THE CURING OF DIALLYLTEREPHTHALATE DETERMINATION OF THE KINETIC TRIPLET *A*, *Ea,app*, ƒ(α) USING THE ISOCONVERSIONAL METHOD

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Abstract

Allyl polymers are important materials for the production of high performance ophthalmic lenses by free-radical bulk polymerization in the casting process. Isoconversional model-free analysis was applied to the isothermal and nonisothermal curing of diallylterephthalate performed by DSC at different sets of heating rates. The results of the kinetic analysis in a form of kinetic triplet (*Ea*, *A*, ƒ(α)) present the variation of the Arrhenius parameters with the calculation method, reaction extent, process mode and heating rates applied. This variation is a sign of the complex and multi-step reaction mechanism. Such a mechanism was approximated with one step $(1-\alpha)^n$ reaction model. With the isokinetic relationship - IKR (compensation effect) in the form of $lnA=aEa,app+b$ it was found out that the isothermal and nonisothermal IKR lines converge to different singular points. From the correlation procedure with the experimental data isothermal narrowest point – NPI was selected as a common point. The curing process in the isothermal and nonisothermal process conditions, respectively, was successfully simulated with the obtained kinetic parameters. The possible alternative reaction paths and the partial diffusion control of the curing process are the reasons for the limiting usage of the model-free kinetic analysis method. This method was mainly used as a preliminary step for further analysis with other methods.

Introduction

Allyl polymers are well known materials for the production of high performance ophthalmic lenses. Interest for better performance and shorter production times of existing and new combinations of monomers are the main reasons to study free-radical bulk polymerization process of relatively simple diallyl system. Diallylterephthalate (DAT) monomer cured with initiator dicyclohexyl peroxy dicarbonate (CHPC) may be an example.

Monomer or pre-polymer mixtures are cured using casting process in a glass or metallic moulds to get almost perfect optic surface without additional processing. In

practice, finished (both surfaces) and semi finished (only front surface) lenses of different geometrical shapes are produced. Finished lenses are 3 to 6 times thinner than semi finished which is 5–15 mm thick.

DAT evolves approximately 350-400 J/g of heat during polymerization. Such high heat evolution joined with the unpleasant geometry is the cause that the heat transfer out of the system becomes limiting factor for the curing process. Because diallyl polymerization expresses no microgelation and no Trommsdorff effect[1] the auto-acceleration effect during polymerization can only be caused by high heat evolution, geometric factors of the product shape and heat transfer to surroundings. Therefore: auto-acceleration as a limiting effect is mainly caused by process conditions. Due to the auto-acceleration effect a hot spots may occur at the centre of a product during nonisothermal curing cycle leading to optical inhomogeneities. Due to this facts, correct determination of the kinetic triplet[2,3] Ea (activation energy), A (Arrhenius preexponential factor) and $f(\alpha)$ (reaction model) is crucial for the reaction modeling and optimization of the curing cycle in a sense of curing time and product quality.

The present study is based on differential scanning calorimetry (DSC) experiments performed only in nonisothermal or dynamic mode. An isothermal experiment as the preferred way to obtain kinetic information is not possible. Heat flow at the isothermal mode is so low that cannot be detected by conventional DSC. Alternative is to perform indirect isothermal method[3] to detect the residual heat nonisothermaly after the samples were exposed to given temperature for a specified time, which is usually referred as – isothermal method II.[3] Such a process is rather slow and time consuming. The drawbacks of the DSC experiments are the detection of heat which evolves from the different reactive processes, what means that calculated results present overall, apparent or effective kinetics. Problems arise also from calculation procedures where different methods give different results due to the compensation effect among Arrhenius parameters,[4, 5] if the temperature dependence of the rate constant $k(T)$ is described by the Arrhenius equation. Compensation effect or isokinetic relationship (IKR)[4] was derived from Arrhenius equation[6] and its form is presented in Eq. 1.

$$\ln A_\xi = b + aE_\xi \qquad (1)$$

The IKR relation is used to find out whether the variations of the activation energy with different factors (ξ), i.e.: reaction model, conversion and heating rate, has a physical background or they are caused by the variations of process conditions or calculation manipulation.

From the concept of the variable apparent activation energy with conversion proposed by Vyazovkin,[7-9] the complex and multi-step reaction mechanism was assumed. But for the purpose of the reaction modeling some simulations with simpler model were applied. One-step reaction order model of *ROn* type was chosen and tested for the reliability.

Experimental

Polymerization mixture was been prepared from commercial technically pure Diallylterephthalate (Daiso co. Japan) and dicyclohexyl peroxy dicarbonate (Laporte, Germany). Clear, homogeneous particle free solution was prepared at room temperature under nitrogen atmosphere. In the curing experiments, 5 % solutions of CHPC in DAT was used. Thermally initiated polymerization was performed in differential scanning calorimeter (DSC) Mettler Toledo 821c at constant atmospheric pressure in nitrogen atmosphere. Dynamic scans were performed at heating rates (β) from 2 to 20 K/min, respectively, in a temperature range of 40–160 ℃ ad N_2 flow of 100 ml/min. DSC samples were placed in 40 μL aluminium crucibles with a perforated lid. Isothermal pre-curing experiments were performed in DSC also at 50 and 60 ℃ respectively. Samples were prepared in the same manner as for dynamic experiments. DSC heating method was constructed of rapid heating (50 K/min) to isothermal curing temperature, curing for certain time at constant tempearure, than rapid cooling (-25 K/min) to start tempeature (25 ℃) and finally dynamic scaned for residual heat at 10 K/min.

