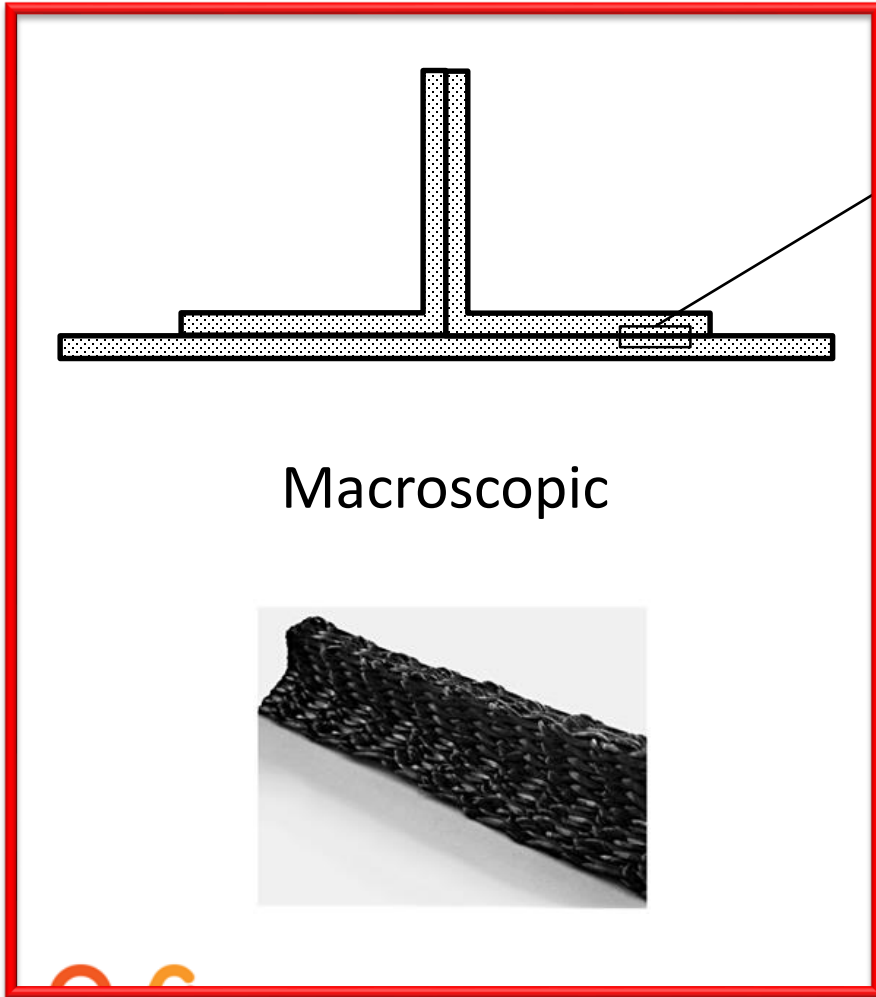
# Liquid Composite Moulding

Physics involved: reinforcement modelling

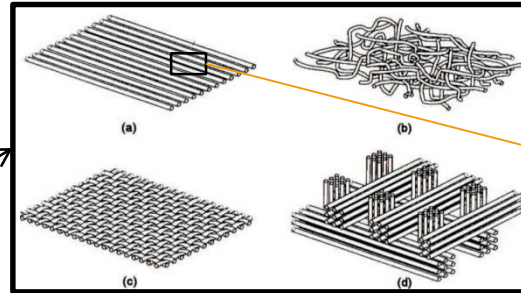


# Liquid Composite Moulding

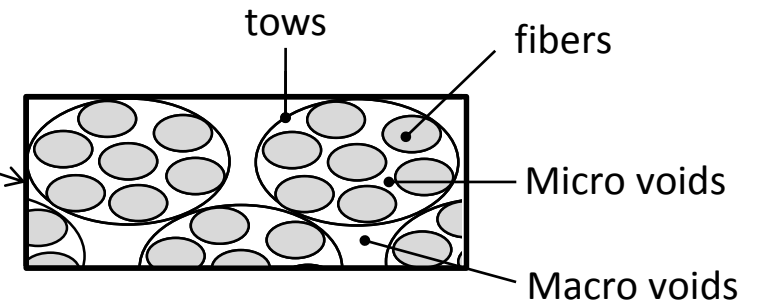
## Physics involved: Preform modelling



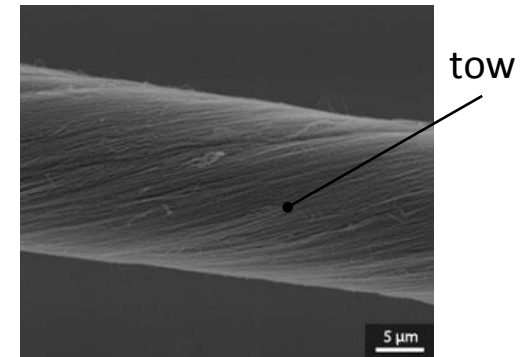
Macroscopic



Meso-scope



Microscopic

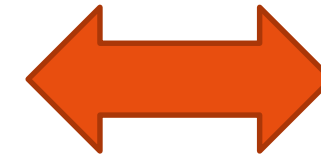
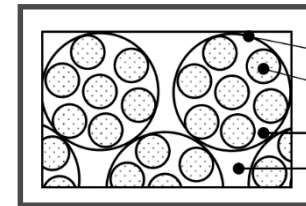
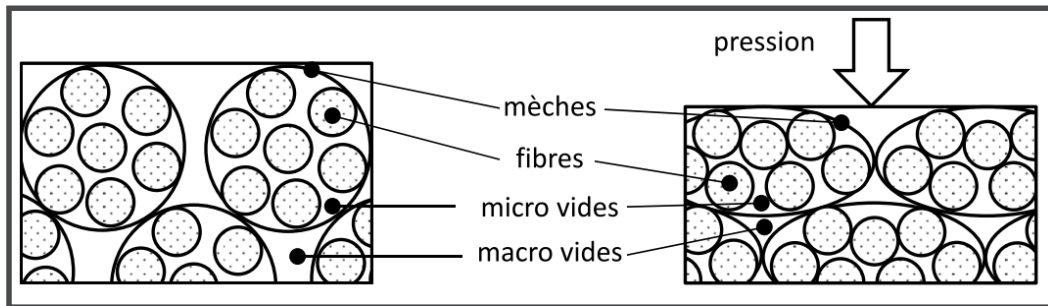
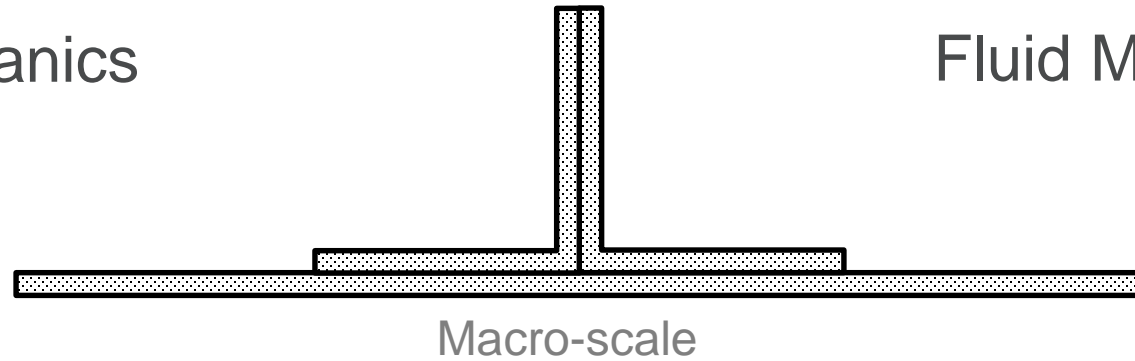


# Preform modelling

## Physics involved: Preform modelling

Solid Mechanics

Fluid Mechanics



Porous medium approximation

Darcy law / permeability

deformable preform made of undeformable filaments

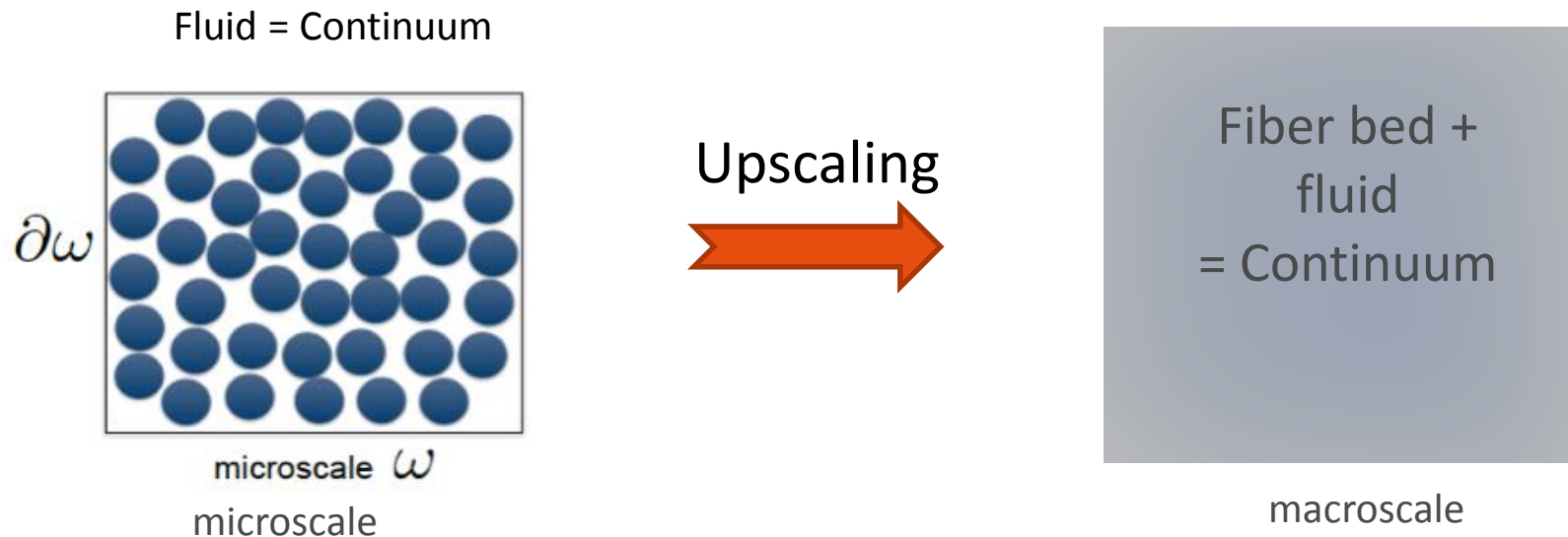
$$J(\vec{x}, t + \Delta t)v_f(\vec{x}, t + \Delta t) = J(\vec{x}, t)v_f(\vec{x}, t)$$



# Fluid Mechanics in porous medium

## Physics involved: Darcian permeability : origin?

Single-phase flow (saturated), negligible inertia (creeping flow), no-slip condition on fibers, single-scale porosity medium, stationary fiber bed, linear & incompressible fluid of constant viscosity



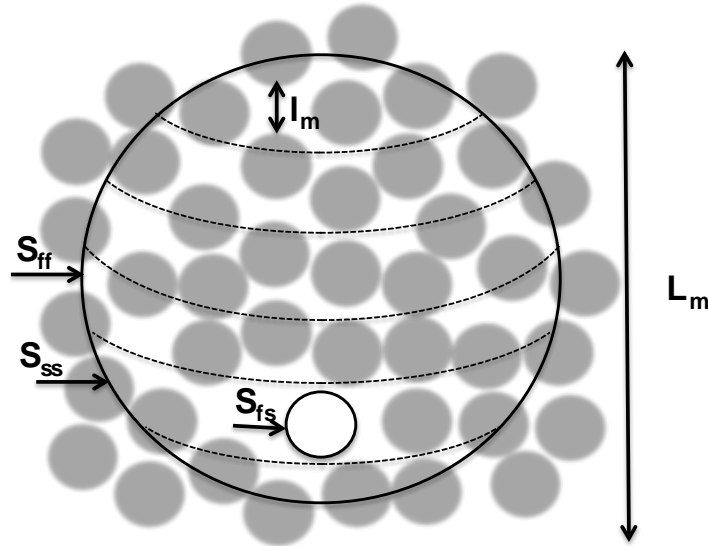
$$\nabla P_f + \eta \nabla^2 \mathbf{v}_f = 0$$

$$\nabla \cdot \mathbf{v}_f = 0$$



# Fluid Mechanics in porous medium

## Physics involved: Darcian permeability : origin?



Upscaling of Stokes equation :

$$\nabla \cdot \langle \boldsymbol{\tau}_f \rangle - \phi_f \nabla \langle P_f \rangle^f - \mathbf{f}_d = 0 \quad (1)$$

↘ Porosity

Where :

$$\boldsymbol{\tau}_f = \eta \left[ \nabla \mathbf{v}_f + (\nabla \mathbf{v}_f)^T \right] = 2\eta \mathbf{D}_f \quad (3)$$

Extra-stress tensor

$$\mathbf{f}_d = -\frac{1}{V} \int_{S_{fs}} \boldsymbol{\sigma}_f \cdot \mathbf{n}_{fs} dS + \nabla \phi_f \langle P_f \rangle^f \quad (4)$$

↘ Drag force

$$\boldsymbol{\sigma}_f = -P_f \mathbf{I} + 2\eta \mathbf{D}_f \quad (5)$$

Total stress tensor for linear fluid

$$l_m \ll L_m$$


$$\langle \boldsymbol{\tau}_f \rangle = \frac{1}{V} \int_{V_f} \boldsymbol{\tau}_f dV \quad (2)$$

$$\langle P_f \rangle^f = \frac{1}{V_f} \int_{V_f} P_f dV$$

At large scale  $\nabla \phi_f \approx 0 \Rightarrow$  Statistically homogeneous porous media

$$\text{Then : } \mathbf{f}_d = -\frac{1}{V} \int_{S_{fs}} \boldsymbol{\sigma}_f \cdot \mathbf{n}_{fs} dS \quad (6)$$

$$\mathbf{f}_d = \frac{\phi_f \eta}{\mathbf{K}} \langle \mathbf{v}_f \rangle \quad (7)$$

 Permeability tensor

$\nabla \cdot \langle \boldsymbol{\tau}_f \rangle \ll \mathbf{f}_d$  if velocity gradients varies smoothly

$$\mathbf{K} = \frac{\phi_f \eta}{-\frac{1}{V} \int_{S_{fs}} \boldsymbol{\sigma}_f \cdot \mathbf{n}_{fs} dS} \langle \mathbf{v}_f \rangle \quad (8) \quad \text{where} \quad \langle \mathbf{v}_f \rangle = \frac{1}{V_f} \int_{V_f} \mathbf{v}_f dV$$

$$\text{Darcy's law : } \langle \mathbf{v}_f \rangle = -\frac{\mathbf{K}}{\eta} \cdot \nabla \langle P_f \rangle^f$$

# Fluid Mechanics in porous medium

Physics involved: resin viscosity

Fibres



+

Organic Matrix



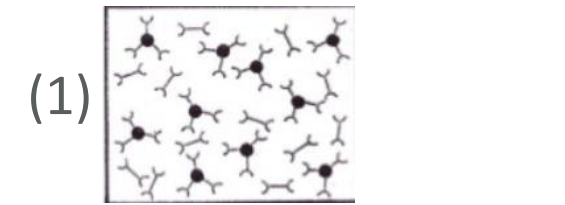
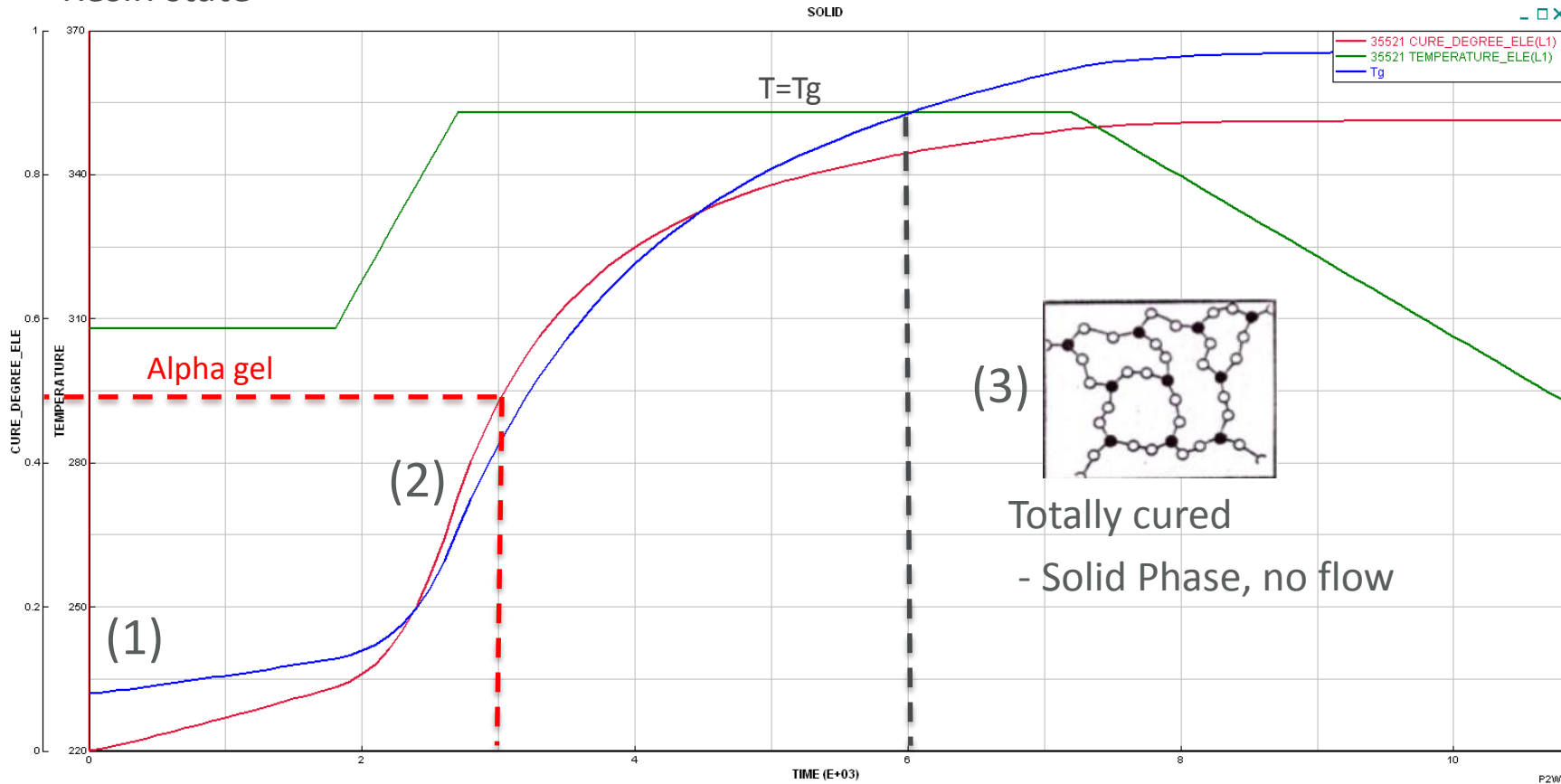
• Thermoset

