Numerical Simulation of Recycled PET Preforms Infrared Heating Including Force Convection Effect in the Industrial ISBM Ovens

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Abstract. Nowadays, injection stretch blow molding (ISBM) process represents the most employed technology to produce plastic bottles. An important step of this process is the heat conditioning stage which is performed within infrared ovens by the use of powerful halogen lamps. Homogenizing the temperature distribution along and inside the preform at the end of this conditioning stage is one of the key parameters to determine the final quality of the bottle (thickness, mechanical properties, transparency…). In this research work, a numerical software has been developed to simulate recycled PET (rPET) preforms infrared heating inside the industrial ISBM ovens, where both rotation and translation of the preform across different heating modules occur. In addition, the presence of a fan system involving a forced convective condition inside the ovens is also considered using a Computational Fluid Dynamics (CFD) approach instead of using a conventional heat transfer coefficient.

Introduction

Classical polyethylene terephthalate (PET) has been adapted for usage in beverage packaging industry since the 1980s. Recently, since the emergence of citizen's consciousness about plastic pollution, recycling PET is the most desirable method providing an opportunity for reductions in oil usage, carbon dioxide emissions and PET waste [1]. Classical PET material is, therefore, little by little replaced by recycled PET (rPET). However, the introduction of recycled content induces important variability in the forming properties (i.e., thermo-mechanical and optical properties…) of the resin, which forces industrial actors of beverage packaging to re-invent their shaping processes with respect to input materials in order to achieve a satisfactory production rate.

The most employed technology for the large-scale production of PET bottle is based on two stages ISBM process [2]. Controlling the temperature distribution in the preform at the end of the conditioning stage in ISBM process with respect to recycled material grades is the main target of this research. This is a key parameter to determine the final quality of the bottle [3,4]. The purpose of this study is to offer a feasible method allowing a complete simulation of IR heating of PET preforms in the context of an industrial ISBM oven, taking into account the dynamics of the preform and hybrid convective conditions inside the industrial oven, which are often lacking from the previous works [5,6]. To do so, a ray tracing method is chosen to simulate thermal radiative energy absorbed inside the semi-transparent preforms. The proposed method allows prediction of changes in IR energy absorption capacity of the materials due to the variability of optical properties. Afterwards, the influences of recycled content in the input materials on the energy efficiency of the IR heating process can be carried out thanks to heat transfer simulations using COMSOL Multiphysics® commercial software.

Understanding air flow involved inside an oven using an air-cooling system is of great importance to determine suitable convective conditions so that the surface temperature distribution of the preform can be controlled. Monteix *et al*. [7] proposed two different experimental methods to estimate the convective coefficient along the preform height: IR thermography and hot wire anemometry. The

authors showed that the two methods presented a large uncertainty. In Ref.[8], the authors proposed a simplified approach for air convection modeling, where a complete 2D simulation were performed in Ansys/Fluent software for the case of the PET sheet. Then, the air flow fields obtained from the 2D simulation was used to calculate a convective heat transfer coefficient correlation along a vertical wall used for 3D simulation of IR heating for PET preform. A recent application of Computational Fluid Dynamics (CFD) to calculate the air flow field in an IR oven can be found in [9]. The CFD model allowed the authors to improve knowledge of the air flow inside the oven, which was then used for the purpose of controlling the flow angle and air volume of the fan system. In this work, we propose a CFD approach for simulation of both natural and forced convection that occur inside an industrial oven, aiming to more precise prediction of the convective heat transfer along the preform height.

Materials and Methods

Materials. Preforms made from virgin and recycled Polyethylene Terephthalate (rPET) resins are used in this study: 100% virgin PET, 50% Eg-rPET and 100% Eg-rPET. According to its origin, the rPET materials is named Eg-rPET, which is taken from Egypt. Virgin PET RAMAPET N180 is supplied by Indorama Ventures Europe. Preforms are produced by injection molding under identical conditions. All preforms used are 18.5g weight, and 2.55 mm thickness, provided by the SIDEL company (see Figure 1).



Figure 1. Preforms made from different materials.

