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2011-01-0248 Modeling of Fuel Permeation in Multilayer Automotive Plastic Fuel Tanks

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ABSTRACT

A numerical simulation model for predicting the fuel hydrocarbon permeation as well as the barrier layer thickness optimization for multilayer plastic fuel tanks is presented. The diffusion model is based on Fick's laws of diffusion for a steady/unsteady state permeation regime through a multilayer polymeric wall under isothermal condition. A continuum approach based on an homogenization technique is used to model solvent diffusion through an n layer film. The hydrocarbon flux determination through the multilayer film is solved using homogenization techniques that ensure continuity of partial pressure at the polymer-polymer inter-diffusion interface. Since the pinch-off zone is known to be the major source of emission per unit area, a method has been developed to automatically detect it at the end of the extrusion blow molding process and the diffusion model is adapted to adequately evaluate the hydrocarbon permeation through this specific area. Finally a gradient-based algorithm has been implemented to get the optimal barrier layer thickness which satisfies the total hydrocarbon fuel emission constraint. The numerical validation in terms of hydrocarbon flux calculation under steady and non steady state is performed on academic case studies by comparing numerical predictions to the analytical ones. The illustration of the methodology and the gain in terms of weight and fuel permeation, during optimization iterations, will be presented for a plastic fuel tank (PFT) case study.

INTRODUCTION

The uses of PFT continue to grow in the automotive industry. One of the few drawbacks of PFTs with regard to steel or aluminum fuel tanks is that a fuel fraction may permeate through a polymer material and cause hydrocarbon emissions. For environmental reasons the emissions have to be kept low to avoid smog and green house effects. Because of this, the government has regulated acceptable levels of evaporative fuel emissions for automotive PFT through the sealed housing evaporative determination (SHED) test. One of the methods used by the automotive industry to meet the SHED is by adding thin layers of a low permeability material such as Ethylene-vinyl alcohol (EVOH). These co-extruded multilayer blow molded fuel tanks are now commonly used. In general, the inner and outer layers of PFTs are made of virgin high-density polyethylene (HDPE), whereas the core of the sheet is made of HDPE regrind. To ensure good hydrocarbon barrier properties, the EVOH layer must be positioned in the core of the structure and cross-linked to the inner HDPE and regrind layer with adhesive tie layers of linear low-density polyethylene (LLDPE), to ensure the required adhesion between EVOH and HDPE [1-2]. With this material layers configuration, the low permeability criterion is achieved over most of the fuel tank surface. However it is still common practice in the thermoplastic forming industry to rely on trial and error to find the right configuration/thickness of the barrier layer required to meet the SHED test. A tool that offers more efficient alternatives based on reliable predictive/virtual analysis of the fuel diffusion throughout multilayer blow molded parts could significantly shorten the design/development cycle by allowing the product prototypes to be analyzed and tested virtually. A first finite element based model that could help a designer to better understand barrier layer properties, was integrated in our BlowView¹ software [3]. The mathematical diffusion model adopted is based on Fick's steady state law to predict hydrocarbon diffusion through a multilayer polymeric wall. Promising results in term of fuel flux and fuel permeation were obtained with this first version of BlowView.

The goal of this work is to generalize the previous permeability model to expand our predictive permeation capabilities for automotive PFTs to both steady and unsteady state regimes. The problem zone for automotive PFTs is the pinch-off zone where EVOH layers (or

¹BlowView is an engineering simulation software developed at IMI-NRC that can handle extrusion blow molding, injection blow molding, stretch blow molding and thermoforming [4-6].

other barrier materials) are highly compressed and can ultimately vanish. Therefore, adequate prediction of fuel permeation in this specific area is of utmost importance. The pinch off zone is automatically detected at the end of the extrusion blow molding process and a modified diffusion model is applied that evaluates adequately the fuel permeation through this specific area under steady/unsteady states regime. Finally the fuel emissions test for PFT is analyzed for both steady and unsteady state via simulation and a sensitivity analysis is performed to show the impact of barrier layer percentage on fuel emissions.

THE PERMEATION MECHANISM

The permeation mechanism occurs in three main phases: The first phase is the absorption of the permeant (fuel) into the polymer that occurs at the upstream side of the polymer wall. The second phase is the diffusion of the permeant from the surface to the core of the polymer due to the concentration gradient. Finally the permeant desorbs on the downstream side of the membranes and is removed from the surface by evaporation to the surrounding air.