• Thermoplastic

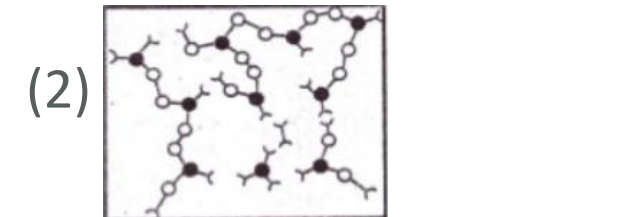
# Fluid Mechanics in porous medium

## Physics involved: Resin Viscosity of thermoset

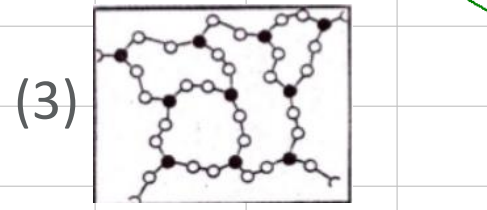
Resin state



Monomers / Oligomers  
 - low viscosity  
 - Newtonian fluid,  $\eta=f(T)$



Partially cured  
 - Viscosity increases rapidly  
 - liquid phase: Newtonian behavior,  $\eta=f(T; \alpha)$   
 - rubbery phase: too high viscosity



Totally cured  
 - Solid Phase, no flow

Resin is liquid      Resin is rubbery      Resin is glassy

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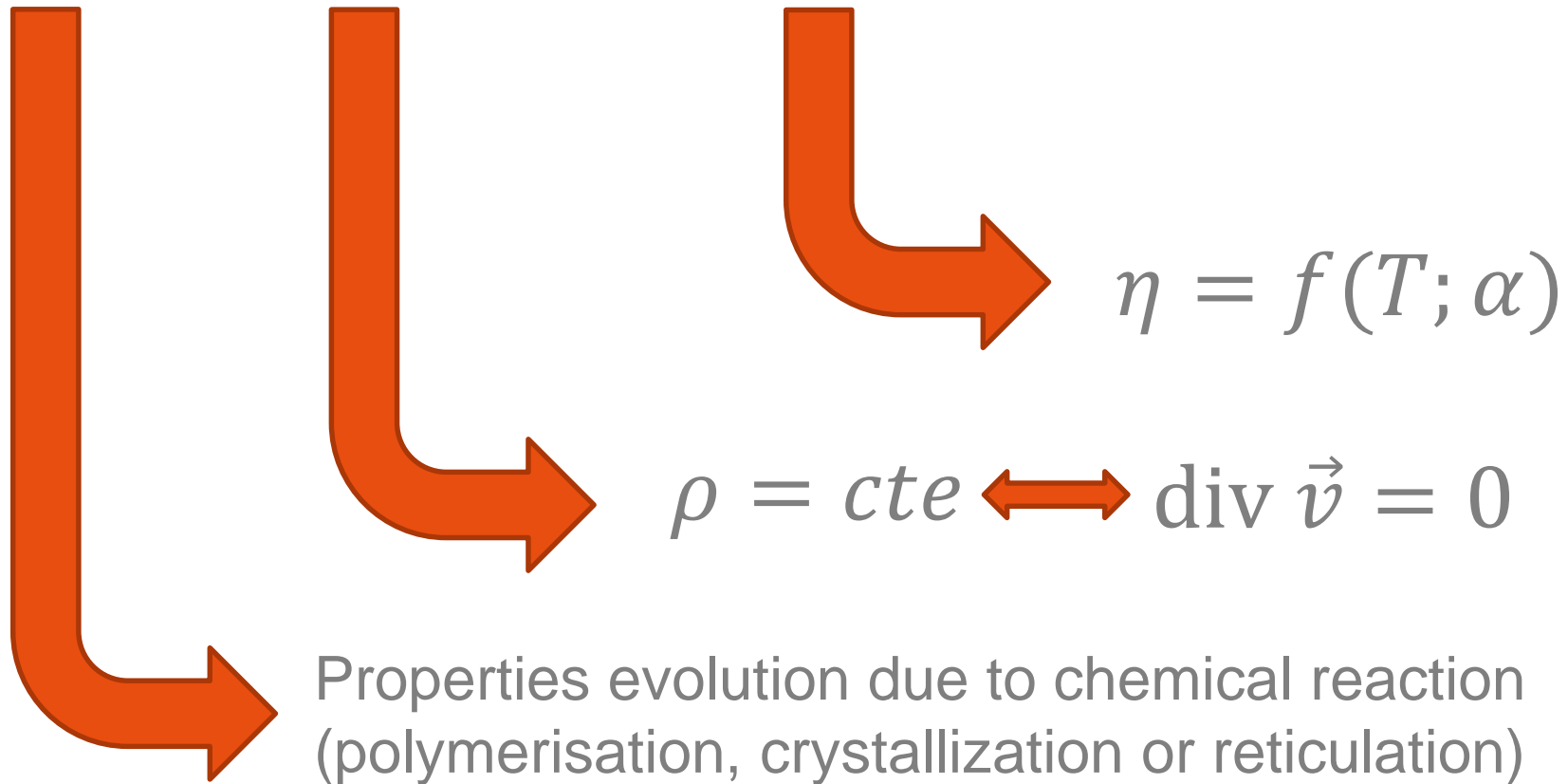
# Liquid Composite Moulding

## Modelling the infusion process in PAM-RTM

# Infusion modelling

## Resin Modelling

- Reactive incompressible Newtonian fluid



# Infusion modelling

## Fluid and Mechanics equations

### Fluid Mechanics

$$\left| \begin{array}{l} \vec{v} = -\frac{\bar{K}}{\eta} (\vec{\nabla} p - \rho \vec{g}) \\ \operatorname{div} \vec{v} = 0 \end{array} \right.$$



$$\operatorname{div} \left( \frac{\bar{K}}{\eta} \vec{\nabla} p \right) = 0$$

Linear finite element method with non-conforming elements

### Solid Mechanics

$$\underline{\operatorname{div}} \underline{\underline{\sigma}} = \underline{f}_v$$

→ Non linear elastic transversally isotropic behaviour

Implicit non linear finite element method



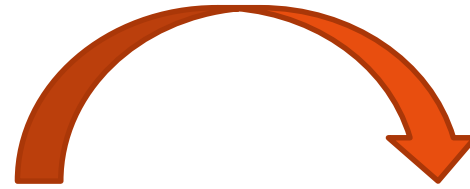
# Infusion modelling

## Fluid and Mechanics equations

Solid Mechanics

Fluid Mechanics

displacements



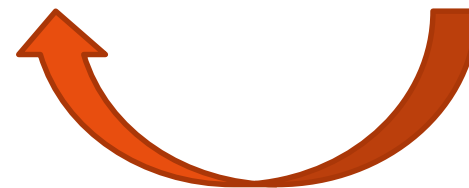
Mesh update  
Fiber ratio update

Terzaghi

$$\overline{\overline{\sigma_{tot}}} = \overline{\overline{\sigma_{eff}}} + sp\overline{\overline{I}}$$



$$\overline{\overline{K}} = F(v_f)$$



Resin pressure

# Infusion modelling

## Thermal Equation

→ chemical  
exothermic  
reaction

$$\rho C_p \frac{\partial T}{\partial t} + \boxed{\rho_r C_{pr} \vec{v} \cdot \vec{\nabla} T} = \text{div}(\bar{\bar{\kappa}} \cdot \vec{\nabla} T) \boxed{+ S}$$

→ Resin flow

$C_p$ : specific heat of the porous medium ( $\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$ )

$\rho$  : volumetric mass density of the porous medium ( $\text{Kg}\cdot\text{m}^{-3}$ )

$C_{pr}$ : specific heat of the resin( $\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$ )

$\rho_r$ : volumetric mass density of the resin ( $\text{Kg}\cdot\text{m}^{-3}$ )

$\vec{v}$ : resin velocity ( $\text{m}\cdot\text{s}^{-1}$ )

$T$ : temperature (K)

$\bar{\bar{\kappa}}$ : thermal conductivity tensor ( $\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ )

$S$ : source term ( $\text{W}\cdot\text{m}^{-3}$ )

# Infusion modelling

## Chemical Reaction Modeling: kinetic law


generic law representing the degree of completion of a  
several chemical sub-reactions

$$\frac{d\alpha}{dt} = \sum_i w_i(t) \frac{d\alpha_i}{dt} = \sum_i w_i(t) f_i(T, \alpha)$$

Example of thermosetting resin reticulation

Kamal-Sorrour model: 
$$\frac{D\alpha}{Dt} = \tilde{K}_i \alpha_i^{n_i} (1 - \alpha_i)^{p_i}$$

Arrhénius law: 
$$\tilde{K}_i = A_i e^{-\frac{E_i}{RT}}$$



# Liquid Composite Moulding

## Material characterization

# ESI PAM-COMPOSITES

## Material characterization for RTM module (Isothermal filling)

### Density of the resin

- Resin supplier

### Viscosity of the resin = $f(\text{time})$

- Rheometer measurement of the viscosity evolution as a function of time at injection temperature

### Permeability tensor of the reinforcements

- In-plane values for shell models
- In-plane and transverse values for solid models



**EASYPERM permeability bench:**  
[https://www.youtube.com/watch?v=YTS0ihjBy\\_Y&feature=youtu.be&list=PLEm2vnZ25o0YUxDvXF0su1wFhK68PycG3](https://www.youtube.com/watch?v=YTS0ihjBy_Y&feature=youtu.be&list=PLEm2vnZ25o0YUxDvXF0su1wFhK68PycG3)

# ESI PAM-COMPOSITES

## Material characterization for RTM module (Heated filling)

Viscosity of the resin =  $f(\text{degree of cure, temperature})$

- Rheometer measurement of the viscosity evolution as a function of time at different temperatures

Kinetic and enthalpy of the resin

- DSC measurements at different temperatures

Specific heat of the resin

- Resin supplier

Conductivity of the resin

- Resin supplier

Density of the resin

- Resin supplier

Conductivity tensor of the reinforcement

- Computed analytically from fiber conductivity

Specific heat of the fiber

- Fiber supplier

Density of the fiber

- Fiber supplier

Permeability tensor of the reinforcements

- In-plane and transverse values



# ESI PAM-COMPOSITES

## Material characterization for Thermal module (Pre-heating & Curing)

### PREHEATING (solids only)

- **Conductivity tensor of the reinforcement**
  - Computed analytically from fiber conductivity
- **Specific heat of the fiber**
  - Fiber supplier
- **Density of the fiber**
  - Fiber supplier

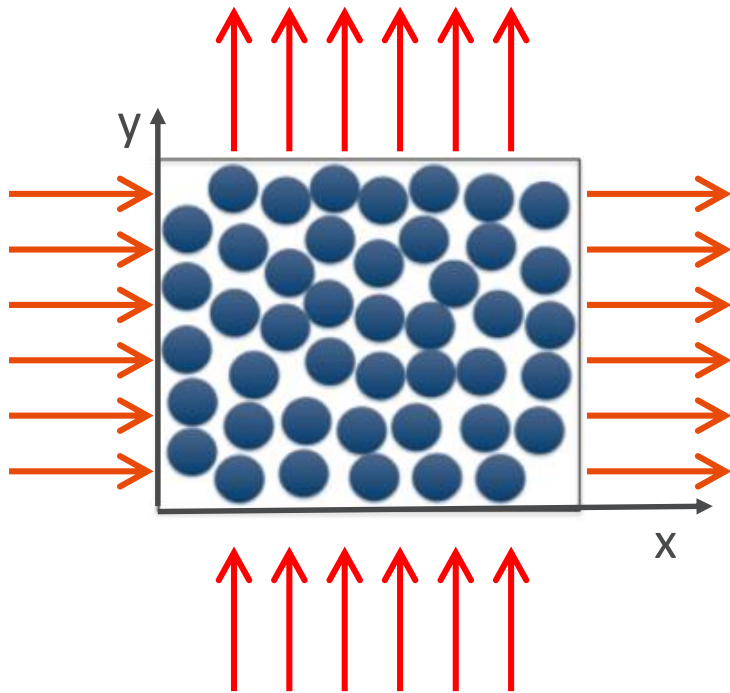
### CURING (solids only)

- **Kinetic and enthalpy of the resin**
  - DSC measurements at different temperatures
- **Specific heat of the resin**
  - Resin supplier
- **Conductivity of the resin**
  - Resin supplier
- **Density of the resin**
  - Resin supplier
- **Conductivity tensor of the reinforcement**
  - Computed analytically from fiber conductivity
- **Specific heat of the fiber**
  - Fiber supplier
- **Density of the fiber**
  - Fiber supplier



## Numerical characterization: Methods to predict K from microstructural data

### 1/ Identification from Darcy's law : **single-scale porous medium**



- Impose appropriate periodic BC (e.g. a given velocity of pressure in the direction  $i$ )

- Solve for  $v_i$  and  $P$  using  $\nabla P_f + \eta \nabla^2 \mathbf{v}_f = 0$  in the fluid domain

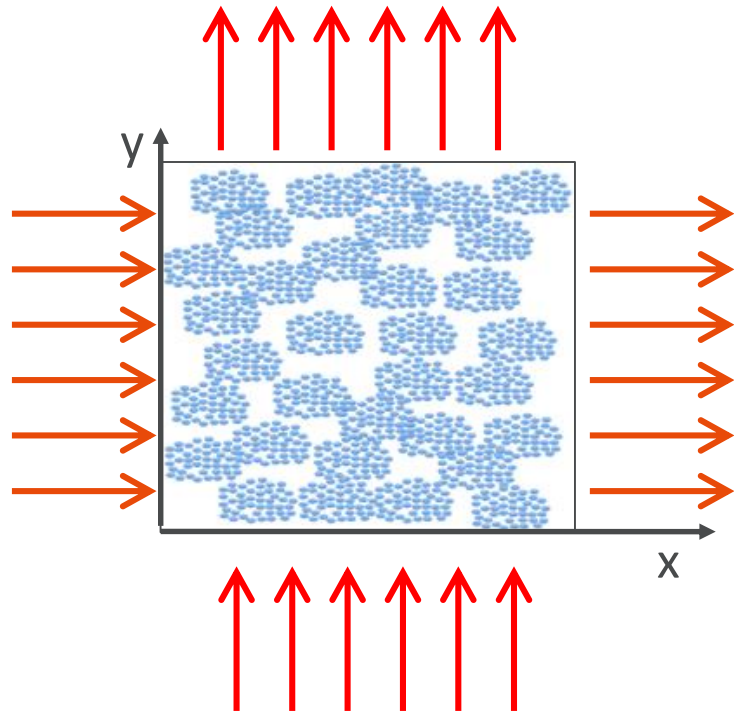
- Compute  $\langle \mathbf{v}_i \rangle = \frac{1}{A} \int_{S_f} \mathbf{v}_f \mathbf{n} dS$

- Compute  $K_i = \frac{\langle \mathbf{v}_i \rangle \eta}{A \nabla P}$



## Numerical characterization: Methods to predict K from microstructural data

### 1/ Identification from Darcy's law : **double-scale porous medium**



- Get the permeability tensor  $\mathbf{K}$  of fiber tows
- Impose appropriate periodic BC (e.g. a given velocity of pressure in the direction  $i$ )

- Solve for  $v_i$  and  $P$  using the Brinkman Eq.

$$-\phi_f \nabla \langle P_f \rangle^f + \eta \nabla^2 \langle \mathbf{v}_f \rangle - \phi_f \eta \mathbf{K}_{tow}^{-1} \cdot \langle \mathbf{v}_f \rangle = 0$$

- Compute  $\langle \mathbf{v}_i \rangle = \frac{1}{A} \int_{S_f} \mathbf{v}_f \mathbf{n} dS$

- Compute  $K_i = \frac{\langle \mathbf{v}_i \rangle \eta}{A \nabla P}$

## Numerical characterization: Methods to predict K from microstructural data

### Example

SEM image

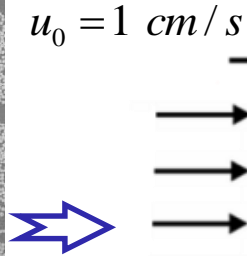
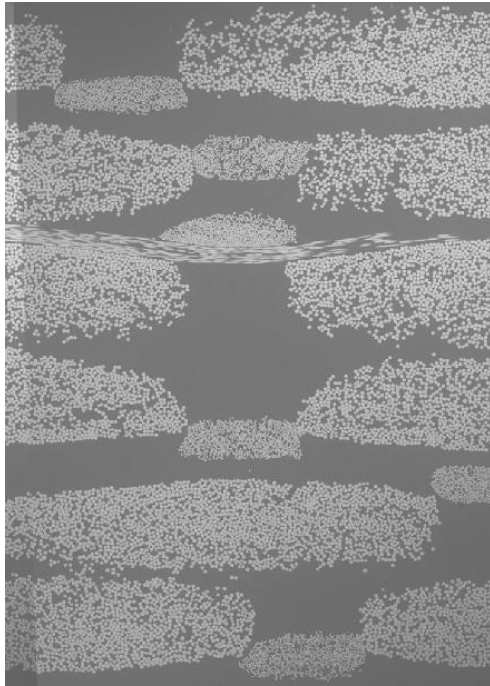
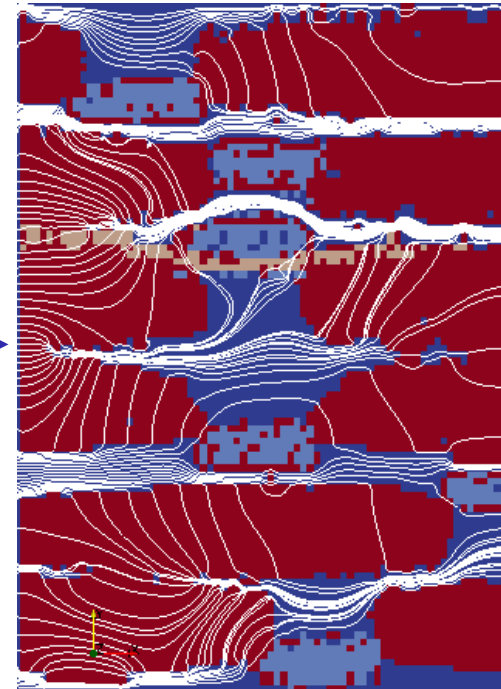


