Numerical Prediction of Stress Evolution During Cooling of Glass Containers Using the Narayanaswamy Model

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Contents

Introduction

- **Glass forming: a delicate process to manufacture containers**
  - Complex thermal phenomena
  - Large deformations of the glass domain during the process
  - Multiphase challenge: solid devices, molten glass, air cooling
- **Motivation for engineering simulation solution**
  - Virtual prototyping for the whole manufacturing process
    - Calculation of the flow pattern, deformation of the free surface, temperature field
    - Prediction of weight variation, stress induced during processing and cooling, possible defect
  - Improvement of existing process and cost-effective innovations

Business drivers

- **Increasing competitive level for containers manufacturing**
  - Globalization of the production market
- **Production of innovative glass containers with**
  - Thinner wall
  - More complex geometries
  - Different materials
- **Reduction of product cycles**
- **Target defect-free production**
- **Emergence of Simulation Driven Product Design**
  - Modeling of the forming, cooling and testing processes

Modelling

- **Calculated quantities**
  - Displacement $\underline{u}$
  - Deformation tensor $\underline{\underline{\varepsilon}}$
  - Stress tensor $\underline{\underline{\sigma}}$
  - Thermal strain Θ
  - Temperature T
  - Fictive temperature T_f
  - Reduced time ξ

Modelling

- **Data**
  - Bulk modulus $K(t) = K_\infty + \sum_{p=1}^{P} K_p \exp[-t/\tau_p]$
  - Shear modulus $G(t) = G_\infty + \sum_{q=1}^{Q} G_q \exp[-t/\lambda_q]$
  - Structural modulus $M(t) = \sum_{r=1}^{R} M_r \exp[-t/\mu_r]$
  - Activation energy A
  - Structural parameter x
  - Reference temperature T_{ref}
  - Density ρ, thermal conductivity κ, heat capacity C_p
  - Liquid and glassy dilatation coefficients α_l and α_g

Modelling

- **Equations (i)**
  - Deformation tensor

$$\underline{\underline{\varepsilon}} = \frac{1}{2}\left[\nabla \underline{u} + (\nabla \underline{u})^T\right]$$

  - Momentum equation

$$\nabla \cdot \underline{\underline{\sigma}} = 0$$

  - Stress constitutive equation

$$\underline{\underline{\sigma}}(t) = \underline{\underline{I}}\int_0^t K[\xi(t)-\xi(\tau)]\frac{d}{d\tau}\left(tr\left(\underline{\underline{\varepsilon}}\right)-\Theta\right)d\tau + 2\int_0^t G[\xi(t)-\xi(\tau)]\frac{d}{d\tau}\left(\underline{\underline{\varepsilon}} - \frac{\underline{\underline{I}}tr\left(\underline{\underline{\varepsilon}}\right)}{3}\right)d\tau$$

Modelling

- **Equations (ii): Narayanaswamy model**
  - Reduced time variable

$$\xi(t)=\int_0^t exp\left[Ax\left[\frac{1}{T_{ref}}-\frac{1}{T(\tau)}\right]+A(1-x)\left[\frac{1}{T_{ref}}-\frac{1}{T_f(\tau)}\right]\right]d\tau$$

  - Fictive temperature

$$T_f(t)=T(t)-\int_0^t M[\xi(t)-\xi(\tau)]\frac{dT(\tau)}{d\tau}d\tau$$

  - Thermal strain

$$\Theta=\int_{T_0}^{T_f} a_l(u)du+\int_{T_f}^{T} a_g(u)du$$

Modelling

- **Interpretation of the Narayanaswamy model**
  – Stress build up:
    - non-uniform cooling
    - -> non-uniform distribution of fictive temperature
    - -> non-uniform distribution of thermal strain
  – Slow cooling, T_f is close to T,
    Low residual stress
  – Fast cooling, T_f can be “frozen” at high values,
    Large residual stress
  – Relaxation mechanism in time

Brown glass

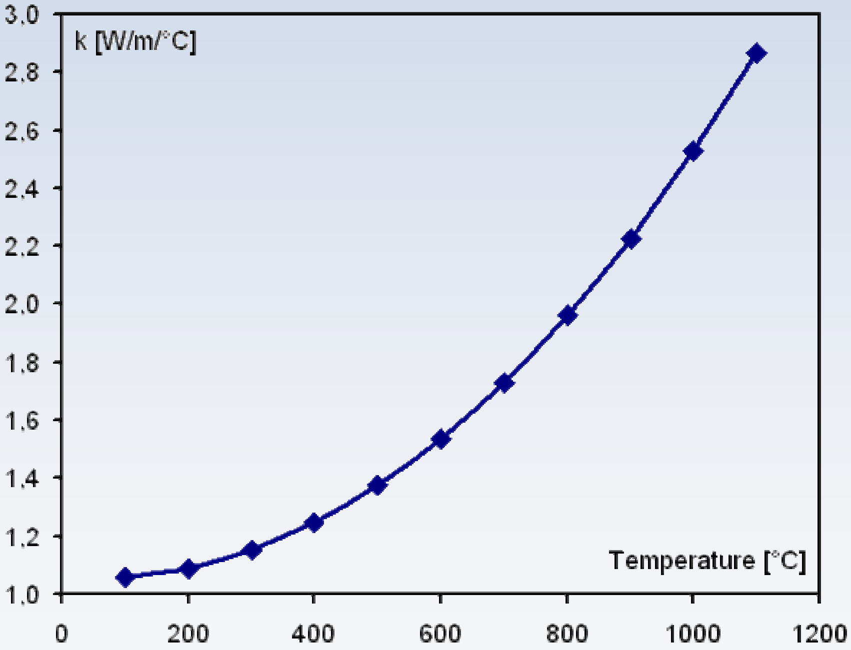
- **Numerical values of the material parameters**
  - Obtaining spectra for glass is expensive, and requires specific equipment;
  - Spectra are measured by
    Laboratory of Glass Properties LLC,
    www.glass-labs.com
    Sankt Peterburg, Russia
    [formerly Thermex Corp.];
  - Time constants typically range from 1 to 10^3 s at high temperature

