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Compensation of in-line metrology of polymer parts based on 3D thermomechanical analyses

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Abstract

The growing demands for quality and flexibility and at the same time production speed challenges conventional metrology. The future tendency is that metrology is an integrated part of the production line and thus is placed in a production environment. This is a challenge since dimensional metrology in a production environment might lead to higher uncertainties due to dynamic variations both in the conditions of the environment and in the conditions of the produced parts. However, many of these effects can be treated as systematic errors if the physical phenomena leading to the deviations can be described. Today, it is very common to compensate for the variations in temperature in a classical 1D manner. However, when temperature gradients and very complex part geometries exist the deformation pattern might not at all follow a linear path. Instead, more advanced three-dimensional thermomechanical numerical models should be applied taking the inherent build-up of residual stresses and warpage into account.

Keywords: Accurate dimensional measurements; numerical modelling; production environment

1. Introduction

In modern production facilities typical parts in the range of 1 – 250 mm are produced with tolerances in the micrometer range \([1, 2]\) and for future manufacturing processes such as micro injection moulding \([3]\) the tolerances could be at nanometer range \([4]\). To deal with such tolerances conventional dimensional metrology uses expensive equipment, costly temperature controlled facilities, long acclimatization times and time consumption during the measurement procedures in order to satisfy todays ISO standard referring to 20\(\text{o}^\circ\)C and 0 N (zero forces acting on the part) \([5]\). However, the growing demands for quality and flexibility and at the same time production speed challenge the conventional metrology. Hence, the metrology in production engineering should be fast, accurate and robust and should ideally be integrated inline and thus be in the production environment \([6]\). Here, the most influencing condition is the temperature of which the ambient in a production environment might be several degrees away from the 20\(\text{o}^\circ\)C reference conditions.

Nomenclature

\(\varphi_p\) specific heat  \(E\) Young’s modulus  \(h\) convective heat transfer coefficient (HTC)  \(k\) thermal conductivity  \(p_i\) external force tensor  \(q\) heat flux  \(T_{\text{ref}}\) reference temperature  \(T_\infty\) ambient temperature  \(T_s\) surface temperature  \(u_i\) displacement tensor  \(a\) coefficient of thermal expansion (CTE)  \(\alpha_T\) thermal diffusivity  \(\delta\) dimensionless change in length  \(\varepsilon_{ij}\) strain tensor  \(\sigma_{ij}\) stress tensor  \(C_{ijkl}\) elastic fourth order tensor  \(\nu\) Poisson’s ratio
Furthermore, the parts itself might be at an elevated temperature due to up-stream manufacturing processes in the production line. The differences in temperature have an influence both on the measuring equipment and on the measured through the material’s coefficient of thermal expansion (CTE). It is very common to compensate for the temperature in the dimensional measurements by applying the equation

\[ \Delta L = L \cdot CTE \cdot \Delta T \]  

(1)

where \( L \) is the measured length and \( \Delta T \) is the temperature difference between the part and the reference. Under normal conditions it is reasonable to use this approach to decrease the uncertainty coming from temperatures. However, the assumptions behind this equation should be considered carefully in order not to make the measurements more uncertain than if not taking this compensation into account. One assumption is that the temperature distribution in the part is uniform. This assumption might hold for measurements after long acclimatization times but at in-line measurements significant temperature gradients might exist in the part due to temperature differences between e.g. a hot manufactured part and a cold fixture. Under those circumstances eq. (1) simply does not hold and would result in considerable errors if being applied. Instead, more advanced three-dimensional thermomechanical numerical models should be used for predicting the deformation of the measurand due to the thermal effects taking the inherent build-up of residual stresses and warpage into account [7]. In the present work 3D thermomechanical analyses are performed in order to construct a more generic expression, which then together with information from a set of sensors (dimensional contact probe and thermocouples on the fixture and on the part) is used to compensate the length dimension measured in-line on classical acrylonitrile butadiene styrene (ABS) polymer bricks at the factory floor.

2. Methodology

2.1. Measuring setup

The fixture is constructed with components manufactured in Invar. It consists of four separate stations that allow for simultaneous measurements of four bricks, see Fig. 1. The stations are equipped with Marposs Red Crown 2 soft touch inductive probes and Omega K-type temperature probes for measuring the fixture and brick temperature. The acquisition system consists of a Marposs Easybox U4T for the inductive probes and an Easybox U4TP for the thermocouples. The OQIS Procella from QDAS is used for the data collection.

The placement of the thermocouples and the contact probe is schematically illustrated in Fig. 2.

Fig. 1. Fixture design consisting of four stations in total.