Image with segmented fibrous regions



Image with segmented regions and calculated flow (streamlines)



3 fiber tows regions (white, dark grey and light grey) :

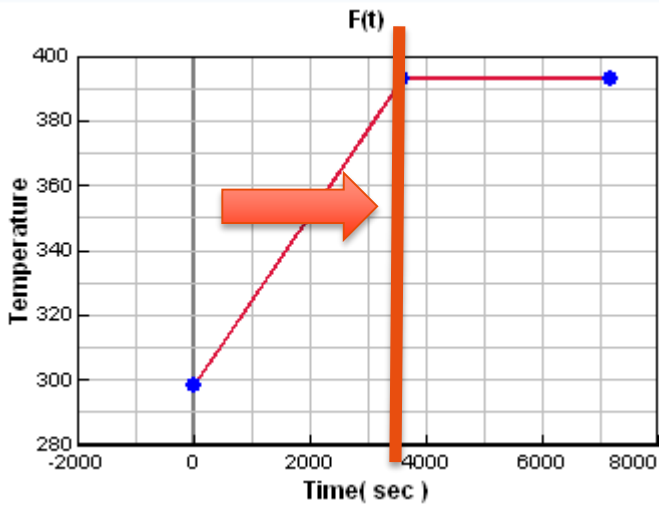
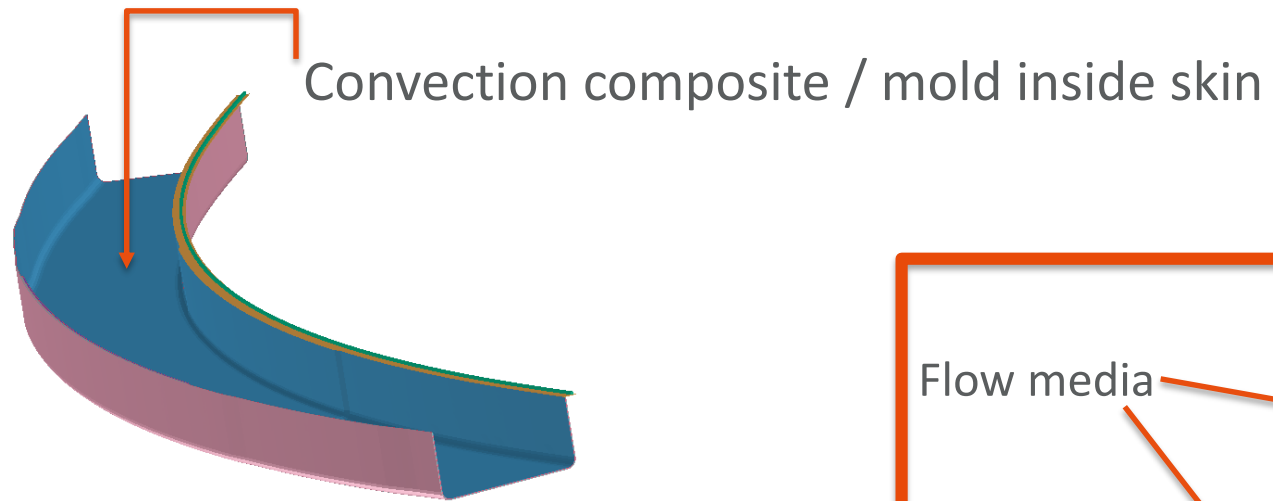
$$\mathbf{K}_1 = \begin{bmatrix} K_{\perp}^1 & 0 \\ 0 & K_{\perp}^1 \end{bmatrix} \quad \mathbf{K}_2 = \begin{bmatrix} K_{//}^2 & 0 \\ 0 & K_{\perp}^2 \end{bmatrix} \quad \mathbf{K}_3 = \begin{bmatrix} K_{\perp}^3 & 0 \\ 0 & K_{\perp}^3 \end{bmatrix}$$

---

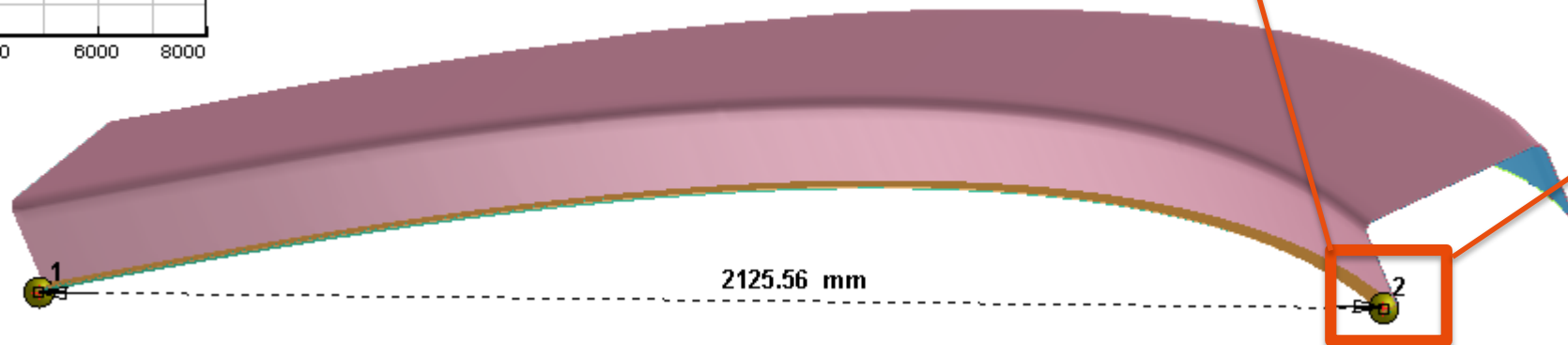
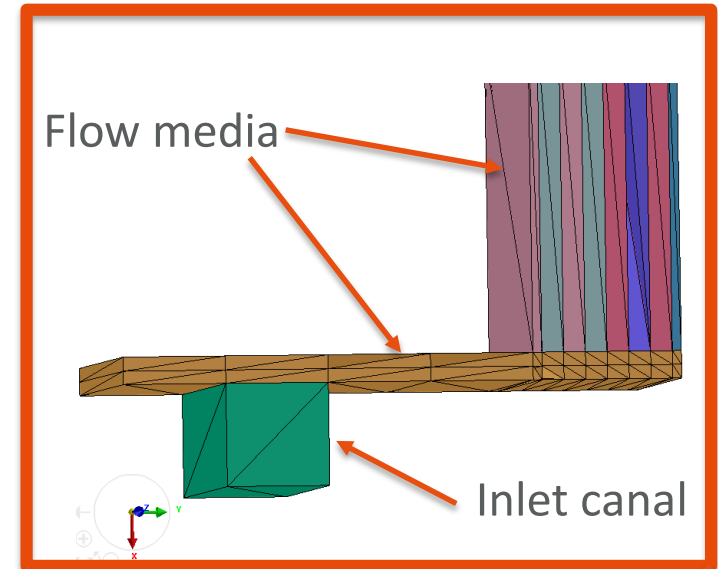
# Liquid Composite Moulding Examples

# C Spar

## Pre-heating model



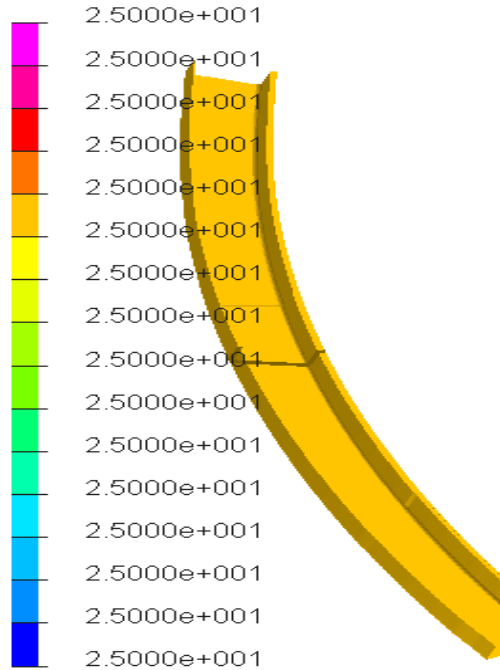
Imposed temperature on the top



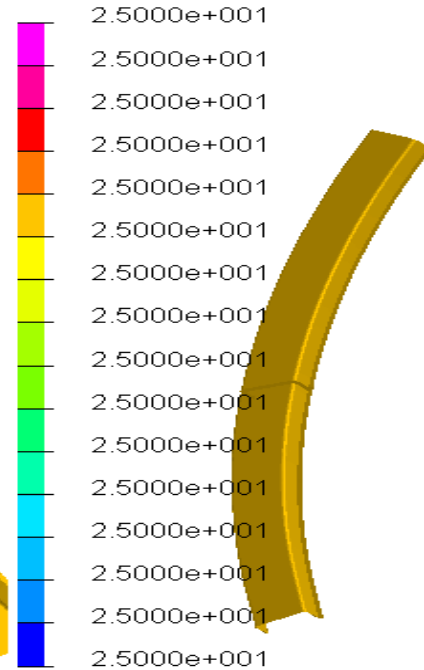
# C Spar

## Pre-heating simulation

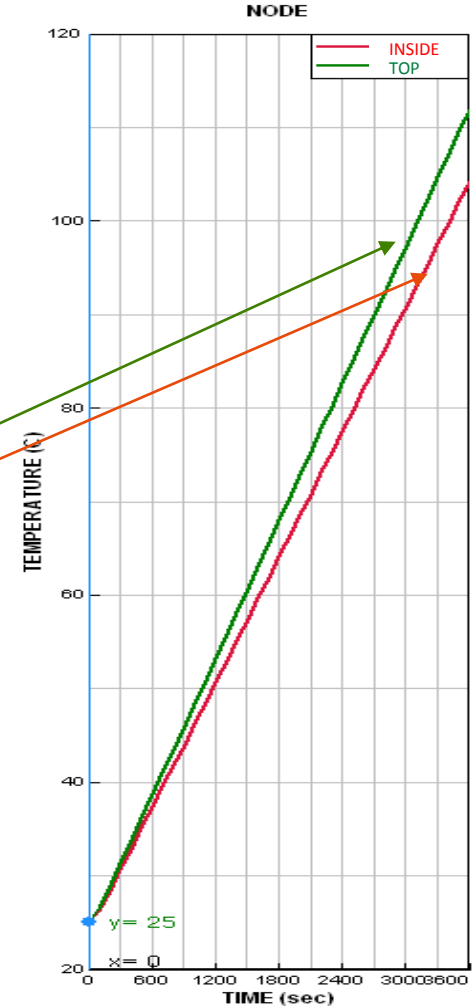
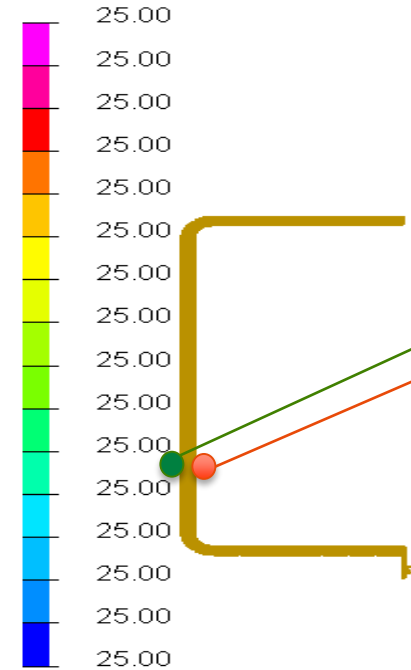
NODE : Temperature ( C ) 1 / 0.000000  
Min = 25 at Node 20925  
Max = 25 at Node 20925



NODE : Temperature ( C ) 1 / 0.000000  
Min = 25 at Node 20925  
Max = 25 at Node 20925



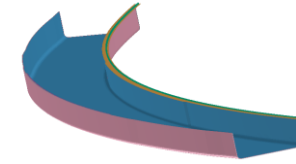
NODE : Temperature ( C ) 1 / 0.000000  
Min = 25 at Node 20925  
Max = 25 at Node 20925



# C Spar

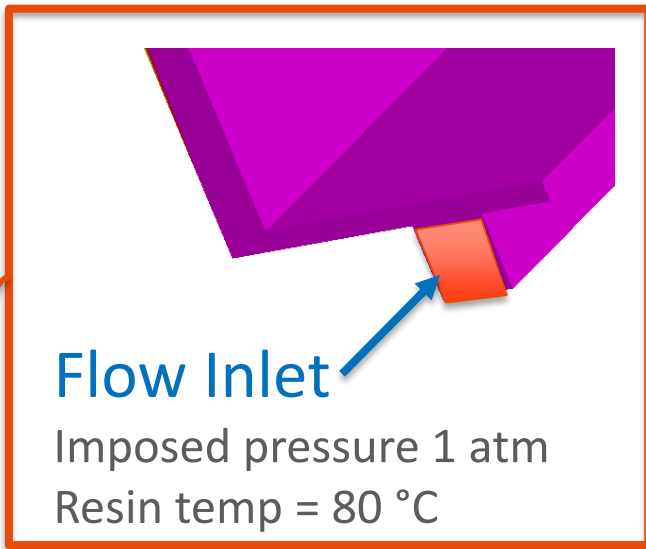
## Heated filling model

## Temperature BC



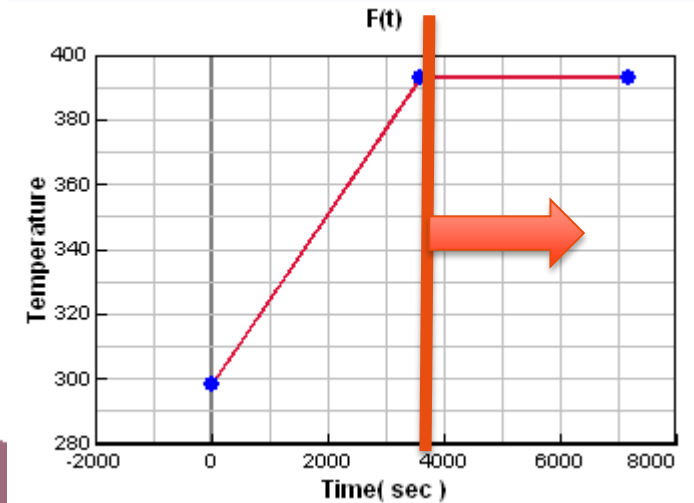
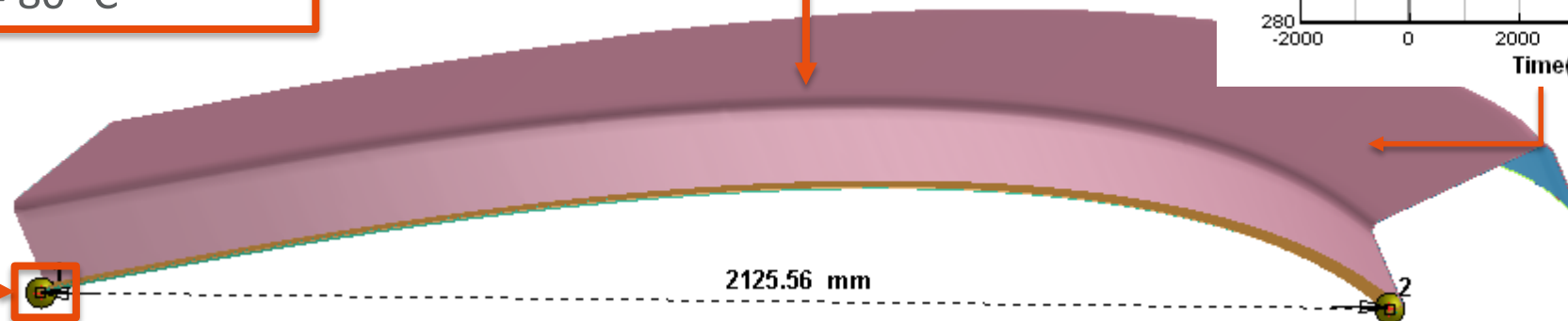
Convection composite / mold inside skin

Imposed temperature on the top



## Mechanical BC

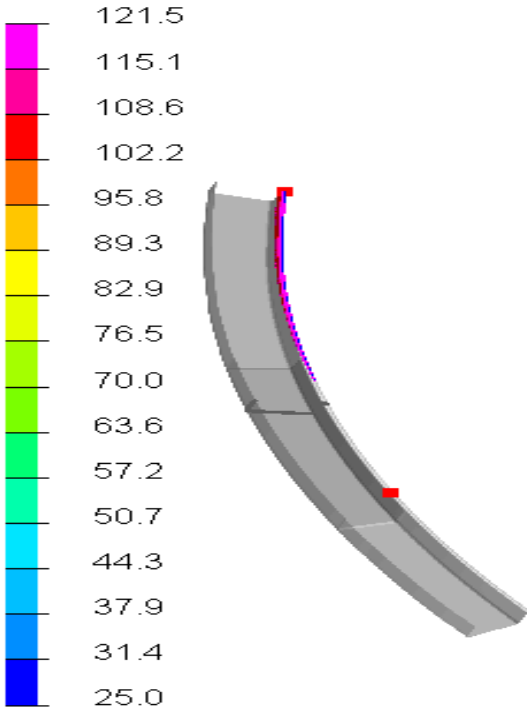
Pressure (1 atm)