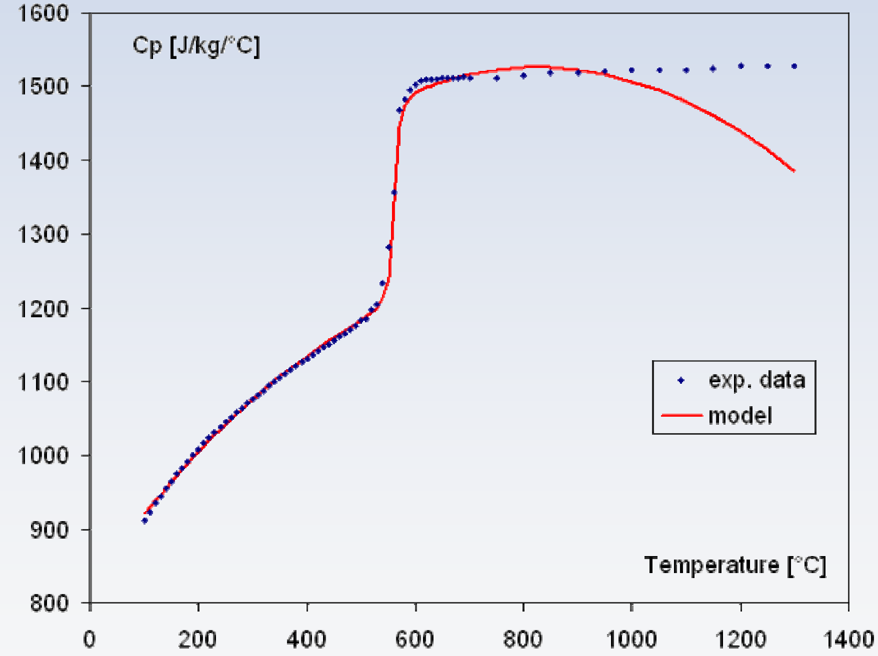
Brown glass

- **Numerical values of the material parameters**
  - Other data
    - ρ = 2,445 kg/m^3
    - k = 1.0586 - 0.139 10^{-3} T - 1.493 10^{-6} T^2 - 0.1146 10^{-9} T^3 W/m/K
    - C_p = 824 + 1.0235 T – 0.621 10^{-3} T^2 J/kg/K + Heaviside function…
    - a_g = 9.5 10^{-6}, a_l = 30 10^{-6}
    - x = 0.58, A = 74,143 K, T_{ref} = 553.1 K

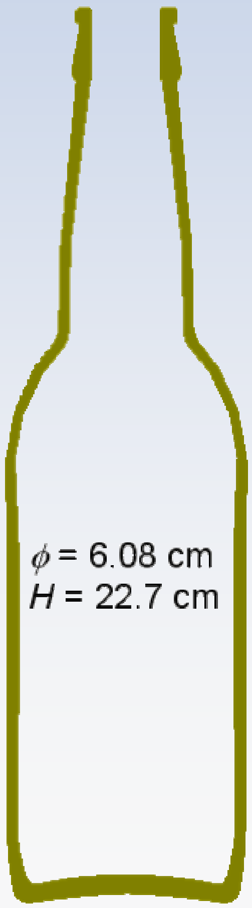
Brown glass

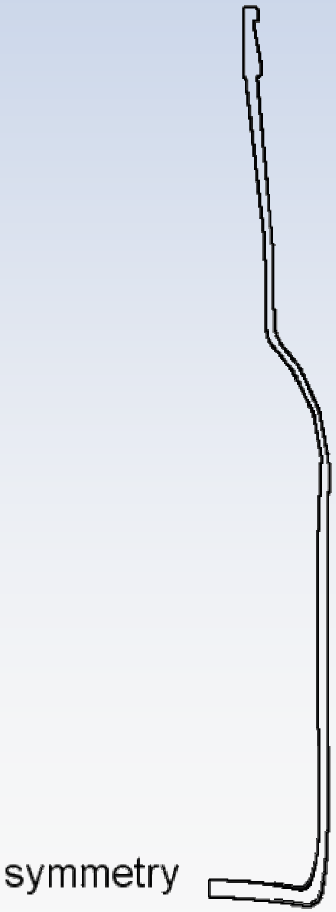
- **Thermal conductivity and heat capacity**





