[0031] Fig. 5 is a bar graph representing the relative distribution of weight fractions as a function of the molecular weight of the discrete component chains of a toluene styrenic telomer distribution described by Beta distribution and formed by process technology of this invention.

[0032] Fig. 6 is a graphical depiction of the relationship of the melt flow index of high impact polystyrene resin compositions formed from brominated styrenic polymers of this invention and the glass transition temperatures of said brominated styrenic polymers used.

[0033] Fig. 7 is a graphical depiction of the relationship of the Vicat of high impact polystyrene resin compositions formed from brominated styrenic polymers of this invention and the glass transition temperatures of said brominated styrenic polymers used.

[0034] Fig. 8 is a graphical depiction of the relationship of the dependency of glass transition temperature of brominated styrenic polymers of this invention on molecular weight as specified as M_w of unbrominated STSTDs of this invention from which the brominated styrenic polymers were formed.

[0035] Fig. 9 is a graphical depiction of the relationship of the Hunter Color Yellowness Index (YI) values of high impact polystyrene resin compositions formed from brominated styrenic polymers of this invention and the thermal color values of said brominated styrenic polymers used.

FURTHER DETAILED DESCRIPTION OF THIS INVENTION

Distributions of Styrenic Telomers of the Invention

[0036] Provided by this invention, among other things, are a number of compositions which comprise telomer distributions in which styrene is the taxogen (polymerizable reagent) and toluene is the telogen (chain transfer agent) which is telomerized in the anionic chain transfer styrene reaction. Four such compositions are as follows:

i) A composition is provided, which comprises a distribution of toluene styrenic telomers of the formula:

(I) $C_6H_5CH_2CH_2\text{-}[(C_6H_5)CHCH_2\text{-}]_nCH_2C_6H_5$

wherein each C_6H_5 is a phenyl group ~~and for each molecule of said formula~~, n is an average number in the range of about 1.5 to about 5.5 with the proviso that 1,3-diphenylpropane, a compound of the above formula in which n is 0, optionally is present in said distribution in an amount of not more than 25 GPC area %, and wherein said distribution is further characterized by having an M_w in the range of about 430 to about

1000, an M_n in the range of about 350 to about 770, an M_z in the range of about 550 to about 1700, a polydispersity in the range of about 1.2 to about 1.65, a standard deviation in the range of about 160 to about 500, and an asymmetry in the range of about 1.3 to about 3.2.

ii) A composition is provided, which comprises a distribution of toluene styrenic telomers of the formula:

(I) $C_6H_5CH_2CH_2$-$[(C_6H_5)CHCH_2$-$]_nCH_2C_6H_5$

wherein each C_6H_5 is a phenyl group ~~and for each molecule of said formula~~, n is an average number in the range of about 2.6 to about 5.5 with the proviso that 1,3-diphenylpropane, a compound of the above formula in which n is 0, optionally is present in said distribution in an amount of not more than 5 GPC area %, and with the further proviso that said distribution optionally further contains toluene in an amount of not more than 0.1 wt %, and wherein said distribution is further characterized by having an M_w in the range of about 630 to about 1060, an M_n in the range of about 460 to about 770, an M_z in the range of about 770 to about 1700, a polydispersity in the range of about 1.2 to about 1.65, a standard deviation in the range of about 250 to about 520, and an asymmetry in the range of about 1.3 to about 2.9.

iii) A composition is provided, which comprises a distribution of toluene styrenic telomers of the formula:

(I) $C_6H_5CH_2CH_2$-$[(C_6H_5)CHCH_2$-$]_nCH_2C_6H_5$

wherein each C_6H_5 is a phenyl group ~~and for each molecule of said formula~~, n is an average number in the range of about 2.8 to about 5.5 with the proviso that 1,3-diphenylpropane, a compound of the above formula in which n is 0, optionally is present in said distribution in an amount of not more than 1 GPC area %, and with the further proviso that said distribution optionally further contains toluene in an amount of not more than 0.1 wt %, and wherein said distribution is further characterized by having an M_w in the range of about 645 to about 1100, an M_n in the range of about 490 to about 770, an M_z in the range of about 780 to about 1760, a polydispersity in the range of about 1.2 to about 1.65, a standard deviation in the range of about 250 to about 530, and an asymmetry in the range of about 1.3 to about 2.8.

iv) A composition is provided, which comprises a distribution of toluene styrenic telomers of the formula:

(I) $C_6H_5CH_2CH_2$-[$(C_6H_5)CHCH_2$-]$_n$$CH_2C_6H_5$

wherein each C_6H_5 is a phenyl group ~~and for each molecule of said formula~~, n is an average number in the range of about 2.9 to about 3.9 with the proviso that 1,3-diphenylpropane, a compound of the above formula in which n is 0, optionally is present in said distribution in an amount of not more than 1 GPC area %, and with the further proviso that said distribution optionally further contains toluene in an amount of not more than 0.1 wt%, and wherein said distribution is further characterized by having an M_w in the range of about 650 to about 750, an M_n in the range of about 500 to about 600, an M_z in the range of about 830 to about 1120, and a polydispersity in the range of about 1.2 to about 1.35. Desirably, the distributions of the compositions described in this paragraph are further characterized by having an M_w in the range of about 690 to about 730, an M_n in the range of about 520 to about 560, an M_z in the range of about 910 to about 960, and a polydispersity in the range of about 1.25 to about 1.32.