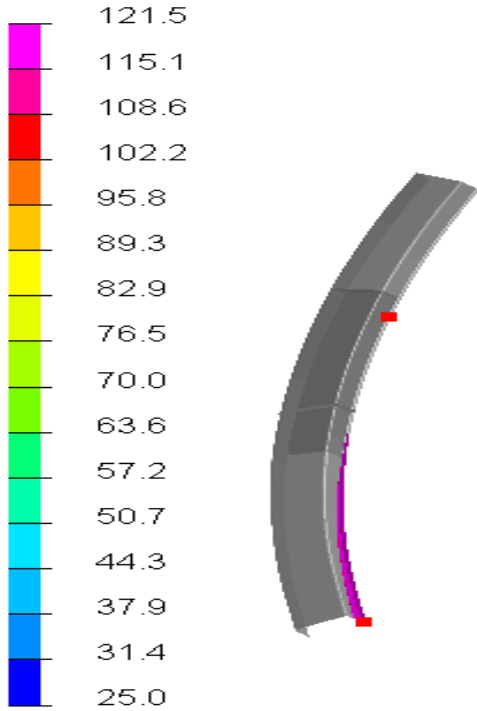
# C Spar

## Heated filling simulation

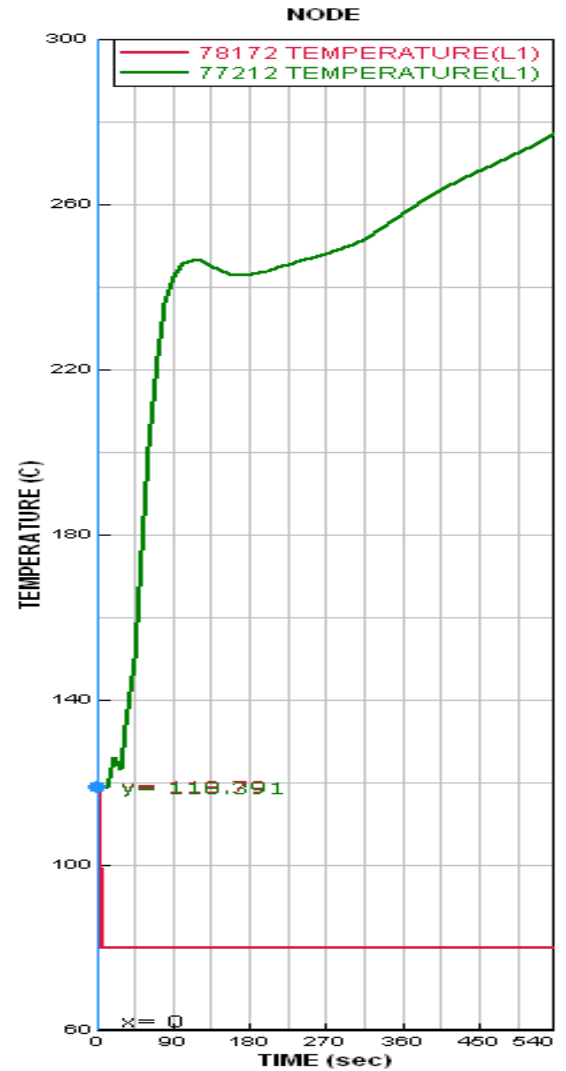
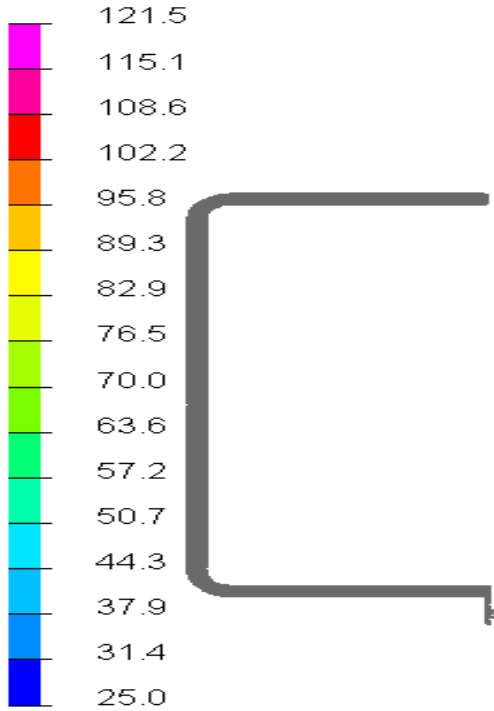
NODE : Temperature ( C ) 1 / 0.000000  
Min = 24.9905 at Node 79615  
Max = 121.491 at Node 76700



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Min = 24.9905 at Node 79615  
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Min = 24.9905 at Node 79615  
Max = 121.491 at Node 76700



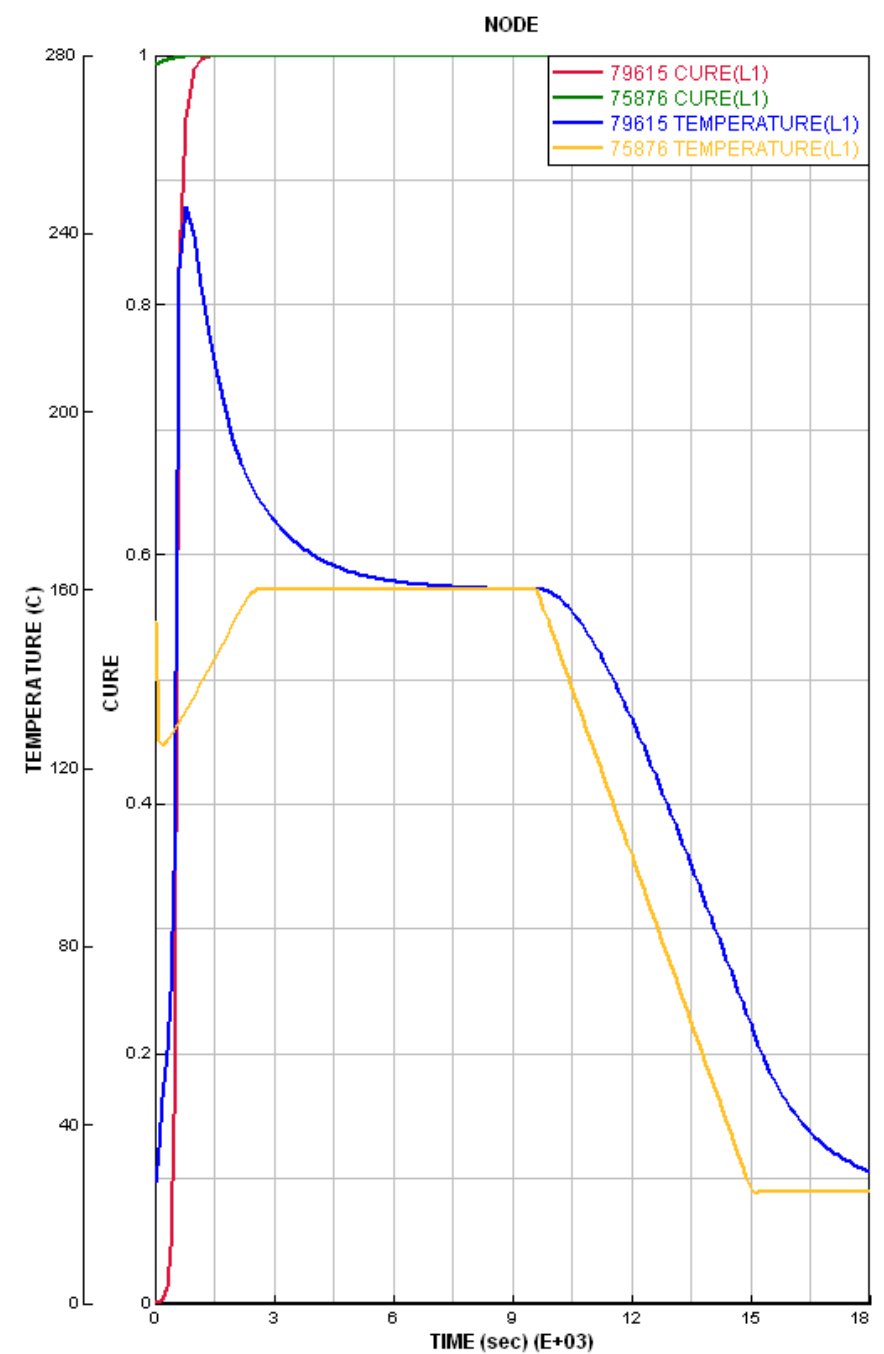
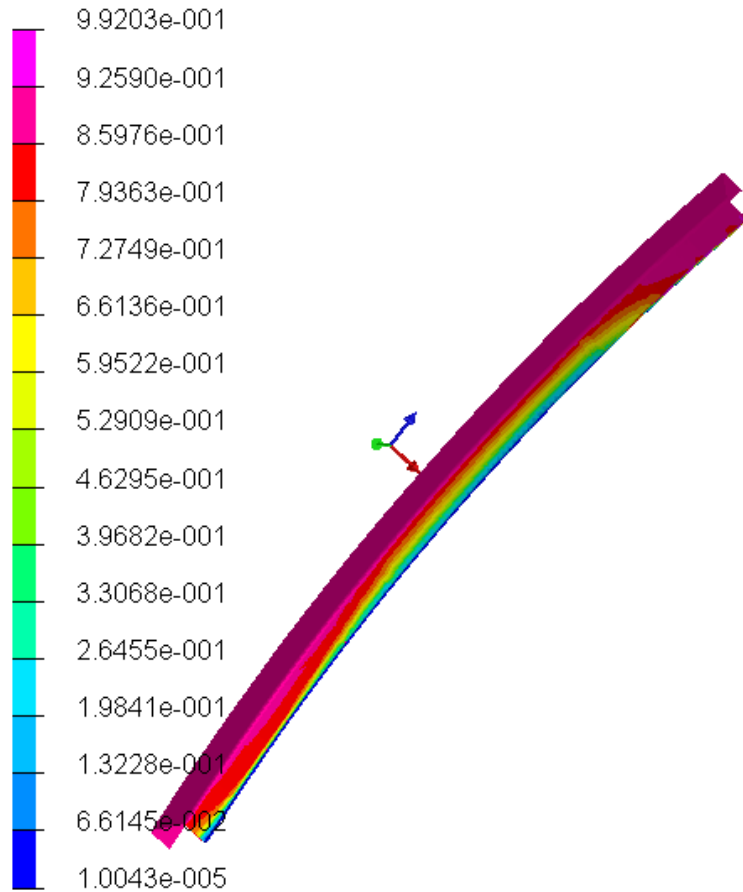
# C Spar

## Curing simulation

curing\U\_spar\_INFUSION\_Curing\_RESULT.erfh5

1 / 0.000000

NODE : CURE  
Min = 1.00431e-005 at Node 79615  
Max = 0.992031 at Node 75876

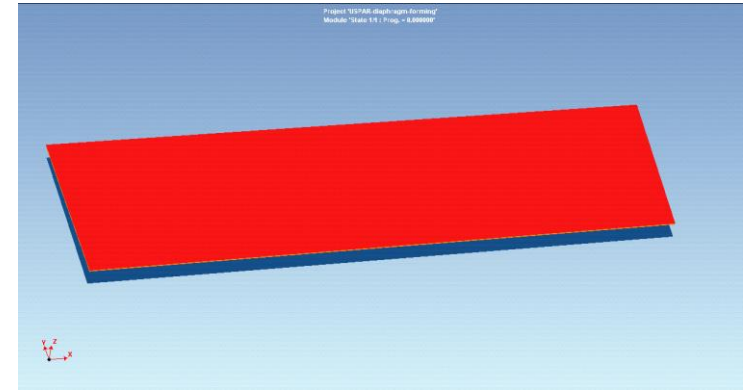
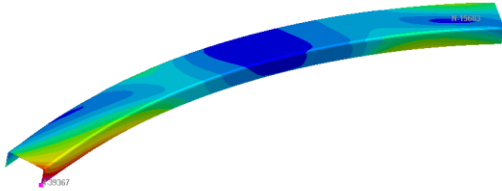
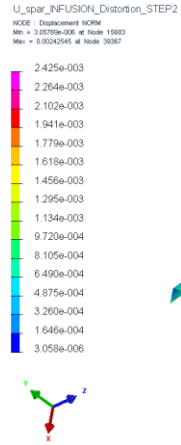




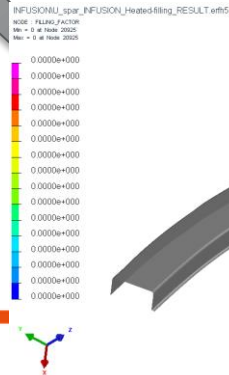


# ESI's PAM-COMPOSITES

Compensated mold



Temperature history  
 Degree of cure history



Fiber direction  
 Thickness variation

---

# CURING & DISTORTION

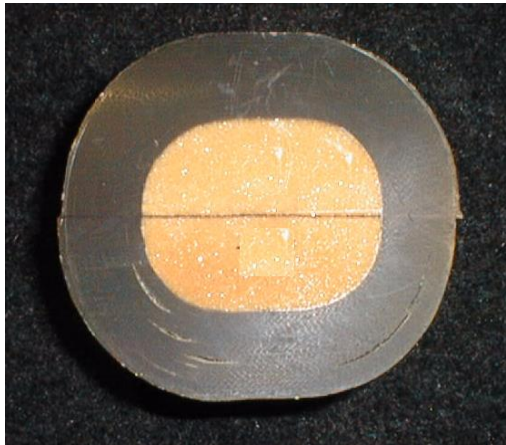
## Industrial issues

# Industrial problematic

## Problem Faced in Manufacture: **assembling problems** and **delamination**



Seattle Times pictures



- How to avoid or minimise distortions and residual stresses ?
- What parameter do I need to modify ?
  - Material
  - Stacking sequences
  - Tooling
  - Temperature history

---

# CURING OF THERMOSETS & DISTORTION

## Why shall we model it ?

**CURING**      With the defined process, is the part going to be fully cured ?  
Are the costs optimised ?

**DISTORTION**      How much does the part deform after tooling removal ?  
How to minimise these deformations ?  
How to quantify the residual stresses ?



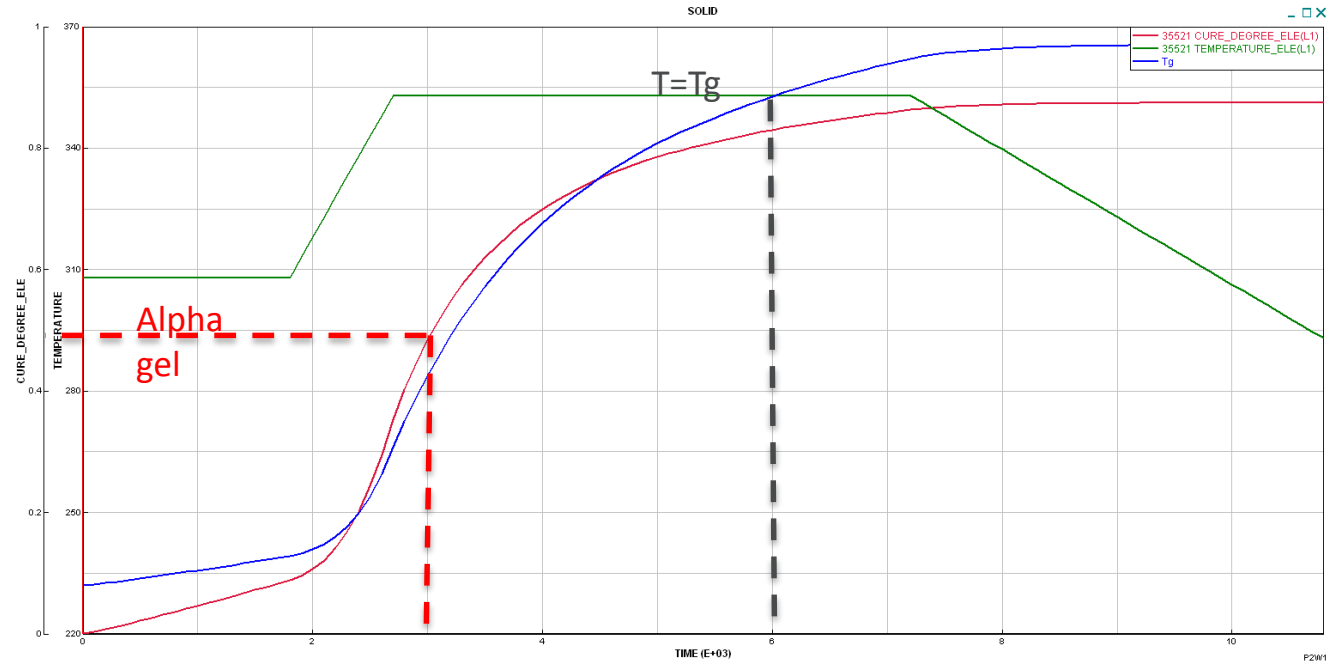
# CURING & DISTORTION

## Material state evolution

# PAM-DISTORTION

## Resin state

- Initially, the resin is a **liquid**. The cross-linking (or **curing**) reaction leads it to a **rubbery** state (after the **gel point**).
- Below the glass transition temperature ( $T_g$ ), the resin is in a **glassy** state.
- The  $T_g$  depends on the degree of cure ( $\alpha$ ).