MATHEMATICAL MODEL

Given the inherently low diffusivity of plastics and the special geometrical configuration of a blow formed part which is relatively thin compared to their surface area, unilateral diffusion is usually assumed to be one dimensional through the thickness. The one-dimensional flux of the permeant transported through the polymer per unit area (A) and unit time (t) is given by Fick's first law [7-8]:

$$J = -D \frac{\partial C}{\partial x} \quad (1.a)$$

The diffusion equation for a constant diffusivity D is given by the following Fick's second law expression:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (1.b)$$

where C is the liquid concentration in the polymer matrix, t is the time, and x the distance through the thickness. The initial and boundary conditions are:

$$t = 0 \quad 0 < x < h \quad C = C_0 \quad (2)$$

$$t > 0 \quad x = 0 \quad C = C_s \quad (3)$$

$$t > 0 \quad x = h \quad C = C_0 \quad (4)$$

The measurement of surface concentrations (C) is not always a simple task. From Henry's law (5) where S is Henry's solubility coefficient (the solubility coefficient of the permeant in the polymer) and p is the vapor pressure of the fuel.

$$C = S \cdot p \quad (5)$$

If the solubility S is assumed to be constant the flux (J) can be expressed in terms of the variation of the vapor pressure, p.

$$J = -P \frac{\partial p}{\partial x} \quad (6)$$

where P is the permeability defined as the product of the solubility and diffusivity coefficients of the material which obeys the Fick's law:

$$P = S \cdot D \quad (7)$$

The set of partial differential equations (1)-(4) can be transformed as follows, [7-11]:

$$S \frac{\partial p}{\partial t} = P \frac{\partial^2 p}{\partial x^2} \quad (8)$$

$$t = 0 \quad 0 < x < h \quad p = p_0 \quad (9)$$

$$t > 0 \quad x = 0 \quad p = p_s \quad (10)$$

$$t > 0 \quad x = h \quad p = p_0 \quad (11)$$

where p_s is the saturated vapor pressure of the fuel.

Permeation through a multilayer polymeric wall

The inter-diffusion variables and hydrocarbon flux determination through the multilayer polymeric materials is solved using homogenization techniques and by assuming continuity of the partial pressure at the polymer/polymer inter-diffusion interface. The penetrate diffusivity and solubility for each layer are assumed to be constant.

Steady-state permeation

Steady state permeation produces a linear piecewise vapor pressure profile in each layer (green dashed line) as illustrated in Figure 1.

Figure 1: Schematic of n layer film for steady-state continuous saturated pressure profiles.

The permeant profile in the polymer layers is obtained by solving the following boundary value problem [12].

$$D_i \cdot S_i \cdot \frac{\partial^2 p_i}{\partial x^2} = 0 \quad \text{where } i = 1, 2, \dots, N \quad (12)$$

with boundary conditions:

$$\begin{cases} p_j(x_{j+1}) = p_{j+1}(x_{j+1}) \\ S_j D_j \frac{\partial p_j}{\partial x} \bigg|_{x_{j+1}} = S_{j+1} D_{j+1} \frac{\partial p_{j+1}}{\partial x} \bigg|_{x_{j+1}} \end{cases} \quad \text{at } x = x_{j+1} \text{ where } j = 1, 2, \dots, N-1 \quad (13)$$

and

$$\begin{aligned} p_1(x_1) &= p_s & \text{at } x = x_1 = 0 & \quad (\text{upstream side}) \\ p_{N+1}(x_{N+1}) &= p_0 & \text{at } x = x_{N+1} = h & \quad (\text{downstream side}) \end{aligned} \quad (14)$$

The interlayer vapor pressure value p_j can be obtained by combining equation (12)-(15), and will produce in the case of a constant diffusivity D_j and solubility S_j the following equation:

$$p_{j+1} = (p_{N+1} - p_1) \cdot \frac{R_{EQ}^j}{R_{EQ}} + p_1 \quad (16)$$

where

$$R_{EQ}^j = \sum_{i=1}^j \left(\frac{h_i}{S_i D_i} \right) \quad \text{for } j = 1, 2, 3, \dots, N \quad (17)$$

and

$$R_{EQ} = \sum_{i=1}^N \left(\frac{h_i}{S_i D_i} \right) \quad (18)$$

where h is the total thickness of the multilayer membrane and h_j the specified thickness of layer i .