- **Geometry, cooling conditions, with blown air**



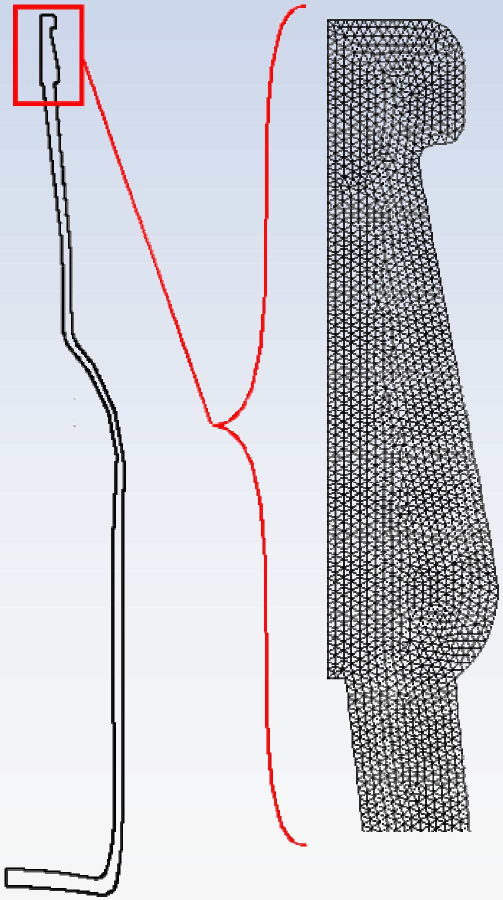


Air temperature: ~ 27°C

Heat transfert coefficient:
$\alpha_{in} / \alpha_{out} = 4/5$

Bottle

- **Finite element discretisation**

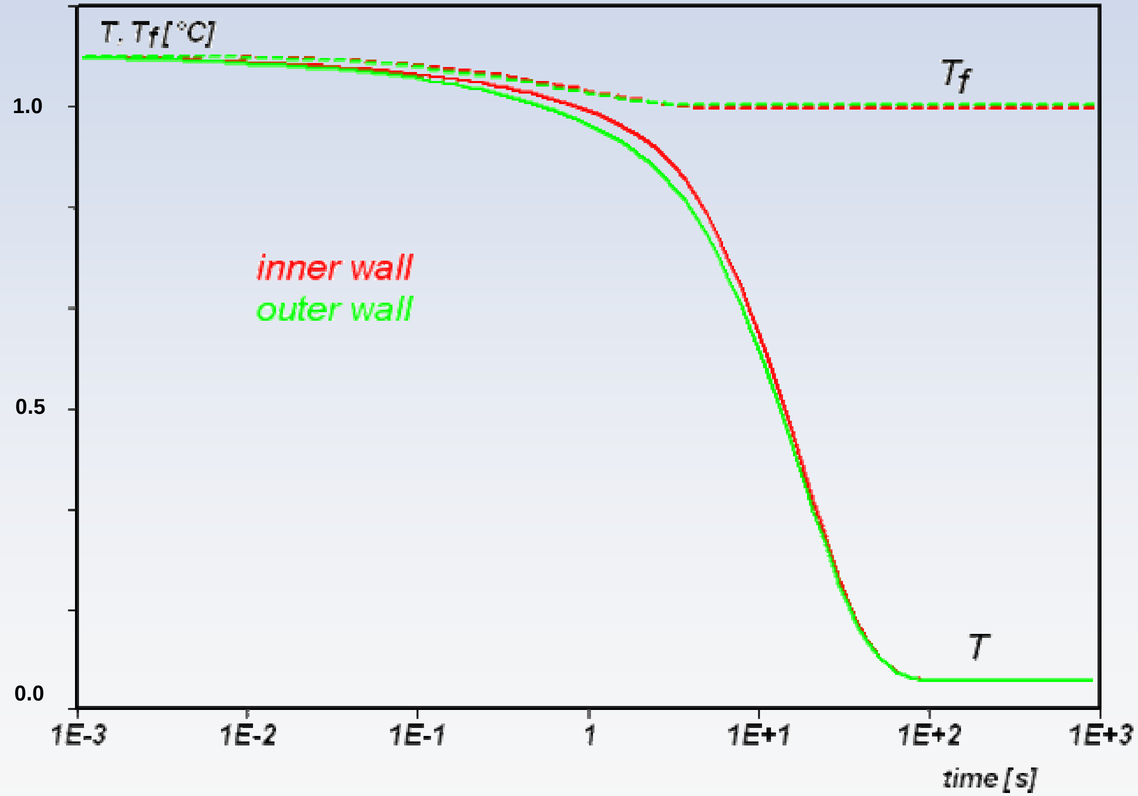


(sample, at the neck)