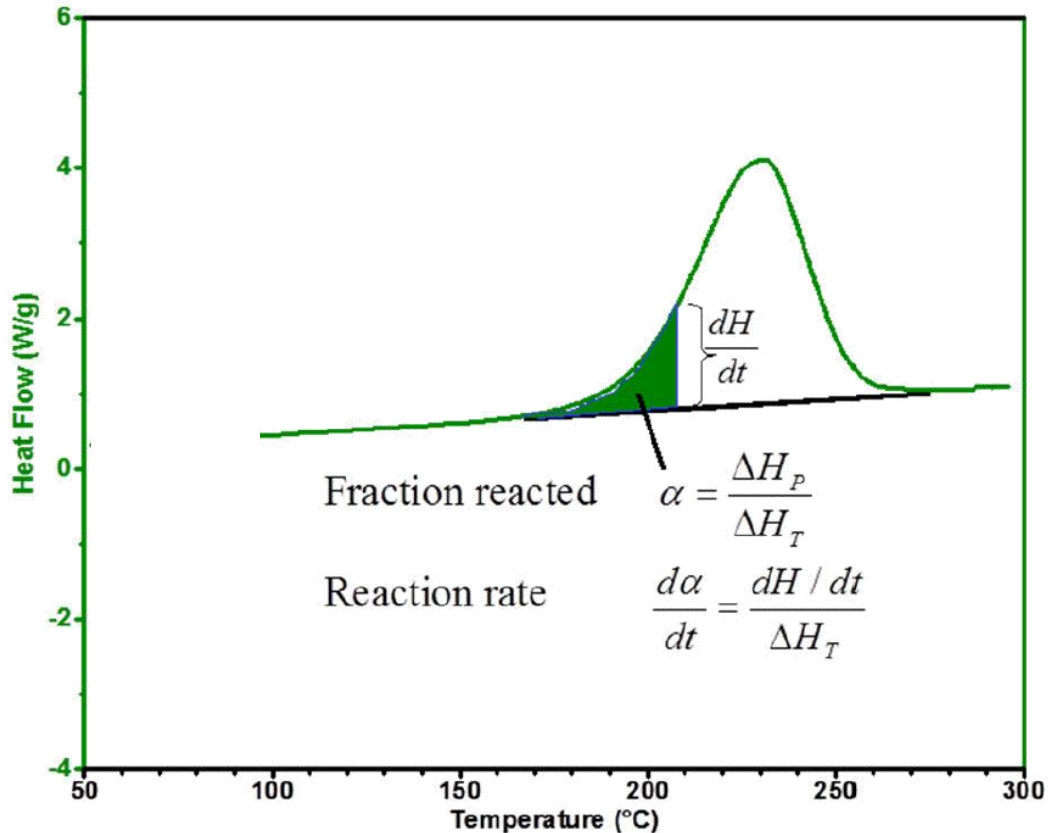
Resin is liquid

Resin is  
rubbery

Resin is glassy

# PAM-DISTORTION

## Differential Scanning Calorimetry



- Gives  $\alpha$  and  $d\alpha/dt$  as functions of time and temperature.
- The cure kinetics can thus be **modelled** (Kamal-Sourour and other models...)

$$\frac{d\alpha}{dt} = f(\alpha, t)$$

- DSC measurements also provide the  $T_g$

Di Benedetto 
$$\frac{T_g - T_{g0}}{T_{g\infty} - T_{g0}} = \frac{\lambda\alpha}{1 - (1 - \lambda) \cdot \alpha}$$

$T_{g0}$ : Glass transition temperature of the uncured system ( $\alpha = 0$ )

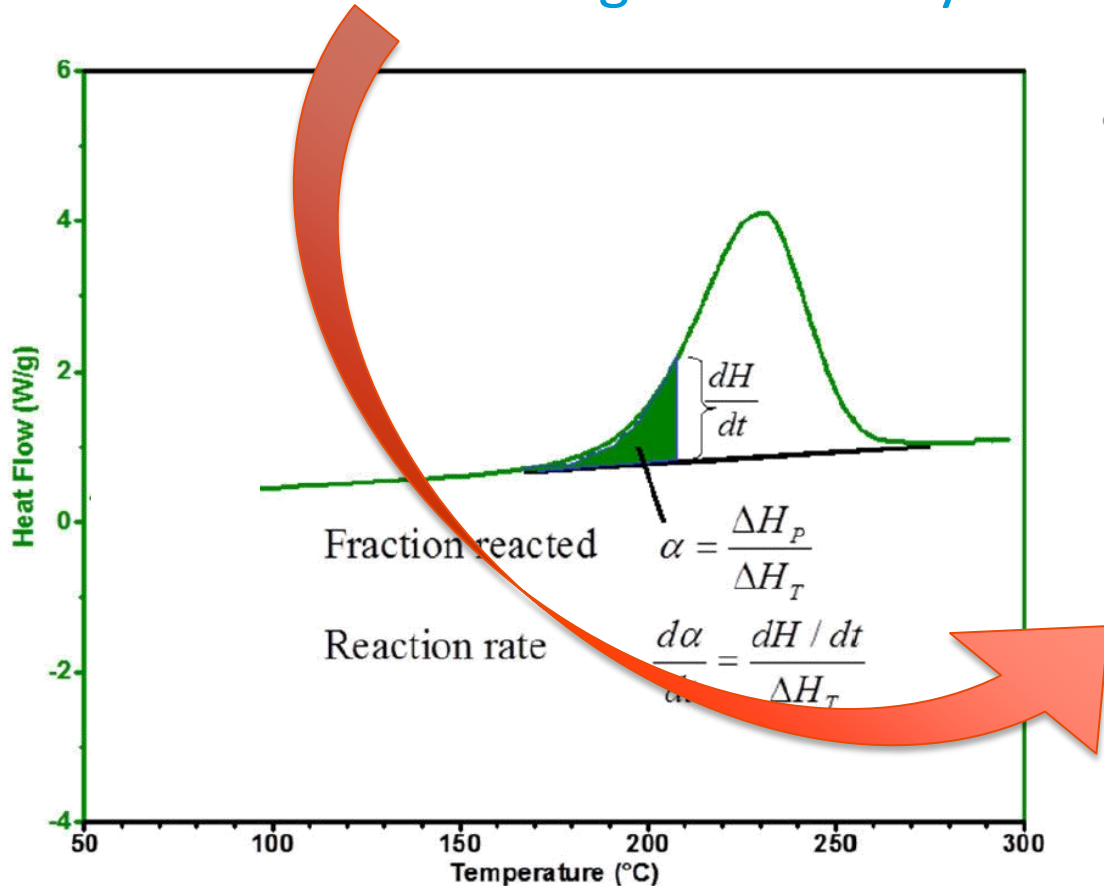
$T_{g\infty}$ : Glass transition temperature of the fully cured system ( $\alpha = 1$ )

$\lambda$ : Material constant



# PAM-DISTORTION

## Differential Scanning Calorimetry



- Gives  $\alpha$  and  $d\alpha/dt$  as functions of time and temperature.
- The cure kinetics can thus be **modelled** (Kamal-Sourour and other models...)

$$\frac{d\alpha}{dt} = f(\alpha, t)$$

- To reduce drastically the **processing time** (for example **the automotive industry**), some **highly reactive resin** are developed, and the curing time can be **below the minute** !
- Accurate characterisation is therefore crucial



# CURING & DISTORTION

## Mechanical behaviour

# PAM-DISTORTION

## Linear Viscoelasticity

- For an **isotropic linear viscoelastic** material, in the 1D case

$$\sigma(t) = \int_0^t E(\alpha, T, t - \tau) : \frac{d}{d\tau} [\varepsilon^{total}(\tau) - \varepsilon^{tc}(\tau)] d\tau$$

With  $\varepsilon^{tc}$  the addition of the thermal **expansion strains** and the **chemical strains (shrinkage)** assumed to be linear

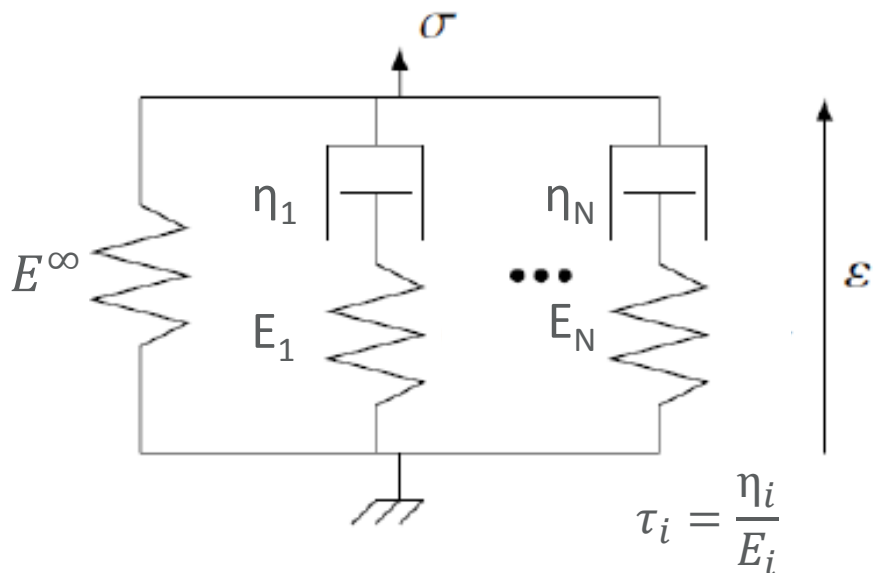
- **Time-temperature superposition** method, sometimes extended to the cure advancement,

$$\sigma(t) = \int_0^t E(\xi(t) - \xi'(\tau)) : \frac{d}{d\tau} [\varepsilon^{total}(\tau) - \varepsilon^{tc}(\tau)] d\tau$$

With the **reduced time variable**  $\xi(t) = \int_0^t \frac{1}{a_T(\alpha, T)} dt$

# PAM-DISTORTION

## Linear Viscoelasticity



**Fig.** Generalised Maxwell model

- For example\* for an epoxy resin characterised with **stress relaxation** tests with **DMA**

$$E(\alpha, \xi) = E^\infty(\alpha) + [E^u(\alpha) - E^\infty(\alpha)] \sum_{i=1}^N W_i(\alpha) \exp\left[\frac{-\xi(\alpha, T)}{\tau_i(\alpha)}\right]$$

- Note that this is not a general model that can represent a priori **ANY** viscoelastic behaviour\*\*.
- Let us assume that this is possible.
- Then, **homogenisation** is needed to estimate the **composite** viscoelastic properties.
- Still **complex** and **costly**: example of numerical homogenisation based on the Laplace-Carson transform \*\*\*

\* Kim YK, White SR. Stress relaxation behaviour of 3501-6 epoxy resin during cure. 1996.

\*\* Bouleau N. Viscoelasticity and Lévy processes. Springer Verlag, 1999.

\*\*\* Lévesque M. et al. Numerical inversion of the Laplace-Carson transform applied to homogenization of randomly reinforced linear viscoelastic media. Comput. Mech 2007.

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# CURING & DISTORTION

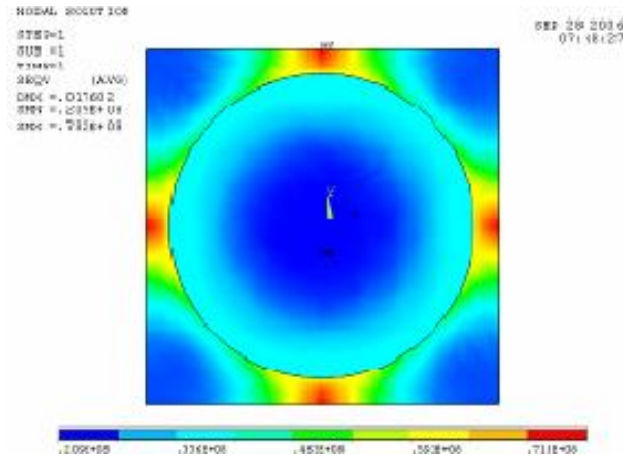
## Identified physical phenomena\*

# CURING & DISTORTION

## Identified physical phenomena

### • Thermal expansion

- ❖ Fibre // matrix CTEs
- ❖ Anisotropic CTE at a ply level
- ❖ Unsymmetric laminates



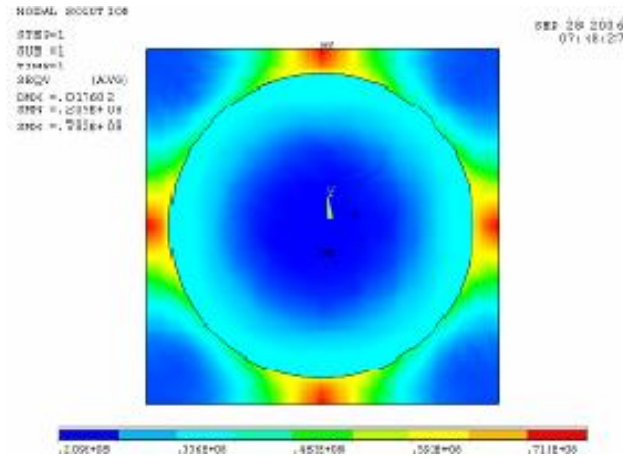
7.4 Curvature in (0/90) unsymmetric laminate due to residual thermal stresses.

# CURING & DISTORTION

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- **Chemical shrinkage**  
(typically about 7% for an epoxy resin)

7.4 Curvature in (0/90) unsymmetric laminate due to residual thermal stresses.

# CURING & DISTORTION

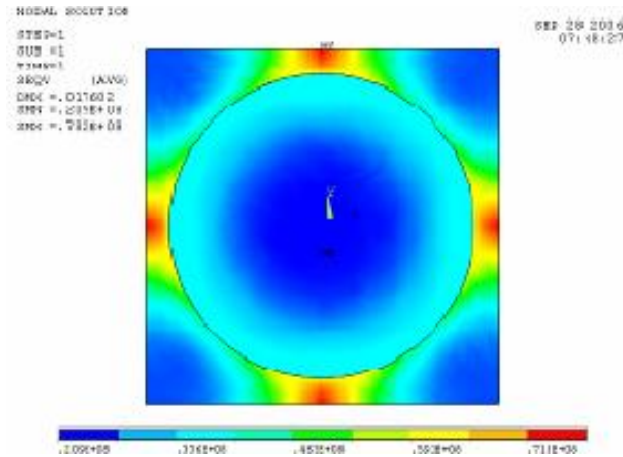
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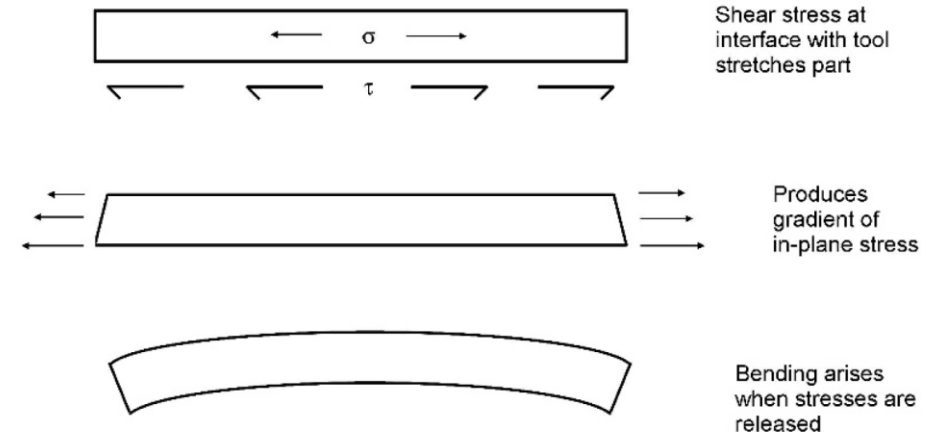
7.4 Curvature in (0/90) unsymmetric laminate due to residual thermal stresses.



- **Chemical shrinkage**  
(typically about 7% for an epoxy resin)

### • Tool part interaction

- ❖ Frictional forces
- ❖ Different CTEs



7.7 Distortion due to shear interaction at tool interface.

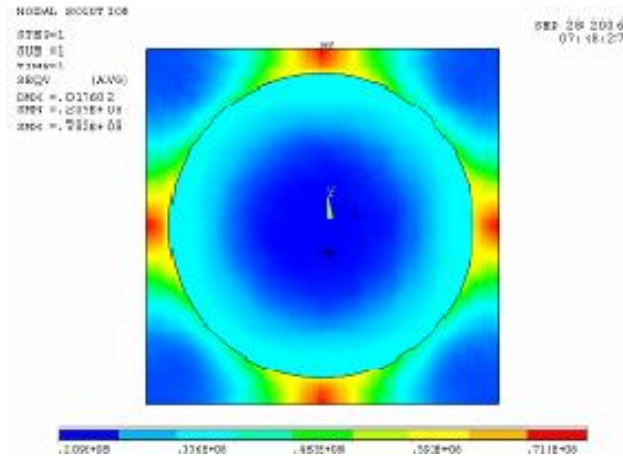


# CURING & DISTORTION

## Identified physical phenomena

### • Thermal expansion

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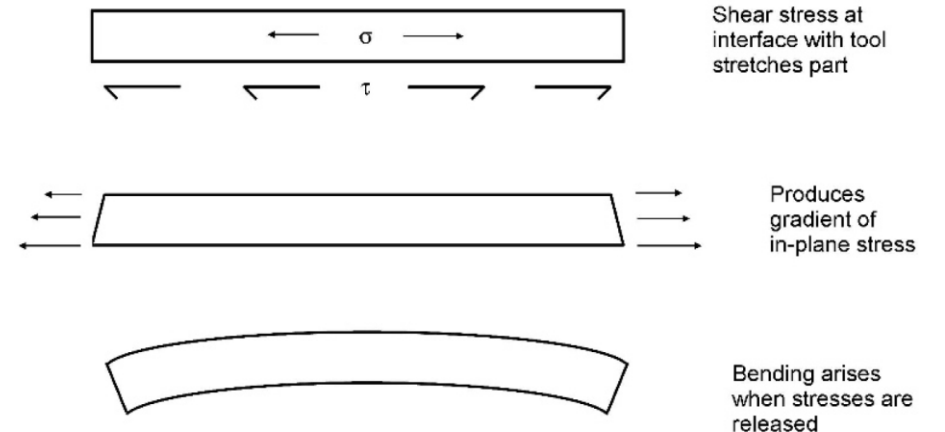
7.4 Curvature in (0/90) unsymmetric laminate due to residual thermal stresses.

- **Others...** (thick parts lead to gradients, heterogeneous fibre content, manufacturing ...)

- **Chemical shrinkage**  
(typically about 7% for an epoxy resin)

### • Tool part interaction

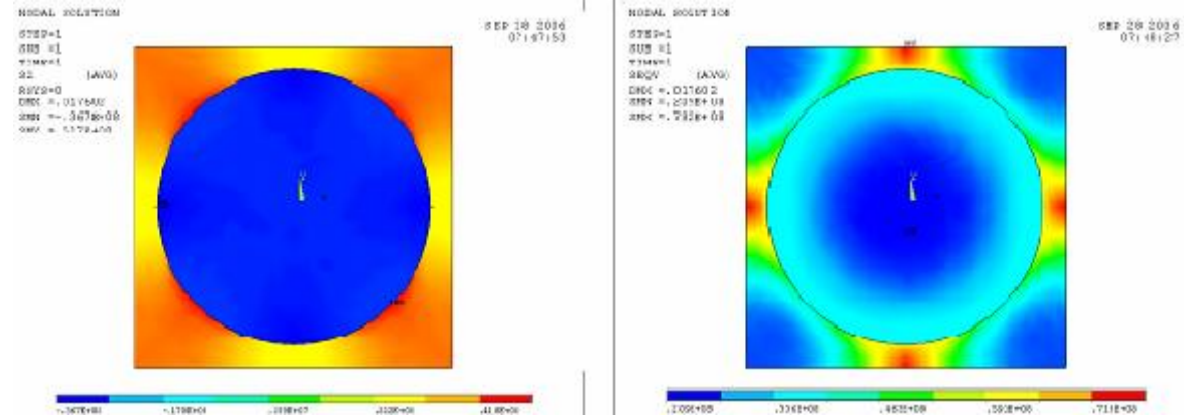
- ❖ Frictional forces
- ❖ Different CTEs



7.7 Distortion due to shear interaction at tool interface.

# A multiscale nature of the problem

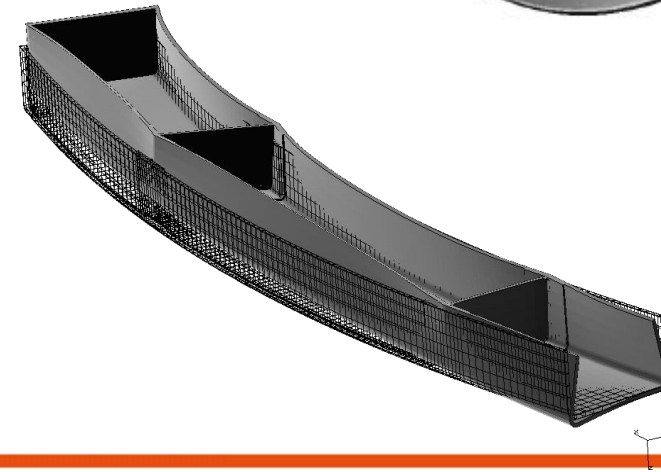
- Micro (Fibre/matrix)