The discontinuous fuel concentration at the inter-diffusion interface is obtained from equation (16):

For the left hand side of the inter-diffusion interface j :

$$C_j^{Left} = S_j \cdot p_j \quad \text{for } j = 2, 3, \dots, N \quad (19)$$

For the right hand side of the inter-diffusion interface j :

$$C_j^{Right} = S_{j+1} \cdot p_j \quad \text{for } j = 2, 3, \dots, N \quad (20)$$

The average concentration at the inter-diffusion interface is obtained by averaging the previous left and right quantities:

$$C_j^{av} = \frac{C_j^{Right} + C_j^{Left}}{2} \quad \text{for } j = 2, 3, \dots, N \quad (21)$$

The concentration at the upstream and downstream side of the polymer membranes is given respectively by the following equations:

$$C_1 = S_1 \cdot p_1 \quad \text{and} \quad C_{N+1} = S_N \cdot p_{N+1} \quad (22)$$

Applying an homogenization technique, assuming continuity of the partial pressure at the inter-diffusion interface, integrating (12) across the total local thickness of the gas tank h , and interpolating between the two saturated vapor pressures, yields the following expression for the fuel permeation rate (FPR):

$$FPR = J = -\frac{P_{EQ}}{h} \cdot (p_{N+1} - p_1) \quad (23)$$

with

$$P_{EQ} = \frac{h}{R_{EQ}} = \frac{h}{\sum_{j=1}^N \frac{h_j}{D_j S_j}} \quad (24)$$

Unsteady-state permeation

Under unsteady-state permeation condition, the analytical expression of the FPR is adapted from [12]:

$$\begin{aligned} FPR = J(t, x) = & -\frac{P_{EQ} \cdot (p_{N+1} - p_1)}{h} + \\ & P_{EQ} \cdot \frac{n\pi}{h} \cdot \frac{2}{h} \sum_{n=1}^{\infty} \exp \left[-D_{EQ} \frac{n^2 \pi^2}{h^2} t \right] \times \cos \left[\frac{n\pi}{h} x \right] \times \int_0^L p_0 \sin \left[\frac{n\pi}{h} x \right] dx + \\ & P_{EQ} \cdot \frac{2}{h} \sum_{n=1}^{\infty} \exp \left[-D_{EQ} \frac{n^2 \pi^2}{h^2} t \right] \times \cos \left[\frac{n\pi}{h} x \right] \times \left(p_{N+1} \cos \left[\frac{n\pi}{h} x \right] - p_1 \right) \end{aligned} \quad (25)$$

with

$$D_{EQ} = \frac{h}{\sum_{j=1}^n \frac{h_j}{D_j}} \quad (26)$$

Note that as time t increases (steady state), the expression for the FPR (25) simplifies to (23).

From the FPR expression, the Fuel Mass Rate (FMR) that permeates through a wall of polymeric membrane area A at the downstream side in time t , is given by the following expressions:

$$FMR = \frac{dM(t, x=h)}{dt} = \int_A J(t, x) \cdot dA = A \cdot J(t, x=h) \quad (27)$$

FINITE ELEMENT FORMULATION

For a thin walled container such as a PFT, all of the previous inter-diffusion variables i.e. p_j , C_j as well as the expression for FPR and MFR are directly applied within each finite element mesh of the co-extruded fuel tank shell.

Therefore for each shell element e with area A_e we can define the quantities below:

$$p_{j+1}^e = (p_{n+1} - p_1) \cdot \frac{R_{EQ}^j}{R_{EQ}} + p_1 \quad (28)$$

where

$$R_{EQ}^j = \sum_{i=1}^j \left(\frac{h_i^e}{S_i D_i} \right) \quad \text{for } j = 1, 2, \dots, N \quad (29a)$$

$$R_{EQ} = \sum_{i=1}^N \left(\frac{h_i^e}{S_i D_i} \right) \quad \text{for } j = 1, 2, \dots, N \quad (29b)$$

and

$$C_j^{Left} = S_j \cdot p_j^e \quad \text{for } j = 2, \dots, N \quad (30a)$$

$$C_j^{Right} = S_{j+1} \cdot p_j \quad \text{for } j = 2, \dots, N \quad (30b)$$

$$C_j^{av} = \frac{C_j^{Right} + C_j^{Left}}{2} \quad \text{for } j = 2, \dots, N \quad (30c)$$