Characterization. Thermal properties of polymers are characterized using laboratory devices which showed a very small dispersion between virgin and recycled grades. The density of polymer is measured by use of a double balance, which provides an average value for all types: $\overline{\rho} = 1.335 \ kg.m^{-3}$. The specific heat capacities of the materials are measured using Differential Scanning Calorimetry, which are temperature-dependent as can be shown in Figure 2a. Thermal conductivity of PET is taken from literature [4], which is also assumed to be constant for all grades: $\overline{k} = 0.25 W.m^{-1}.K^{-1}$.

Optical properties of the materials are measured using a Fourier Transform Infrared spectrometer (FT-IR Bruker Vertex 70) over the spectral range $[0.4 - 25] \ \mu m$. Results from the spectral transmissivity (τ_λ) and the spectral reflectivity (ρ_λ) measurements allow us to calculate the spectral absorption coefficient (κ_λ) according to the Beer–Lambert law (Eq.1):

$$\tau_\lambda = (1 - \rho_\lambda)e^{-\kappa_\lambda d} \tag{1}$$

Where d is the sample thickness. The results of κ_λ with respect to semi-transparent materials can be seen in Figure 2b. All the preforms are opaque in the spectral range $[2.72 - 25] \ \mu m,$ so that the computation of the absorption coefficient tends to an infinite value in this spectral range. It is important to note that the differences in optical properties of the resins due to effects of recycled content are mostly found in the spectral range $[0.4 – 1.65] \ \mu m$. Considering a typical IR lamps using for ISBM process, with a filament temperature of 2400K, this spectral range encompasses about 47%

of radiative energy emitted by the filament regarding to Planck's law [10]. This mean that variability in absorption characteristics in this spectral range may have a significant effect on the amount of absorbed IR energy inside materials.
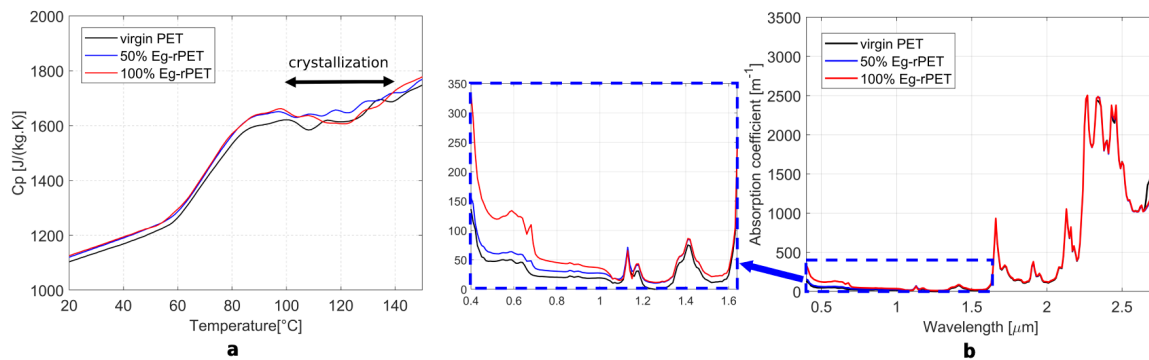
**Figure 2.** Properties of materials used (a) Specific heat capacity and (b) Absorption coefficient.

Radiation exchange. Thermal radiative interactions between the components constituting the oven (i.e., IR halogen lamps and reflectors) and a static preform is simulated thanks to a ray tracing method using an in-house software so-called RAYHEAT [5]. The proposed method allows calculation of absorbed radiative energy inside a semi-transparent media using the Beer-Lambert's law, which results in a volumetric heat source computed within each three-dimensional mesh element. This method allows to take into account changes in IR energy absorption capacity of the materials due to variability of optical properties. For ray tracing simulation, each IR halogen lamps is decomposed into two independent radiative sources: the tungsten filament and the quartz tube. Radiative characteristics of IR lamps used in this application are shown in Table 1. Radiative emission from the cylindrical surface of the sources are assumed to be isotropic. Thanks to this assumption, the discretization of the rays on the emitted surface and the ray's directions are determined adopting a stochastic approach. For each source, 2 million rays are computed [5]. The support of the preform is also modeled as an aluminum body, which allows more accurate prediction of the heat exchange near the preform neck. Since the aluminum is opaque, IR energy illuminated from the lamps results in a local radiative heat flux on the aluminum surface.

Table 1. Radiative characteristics of IR lamps.