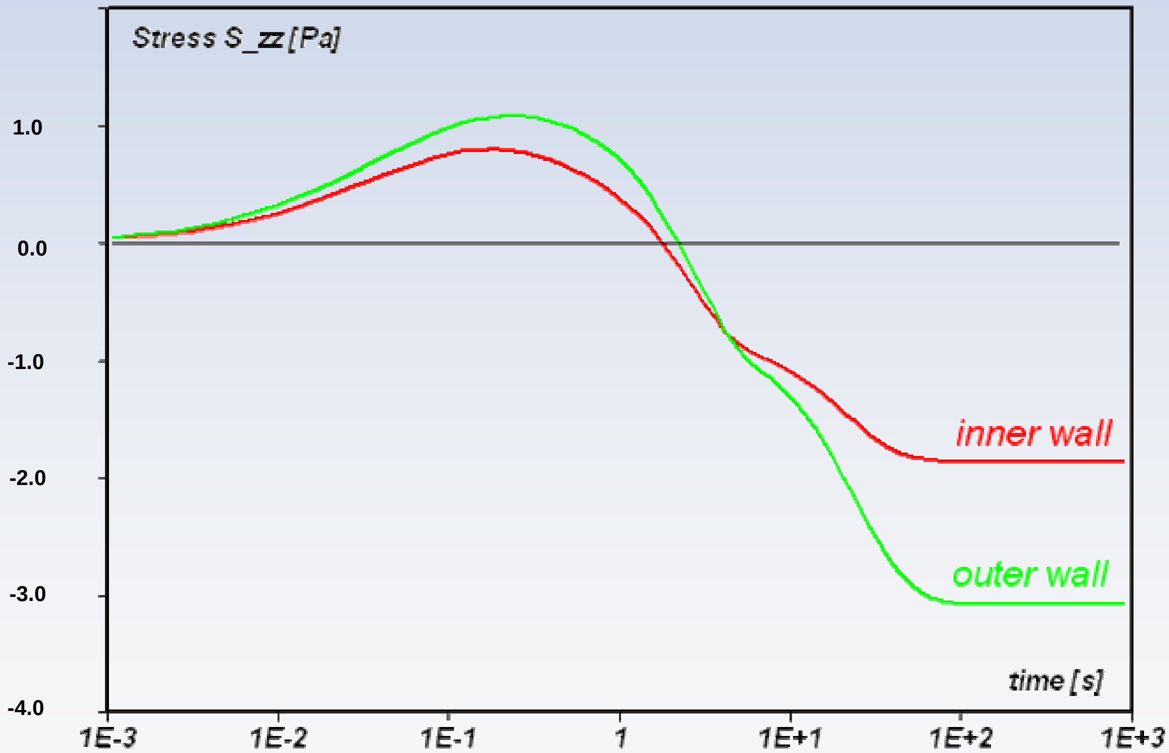
Total:
24,396 elements
50,865 nodes for T