The weight of the samples has been measured accurately in a range of 3-12 mg. The sample mass was selected according to recommendation from ASTM 698[10] that peak of heat flow at given geometry and mass (40μL Al crucible) should not exceed 8 mW to avoid auto acceleration. Measurement procedures were performed according to ASTM E 698 and E 2041.[11]

Pre-cured samples of polymer mixture at isothermal conditions were prepared in DSC under N_2 atmosphere. The samples were scanned for residual heat evolution

immediately after isothermal curing without removing the sample inside the same temperature program.

The initiation of the polymerization was conducted by the thermal decomposition of the CHPC, which is highly exothermic process and overlapped by the polymerization process. To obtain heat of the polymerization only, the heat of initiator decomposition was subtracted from the overall heat of the polymerization. Heat of the decomposition of the CHPC was evaluated in the DSC at the same conditions and concentration as studied sample. Dibutyl phthalate (DBP) was used as a neutral but rather similar solvent[12] to the DAT to simulate thermal decomposition of CHPC without polymerization.

Results and discussion

I. Nonisothermal method

To apply isoconversional model free kinetics experiments should be performed at different heating rates.
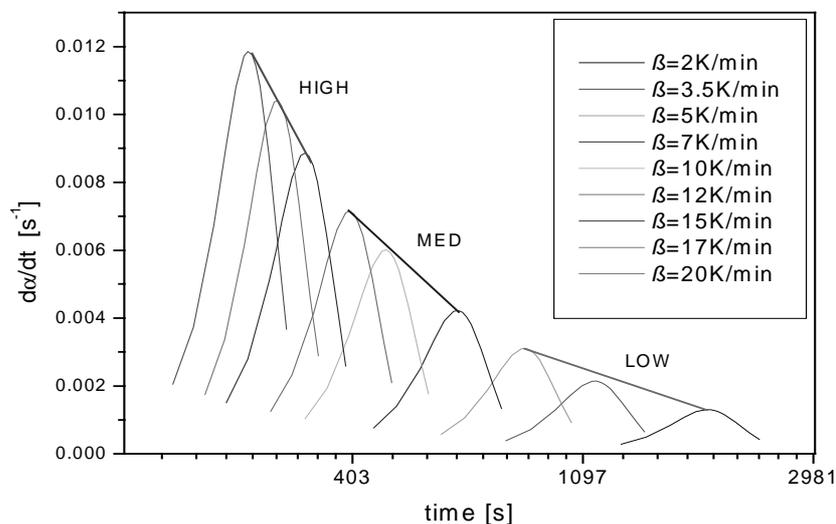

Figure 1. Three sets of scanning rates and achieved reaction rates.

To select consistent reaction rates the interval inside 2-20 K/min was divided into three sections as shown in Figure 1 where normalized DSC scans are represented. Low section (LOW) is represented by 2, 3.5 and 5 K/min, medium section (MED) is represented by 7, 10 and 12 K/min and high section (HIGH) by 15, 17 and 20 K/min.

Achieved maximum reaction rates in the LOW part where around $2 \cdot 10^{-3}$ s^{-1}, in the MED part around $6 \cdot 10^{-3}$ s^{-1} and in the HIGH part around $10 \cdot 10^{-3}$ s^{-1}. The maximum reaction rates varied in the range from 1:5, and were kept above auto-accelerating range with the variation of the sample mass.

To establish the kinetic parameters of the curing system from DSC data some assumptions should be accepted: reaction extent is associated with conversion (α) and the conversion rate (*dα/dt*) is proportional to the measured heat flow (*dQ/dt*) Eq. 2. Measured heat flow (*dQ/dt*) in mW was normalized with the sample mass and the total heat of the reaction *(Q$_{tot}$)* obtained with the integration of the total peak area.

Isoconversional kinetic analysis was performed using differential equations proposed by Friedman[13] (Eq. 3), which allows "model-free" calculation of apparent activation energy from the slopes of the lines when *ln dα/dt* is plotted against *1/T* at different α as shown Figure 2.
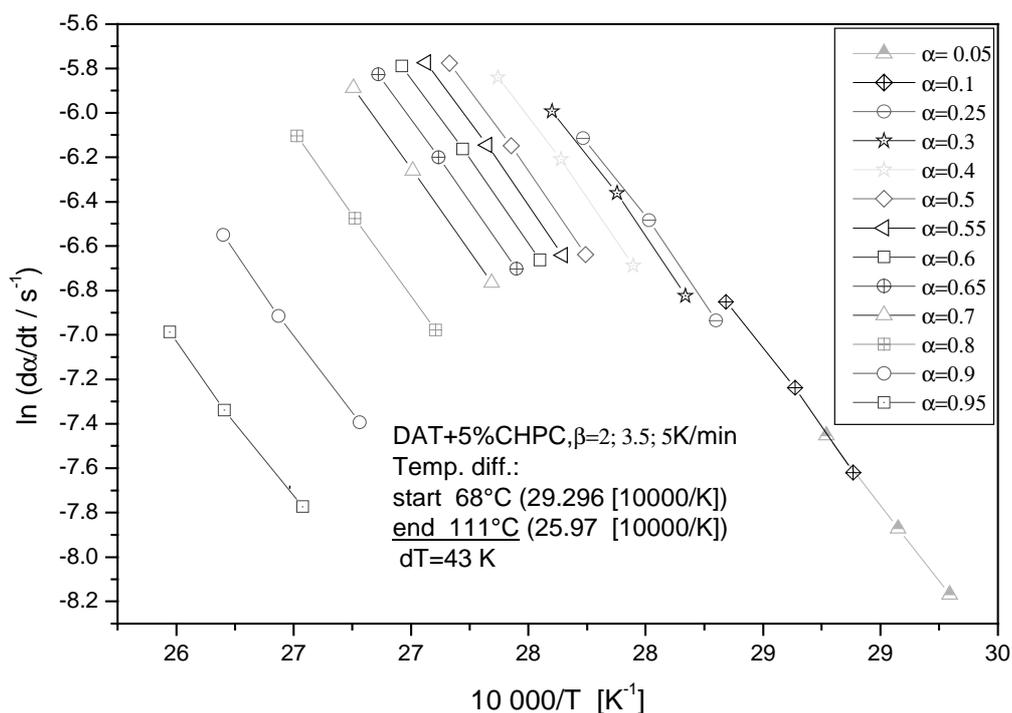