Parameter	Symbol	Unit	Lamp 1	Lamp 2	Lamp 3	Lamp 4	Lamp 5	Lamp 6
Electrical power	P_e	W	1000	1000	450	300	750	900
Filament temperature	T_f	K	2433.4	2433.4	2035.9	1858.6	2281.9	2376.7
Quartz temperature	T_q	K	675.9	675.9	584.9	547.3	640.2	662.4
Filament power	P_f	W	838.4	838.4	352.0	223.0	615.6	749.1
Quartz power	P_q	W	57.6	57.6	35.3	27.8	48.2	54.0
Length of lamps	L	m			272e-3			
Diameter of filament	d_f	m			1.97e-3			
Diameter of quartz	d_q	m			10.4e-3			

The rotation of the preform is considered by using an interpolation function associated with a rotated coordinate system (O, x1, y1, z1) with respect to the reference system (O, x, y, z). This interpolation function results in a time-dependent periodic heat source distribution around the preform circumference (see Figure 3).

In order to model the translation of the preform, multiple ray tracing calculations are performed with respect to different positions of the preform with regard to the oven's module. These calculated radiative heat sources are stored, then the translation of the preform inside the oven is performed using a linear interpolation.
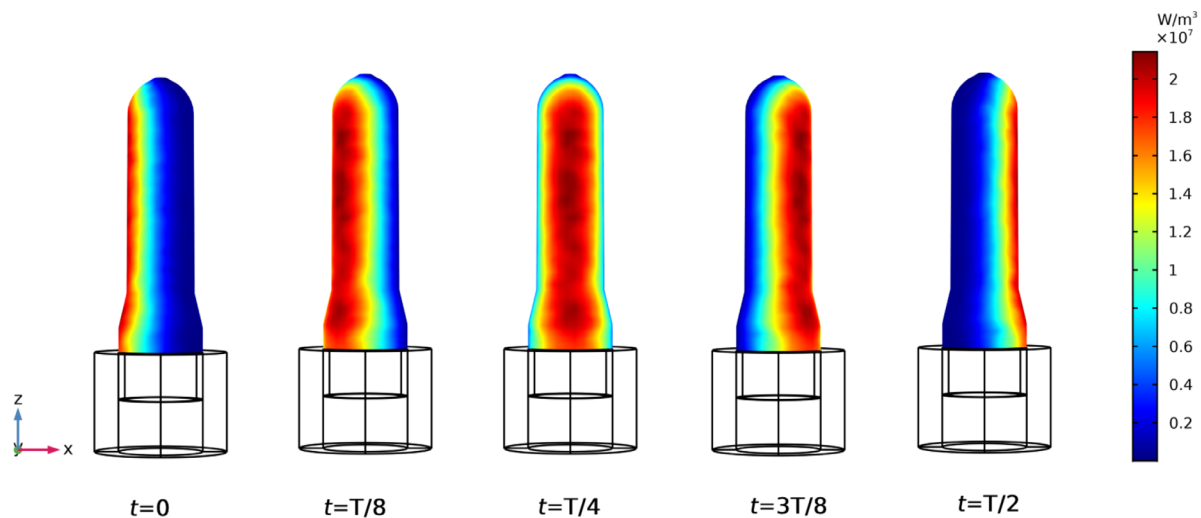
Figure 3. Time-dependent periodic radiative source around the preform circumference. T stands for the preform rotation cycle.

Heating simulation. Results from the previous computations are transferred as boundary conditions to the heat transfer simulation, which is performed in COMSOL Multiphysics® commercial software. In this step, IR heating of rPET preforms is simulated considering the absorption of the IR radiation, the heat conduction within the materials, the surface-to-ambient radiative emission and the air-cooling convection on the material surface. To do so, the continuity equation, the Navier-Stokes equations and the energy balance equation are solved within a finite control volume around the preform (see Figure 4). The final result of the heating simulation is a three-dimensional temperature distribution of the preform (and also the velocity and pressure fields of the air flow, if required). In the following, we focus on the modelling of the air-cooling convection in the context of an industrial ISBM ovens, where the preforms are transferred across different heating modules. In this situation, convective condition varies consecutively inside and outside the heating module. Inside the modules, the presence of fan system involves forced convective condition, whereas outside the modules, natural convection occurs. Figure 4 shows the differences in boundary conditions applied for flow simulation between the natural and forced convection. In an industrial context, based on position of the preform with respect to the heating modules, the boundary condition must be changed accordingly.