Bottle

- **Simulation 1: blown air cooling**



- **Simulation 1: blown air cooling**



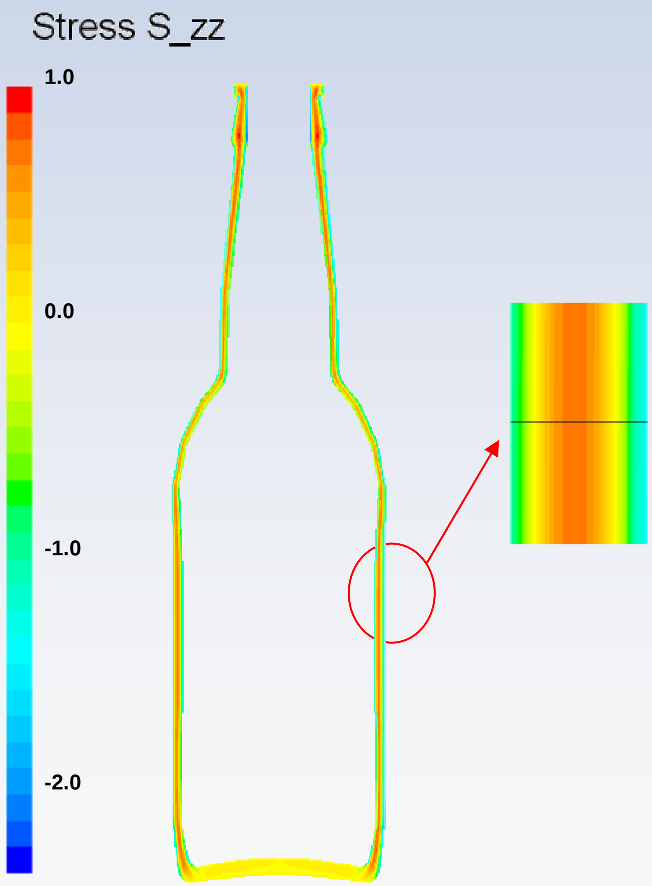
Bottle

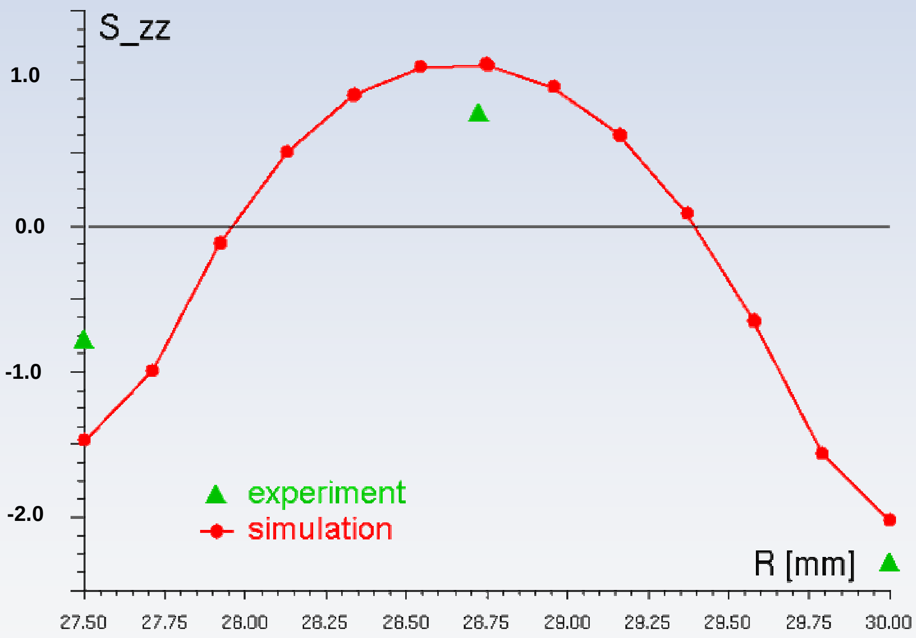
- **Measurements of surface stress**
  - Equipment used
    - Automatic polariscope AP-02 SM
      [Laboratory of Photoelasticity
      Institute of Cybernetics at TTU, Tallinn, Estonia]
    - based on birefringence
  - Measurements indicate about:

Time [s]	Non-dimensionalized S_{zz} component [Mpa]		
	Inner surface	Centre	Outer surface
20	-0.71	0.62	-2.14
10^4	-1.52	1.00	-2.95