Figure 2. Model free determination of *Ea,app* at different α (Eq. 3).

$$\frac{d\alpha}{dt} = \frac{dQ}{dt} \cdot \frac{1}{Q_{tot}} = k(T) \cdot f(\alpha) = A \cdot \exp(-Ea, app / R \cdot T) \cdot f(\alpha) \qquad (2)$$

$$\ln(d\alpha / dt)_{\alpha} = \ln[A_{\alpha} \cdot f(\alpha)] - Ea_{\alpha, app} / R \cdot T \qquad (3)$$

To calculate the Arrhenius preexponential factor *A* from the Eq. 3 the reaction model $f(\alpha)$ should be determined. The proposed one step reaction model of *ROn* type was used:

$$f(\alpha) = (1-\alpha)^n \tag{4}$$

Málek[14] proposed a method to test the reliability of the reaction model with the help of two auxiliary functions *y(α)* and *z(α)* that can be calculated from the experimental data according to Eqs. 5 and 6.

$$y(\alpha)=(d\alpha/dt)\,e^x \tag{5}$$

$$z(\alpha)= \pi(x)\,(d\alpha/dt)\,T/\beta \tag{6}$$

Where $x = Ea,app/RT$ and $\pi(x)$ is the temperature integral approximation (Appendix A) according to Senum and Yang.[15] The functions were normalized within (0,1) interval and are presented in Figure 3. Function *y(α)* has a maximum at α_{max}^y and it is concave. The condition of $\alpha_{max}^y < \alpha_{max}^z$ and $\alpha_{max}^z < 0.633$ proposed by Málek[14,16] should be an indication of the *ROn (n >1)* model.
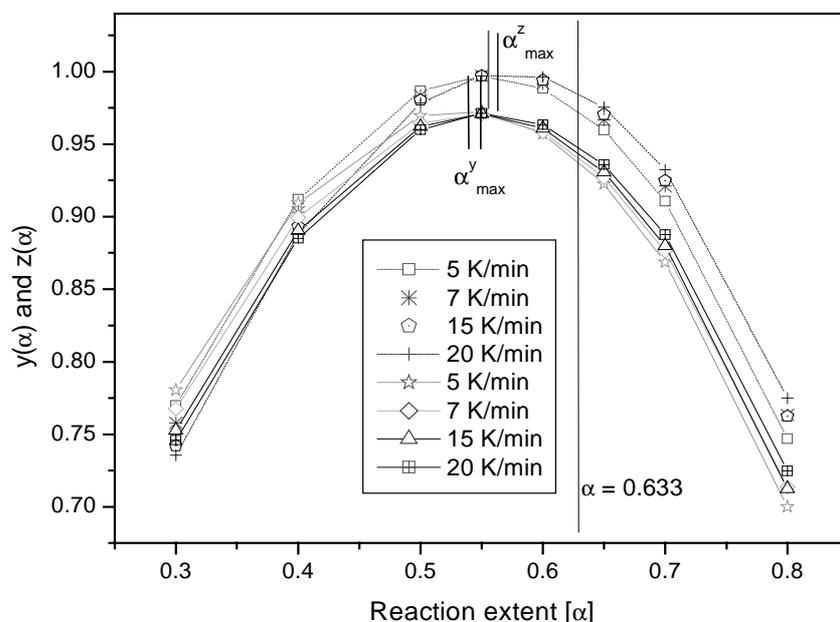

Figure 3. Plot of the *y(α)* and *z(α)* and the corresponding positions of α_{max}^z and α_{max}^y.

To determine the reaction order *n*, for the chosen model (Eq. 4), single heating rate method (SHR) and multilinear regression[17] were applied in the whole range of used heating rates. The variation of the reaction order shown in Figure 4 is within ± 5 % and may be taken as an independent of heating rate with average value of 1.33.
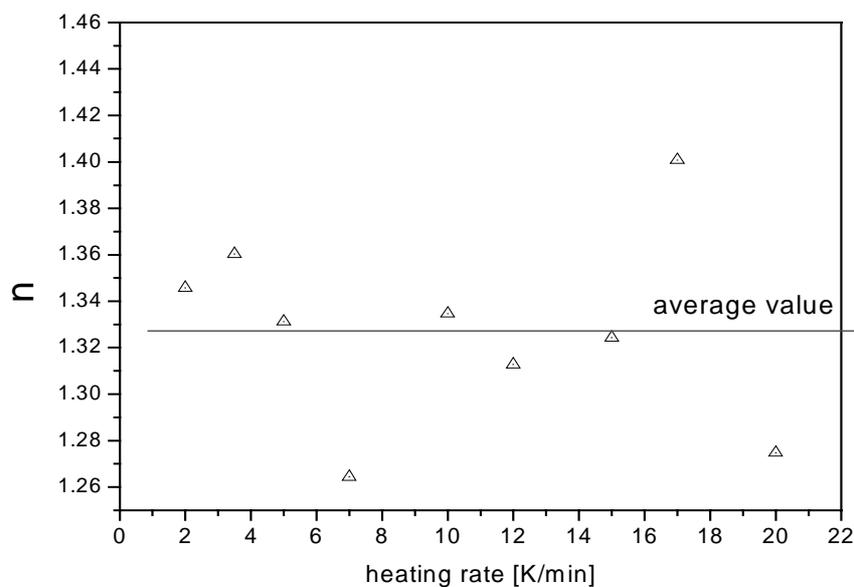

Figure 4. Reaction order n at different *β* calculated with SHR method by multilinear regression.