- Meso (Ply)

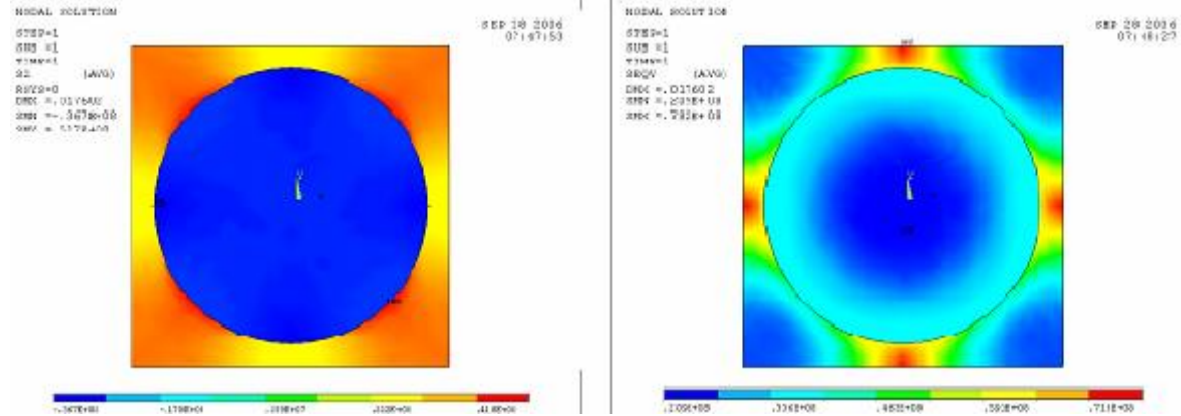


- Macro (Laminate)



# A multiscale nature of the problem

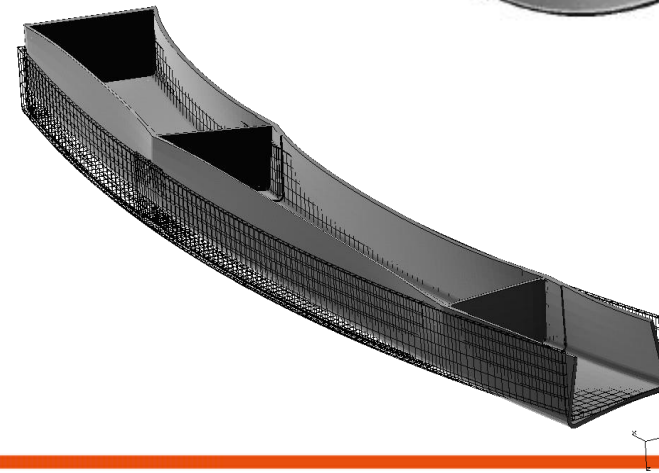
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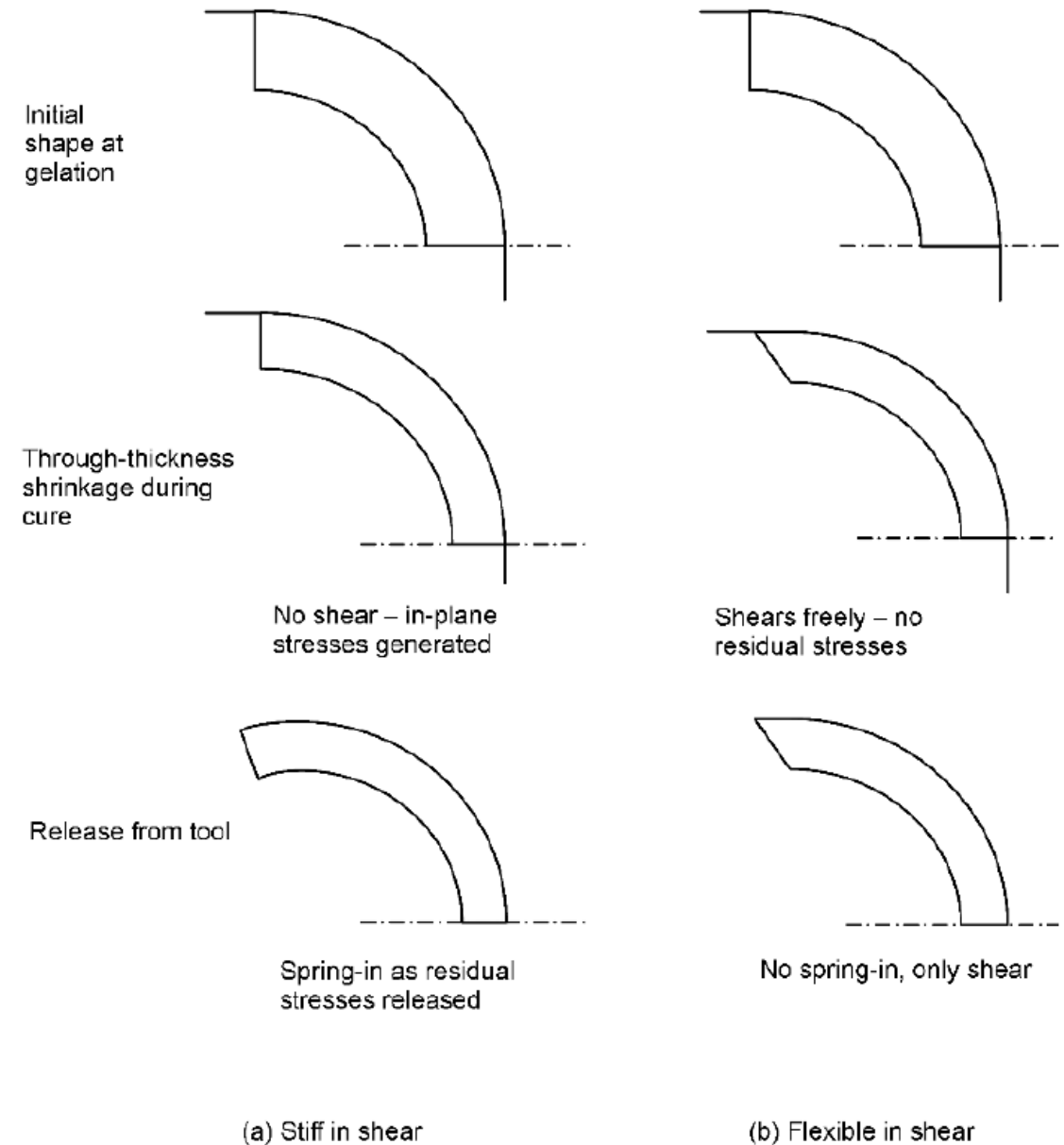


# Spring in of curved parts

In the **elastic case, without chemical shrinkage,**

$$\frac{\Delta\theta}{\theta} = (\alpha_I - \alpha_T)\Delta T$$

Where  $\Delta\theta$  is the change in angle  $\theta$ , and the  $\alpha$ 's are the CTEs (in-plane and through-thickness).



## 7.10 Change of angle due to a through-thickness contraction.

---

# CURING & DISTORTION

## Modelling the composite material behaviour

# Constitutive law

## • Elastic Models

- based on CTE orthotropy
- Material stiffness is constant
- Offer good insight in general, but are not sophisticated enough to become accurate

$$\sigma = \mathcal{C} : \varepsilon$$

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## • CHILE Models (Cure Hardening Instantaneously Linear Elastic)

- Incrementally elastic
- Material stiffness function of temperature and degree of cure
- Easy to characterise and to implement

$$\sigma(t) = \int_0^t C(T(\tau), \alpha(\tau)) : \frac{d\varepsilon}{d\tau} d\tau$$

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## • Viscoelastic Models

- Known as polymer behaviour. Especially pronounced for partially cured polymers at high temperatures in a cure cycle.

$$\sigma(t) = \int_0^t \mathcal{C}(t - \tau) : \frac{d\varepsilon}{d\tau} d\tau$$



# Constitutive law

Attractive

Computational cost



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$$\sigma(t) = \int_0^t \mathcal{C}(t - \tau) : \frac{d\varepsilon}{d\tau} d\tau$$

Global Accuracy



# Constitutive law

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PAM-DISTORTION

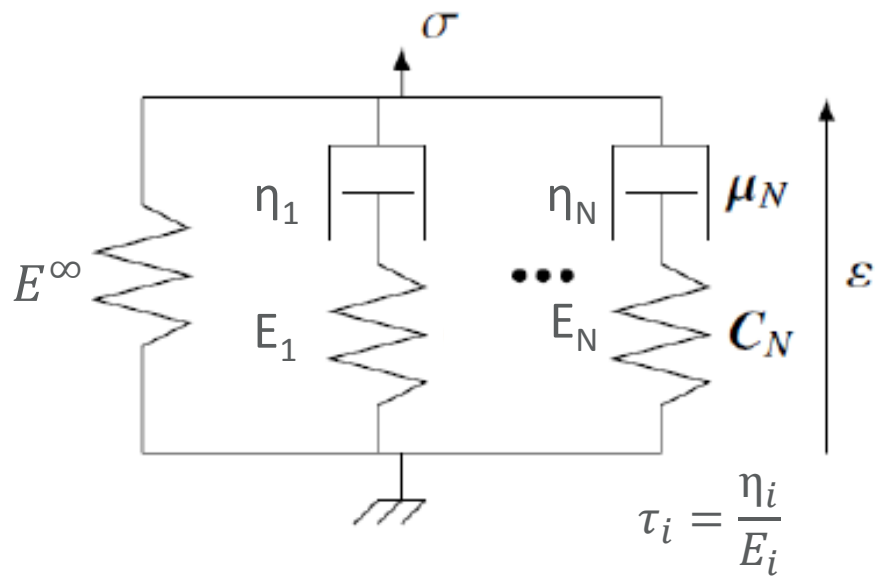
Simplified viscoelastic formulation

## • Viscoelastic Models

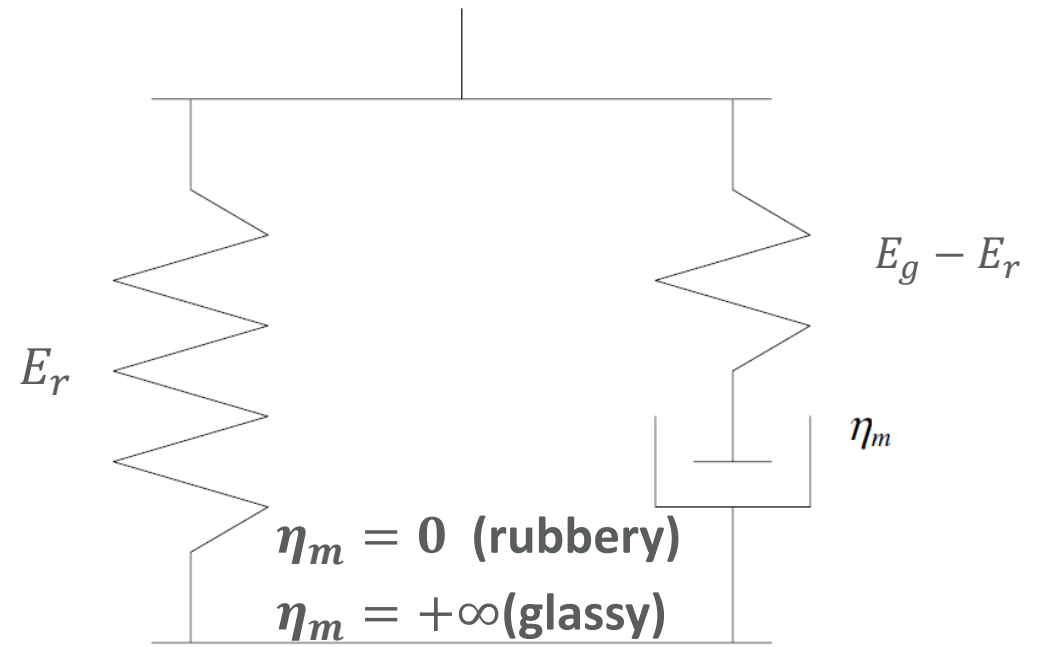
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$$\sigma(t) = \int_0^t C(t - \tau) : \frac{d\varepsilon}{d\tau} d\tau$$

# Introduction of a simplified formulation



**Fig. Generalised Maxwell model**



**Fig. Simplified model**

# Introduction of a simplified formulation

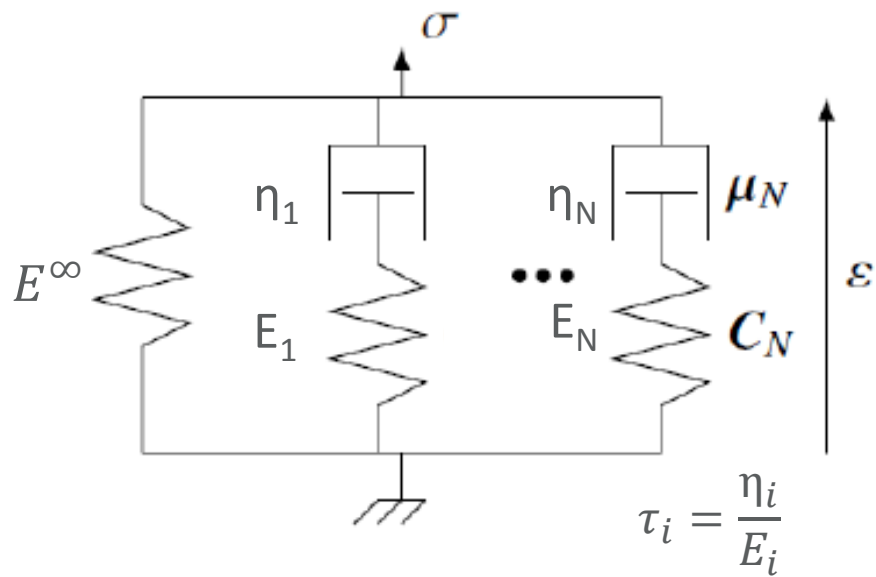


Fig. Generalised Maxwell model

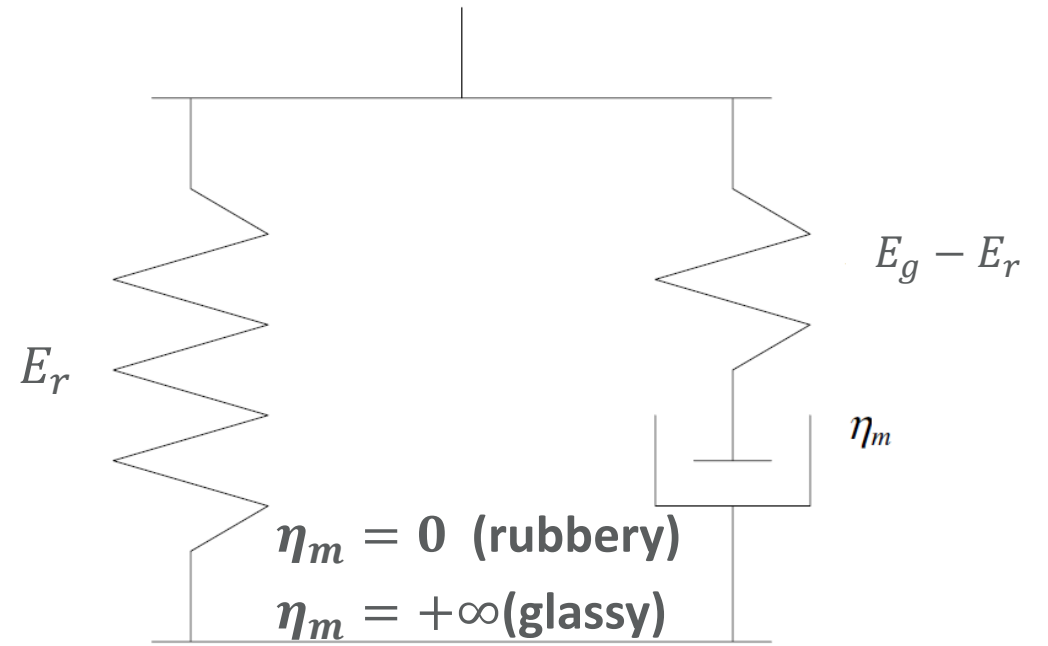
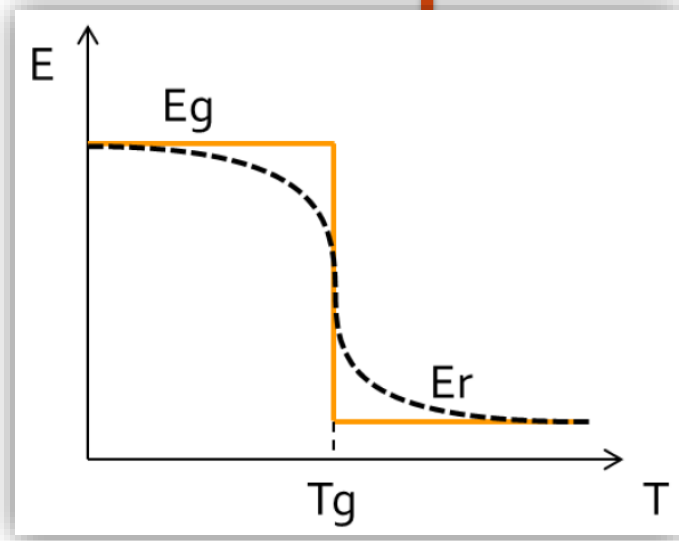


Fig. Simplified model



# Introduction of a simplified formulation

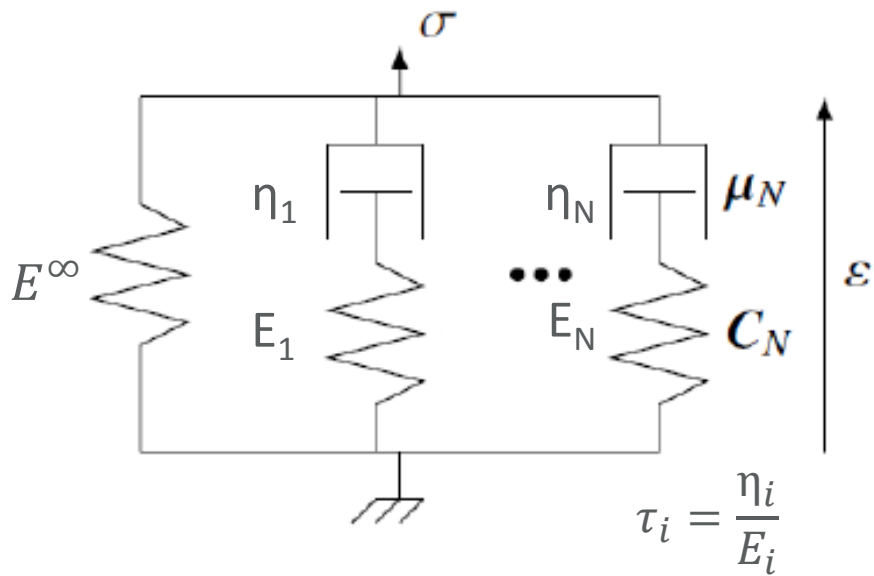


Fig. Generalised Maxwell model

$$\sigma(t) = \int_0^t E(\xi(t) - \xi'(\tau)) : \frac{d}{d\tau} [\varepsilon^{total}(\tau) - \varepsilon^{tc}(\tau)] d\tau$$

$$E(\alpha, \xi) = E^\infty(\alpha) + [E^u(\alpha) - E^\infty(\alpha)] \sum_{i=1}^N W_i(\alpha) \exp\left[\frac{-\xi(\alpha, T)}{\tau_i(\alpha)}\right]$$