2.2. 3D thermomechanical model

The thermomechanical model has to solve for two different field quantities: the transient temperature field and the transient displacement field. The simulation is performed sequentially, such that the temperature field is solved in a separate model, and temperatures from this model are subsequently transferred to a mechanical model, where they are the driving force for the thermal strains leading to the overall displacement field. The thermal model serves two different purposes. First of all, it should be able to reconstruct the overall temperature field based on the measured temperature in the specific point of the part. Secondly, it should be able to predict the transient temperature evolution in the part based on the surrounding conditions (in this case only the surrounding temperatures). The basic field equation that has to be solved is the standard heat conduction equation by Fourier

\[ \rho c_p \dot{T} = (k T_{ij}) \]  

(2)

This is solved via the finite element method and results in the transient temperature field in discretized points (nodes) in the body of the part. The influence from the surroundings is in this case modelled via Newton’s law of cooling, which is applied as boundary condition on the surface

\[ q/A = h(T_{in} - T_s) \]  

(3)
The purpose of the mechanical model is on basis of the transient temperature distribution found in the thermal model, to predict the length of the brick at any temperature and time (and hence also in the reference conditions). The basic field equations that have to be solved are the three static equilibrium equations
\[ \sigma_{ij} + p_j = 0 \]  
(4)

Hooke’s law and linear decomposition of the strain tensor as well as small strain theory are applied together with the expression for the thermal strain

\[ \varepsilon^{\text{tot}}_{ij} = \varepsilon^{\text{el}}_{ij} + \varepsilon^{\text{th}}_{ij} \]

\[ \sigma_{ij} = C_{ijkl} \varepsilon^{\text{el}}_{jk} = C_{ijkl} \left( \varepsilon^{\text{tot}}_{ij} - \varepsilon^{\text{th}}_{ij} \right) \]

\[ C_{ijkl} = \frac{E}{1 + \nu} \left[ \frac{1}{2} \delta_{ij} \delta_{jl} + \delta_{ij} \delta_{jk} - \frac{\nu}{1 - 2\nu} \delta_{ij} \delta_{kl} \right] \]

\[ \varepsilon^{\text{el}}_{ij} = \frac{1}{2} \left( u_{i,j} + u_{j,i} \right) \]

\[ \varepsilon^{\text{th}}(T_i \rightarrow T_f) = \int_{T_i}^{T_f} \alpha dT \]

These equations should be solved together with a set of proper boundary conditions, making the equation system statically determined. The equations are solved via the finite element method, which returns a solution of the three displacements at every node in the discretized geometry of the part. The length between the two reference points of the brick can then directly be extracted from the simulation results.

2.3. Deriving the generic expression for real time compensation

The derivation of the expression from the 3D thermomechanical analyses is based on knowledge from classical heat conduction theory. Since the cooling pattern of the brick mounted in the fixture to a large extend is one dimensional with the dominating thermal gradient in the direction of the fixture i.e. in the “height direction of the brick” (see Fig. 1), the basic principles behind classical one dimensional solutions are considered. A classical 1D solution of the heat conduction equation comes from considering a semi-infinite solid with fixed surface temperature, which means that eq. (2) subjected to the boundary conditions \( T(0,t) = T_i \), \( T(\infty, t) = T_f \) and the initial condition \( T(x,0) = T_i \) may be solved by Laplace transformation to yield the solution

\[ \theta = \frac{T(x,t) - T_i}{T_f - T_i} = \text{erf} \left( \frac{x}{\sqrt{4\alpha T_i}} \right) \]

(6)

where \( \text{erf}(x) \) is the Gaussian error function. Expressing the temperature for the present case in a similar manner on dimensionless form makes it versatile since it holds a wide range of solutions with respect to the choice of initial and surrounding temperatures. A similar dependence should be extracted from the 3D thermomechanical model. Eight simulations with different starting temperatures, fixture temperatures and heat transfer coefficients resembling the thermal contact to the fixture were therefore performed in order to derive the dimensionless form analogous to the analytical solution presented in eq. (6), see Table 1. In Fig. 2, the meshed geometry used for the thermomechanical analyses in ABAQUS, is shown. For the thermal calculation the boundary conditions were prescribed via a HTC value for the surrounding air of 10 W/m²K and the values given in Table 2 for the HTC to the fixture in the bottom of the brick. The basic thermal properties of the ABS materials were chosen to be \( k = 0.2 \) W/m K, \( \rho = 1000 \) kg/m³ and \( c_p = 1000 \) J/kg K. The ambient temperature was prescribed to be the fixture temperature in Table 2.

<table>
<thead>
<tr>
<th>Simulation number</th>
<th>Fixture temperature [°C]</th>
<th>Initial temperature [°C]</th>
<th>HTC fixture [W/m²K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>15</td>
<td>30</td>
<td>500</td>
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<tr>
<td>2</td>
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<td>30</td>
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<td>25</td>
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<td>1000</td>
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</tbody>
</table>

The temperature from the simulations were reported in 11 specific nodes from bottom to top along the sidewall of the brick (x-direction in Fig. 3), see also Fig. 2. Those curves were then converted into dimensionless form by using the knowledge from the 1-D solution eq. (6), see Fig. 4.
In a similar manner, the resulting displacement from the mechanical analysis in terms of the change in dimension of the brick between two reference points (see Fig. 2) should be non-dimensionalized, which after some consideration was found to be accomplished via the following equation

$$\delta = \frac{\Delta L(z) \cdot \text{CTE} \cdot L \cdot (T_i - T_{ref})}{\text{CTE} \cdot L \cdot (T_f - T_i)}$$  \hspace{1cm} (7)

The expression of this dimensionless change in length resembles very much the philosophy behind the dimensionless temperature. In the very beginning of the measurement, the uniform temperature distribution results in a difference in length corresponding to the difference between the reference and the initial temperature. In the same manner, when the temperature of the brick is equal to the fixture temperature, the difference lies between the fixture and the reference temperature. The two dimensionless quantities ($\hat{\delta}$ and $\hat{\theta}$) can then be combined such that the dimensionless change in length is plotted as a function of the dimensionless temperature, see Fig. 5.