With the estimated reaction order the preexponential factor *A* can be calculated according to Eq. 3. The results of Friedman isoconversional analysis at different extent of the reaction (α) are represented in Figure 5.

From the dependence of the *Ea,app* with reaction extent (Figure 5) it may be concluded that the reaction under consideration is a typical complex multi-step reaction.[18] A useful characteristic of this reaction system is that the complex mechanism may be simplified with the one step reaction order model as it was shown above. Simple, and still accurate enough, the reaction model does not contribute to the understanding of reaction mechanism but gives rise to the modeling of the reaction at different process conditions with good predictive power.

From the first part of the calculation, three sets of pairs of *Ea,app* and *A* are available according to Figure 5. Variation of the Arrhenius parameters with conversion and heating rate, at selected one step reaction model is caused by the compensation

effect (IKR) or simply by calculation procedure, and not the reaction mechanism. The criterion to consider whether the IKR is true or false is the ability of the ξ factor from the Eq. 1 to affect the temperature dependence of a single-step reaction[4] rate.
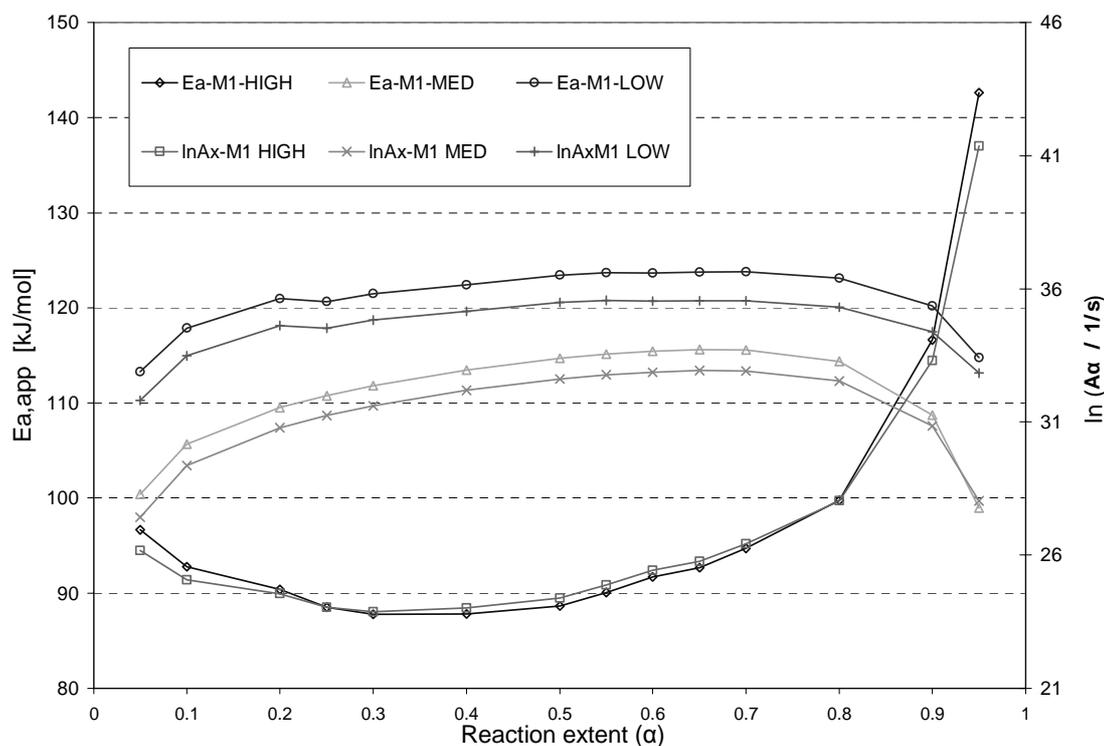

Figure 5. Variation of *Ea,app* and *A* with α at various *β* range.

In the analysis of the nonisothermal kinetics, three types of IKR may appear due to variation of: (i) reaction model, (ii) conversion and (iii) heating rate. Due to the chosen reaction model and invariate Eq. 3, only the latter effects should be considered.

From the theory[4] , the IKR type (iii)-heating rate dependency is caused by a change in the temperature region within the variation of *β*. From Figure 6 it is evident that the relationship is linear with very small variation of the slopes. Lines tend to converge to the same point what could be used as a singular value of the kinetic triplet.

The point of convergence may be find out with the extension of the calculated lines of the IKR through the whole range of *Ea,app*. The lines do not converge to common intersection but to the narrowest point (NP) as shown in Figure 6. This point was taken as a characteristic singular point. The convergence point is very narrow inside