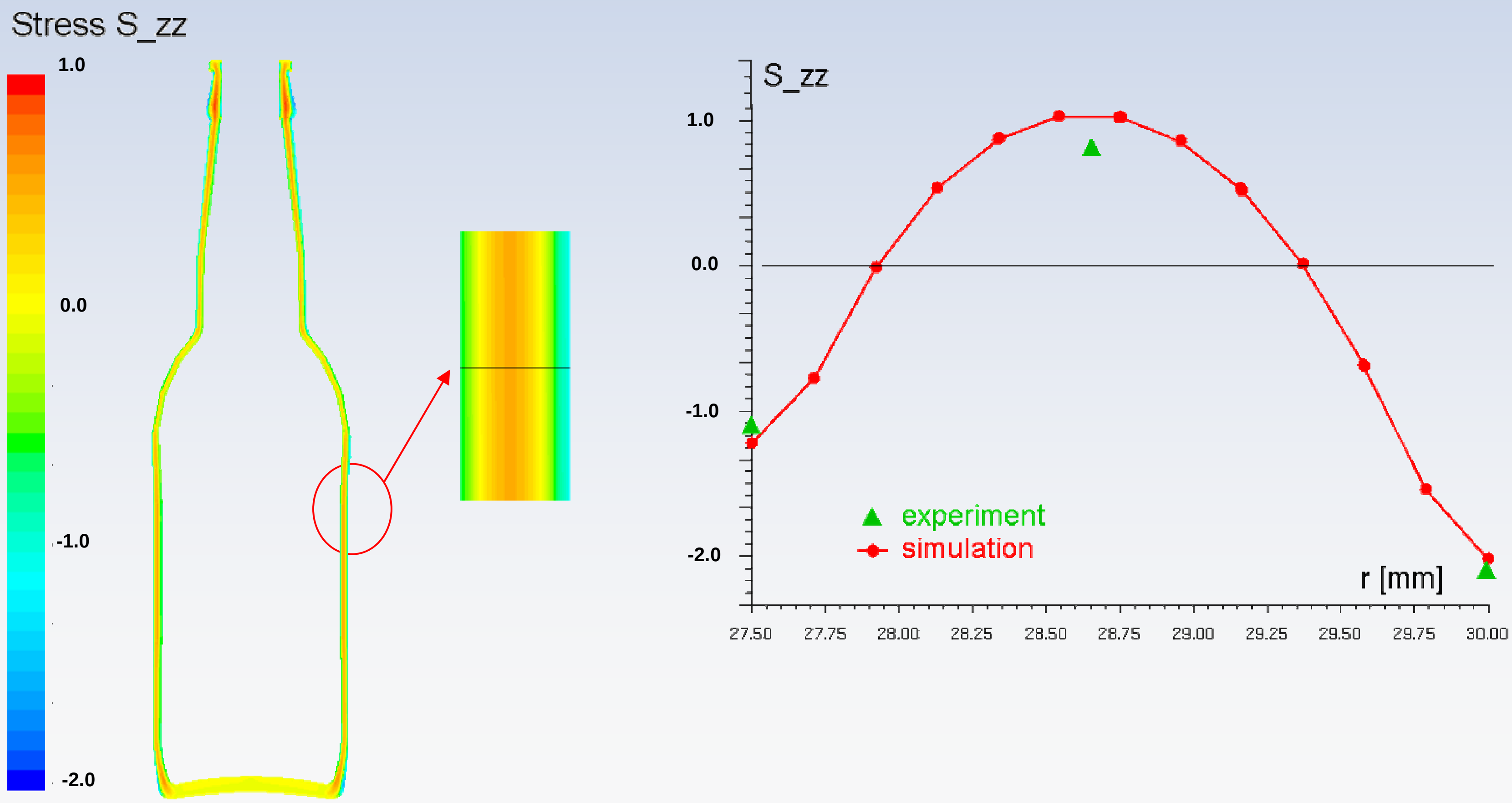
Bottle

- **Simulation 1: blown air cooling, <u>at t = 20 s</u>:**





- **Simulation 1: blown air cooling, at $t = 10^4$ s:**

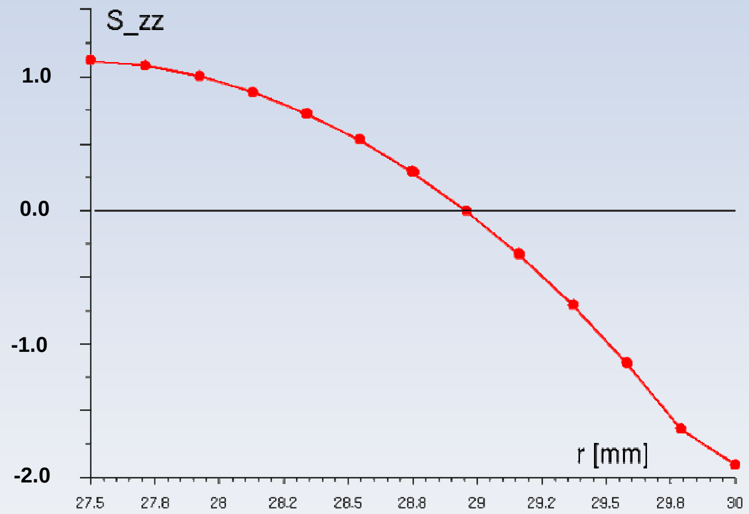


Bottle

- **departure w/r to experiments at 20s:**
  - uncertainty on the cooling parameters
  - uncertainty on the distribution of cooling
  - calibration issues
  - short time interval for measurement

Bottle

- **Simulation 2: outside radiation only**



  - Occurrence of positive stress at the inner surface of the bottle
  - Cause of defect (risk of fracture)
  - Operating condition to reject

Bottle

- **Observations from the physics**
  - Cooling needed on both inner and outer surfaces
  - Prediction of compression state after 20 s
  - Results in agreement with experimental data
- **Observation from the computation**
  - Calculation time: 1.5 h on Dell SC1435
    Processor: AMD 2220 SE 2.8GHz
  - 61 steps for 20 s of experimental time
  - [193 steps for 10^4 s of experimental time]

Conclusion

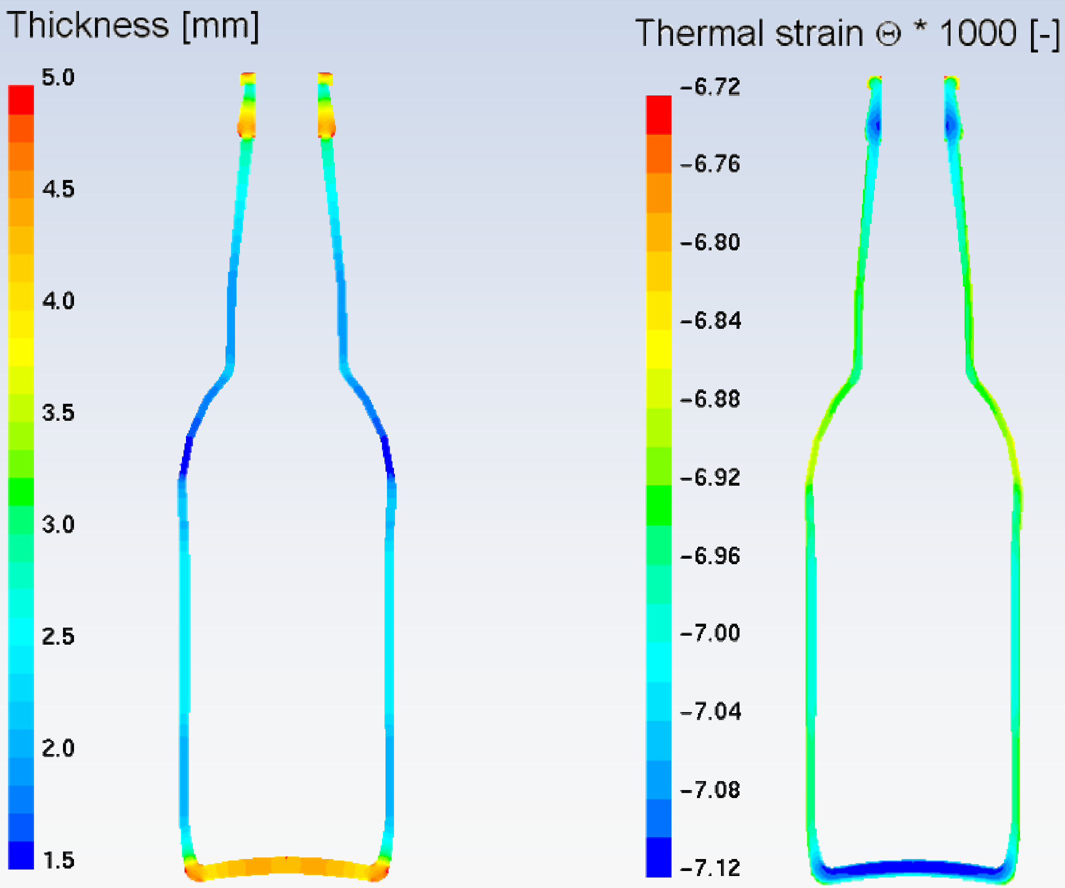
- **Implementation of the Narayanaswamy model**
- **Validation vs. existing results**
- **Application to an industrially relevant case**
- **Comparison with experimental data**
- **Challenge of getting material data**