In the case of natural convection, an open boundary is applied for the flow on the top and lateral walls of the control volume which allows free incoming and outgoing flows. While on the preform and support surfaces and on the bottom wall we apply a "no slip" condition.

In the case of forced convection, a normal inflow velocity of air v_{inlet}=2 [m/s] is imposed at the inlet. At the outlet (i.e., the opposite wall to the inlet), we impose a static pressure equal to zero (relative to P_{atm}) $P_{outlet} = 0$. On the top and lateral walls of the control volume, a slip wall condition is applied, which has no viscous effect that hinders the flow at the wall.

It is appropriate to build a hybrid mesh for simulation, structured mesh at the boundary layers near to the walls and unstructured mesh in other volumes. For this application, over 200 000 mesh elements are generated.

Before applying for hybrid convective conditions in an industrial ISBM ovens, case studies are performed for each single condition. Simulations are done for an IR heating process of 60s (the preform is heated during 50s and then cooled down during 10s). The CPU time (AMD Ryzen Threadripper 3960X 24-Core Processor, 64.0 Gb of RAM) for one simulation is about 10 hours. Figure 4 shows the results of the flow velocity at the end of 60s. In both cases, the simulated results provide detail descriptions of the air flow inside the oven. In the case of natural convection, the flow

is driven by the buoyancy force, yielding the vertical air currents along the preform walls. On the other hand, forced convection flow is driven by the imposed velocity, which results in a very different velocity fields in front and behind the preform, as well as along the preform longitudinal direction.
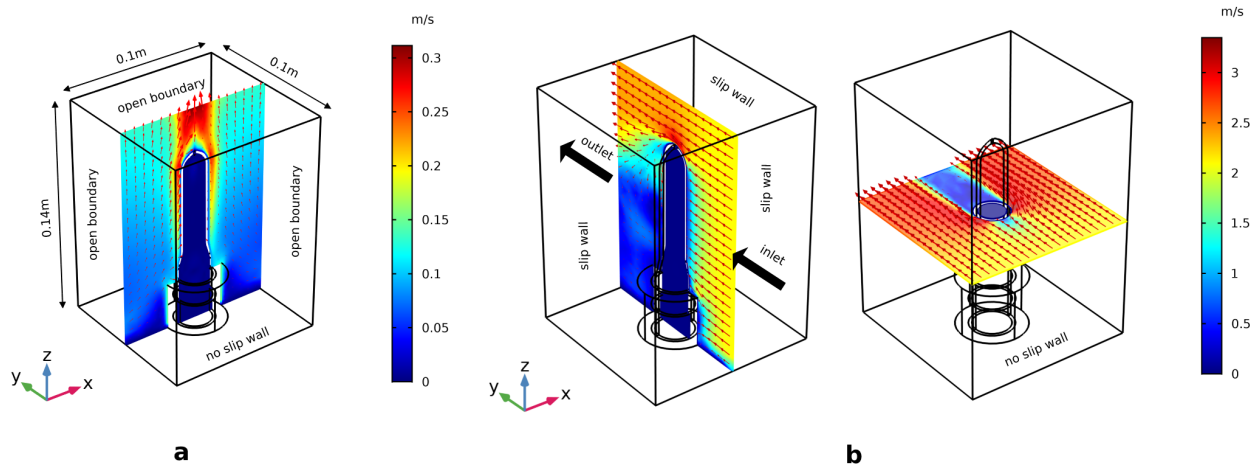
Figure 4. Flow boundary conditions and velocity field resulted from CFD approach (a) Natural convection (b) Forced convection with v_{inlet}=2 [m/s].