the range of ±0.3% for both variables. With the use of parameters from the narrowest point (NP) variations with the conversion (IKR (ii)) and with the heating rate (IKR (iii)) are eliminated.
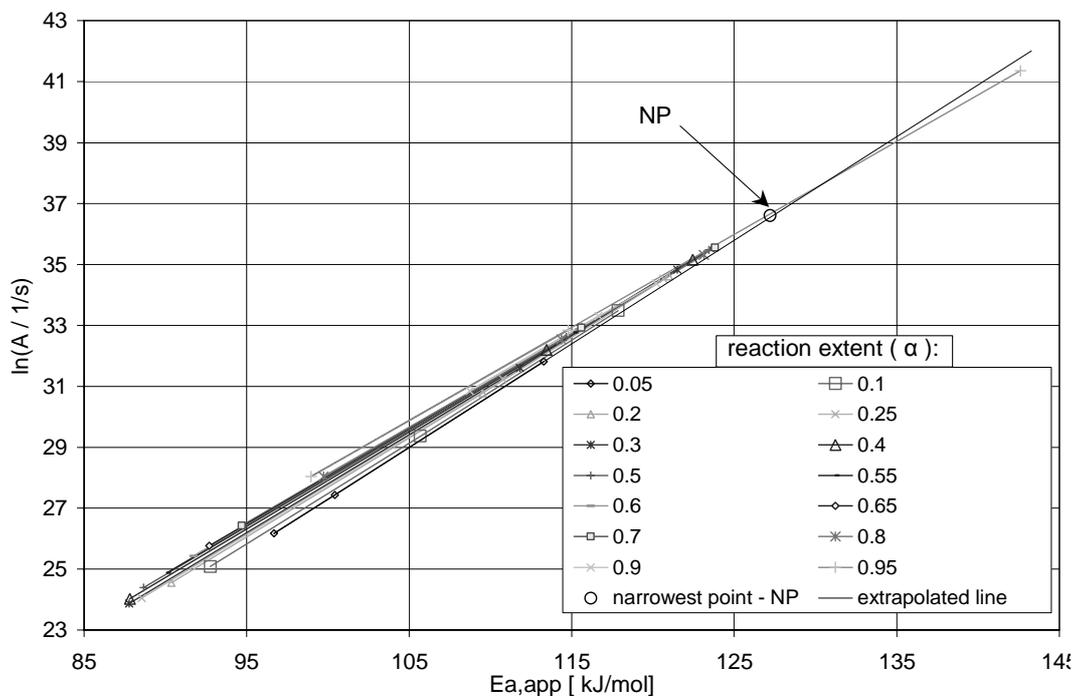

Figure 6. Variation of *lnA* and *Ea,app* at different α at LOW, MED and HIGH set of *β*.

II. Isothermal method - II

Importance of the curing at isothermal conditions comes from the industrial curing process, which consists of nonisothermal and isothermal segments. Isothermal segments occupy 85% of all curing time of the industrial curing cycle. Because of this fact, curing at isothermal conditions should be the main criterion used in the further procedure of searching for a common kinetic triplet. Polymerization system with DAT monomer, as it was discussed at the beginning, cannot be analyzed in the isothermal regime directly with the DSC method. The residual heat method referred as – isothermal method II[3] was therefore applied.

Samples of monomer mixtures with initiator were cured isothermally up to a certain time and than nonisothermaly scanned at heating rate of *10K/min* to detect the residual heat. Degree of conversion was calculated on a base of Q_{tot}, (total heat released

of the uncured samples at the same conditions). The IKR relation for the isothermal cure conditions, contrary to nonisothermal ones, cannot be calculated from experimental data directly because reaction rate cannot be recorded. By rearranging Eq. 3 and combining it with Eq. 1 one may obtained the following expression:

$$\ln\left[\frac{(d\alpha/dt)_\alpha}{f(\alpha)}\right] + \frac{1}{R \cdot T} \cdot Ea, app_\alpha = \ln A_\alpha = aEa, app_\alpha + b \tag{7}$$

Using Eq. 7 and applying it on the isothermal data the slope may be calculated directly as *a=1/RT*. Intercept may be determined with the fitting procedure of the reaction model with the experimental data at different *Ea,app* to find related preexponential factor *A*. The data were collected for the samples cured at 50, 60 and 70 °C.

Compensation effect for the isothermally precured samples is presented in Figure 7. The behavior of the lines group is almost the same as for nonisothermal curing with the narrowest point signed as NPI.
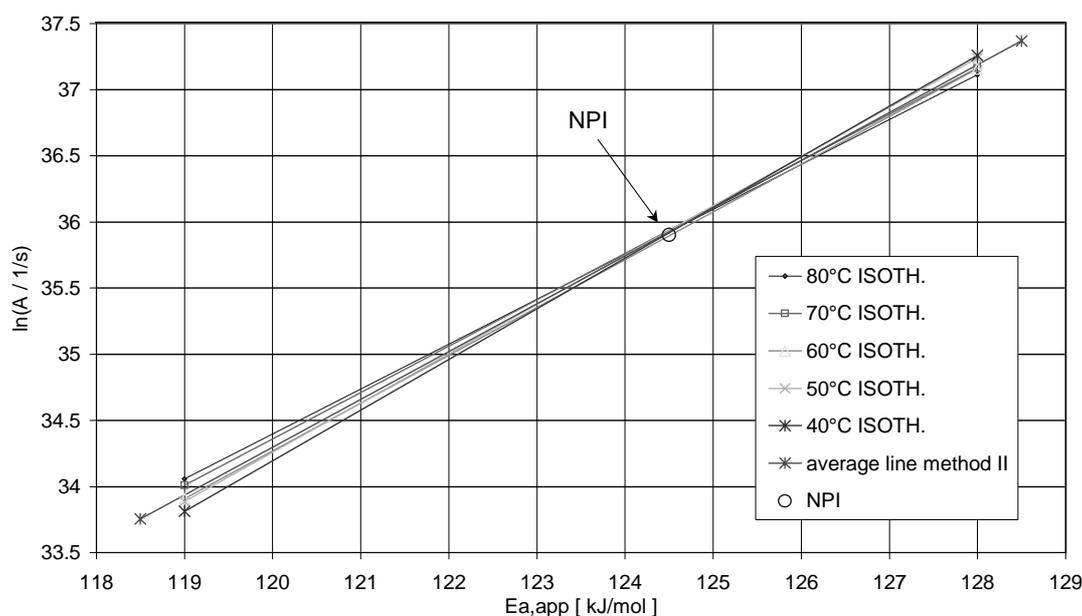

Figure 7. IKR lines for the isothermally precured samples and its narrowest point NPI.