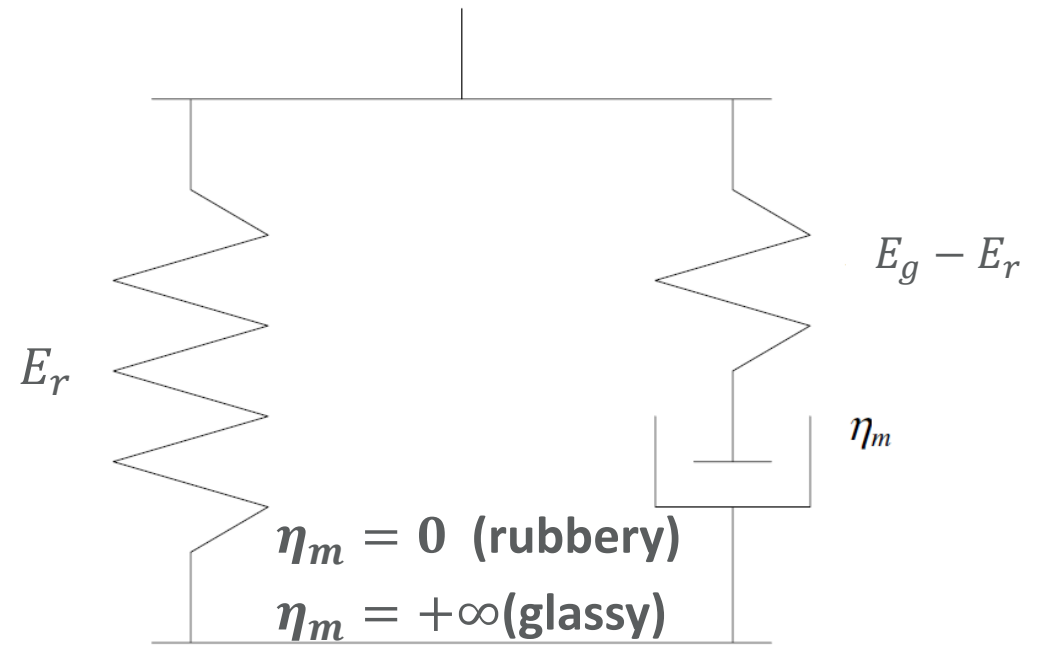


Fig. Simplified model

**In glassy state**

$$\sigma(t) = E_g [\varepsilon^{total} - \varepsilon^{tc}] - (E_g - E_r) \cdot [\varepsilon^{total} - \varepsilon^{tc}]_{vit}$$

**In rubbery state**

$$\sigma(t) = E_r [\varepsilon^{total} - \varepsilon^{tc}]$$

# Introduction of a simplified formulation

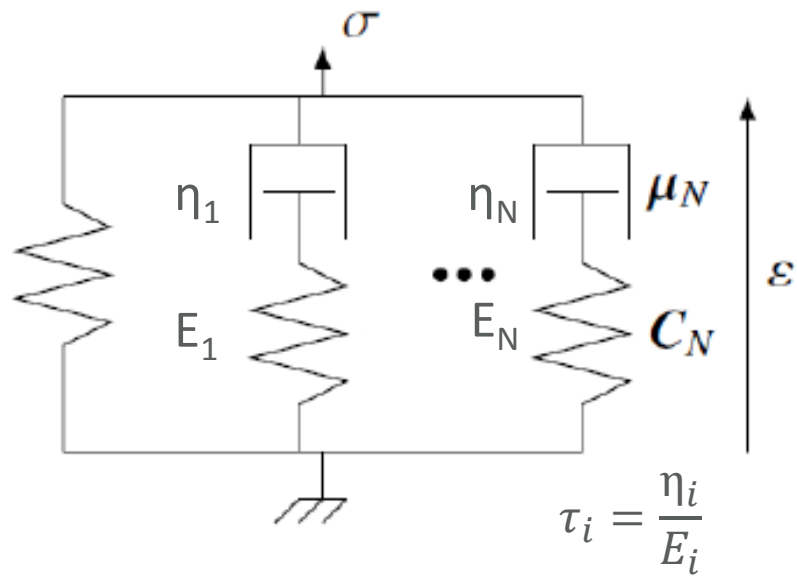


Fig. Generalised Maxwell model

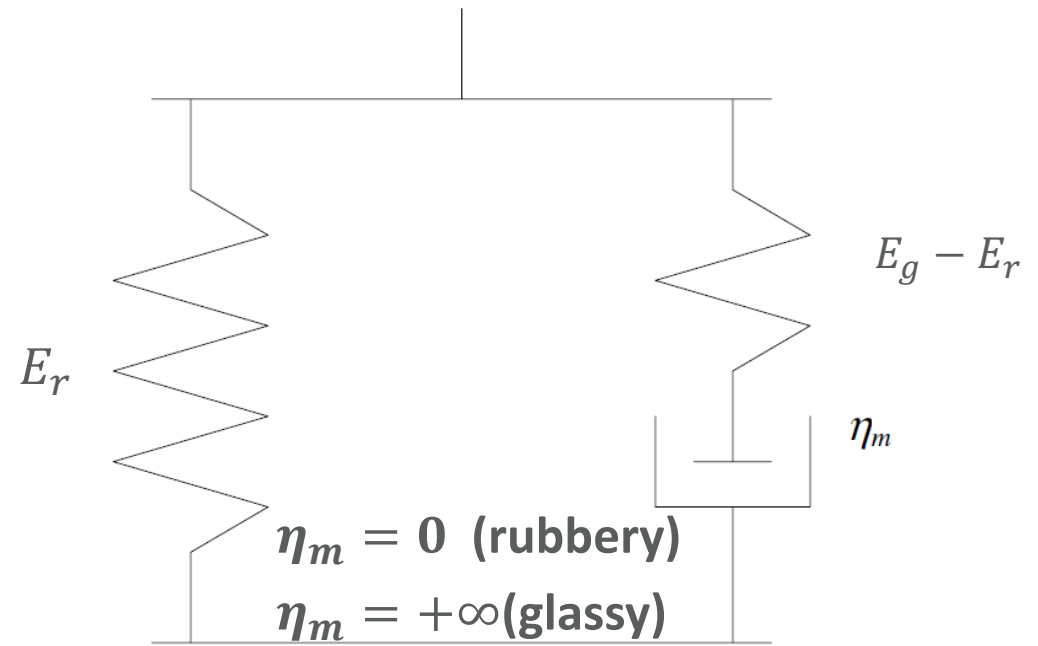


Fig. Simplified model

## A fully viscoelastic approach

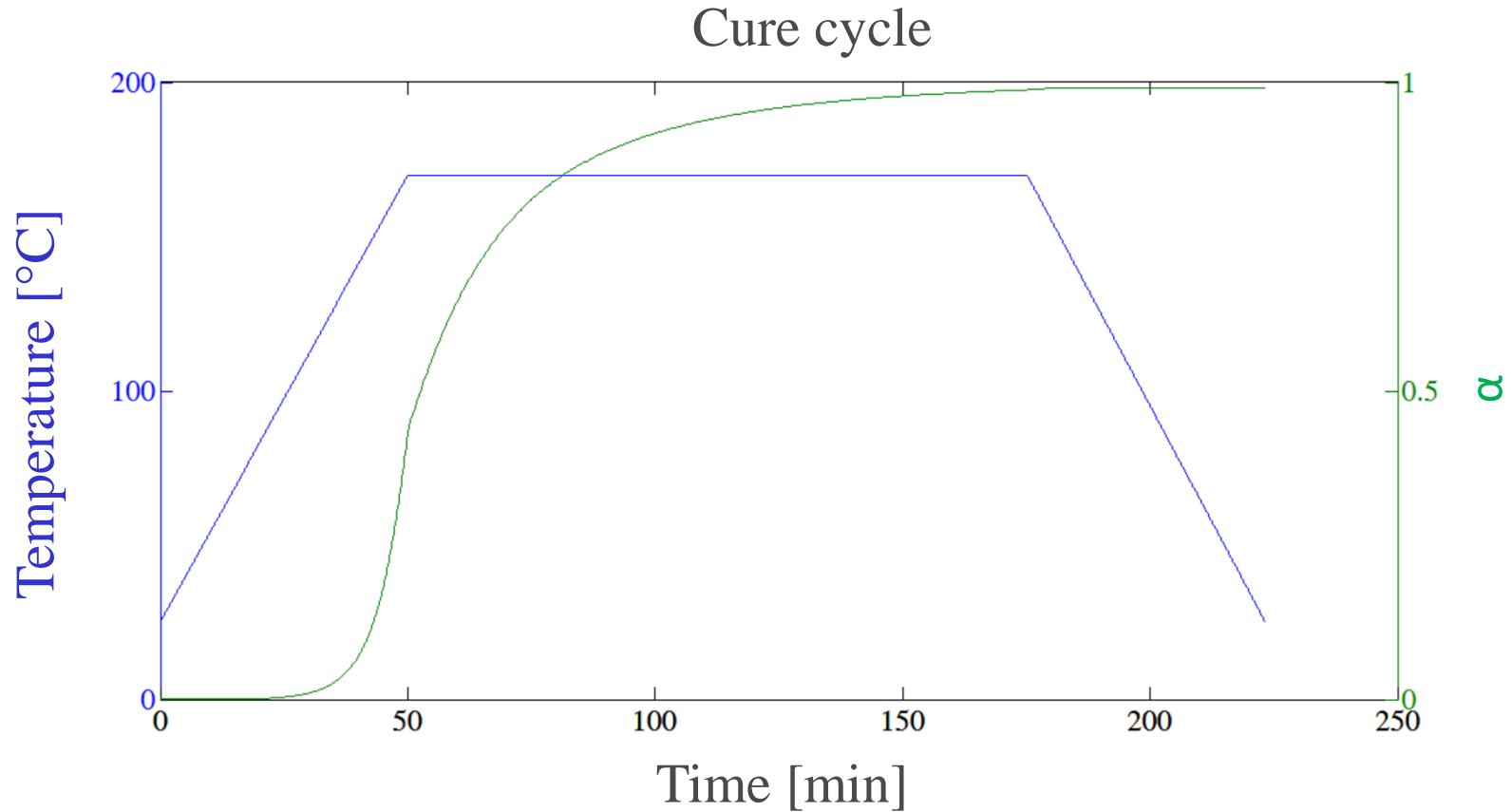
- Rich model, temperature and degree of cure dependent
- Complex and costly
- Numerically and in terms of material characterisation

## ESI pragmatic approach based on Svanberg\* formulation

- Simpler formulation with constant moduli
- Processing time assumed very large compared to material characteristic relaxation times
- Much less characterisation needed
- Very large structure simulation affordable

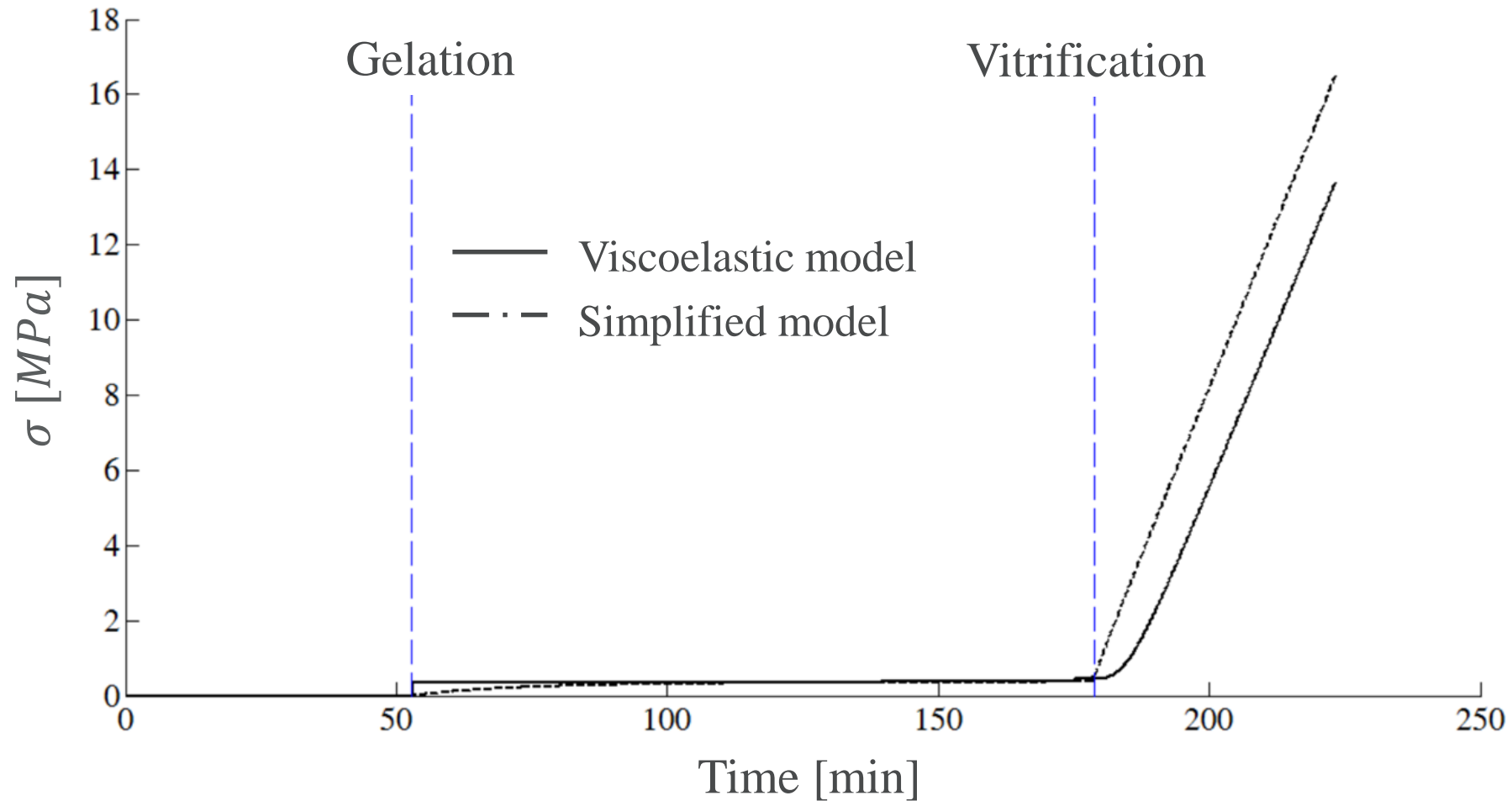
# Illustration of a 0D case

- Simulation of a fully constrained block of a characterised polymer



# Illustration of a 0D case

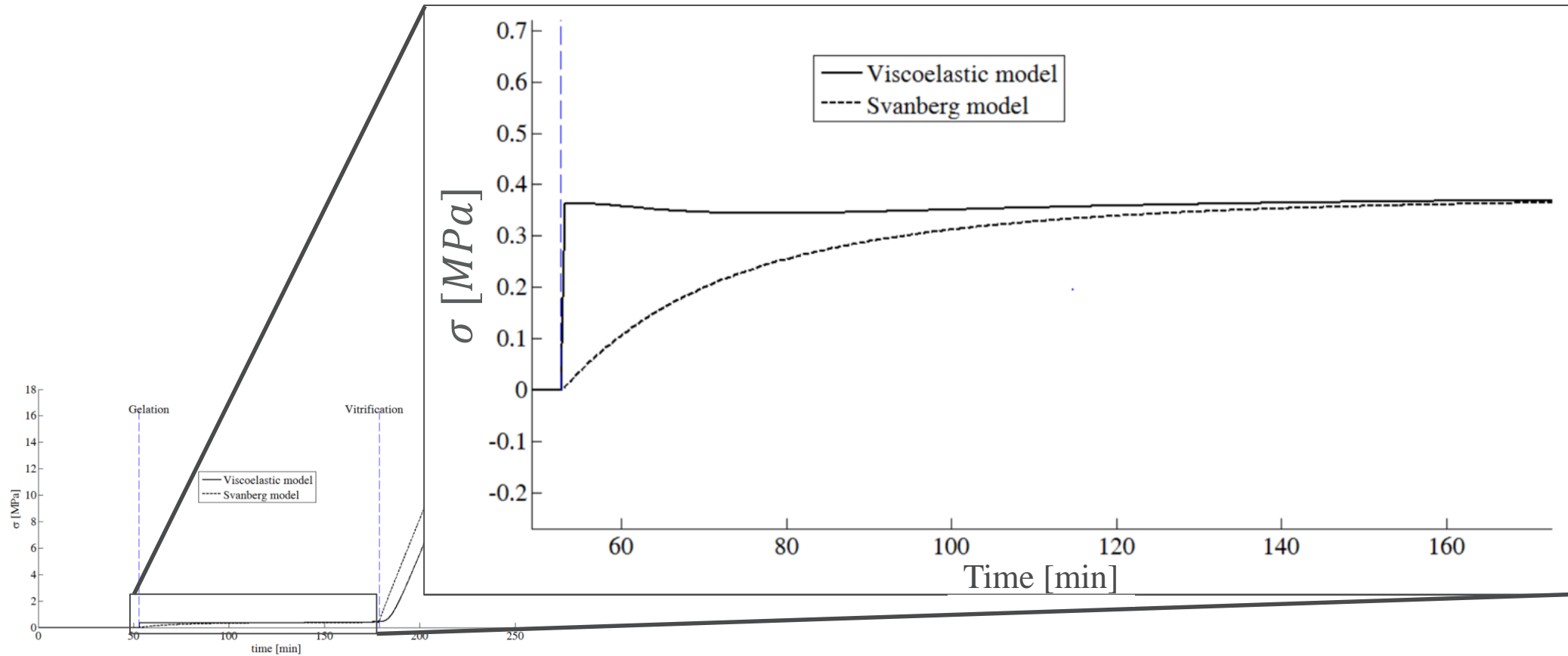
- Simulation of a fully constrained block of a characterised polymer



