





Cost-Effective Computational Method for Radiation Heat Transfer in Semi-Crystalline Polymers

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INTRODUCTION



THERMOFORMING OF THERMOPLASTICS



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OUTLINE



□ Introduction & Problem statement

- □ Experimental analyses
- □ Background of the numerical model
- □ Numerical experimental comparisons: IR-heating of PE plate
- Conclusions





RADIATION TRANSPORT IN SEMI-CRYSTALLINE POLYMERS



 Radiation heat transfer equation (RTE) offers a complete solution of radiation transport in optically homogeneous or heterogenous media:

$$\frac{dI_{\lambda}}{dS} = -\beta_{\lambda}(S)I_{\lambda}(S) + \kappa_{\lambda}(S)I_{\lambda b}(S) + \frac{D_{\lambda}}{4\pi}\int_{\Omega_{i}=0}^{4\pi}I_{\lambda}(S,\Omega_{i})\varphi_{\lambda}(\Omega,\Omega_{i})d\Omega_{i}$$

Spatial distributions of scattered light

• The attenuation of radiation due to both optical scattering and absorption may be computed using Beer-Lambert Law:

$$\frac{dI_{\lambda}}{dS} = -\beta_{\lambda}(S)I_{\lambda}(S) = -(\kappa_{\lambda}(S) + D_{\lambda}(S))I_{\lambda}(S)$$

$$\nabla \cdot q_r(S) = \int_0^\infty -\beta_\lambda I_\lambda(0) e^{-\beta_\lambda S} d\lambda = \int_0^\infty -(\kappa_\lambda + D_\lambda) I_\lambda(0) e^{-(\kappa_\lambda + D_\lambda)S} d\lambda$$



- Optical scattering behavior is spectral-dependent, where also a scatterer in unfilled semi-crystalline polymer may evolve under varying temperature
- Prediction of absorption may thus be quite complex due to the evolution of spatial distributions of scattered light under heating



TEMPERATURE-DEPENDENT OPTICAL PROPERTIES OF PE



Φ^s

FT-IR Analyses

Port - 2 🔻

Sample

 The significant difference between directional-directional (T_λ^{i, r}) and directionalhemispherical transmittance (T_λ^{i, ^}) of PE due to optical scattering

- Spectral-dependenc in optical scattering, especially for $\lambda{<}2~\mu\text{m}$





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TEMPERATURE-DEPENDENT OPTICAL PROPERTIES OF PE



- Temperature dependent $T_{\lambda}^{i,r}$ measurements between 25° and 128°C, demonstrated that optical scattering becomes weaker.
- The dramatic change in thermo-optical properties of semi-crystalline polymers close to melting range



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Boztepe et al., 25ème Congrès Français Thermique (2017)



Geiger et al., *Production Engineering* (2009)

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TEMPERATURE-DEPENDENT TRANSMISSION AND REFLECTION TESTS



- Temperature dependent T_{λ}^{i} and R_{λ}^{i} measurements to obtain temperature-dependent extinction coefficient (β_{λ} (T)) of PE
- Identical quenched PE in liquid nitrogen (LN_2) samples were prepared in three different thicknesses
- Preliminary tests were performed on both heating devices

Test type	Test Device	Spectral Range (µm)	Sample thickness (mm)	Nr. of temperature steps (25°C-128°C)
Τ _λ ^{<i>i</i>, ^ (T)}	FT-IR Spectrometer (Perkin Elmer 900VIS)	0.25 - 2.5	0.25 0.5 and	14
R _λ ^{<i>i</i>, ^ (T)}	Directional-hemispherical reflectometer (SOC100-HDR)	1 - 25	0.25 , 0.5 and 0.75	10



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- The increase in $T_{\lambda}^{i, \gamma}$ is very small until 97°C where also it is more pronounced after ~116°C
- Generally $T_{\lambda}^{i, \uparrow}(128^{\circ}C) \approx T_{\lambda}^{i, \uparrow}(126^{\circ}C) \rightarrow$ The measurements at last temperature step was neglected.



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TEMPERATURE-DEPENDENT $R_{\lambda}^{i, \uparrow}$ TESTS



- Inverse relation between temperature and $R_{\lambda}^{i, \gamma}$ was all the samples.
- The slight decrease in $R_{\lambda}^{i, \gamma}$ is distinctive after 110°C, therefore 2 assumptions were made for β_{λ} (T) calculations:
- 1- R_{λ}^{i} (@25°C) for the temperature until 110°C 2- Averaged R_{λ}^{i} for the measurements 110°C <T<128°C





DETERMINATION OF β_{λ} (T)