Average compensation lines for nonisothermal conditions and isothermally precured samples are presented together in Figure 8 to obtain a singular kinetic pair of *Ea,app* and *A*. There is no evidence that such activation energy may be attributed to the classical concept of energy associated with the transformation of inactive molecules into active one.

There are many pairs of *Ea,app* and *A* describing the kinetic process under the study but only few may be interpreted mechanistically or even physically. Average nonisothermal line was calculated from IKR data from Figure 6.

Kinetic parameters from nonisothermal average IKR line on Figure 6 give most reliable simulations at NP point. Deviation of the calculated results from experimental one progress with lower value of *Ea,app*. Deviation higher than ±5% was taken as a limiting value Figure 8.

Average line of the isothermally precured samples continues through all of the range because results calculated with pairs of [*Ea,app*, *A*] from the line do not deviate significantly from experimental one.
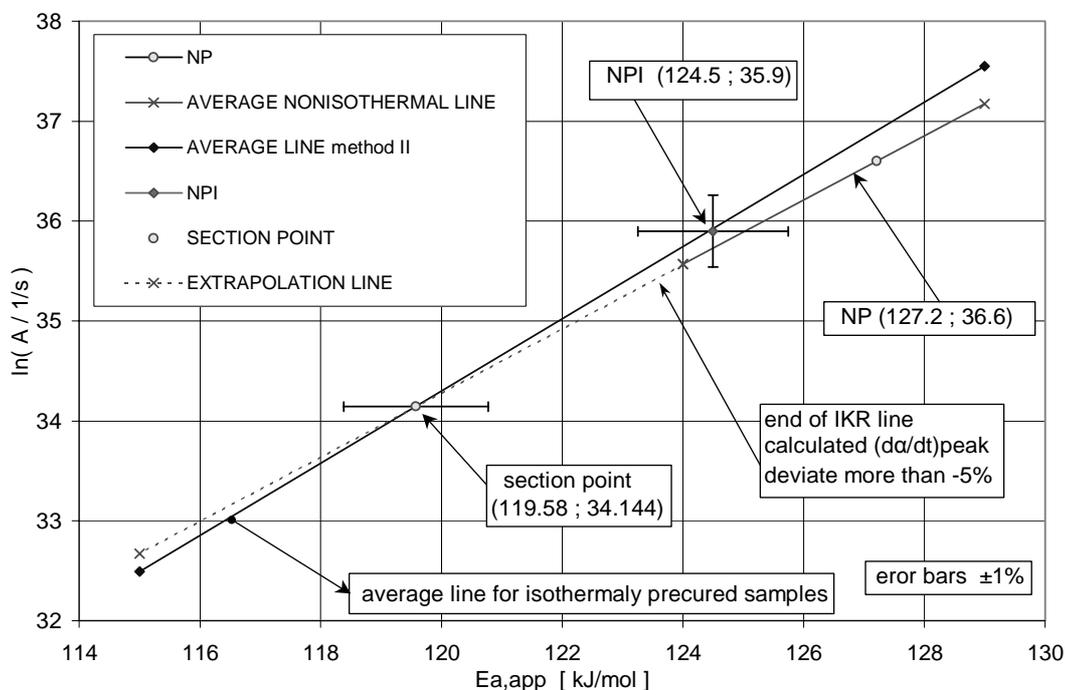

Figure 8. IKR for nonisothermal conditions and isothermally precured samples.

The extrapolation of the nonisothermal line intersects with the line of precured samples, but because the intersection is out of the range of nonisothermal results it cannot be taken as common point.

Two points from the Figure 8 may finally be taken into the consideration: the NPI point from isothermally precured samples and the NP point from nonisothermal curing regime. The correlation among set of experimental and calculated results of the curing extent may be used as one of the criterion for selecting NPI or NP as a common point. Another criterion should be the isothermal regime which represents most of curing time of industrial process. The best correlation at isothermal curing conditions are necessary to ensure the smallest error when industrial process will be tested. Results of the correlation procedure are represented in the Table 1.

Results from the Table 1 show that kinetic triplet at NPI point give the best results for both conditions.

Table 1. Correlation among experimental and simulated reaction extent for each triplet at NPI and NP point.

triplet at:		NPI	NP
$f(\alpha) = (1-\alpha)^{1.33}$			
Ea,app	[kJ/mol]	124.5	127.2
Ao	[1/s]	3.90E+15	7.86E+15
Correlation for **isothermaly** precured samples	r^2	0.998153	0.995083
Correlation for **nonisothermaly** cured samples, average value for $\beta = 2$ -20 k/min	r^2	0.994655	0.989112
Average value		**0.996404**	0.992098

Results in the table seems to be confuse in the first moment, while simulations at NPI give better results as original at NP. This is a consequence of the more scattered results of nine samples and its wide range of β applied. The last reason, to select NPI as a common point, is the prevailing part of isothermal conditions inside the industrial curing cycle. Kinetic triplet at NPI, *Ea,app=124.5* kJ/mol, *A=3.9E15* 1/sec and $f(\alpha)=(1-x)^n$ with

n=1.33 was selected as a common point for isothermal and nonisothermal curing simulations.