The elementary FPR is given by:

$$FPR^e = J^e(t, x) = \frac{P_{EQ} \cdot (p_{N+1} - p_1)}{h} +$$

$$P_{EQ}^e \cdot \frac{n\pi}{h} \cdot \frac{2}{h} \sum_{n=1}^{\infty} \exp \left[-D_{EQ}^e \left(\frac{n\pi}{h^e} \right)^2 t \right] \times \cos \left[\frac{n\pi}{h^e} x \right] \times \int_0^L p_0 \sin \left[\frac{n\pi}{h^e} x \right] dx +$$

$$P_{EQ} \cdot \frac{2}{h} \sum_{n=1}^{\infty} \exp \left[-D_{EQ}^e \left(\frac{n\pi}{h^e} \right)^2 t \right] \times \cos \left[\frac{n\pi}{h^e} x \right] \times \left(p_{N+1} \cos \left[\frac{n\pi}{h^e} x \right] - p_1 \right) \quad (31)$$

with

$$P_{EQ}^e = \frac{h^e}{\sum_{j=1}^n \frac{h_j^e}{D_j S_j}} \quad \text{and} \quad D_{EQ}^e = \frac{h^e}{\sum_{j=1}^n \frac{h_j^e}{D_j}} \quad (32)$$

h^e and h_j^e being respectively the total thickness and the thickness of layer j for the current finite element e .

The elementary FMR of finite element e with area A_e is given by the following:

$$FMR^e = \left. \frac{dM(t, x)}{dt} \right|_e = \int_{A^e} J^e(t, x) \cdot dA \quad (33)$$

The total FMR through the entire gas tank wall on its downstream side is given by summing the elementary contribution of each finite element.

$$FMR = \left. \frac{dM(t, x = h)}{dt} \right|^{Total} = \sum_{e=1}^{nElem} \int_{A^e} J^e(t, x = h) \cdot dA \quad (34)$$

The total thickness h^e and the layer thickness distributions h_i^e were obtained from BlowView. The software simulates the whole process, i.e. the multilayer co-extruded parison taking into account the non-isothermal sag and swell phenomenon, the parison stretching at the bottom using spreading pins, the mold clamping and the parison inflation.

Pinch-off zone treatment

According to the experimental observations in [13-14], the pinch-off zone of fuel tanks revealed zones where the EVOH barrier layer became too thin or even disappeared completely. Therefore, a special treatment of the permeation of these zones is required in order to adapt locally the elementary expression of FMR. We first need to identify all the mesh elements located near the pinch-off tip zone. An automatic procedure has been developed and implemented in BlowView for this purpose: For each pinch-off finite element e , the expressions of the FMR transported through the elementary area A_e is evaluated as in equation (30), but with the barrier layer property in the elementary expression of P_{EQ} and D_{EQ} (equation 32) removed as follows:

$$P_{EQ}^e = \frac{h^e}{\sum_{j=1}^n \frac{h_j^e}{D_j S_j}} \quad \text{and} \quad D_{EQ}^e = \frac{h^e}{\sum_{j=1}^n \frac{h_j^e}{D_j}} \quad \text{with } j \neq j_{EVOH} \quad (35)$$

BARRIER LAYER AND WEIGHT OPTIMIZATION PROCEDURE

In this section we describe the main components and the implementation of the BlowDesign optimization software developed at IMI which is integrated in BlowView [15]. The software manipulates design variables or processing parameters such as die gap opening profiles, die geometry and flowrate in order to minimize the parison weight subject to process constraints such as extrusion time and parison length. At each optimization iteration, BlowDesign manipulates the design variables to minimize the objective function, which is defined for PFTs as being the weight subjected to a minimum inflated parison thickness (T_{min}) or part thickness constraint (T_{min}). To achieve this objective, the following optimization scheme is used:

$$\text{Objective function:} \quad \min F(X) = \text{weight} = \frac{\sum_{i=1}^{nElem} \rho T_i}{nElem} \quad (36)$$

Constraints:

$$L_p = \text{constant} \quad (37a)$$

$$T_i > T_{min} \quad (37b)$$

$$X_{min} < X < X_{max} \quad (37c)$$

Manipulated function:

$$X = \{\Theta_i(t), \Delta Gap(\theta), Q, P_b\} \quad (37d)$$

where L_p , T_i , $\Delta Gap(\theta)$, Q , P_b and $\Theta_i(t)$ are the targeted parison length, the nodal parison thickness, the circumferential die gap, the flowrate, the pre-blow pressure and the programming profile respectively.