In order to evaluate the proposed approach, CFD simulations are compared with classical heat transfer coefficient correlation for vertical thin cylinder proposed in [10]. Figure 5a represents a comparison of the predicted distribution of the convection coefficient, h_c, along the height of the preform, and Figure 5b compares the temperature profiles along the preform height of both approaches. It is clearly seen that, for the case of natural convection, the discrepancy of h_c between the two approaches is not noticeable, thus both results produce almost the same profile of temperature along the preform height. Nevertheless, for the case of forced convection where the air flow is more complex, the discrepancy of h_c between the two approaches becomes obvious along the preform height, which produces a considerable difference in the temperature profile between the two approaches.
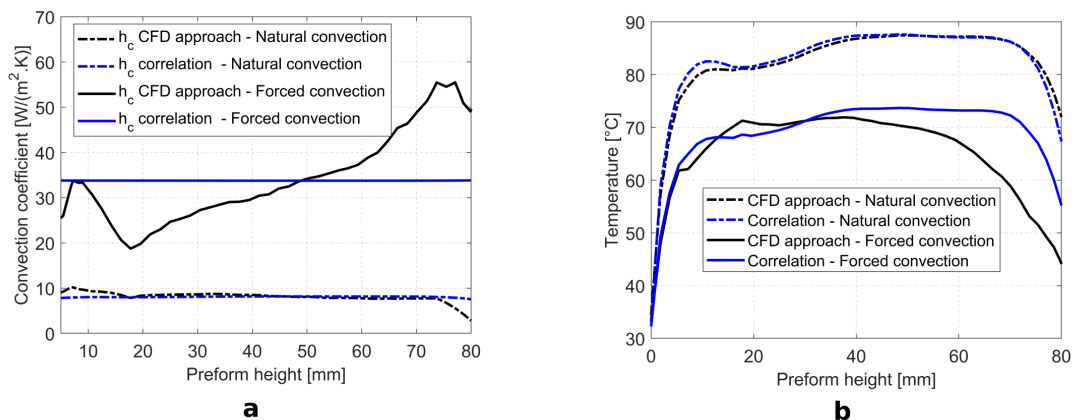

Figure 5. (a) Heat transfer coefficient along the preform height (b) Simulated external temperature profile along the preform height.

Results and Discussion

Experimental validation. As a first step, the numerical model is validated using a research set-up designed to reproduce an industrial machine. The oven has only one heating module, which is constituted of six IR halogen lamps and which radiative characteristics are listed previously in Table 1. A white ceramic Saint-Gobain SilPower reflector is located behind the lamps, which behaves as a

Lambertian surface. The preform is originally placed outside the heating module, at 0.45m with respect to the module center. Then, it is transferred by translation into the heating module and stays at the module center throughout the heating process. During the heating stage, the preform rotates axially with a rotational speed of 1.15 rounds per second. The translation velocity is equal to 0.18 [m/s]. The heating module is open, which means that the preform can absorb IR energy emitted at grazing angles, outside the module, during its translation. As soon as the preform arrives the module center, it is heated during $50s$ and then cooled down by natural convection during $10s$. There is no ventilation fan system in the oven. Figure 6 shows a good agreement between simulations and measurements for a typical case of virgin PET. It can be deduced that the numerical model successfully predicts both the heat-up rate during the IR heating stage and the temperature profile along the preform height.