For practical representation the difference among measured and calculated conversion using NPI point isothermal and nonisothermal curing for typical samples are shown on Figure 9.
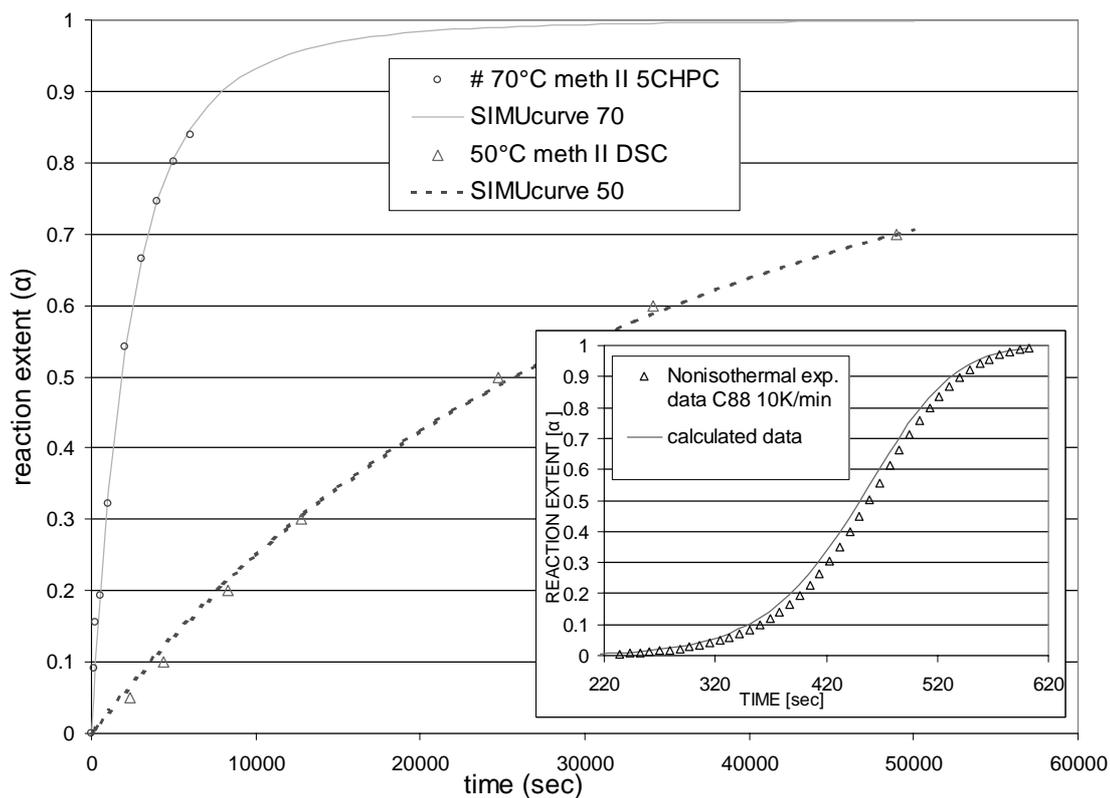

Figure 9. Isothermal and nonisothermal (inset) experimental data and simulated results.

III. Testing the industrial process

Once the common kinetic triplet was established and tested the results may be verified in the industrial curing process. Industrial curing cycle is constructed as a exponential curve in the *Temp=f*(time) diagram. The cycle was divided into the 19 nonisothermal and isothermal segments (inset on Figure 10). Cycle start from 25 ℃, nonisothermal segments between isothermal one are constructed with *β* = 0.5 and 2 K/min. Whole cycle is 17 hours and 25 minutes long and it finishes at 140 ℃, so that

post-curing process is not necessary. Cycle is constructed with some main assumptions that should be accomplished:

- there should be no self-acceleration inside reaction mass,
- the temperature profile should be homogeneous inside the shape without hot spots,
- the cured polymer should express no residual heat release in DSC after cure,
- conversion of the (C=C) bond in final polymer measured with FTIR spectrometer should be homogeneous inside the shape.

Inside the curing cycle seven testing points were selected. At each test point temperature program was stopped and samples were tested for residual heat release in DSC. With the selected common kinetic triplet conversion at each test point reaction extent was calculated. Figure 10 shows the correlation among calculated and measured conversion (residual heat method). Good agreement confirms the correct kinetic triplet selection and gives rise to use these parameters for the process redesign and optimization.
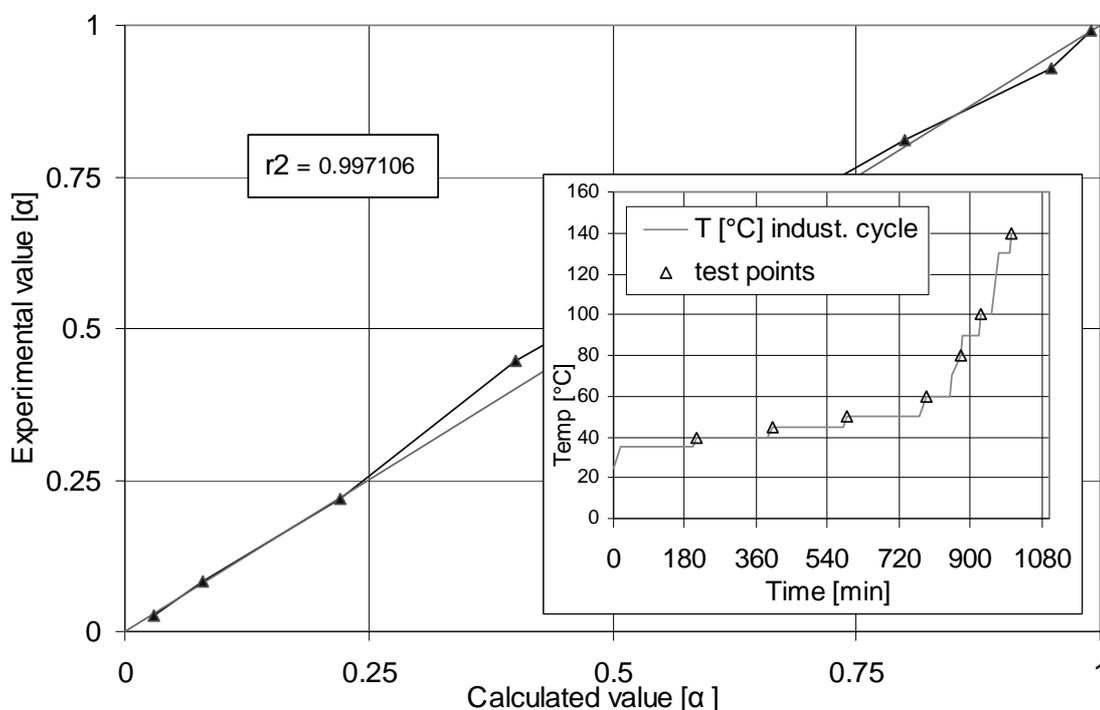