Each curve on this figure then corresponds to a correlation between temperature and displacement for a temperature extracted at a specific point on the sidewall of the brick. The somewhat resemblance with a straight line for $x = 1$ mm would to some extend correspond to eq. (1) since the transient temperature and the transient displacement at the same $x$ – coordinate is close to behaving like in 1D. One of the curves corresponds to the actual measurement at $x = 5$ mm (see Fig. 2), which is where the transient temperature of the brick is measured in the fixture. This curve gives the correlation between temperature and change in length and should be used for compensating the measured length. This is done by an exponential fit yielding the expression

$$\delta_{fit} = a \exp(b \theta) + c \exp(d \theta)$$ \hspace{1cm} (8)

with the coefficients $[a = 1.011, b = -0.012, c = -0.558, d = -8.860]$. This expression will henceforth be termed the “adjusted 1D formula”.

3. Application

At the production line the polymer bricks are ejected from the injection moulding machine and via a conveyor belt they end up in a container, see Fig. 6. A thermographic image was taken of the bricks in the container in order to quantify the temperature differences of the collected bricks, see Fig. 7.
As observed from the thermographic image the bricks have a wide range of temperatures, depending on the time from ejection. This further highlights the importance of having a versatile compensation calculation, which can take these differences in temperature into account when predicting the dimensions at reference conditions. For this particular application, the bricks are picked up from the container and placed in the fixture (Fig. 1) where the length dimension, the temperature of the brick and the temperature of the fixture is measured dynamically over ten minutes. The bricks are measured approximately five to ten minutes after production. In Fig. 8, the raw data in terms of transient part temperatures and dimensions, are shown for the 24 bricks measured in total. Here an initial temperature of 23 – 33°C and length changes ranging from 3 to 16 μm is observed, which then should be used as input for the compensation together with the measured ambient temperature, in order to get the value of the length at reference state (20°C).

4. Results

One of the main results in this study is the comparison of predicted transient deformation obtained from the presented methods, i.e. 1D classical compensation, 3D thermomechanical analysis and the developed adjusted 1D formula, see Fig. 9. The results presented in this figure is the most extreme case of the measurements with an initial temperature of 33°C for the polymer part. First of all, it is observed that the prediction with the classical 1D equation would just follow the transient of the measured temperature, as also was expected. The 3D thermomechanical model is however able to simulate the differences in time constants between the transient temperature and length variation. The reason for this behavior is warpage of the brick mounted in the fixture due to the non-uniform cooling as a result of the one-sided contact with the Invar fixture in combination with the length measurement being performed only 1 mm away from this surface, see Fig. 2. The adjusted 1D formula shows to give results very similar to the simulation performed in ABAQUS.

![Fig. 8. The in-line measured transient temperature and length of 24 ABS bricks the in total. a) the measured temperature evolution of the brick, b) the measured change in length of the brick during the 10 minutes.](image)

![Fig. 9. Comparison of the measured transient behavior with results from the 3D thermomechanical analysis performed in ABAQUS, the developed adjusted 1D formula (eq. (8)) and the classical 1D eq. (1).](image)

For all the measured bricks the residual i.e. the difference between the measured and predicted transient behavior is calculated based on the adjusted 1D formula and the classical 1D compensation, respectively, see Fig. 10.

![Fig. 10. The residual from all the 24 measurements comparing the measured and calculated transient behavior from the 1D classical equation and from the adjusted 1D formula developed in this work, respectively.](image)
Here, the benefits of the developed approach is clearly illustrated, with a maximum deviation from the adjusted 1D formula of around 3 µm and a maximum deviation from the 1D classical compensation of around 13 µm. The error is largest in the beginning of the measurements which could be explained by the large thermal gradients present initially within the part and as the temperature field becomes more and more uniform, the two solutions approach each other. This naturally leads to the question on the relevance of the proposed method, because the 1D classical method serves a good job if the measurement are just performed 300 s later than what was done in this particular case. However, the chosen case is just a demonstration of the method in general, and for more complex or larger parts, the acclimatization time (until a uniform temperature in the part is reached) might take so long time that it will not be able to reach that state at the production line.

5. Conclusion

A new method for thermal compensation in dimensional metrology of polymer parts in a production environment based on 3D thermomechanical analyses has been developed. Knowledge from classical heat transfer theory was used to derive a more generic expression for the compensation from the transient 3D temperature and displacement fields, based on dimensionless values. The developed adjusted 1D formula was then used for length compensation on 24 samples measured in-line. The results revealed a significant improvement in capturing the transient behavior of the polymer brick with a reduced error from 13 µm to 3 µm, applying the developed formula instead of using the more classical 1D thermal compensation.

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