- β_{λ} (T) was calculated using SQP algortihm in MATLAB
 - 12 computions were performed regarding numerical inputs created for 12 temperature steps (up to 126°C)
 - **12 different** $\beta_{\lambda}(T)$ values were calculated \rightarrow Numerical input for radiative source term $(\nabla \cdot q_r)$ computations





DETERMINATION OF β_{λ} (T)



- A typical IR-lamp temperature is around 2000 2600 K The effect of significant increase in $T_{\lambda}^{i, \gamma}$ (°C) for VIS and early NIR ranges (0.5 1.6 µm) is seen in β_{λ} (T) Regarding to Wien's displacement law: $\lambda_{max} * T_{IR-lamp} = 2897.7686 \mu mK$ In terms of radiation physics, the change in this spectrum should have an effect on the temperature field predictions on PE
- 95% of the blackbody emissive power ($E_{\lambda b}$) is between $0.5\lambda_{max} < E_{\lambda b} < 5\lambda_{max}$





MODELING BACKGROUND -(TEMPERATURE-DEPENDENT THERMOPHYSICAL PROPERTIES)



- Temperature-dependent conductivity (k) of PE was adopted from literature and assumed isotropic.
- Apparent specific heat ($C_{p,apparent}$) of PE was determined \rightarrow Calorimetric DSC analyses using LN₂ quenched PE samples
- The total energy required both for increasing T(C) for unit mass of polymer and partial melting of crystalline phase registered by DSC signals





MODELING BACKGROUND -(TEMPERATURE-DEPENDENT THERMOPHYSICAL PROPERTIES)



 $X_{c}(\%) = \frac{\Delta H_{m}}{\Delta H_{m}^{0}}(\%)$

- The model considers the change in density (ρ) of PE considering a two-phase model:
 - The degree of crystallinity (X $_{\rm c}$ (%)) of PE was determined from the DSC melting endotherm \rightarrow
- Temperature-dependent melt ratio (α_{melt}) was calculated based on melting endotherm and used as numerical input



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IR-HEATING OF PE PLATE (EXPERIMENTAL)



- IR-heating of PE plate (78x78x2.2mm) was performed using an IR-lamp (1 kW) at its nominal power (P_{IR-lamp} = 100%)
- Two thermocouples (TC) were attached on the back surface of the plate (positioned 4 and 9 mm away from the edge)
- The back surface was also monitored via IR-camera (AGEMA 880LW) once the back surface is at steady-state temperature





IR-HEATING OF PE PLATE (NUMERICAL)



- A parametric case study was carried out performing two different simulation cases.
- The aim is to investigate two different points:
 - 1 The accuracy of close-loop iterative simulations using β_{λ} (T)
 - 2 The effect of ignorance the temperature-dependent optical properties of PE on the temperature field predictions

	Radiation absorption in polymer medium
Simulation Case - 1 (C1)	Constant radiation absorption with <i>∇</i> .qr (25 °C)
Simulation Case - 2 (C2)	Temperature-dependent radiation absorption with V.q _r [T,x,y,z]) between 25 and 128°C

- Except abla.qr, all the boundary conditions and meshing properties were kept identical
- The boundary conditions chosen identical to the IR-heating experiments
- Numerical simulations were carried out for heating up to 600 seconds ←

Obtained from IR-heating experiments



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NUMERICAL-EXPERIMENTAL COMPARISONS (STEADY-STATE)



- Vertical and horizontal profiles were defined on both IR-thermography and the numerical simulations
- The temperature profiles were compared considering the steady state condition at 600 seconds



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NUMERICAL-EXPERIMENTAL COMPARISONS (STEADY-STATE)



- C-2 built with β_{λ} (T) closely predicts the temperature in the middle zones (between 15 to 55 mm)
- Somewhat overestimation of temperature was observed close to the edge → Perfect contact assumption for PE plate-barrier





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NUMERICAL-EXPERIMENTAL COMPARISONS (REAL-TIME)



- Real-time temperature measurements: TC recordings and IR-heating were started simultaneously
- The temperature evolution on over time was compared to simulation results obtained on the exact geometrical positions of TCs



Potential conduction losses between barrier and the plate may be underestimated

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CONCLUSIONS



- A numerical model that proposes an approach to consider the optical scattering and the change in its behavior under heating condition indirectly, without modeling how the light scatters inside of polymer medium
- Under varying temperature, the scattering behavior evolves due to microcrystalline structure evolutions
- Temperature-dependent β_{λ} (T) of PE was experimentally determined and used as numerical input in the closed-loop iterative model.
- **D** Thanks to this, absorption characteristics of PE medium was updated at mesh scale regarding to $\beta_{\lambda}(T)$
- The model closely predicts temperature in the middle zones of PE plate while overestimation of temperature was observed close to the plate edge
- □ Thermal contact resistance value between barrier and the plate is required









THANK YOU FOR YOUR ATTENTION!

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