PERMEATION TEST VALIDATION

An important contribution of this work is to establish a procedure to provide a more rigorous comparison of analytical and finite-element based computational models. The driving principle is that numerical data should be validated relative to a real-world benchmark. For this purpose, a three-layer polymeric wall with a total thickness h and a lateral area A is exposed to a permeant saturated vapor pressure p_s on the upstream side and to a lower pressure p_0 on the other side is proposed Figure (2).

Figure 2: Multilayer square polymer membrane (Two HDPE layers (blue ones) separated by a EVOH layer (red one)).

Throughout this example, the permeability of HDPE is normalized as $P_{HDPE} = 1$. From [1-2] and [17], the permeability of EVOH is estimated to be at least 1000 to 10000 times less than that of HDPE. For a thickness $h = 0.1$ m, a lateral area $A = 1$ m², an upstream and downstream permeant vapor pressure of $p_s = 1$ and $p_0 = 0$ respectively is applied on each side of the laminate. Figure 3 illustrates the evolution of the MFR versus time on the downstream side ($Z=h$) of the multilayer polymer membrane. The FMR profiles are presented for different values of P_{EVOH} permeability of 10^{-3} , 2×10^{-3} and 5×10^{-4} respectively. The volume fraction of the EVOH barrier layer is set to 3%. The analytical results are based on equations (25-27) and the numerical predictions are obtained from equation (34) using a 36 triangular elements (6x6) mesh.

Figure 3: Time evolution of the fuel mass rate for the three-layer laminate incorporating a barrier layer with permeability coefficients $P_{EVOH} = 10^{-3}$, 2×10^{-3} and 5×10^{-4} . Portion of EVOH: $X = 3\%$.

As expected (Figure 3) a decrease in barrier layer permeability leads to a significant reduction of the FMR (permeation). On the other hand, a decrease in barrier layer permeability leads to an increase of the time required to reach the steady state FMR. These observations are valid for both analytical and numerical results. Figure 3 also shows that the numerical predictions correlate closely to the analytical results, showing a robust finite element implementation.

Figure 4 and 5 illustrate the evolutions of the FMR through the multilayer polymeric membrane based on the volume fraction of the barrier layer in the steady state. In Figure 4, for a volume fraction of the EVOH layer of $X\%$ the volume fraction of each HDPE layer is set to $50 - X/2\%$ on each side. The permeability of the EVOH layer is set to: $P_{EVOH} = 10^{-3}$, 5×10^{-4} and, 10^{-4} respectively.

In Figure 5, the volume fraction of the EVOH layer is fixed at $X = 3\%$, 6% and 9% respectively and the permeability of the EVOH layer varies from 10^{-4} to 1. The results are compared to the analytical solution when the steady state regime is reached.

Figure 4: Fuel mass rate through a three-layer laminate (PHDPE = 1) incorporating a barrier layer with permeability coefficients $P_{EVOH} = 10^{-3}$, 5×10^{-4} and, 10^{-4} .

Figure 5: Fuel mass rate through a three-layer laminate (PHDPE = 1) incorporating a barrier layer with percentages $X = 3\%$, 6% and, 9% and permeability coefficients P_{EVOH} varying from 10^{-4} to 1.

As shown in Figure 4, the increase in the barrier layer volume fraction leads to a significant reduction of the FMR (permeation). The FMR can be reduced by a factor of approximately 100 to 1000 by using 10% of EVOH depending on its permeability. Moreover, a slight (1-3 %) variation of the barrier layer thickness has a significant impact on the FMR. On the other hand, the effectiveness of an improved barrier resistance decreases as the barrier thickness increases beyond 5 %. From Figure 5, we notice that for low permeability values ($P_{EVOH} < 10^{-3}$) the FMR is less dependent on the percentage of the barrier layer, in contrast to what can be observed in the higher range of permeability values ($P_{EVOH} > 10^{-2}$ to 10^{-1}). These observations apply to both analytical and numerical results.

