



TXS 'EP' Blend Module

1. BLEND PROCESSING

A new material type (EP Blend) and a new process module (EP Blend Processing) has been incorporated to TXS. The new material and process module was made available in 1Q, 2004.

1.1. EP Blend material type

The new material type, a binary blend of a soft elastomer and an ordinary thermoplastic resin, is defined based on the separate definitions of two different resin type materials:

- material A (the elastomer) defined as a melt-only polymer resin with a softening point below the intended feed temperature (cf. *TXS User Manual*, § 5.3.1),
- material B (the plastomer) defined as an ordinary polymer resin, with solid and melt properties,

Physical properties and viscosity parameter of both materials A and B are set with TXM. In particular, all available models for shear and temperature dependence of the viscosity, and all melt properties (density, specific heat, thermal conductivity) will be available for both materials. Melting point, melting range, heat of fusion, crystallinity, and all solid properties (density, specific heat, thermal conductivity) will be available for the plastomer (B).

Consequently, specification of an EP blend material will require the selection of both components from a list of previously defined polymer resins. In addition the specification of the new material will require the setting of a series of blend properties

- **Composition range.** Feed composition will be limited to a range specified in the blend definition. Maximum range allowed will be 1-99%.
- **Viscosity model ($T < T_m$).** Functional expression to relate the viscosity of the blend to the viscosity of elastomer and the concentration of the solid plastomer at temperatures below the melting point of the later. The model will be used by TXS to compute melt viscosity in the process simulations after the feed port and before the softening of the plastomer. The following options will be available:

Polynomial. In this case the viscosity of the blend will be represented by:

$$\eta_{EP}(\dot{\gamma}, T, w) = (1 + a\phi + b\phi^2)\eta_E(\dot{\gamma}, T) \quad (1)$$

where η_{EP} and η_E are the viscosity of the blend and the elastomer, respectively, $\dot{\gamma}$ and T are the prevailing shear rate and temperature, w and ϕ are the mass and volume fraction of

plastomer, and a and b are empirical fitting constants characteristic of the blend. The volume and mass fractions are related through:

$$\phi = \left(1 + \frac{1-w}{w} \cdot \frac{\rho_S^{(P)}}{\rho_M^{(E)}} \right)^{-1} \quad (2)$$

where $\rho_M^{(E)}$ is the elastomer's density and $\rho_S^{(P)}$ is the solid plastomer's density.

Modified Maron-Pierce. In this case the viscosity of the blend will be represented by:

$$\eta_{EP}(\dot{\gamma}, T, w) = \frac{\eta_E(\dot{\gamma}^*, T)}{(1-a\phi)^2} \quad (3)$$

where η_{EP} and η_E are the viscosity of the blend and the elastomer, respectively, $\dot{\gamma}$ and T are the prevailing shear rate and temperature, w and ϕ are the mass and volume fraction of plastomer, and a is an empirical fitting constant characteristic of the blend. The viscosity of the elastomer will be evaluated at the modified shear rate:

$$\dot{\gamma}^* = \frac{\dot{\gamma}}{1-b\phi} \quad (4)$$

where b is an empirical fitting constant characteristic of the blend.

- **Viscosity model ($T > T_m$).** Functional expression to relate the viscosity of the blend to the viscosities and concentrations of elastomer and plastomer at temperatures below the melting point of the later. The selected model will be used by TXS to compute melt viscosity in the process simulations after the softening of the plastomer. One model will be available:

Log Average. The viscosity of the blend is represented by:

$$\log \eta_{EP} = c_E(1-\phi)\log \eta_E + c_P\phi \log \eta_P + c_{EP}(1-\phi)\phi \log \eta_E \log \eta_P \quad (5)$$

where ϕ is the volume fraction of plastomer in the blend, η_{EP} , η_E , and η_P are the viscosities of the blend, the elastomer, and the plastomer, respectively, at the prevailing shear rate and temperature, and c_E , c_P , and c_{EP} are empirical fitting constant characteristic of the blend. The volume fraction (ϕ) is related to the mass fraction (w) through:

$$\phi = \left(1 + \frac{1-w}{w} \cdot \frac{\rho_M^{(P)}}{\rho_M^{(E)}} \right)^{-1} \quad (6)$$

where $\rho_M^{(E)}$ is the elastomer's density and $\rho_M^{(P)}$ is the molten plastomer's density.

- **Melt temperature shift.**

The blend specification will permit the setting of a concentration dependent shift melting or softening point of the elastomer:

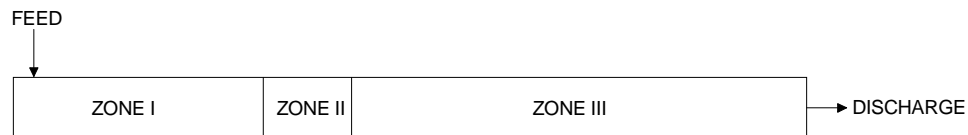
$$T_m = T_m^{(P)} + \phi \Delta T_m^{(EP)} \quad (7)$$

1.2. EP Blend processing module

A new custom-processing module was developed to simulate the processing of EP blend materials. A single feed port allows the feeding of a blend of a soft elastomer (A) and a solid thermoplastic (B) at a temperature below the initial melting/softening point of B. Multiple liquid injection ports are also supported. The operating conditions settings (throughput, screw speed, feed temperature and pressure, head pressure, and barrel temperature profile) are available as usual, with the addition of one more item: mass fraction (%) of component B (the thermoplastic) in the feed.

The simulation proceeds in three steps:

- Zone I, from the feed to the initial melting point of material B. The material is a dispersion of solid particles of material B in material A. Viscosity will be computed using a specific model and viscosity parameters; cf. eq. (1)-(6) above.
- Zone II, from the initial to the final melting point of material B. The material is a dispersion of solid particles of material B in material A. A new (to TXS) dissipative mix-melting model will be implemented. This model includes energy contributions from viscous dissipation of the blend of material A and partially molten material B, as well as heat transfer from the barrel. A contribution for plastic deformation of solid material B, *although not recommended*, could be added via an empirical adjustable parameter.
- Zone III, from the final melting point of material B to the discharge. The material is a mixture of molten material B and material A. Viscosity will be computed using a specific model and viscosity parameters; cf. eq. (7)-(8) above.



The new material and process module includes a set of empirical adjustable parameters to manipulate energy dissipation and heat transfer in the three processing zones separately.