- **Filling the gap between glass forming and structural modeling**
  - Seamless interface between ANSYS POLYFLOW and ANSYS Mechanical

Some references

- **The model**
  - R.S. Chambers, Numerical integration of the hereditary integrals in a viscoelastic model for glass, J. Am. Ceram. Soc., 75 (1992) 2213-2218 Third level text
  - O. S. Narayanaswamy, A Model of Structural Relaxation in Glass, J. Am. Ceram. Soc., 54 (1971) 491-498
  - A. Markovsky and T.F. Soules, An efficient and stable algorithm for calculating fictive temperatures, J. Am. Ceram. Soc., 67 (1984) C-66-C-67
- **The software implementation**
  - POLYFLOW version 3.12, user's manual, ANSYS Inc, Canonsburg, PA

- **Simulation 1: blown air cooling**



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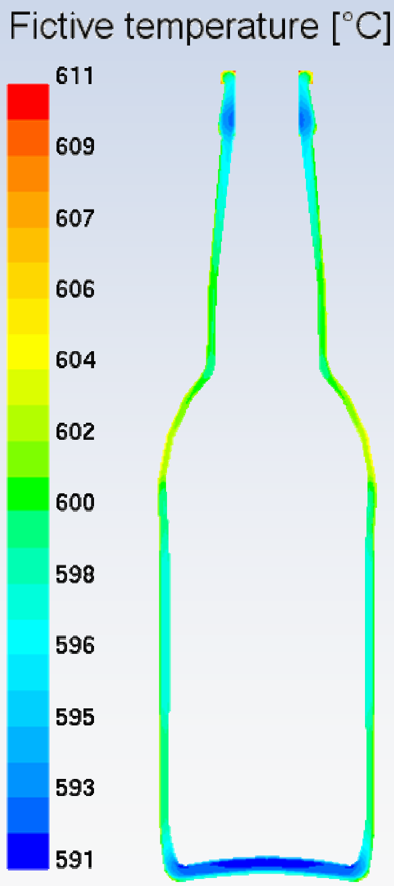
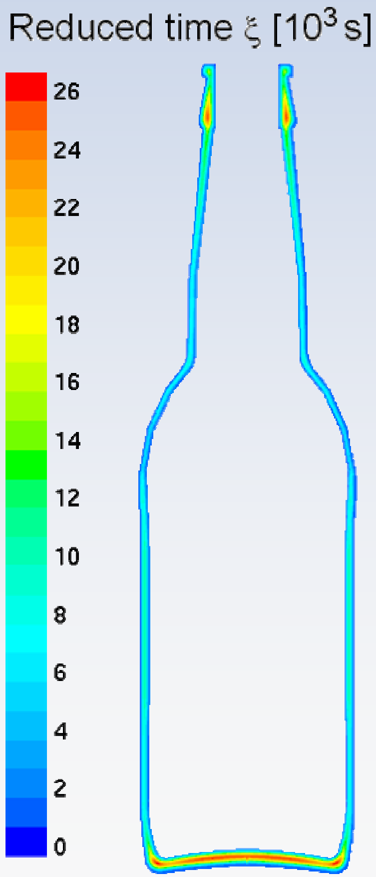
- **Simulation 1: blown air cooling**