Figure 6 illustrates the distribution of the vapor pressure through the multilayer thickness in the steady state. The vapor pressure profiles are reported for different values of EVOH permeability ($P_{EVOH} = 1$, 10^{-1} , 10^{-2} and 10^{-4} respectively) with a volume fraction of the EVOH barrier layer set to 3%. As can be seen, the lower the permeability of EVOH, the higher the upstream side value of the vapor pressure of the EVOH barrier layer is. However the exact opposite is observed on the downstream side of the barrier layer. Also the lower the permeability coefficient, the higher the vapor pressure gradient in the EVOH layer is. These observations are valid for both analytical and numerical results. It is important to notice here, that the vapor profile for $P_{EVOH} = 1$ corresponds to the case where there is no barrier layer in our multilayer laminate, which describes the pinch-off area. In these Figures numerical predictions are very close to analytical results, showing a robust finite element implementation.

Figure 6: Vapor pressure distribution through the thickness.

PLASTIC FUEL TANK ANALYSIS

To illustrate the permeation prediction in terms of mass fuel rate time evolution and fuel vapor pressure/concentration distribution, a typical plastic fuel tank layer percentage was used [3]. The initial design of the PFT is composed of 6 layers of polymeric materials as illustrated in Table I.

Table 1. Percentage, diffusion and solubility coefficients of each polymeric layer used in PFT from Upstream side to Downstream side [3].

PFT Layers of Initial design	Layer Percentage [%]	Diffusion Coefficient [m ² /s]	Solubility Coefficient [g/g]	
Outer HDPE	24.7	5.5e ⁻¹²	6.8e ⁻²	<div>Upstream Side</div>
Outer LLDPE adhesive	2.5	8.2e ⁻¹²	1.49e ⁻¹	
EVOH Barrier	0.3	5.0e ⁻¹³	5.0e ⁻⁴	
Inner LLDPE adhesive	2.5	8.2e ⁻¹²	1.49e ⁻¹	
Inner HDPE	50.0	5.5e ⁻¹²	6.8e ⁻²	
Outer HDPE	20.0	5.5e ⁻¹²	6.8e ⁻²	Downstream Side

Figure 7 shows typical finite element meshes used to model the parison extrusion, inflation and finally the deflashed part. It is important to notice here, that the permeability analysis is done on the deflashed part where the pinch off zone elements have been tagged in order to apply the adapted permeation analysis in this zone.

Figure 7: Typical finite element meshes used for the simulation of the extrusion blow molding [3].

Figure 8 illustrates the initial thickness distribution of the PFT. The hydrocarbon emission fluxes per unit area (FPR [mg/day/m²]) for different permeation times are depicted on Figure 9. Knowing the total surface area of the tank shell and the pinch-off zone, the daily MFR [mg/day] can be evaluated after different permeation times. One can notice that the initial design (0.3 % of EVOH) does not satisfy the daily permeation constraint which is usually set to 10 mg/day. Indeed, the daily MFR is already greater than the permeation constraint after 7 days of permeation. The daily MFR reaches a plateau value (steady state daily MFR) only after approximately 100 days. From Figure 8, it can also be observed that where the PFT thickness is small, the permeation is high and vice-versa, which is consistent in physical terms.

Figure 8. Thickness distributions and FPR at the Steady State for the initial design.

Figure 9. FPR distributions for different times for the initial design (0.3 % EVOH).

Since the initial design does not satisfy the daily permeation constraint the optimization procedure is performed, in order to minimize the weight and to meet the daily fuel permeation rate. For each optimization iteration, BlowDesign adjusts the design variables to minimize the objective function (36), which is defined as the PFT weight subjected to a minimum inflated parison thickness constraint (T_{min}), which in the plastic fuel tank industry is around 3.0 mm. Thereafter, for a specified thickness distribution, a gradient-based algorithm is used to update the percentage thickness of the barrier layer to converge towards the steady-state daily permeation constraint (10 mg/day).