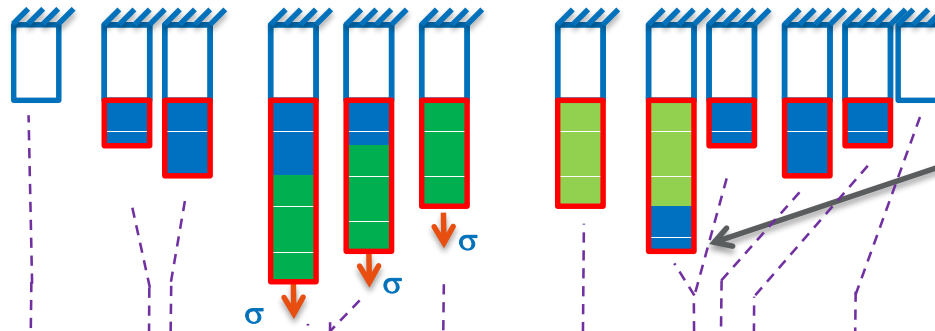


# Illustration of a 0D case

- Simulation of a fully constrained block of a characterised polymer



Fully cured rod of neat resin subjected to simultaneous temperatures changes and mechanical load

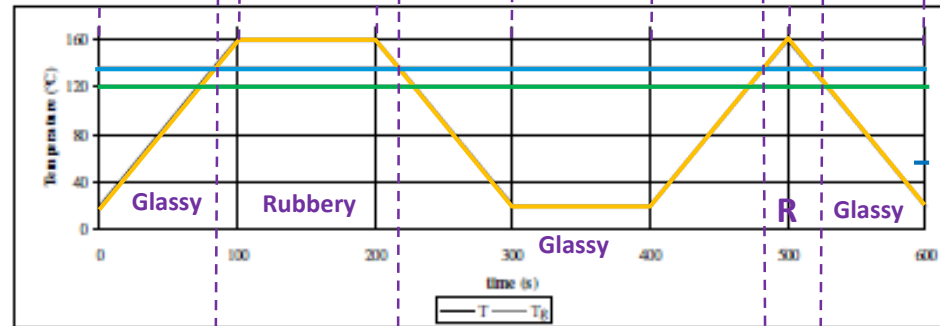


Instantaneous Relaxation of frozen strain

Expansion strain  
 Mechanical strain with Frozen strain  
 Total strain

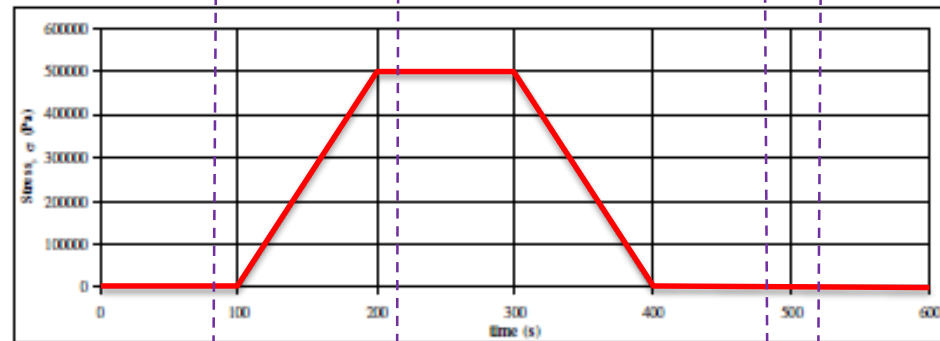
Applied Temperature

$T_g$



$\alpha=1$

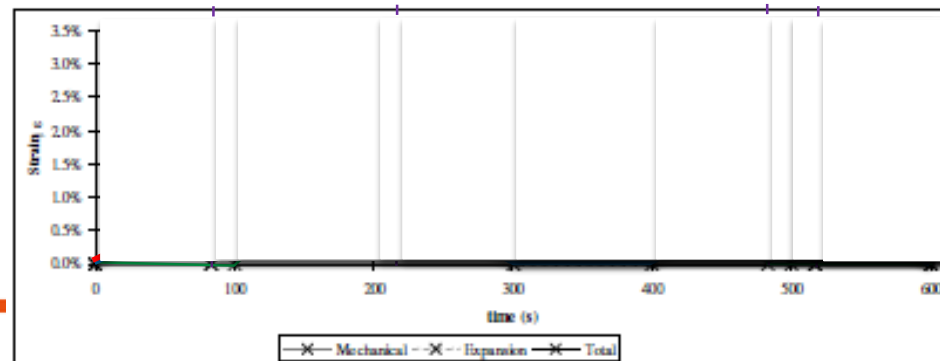
Applied Stress



Expansion strain =  
 Thermal strain + Chemical strain ( $\alpha : 0 \rightarrow 1$ )

Mechanical strain

Total strain



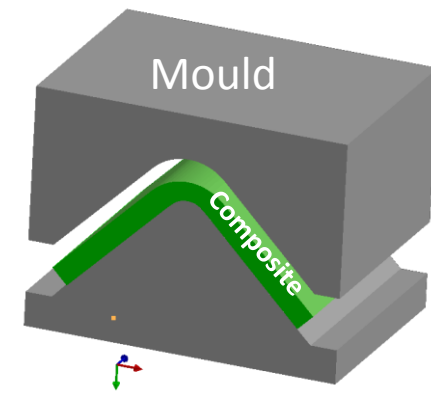


# CURING & DISTORTION

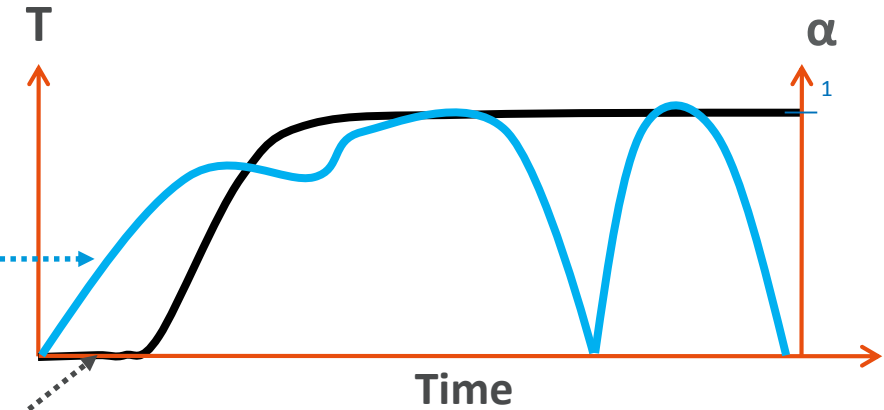
## Simulation workflow

# Typical workflow

- After a curing simulation, ...



Element thermo-chemical history



Orthotropic  
conduction

Exothermic  
curing reaction

Heat transfer

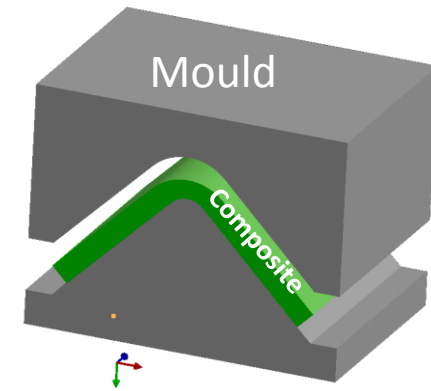
$$\rho C_p \frac{\partial T}{\partial t} = -\nabla \cdot (\bar{\bar{K}} \vec{\nabla} T) + \rho_m H_{tot} \frac{\partial \alpha}{\partial t} (1 - V_f)$$

Cure kinetics

$$\frac{d\alpha}{dt} = \sum_i w_i(t) \frac{d\alpha_i}{dt} = \sum_i w_i(t) f_i(T, \alpha)$$

# Typical workflow

- After a **curing simulation**, a **distortion simulation** is run



$(T, \alpha)$

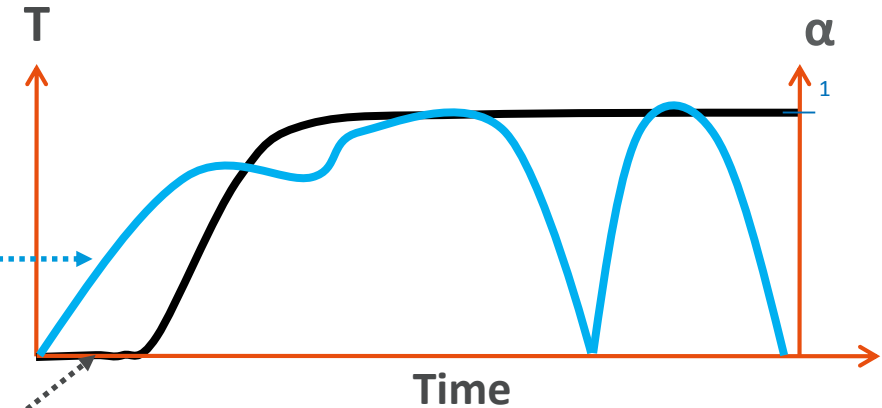
Orthotropic conduction

Exothermic curing reaction

Heat transfer

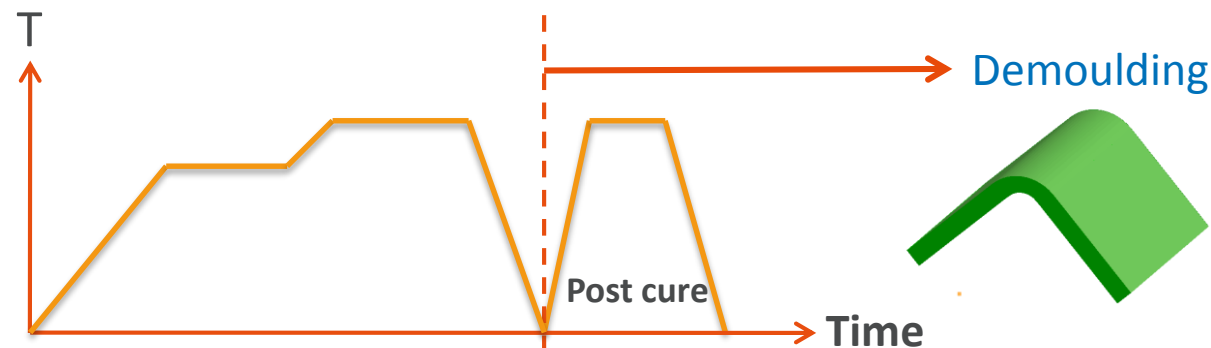
$$\rho C_p \frac{\partial T}{\partial t} = -\nabla \cdot (\bar{\bar{K}} \vec{\nabla} T) + \rho_m H_{tot} \frac{\partial \alpha}{\partial t} (1 - V_f)$$

Element thermo-chemical history

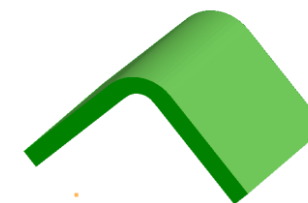


Cure kinetics

$$\frac{d\alpha}{dt} = \sum_i w_i(t) \frac{d\alpha_i}{dt} = \sum_i w_i(t) f_i(T, \alpha)$$



Mechanical equilibrium



Imposed temperature cycle over part surfaces

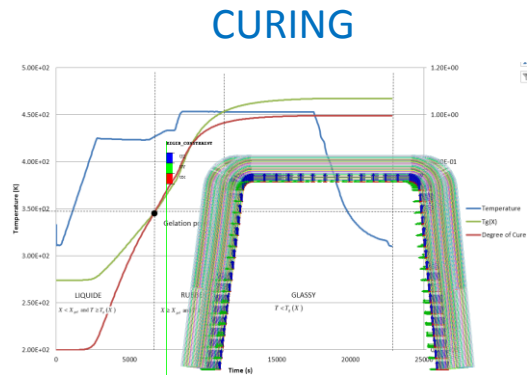
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# CURING & DISTORTION

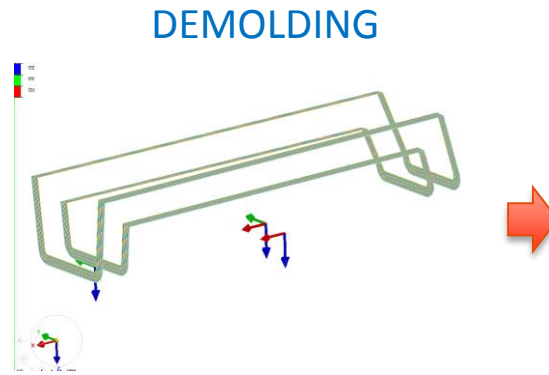
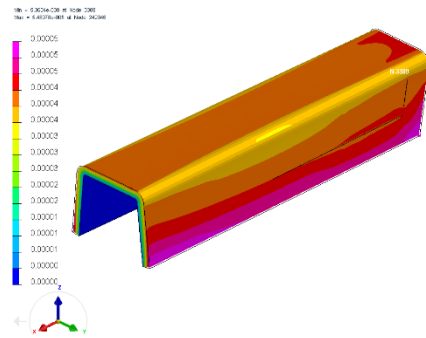
## Example

# C spar

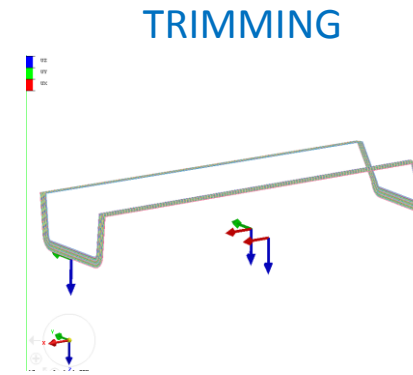
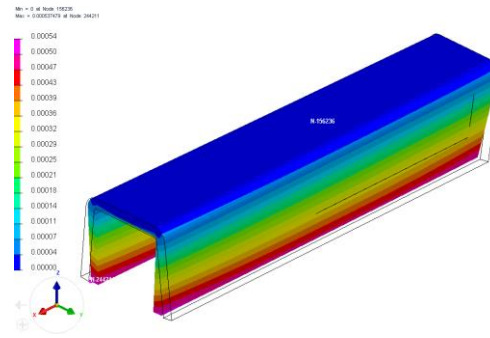
## Distortion analysis



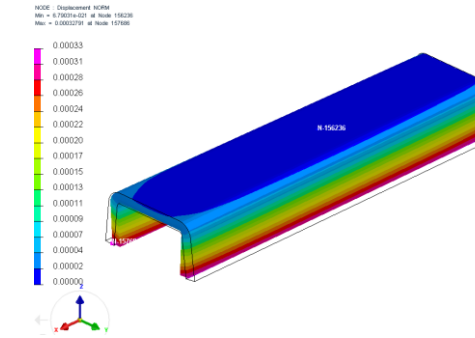
•PHASE1: inner surface of the C-Spar in contact with the mold is fixed during curing



PHASE 2: Isostatic conditions are defined on the upper side of the C-Spar



PHASE 3: Isostatic conditions are defined on the upper side of the C-Spar



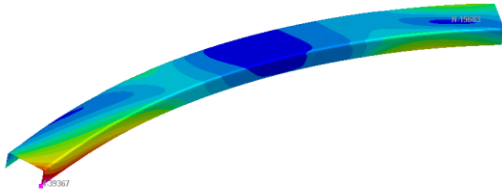
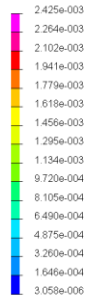
Global displacement of the C-Spar (x20)

# ESI's PAM-COMPOSITES

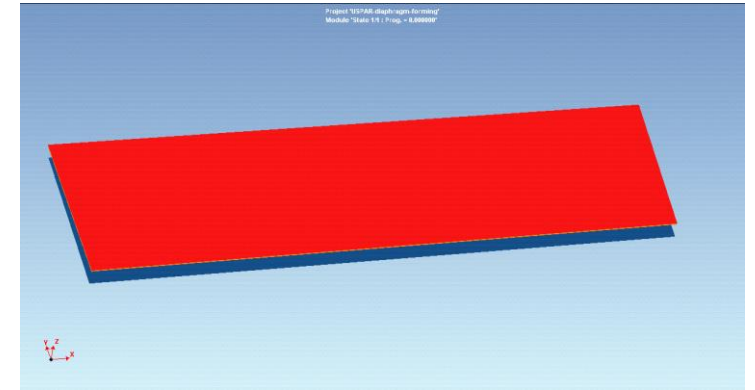
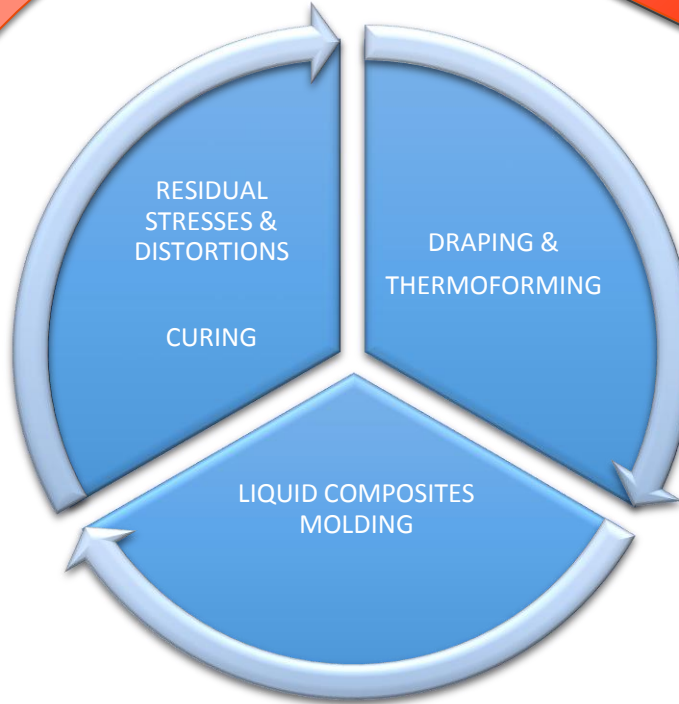
Compensated mold

esi | PAM-COMPOSITES

U\_spar\_INFUSION\_Distortion\_STEP2  
 NODE : Displacement NORM  
 Min = 3.05709e-006 at Node 1593  
 Max = 0.0024256 at Node 3037

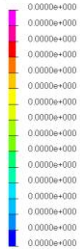


1 / 18000000.00



Fiber direction  
 Thickness variation  
 ( $V_f$ )

INFUSION\_U\_spar\_INFUSION\_HeatedFilling\_RESULT.ans  
 NODE : FILLING\_FACTOR  
 Min = 0 at Node 2025  
 Max = 0 at Node 2025



1 / 0.000000







**Thank you  
for listening**



**Do you have any question ?**

# Do you have any question ?