Preform temperature profiles were recorded by a FLIR A655sc IR camera, operating in the spectral range $[7.5 - 14]\ \mu m$. In this range, all the PET grades used behavior as an opaque body, allowing for surface temperature measurements. Also inferred by spectrometry, an average emissivity of all PET grades $\bar{\varepsilon}$=0.94 is used for all measurements. The measurement uncertainty associated with the temperature range of polymer [20-120]°C, provided by the IR camera supplier, is equal to ± 2°C. This value is used to build the error bars.
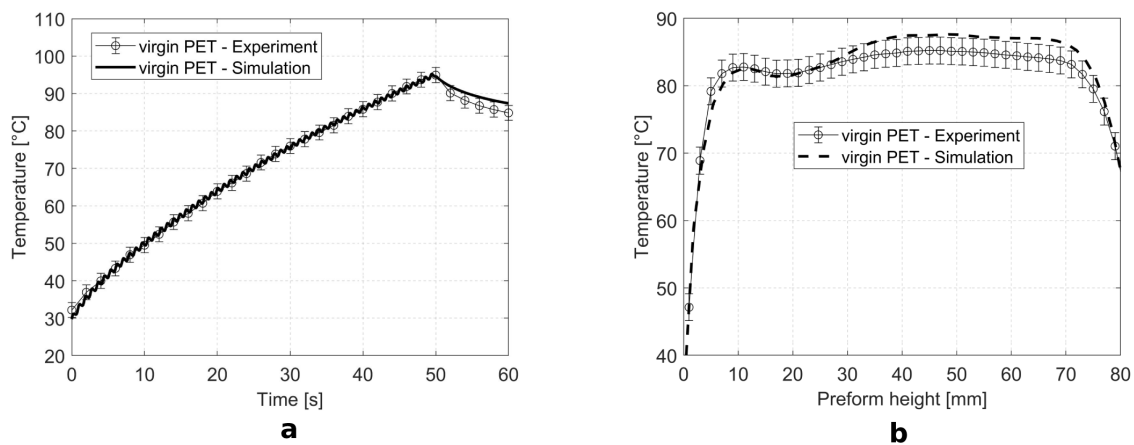
Figure 6. Confrontation between simulated and measured results (a) Evolution of the temperature at the midpoint (b) Temperature profile along the preform height.
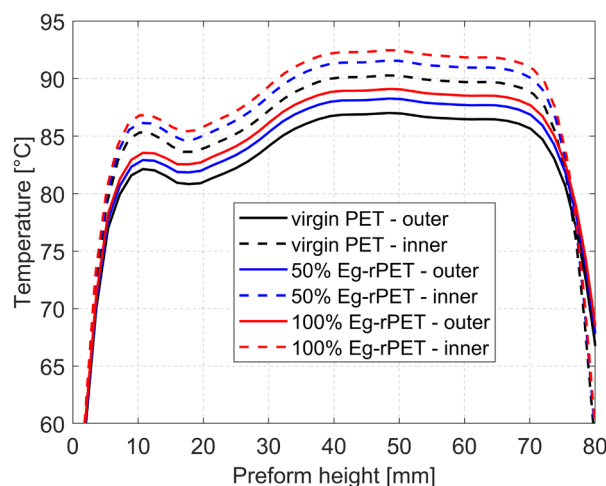
Figure 7. Simulated temperature profile along the preform height of different material grades.

Influence of recycled content. In a second step, we investigate the influence of the recycled content in material grades on the energy efficiency of the IR heating process. To do so, simulations are performed for 3 different material grades: virgin PET, 50% Eg-rPET and 100% Eg-rPET. In Figure 7, the inner and outer longitudinal temperature profiles of preforms made from 3 material grades are compared. The difference in temperature can be attributed to the difference in the optical properties of the examined materials in the process relevant spectral range. The 100% Eg-rPET has the highest absorption coefficient, and thus absorbs the most IR energy resulting in highest temperature. While the virgin PET has the lowest absorption coefficient, then absorbs the least IR energy resulting in lowest temperature. It is clearly seen that, at the end of process, temperatures on the inner surface are higher than on the outer surface. This is because during the 10s of the preform cooling time, heat losses due to natural convection and surface-to-ambient radiative are crucial on the outer surface, whereas the inner surface is still heated by heat conduction. Actually, this gradient temperature is crucial for the next stretch blow molding process, where the blowing rate at the inner surface is much higher compared to the outer surface due to the thickness of the preforms.

Conclusion

A numerical software has been developed in order to simulate rPET preforms infrared heating in ISBM process. The implementation aims to mimic the dynamic of the preform inside an industrial ISBM ovens, including the rotation and the translation across multiple heating modules. Both the natural and forced convective conditions that occur inside the industrial oven are considered using a CFD approach. In comparison with a classical heat transfer coefficient, the proposed CFD approach predicts more in details the local effects of air flow surrounding the preform. Notably, in the case of forced convection where the classical heat transfer coefficient correlation for vertical thin cylinder is not enough to predict the complexity of air flow around the preform. There is a good agreement between the numerical and experimental results producing in our laboratory oven.

In a second step, the influence of recycled content on the energy efficiency of the IR heating process is investigated. The results point out that the numerical software is sensitive enough to successfully predict change in temperature due to the recycling rate, thus, this could be a helpful tool to optimize the energy cost for the ISBM industry when dealing with the use of rPET as input materials.

In further works, we intend to validate the forced convective heat transfer coefficient calculated using the proposed CFD approach by experimental measurement, then, further extend the applications of the numerical software for real industrial ISBM oven.

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