The mandrel die gap opening vs. extrusion programming profile for different optimization iterations are presented in Figure 10. Figure 11 and 12 presents respectively the thickness distribution and the FPR at the steady state (~173 days) for the initial design, iteration 10 and iteration 20 (optimized design).

Figure 10: Die Gap opening vs. Programming Profile for Optimization iteration: 4, 10 and 20.

Figure 11: Thickness distribution for the Initial design, iteration 10 and the optimized design (iteration 20)

Figure 12: Steady state FPR for the Initial design, iteration 10 and the optimized design (iteration 20).

The part weight has been reduced after 20 optimization iterations from 22.9 kg to 18.18 kg and satisfies the minimum thickness constraint of 3 mm (Figure 11). The thickness of the PFT for the optimal design is more uniform with an average value around 3-4 mm except at the top of the PFT. We can notice that the less the weight the less and more uniform the thickness becomes. However, as the thickness decreases the percentage of EVOH increases in order to satisfy the daily permeation constraint. In Figure 12, the gradient-based algorithm has adjusted the percentage of EVOH to 5.17 % (instead of the 0.3% used in the initial design) in order to satisfy the daily permeation constraint of 10 mg/day for the given thickness distribution. As expected, the maximum FPR is located in the pinch off zone at the top and the bottom of the PFT. This is due to the fact that the pinch-off zone of the PFK is where the EVOH barrier layer becomes very thin or even disappears completely.

a) Initial design (0.3 % of EVOH)

b) Final design (5.17% of EVOH)

Figure 13. Daily MFR Time evolution

Figure 13 presents the effect of the adapted numerical treatment of the pinch off zone on the daily MFR Time evolution for the initial and final design with and without special treatment of pinch off zone. For the initial design the daily MFR exceeds 10 mg/day after 7 days. However, a plateau of 85 mg/day is reached after around 90 days of permeation. Because of the low percentage of EVOH (0.3%) there is no significant difference between the analysis with and without the pinch-off treatment. For the final design with an optimal barrier layer percentage (5.17% of EVOH) the plateau values of the daily MFR are 8 and 10.05 mg/day for the analysis without pinch off and with pinch off respectively, showing clearly that with the adapted pinch off zone treatment we satisfy the daily permeation constraint.

The Fuel vapor pressure distribution in the inter-polymer layers in the steady state is presented in Figure 14 for the optimal part design. At the top and bottom pinch-off zones, we observe that for the inter-layers interfaces located on the upstream side of the EVOH barrier layer (HDPE-LLDPE and LLDPE-EVOH) the vapor pressure at the pinch off zone is lower than the vapor pressure on the reminder of the PFT shell. However, for inter-layers interfaces located on the downstream side of the EVOH barrier (EVOH-LLDPE, LLDPE-HDPE and HDPE-HDPE) the exact opposite is observed. This vapor pressure behavior could be explained by the fact that the permeability resistance in the pinch-off zone is lower than in the reminder of the PFT shell. This difference in the permeability resistance explains why the vapor pressure drop in the pinch zone is greater than in the shell. This phenomenon can also be seen in Figure 6.

Figure 14. Fuel vapor pressure inter-polymer layers distributions at the steady state for the final design.

CONCLUSIONS

A finite element based numerical simulation model for the prediction of fuel permeation through multilayer polymeric material under steady and unsteady regime that incorporates a novel method for the treatment of the diffusion in the pinch-off zone was developed. The accuracy of the proposed model was verified by comparing predicted and analytical results for a three-layer HDPE laminate. Very good agreement was found between analytical and numerical results.

This permeability model was incorporated in BlowDesign to optimize the barrier layer percentage by manipulating the % of EVOH to satisfy the daily permeation rate constraint. For the gas tank studied, we found that 5.17% of EVOH was necessary to meet a typical 10 mg daily emission constraint as is presently used in the industry. For a given laminate thickness, small increases in the thickness of the barrier layer have profound influences on the permeability when the barrier layer is thin (1-3 % of EVOH). However, the effectiveness of the barrier layer decreases as it increases in thickness. We have also noticed that when the weight and thickness is decreased the percentage of the EVOH needs to increase in order to satisfy the permeation constraint. The barrier layer percentage was found to be the primary factor for the reduction of the evaporative fuel emissions.

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