[0037] Particularly preferred embodiments of this invention are ACTSRs that yield TSTDs which can be reasonably described (modeled) by both equation (1) below. Equation (1) is known as the Weibull probability density function (PDF). Equation (1) is evaluated for discrete values of x_i. Such a typical Weibull distribution is represented by Fig. 4. Such calculations for the Weibull PDF are conveniently made through the use of modern spreadsheet software programs that contain the Weibull PDF among their built in ensemble of statistical functions. Equation (2) provides the normalized weight fraction X_i for telomer component chain x_i. From equations (2) and (3) the mole fraction, n_i, is calculated over the range x_i from $x_i = 1$ to at least $x_i = (M_w + 6\sigma)/104$. From n_i and M_i (the molecular weight of polymer component chain x_i), values for M_n, M_w and M_z are calculated from the Weibull distribution, according to the equations for those parameters presented in Table 2 above. The model "fit" or accuracy is in turn evaluated based on comparison of values generated for PDI, standard deviation (σ_n), skewness $_nU_3$ and asymmetry ($_n\alpha_3$) with those generated from the experimentally determined values (GPC analytical results).

CLAIMS

1. A composition which comprises a toluene styrenic telomer distribution of the formula:

(I) $C_6H_5CH_2CH_2$-$[(C_6H_5)CHCH_2-]_{n_{average}}CH_2C_6H_5$

wherein each C_6H_5 is a phenyl group ~~and for each molecule of said formula~~, n is an average number in the range of 2.9 to 3.9 with the proviso that 1,3-diphenylpropane, a compound of the above formula in which n is 0, optionally is present in said distribution in an amount of not more than 25 GPC area %, and with the further proviso that said distribution optionally further contains toluene in an amount of not more than 0.1 GPC area %, and wherein said distribution is further characterized by having an M_w in the range of 650 to 750, an M_n in the range of 500 to 600, an M_z in the range of 830 to 1120, and a polydispersity in the range of 1.2 to 1.35, a standard deviation in the range of 160 to 500, and an asymmetry in the range of 1.3 to 3.2.

2. A composition as in Claim 1 wherein said distribution is further characterized by having an M_w in the range of 690 to 715, an M_n in the range of 520 to 560, an M_z in the range of 910 to 960, and a polydispersity in the range of 1.25 to 1.32.

3. A process for producing a toluene styrenic telomer distribution, which process comprises:

I) feeding styrene through a small orifice with a feed velocity greater than 10 feet/second into an agitated reaction mixture formed from components comprising toluene, alkyllithium, and optionally Group IA or IIA co-catalyst and TMEDA, at rates of (i) moles of styrene/moles of toluene/hour in the range of 0.3 to 1.5 and (ii) moles of styrene/moles of alkyllithium/hour in the range of 40 to 110; with a molar ratio of styrene:toluene in the range of 0.75 to 4, a molar ratio of styrene:alkyllithium in the range of 150 to 350, and a molar ratio of TMEDA:alkyllithium in the range of 2.2 to 8;

feeds occurring either above the surface or subsurface to a liquid phase in the bromination reaction mixture.

14. A process as in any of Claims 12 or 13 wherein said aluminum halide bromination catalyst is aluminum tribromide or aluminum trichloride or a mixture of aluminum tribromide and aluminum trichloride and where the brominating agent is bromine.

15. A process as in Claim 14 wherein the solvent is comprised predominately of bromochloromethane.

16. A process as in any of Claims 12 or 13 wherein the process further comprises (1) quenching the reaction mixture in water containing hydrazine hydrate to deactivate the bromination catalyst, and to quench bromine, thereby forming an aqueous phase and an organic phase to which is optionally added and then separating the organic phase from the aqueous phase. (2) subsequent to the quenching, washing the separated organic phase or with aqueous NaOH, optionally containing $NaBH_4$ in order to reduce the content of N-bromoamines that may be present, such washing(s) occurring at a temperature within the range of from 20° to 65°C.

~~17. A composition which comprises a toluene styrenic telomer distribution wherein said toluene styrenic telomer distribution has an M_w in the range of 600 to 820, an M_n in the range of 430 to 550, an M_z in the range of 790 to about 1140, with a polydispersity index in the range of 1.3 to 1.5, a standard deviation in the range of 250 to 475, and an asymmetry in the range of 1.6 to 1.9.~~