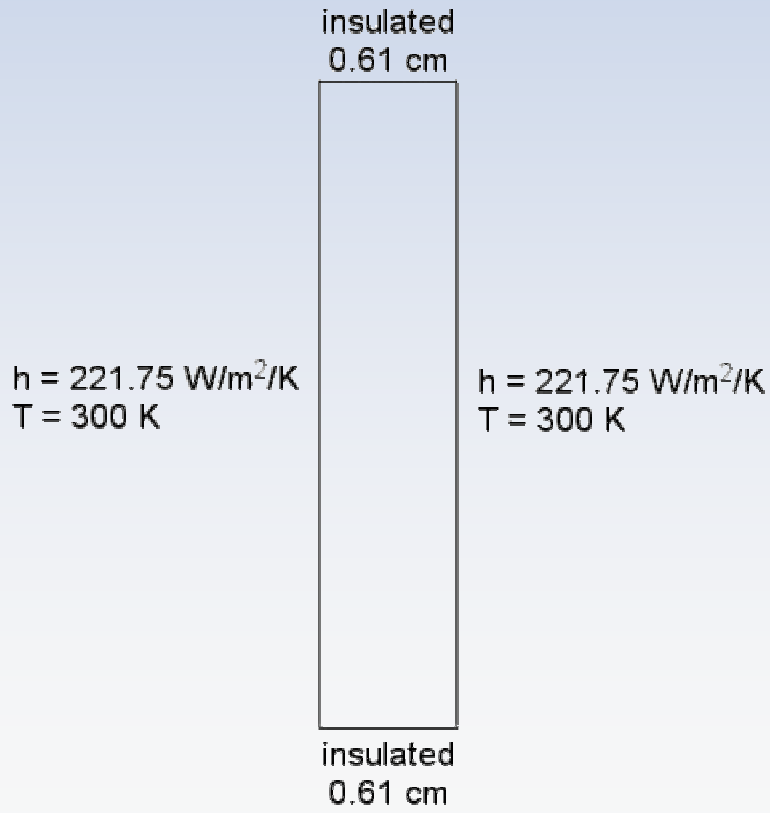


Numerical treatment

- **Approach suggested by Chambers et al.**
  - Time marching scheme
  - Calculation of temperature field
  - Calculation of fictive temperature and auxiliary fields
  - Calculation of thermal strain
  - Calculation of stresses and deformation

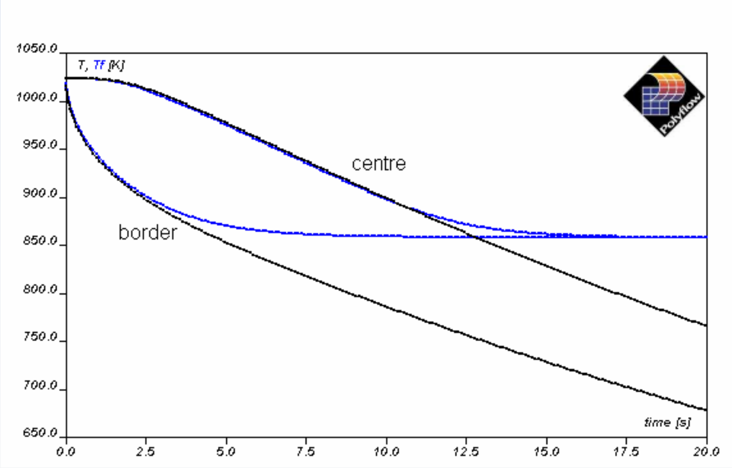
Validation vs. ANSYS

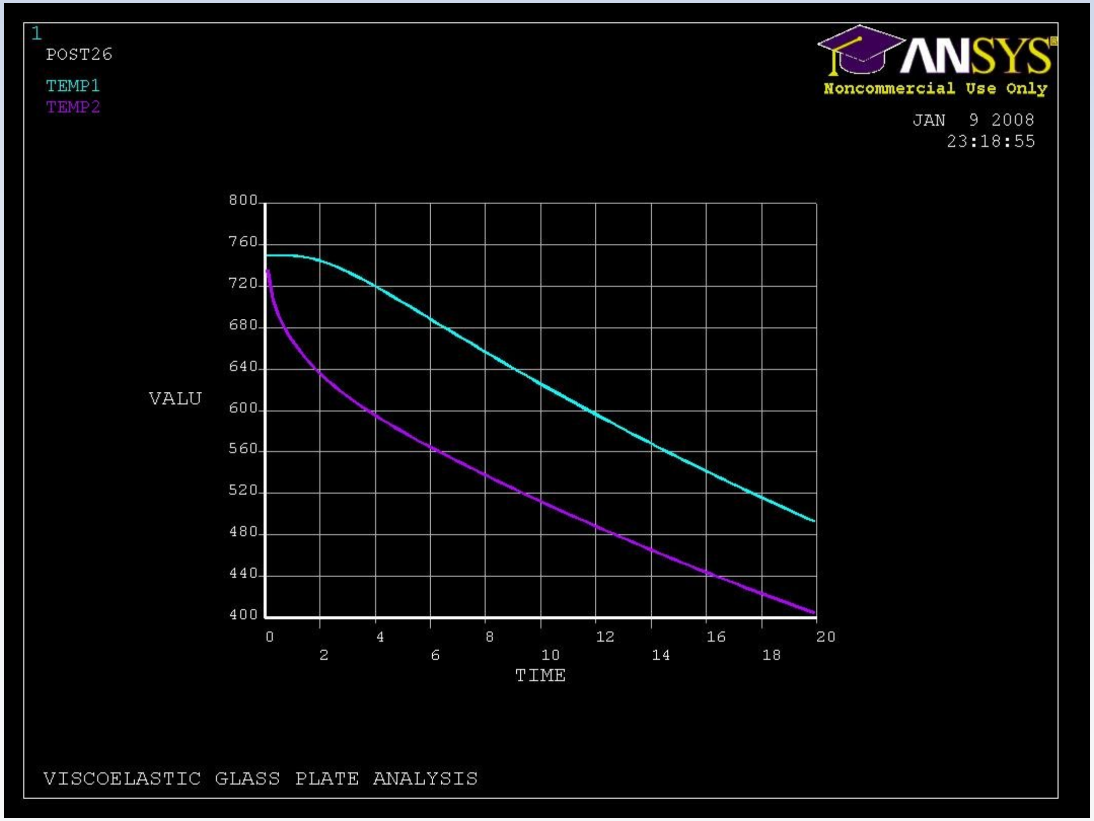
- **Cooling of a plate: definition**



Validation vs. ANSYS

- **Cooling of a plate: temperature calculations**





Validation vs. ANSYS

- **Cooling of a plate: stress calculations**