Figure 10. Industrial curing cycle and correlation among calculated and measured conversion.

Conclusions

It is possible to construct reliable unifying kinetic triplet from relatively dispersed originally evaluated kinetic parameters using compensation effect. Therefore, such a procedure does not help to understand the reaction mechanism better and this is the main reason why compensation effect is still controversial.[18] There is obvious, that IKR (i) caused by application of different reaction models is artificial an cannot be true,[4] otherwise IKR (ii) caused by conversion changes and IKR (iii) caused by heating rate may be interpreted as real one. It is known[4] that latter two IKR`s may be misinterpreted as true one what may also be concluded from the case under consideration. Namely, when the compensation effect is able to compensate from dispersed results to common point it may also compensate in "opposite" way. For example, false results (like mathematical manipulation) may be "compensated" as true one and opposite, true results as the false one. The compensation procedure presented in this work may be expressed as "one way" compensation from results to "artificial", but as it was shown above, useful common point. On the other hand, no evidence of the theoretical meaning of this point was found. Such a common point can hardly be recognized as an important mechanistic characteristics of the reaction system. From the mechanistic point of view of the kinetic study, the IKR seems to be unreliable and attention should be brought to basic results in Figure 8.

Results from Figure 8 should be analyzed in the light of regarding the use of model-free analysis kinetics that comes from recently published article.[19] The authors stress out some conditions which are required for the reliable use of this technique. The following conditions should not be present:

1) combinations of exothermal and endothermal signals in DSC measurements,
2) processes with branched reaction paths,
3) partial diffusion control of the process,
4) back reactions and
5) distinct variations of the process stoichiometries.

Results from our measurements of the temperature modulated DSC (TMDSC) of the 5 % CHPC-DAT system confirm that only exothermal nonreverse signal is presented meaning that (1) and (4) are not present. Because of rather simple reaction stoichiometries significant variations are not probable and (5) may be eliminated, too.

Different reaction paths (2) and partial diffusion control (3) are, according to present state of knowledge,[20] possible. From this, it may be concluded that mentioned restrictions importantly limits the use of model-free analysis. Further mechanistic studies are directed to use non-linear regression and model-fit method,[19] where these restrictions are not valid. The evaluated results from model-free analysis are important starting values for the calculation procedure and may serve as an important preliminary step.

Acknowledgement

References

1. A. Matsumoto, D. Mitomi, H. Aota, J. Ikeda, *Polymer* **2000**, *41*, 1321–1324.
2. J. Jang, J. Yi, *Polymer Journal* **1995**, *27*, 404–413.
3. R. B. Prime, Thermosets, in E. A. Turi (Ed.), *Thermal Characterization of Polymeric Materials*, 2nd Edition, Academic Press, New York, 1997, pp 1380–1766.
4. S. Vyazovkin, W. Linert, *Chemical Physics* **1995**, *193*, 109–118.
5. J. M. Salla, X. Ramis, J. M. Morancho, A. Cadenato, *Thermochim. Acta* **2002**, *388*, 355–370.
6. S. Vyazovkin, C. A. Wihgt, *Thermochim. Acta* **1999**, *340-341*, 53–68.
7. S. Vyazovkin, A. I. Lesnikovich, *Thermochim. Acta* **1990**, *165*, 273–280.
8. S. Vyazovkin, *Thermochim. Acta* **1992**, *211*, 181–187.
9. S. Vyazovkin, *Int. Rev. Phys. Chem.* **2000**, *19*, 45–68.
10. Standard Test Method for *Arrhenius Kinetic Constants for Thermally Unstabile Materials*, ASTM E698-99, 1999, ASTM, Philadelphia.
11. Standard Test Method for *Estimating Kinetic Parameters by Differential Scanning Calorimeter Using the Borchardt and Daniels Method*, ASTM E2041-99, 1999, ASTM, Philadelphia.
12. V. I. Arulin, L. I. Efimov, V. P. Zubov, *Vysokomol. Soedin.* **1975**, *Ser. B 17*, 420–429.
13. H. Friedman, *J. Polym. Sci.* **1963**, *C 6*, 183–199.
14. J. Málek, *J. Thermal. Anal.* **1992**, *38*, 71–88.
15. I. Senum, R. T. Yang, *J. Thermal Anal.* **1977**, *11*, 445–462.
16. J. Málek, *Thermochim. Acta* **2000**, *355*, 239–253.
17. R. Serra, J. Sempere, R. Nomen, *Thermochim. Acta* **1998**, *316*, 37–45.
18. M. E. Brown, A. K. Galwey, *Thermochim. Acta* **2002**, *387*, 173–183.
19. J. R. Opfermann, E. Kaiserberger, H. J. Flammersheim, *Thermochim. Acta* **2002**, *391*, 119–127.
20. D. J. T. Hill, H. J. O'Donnell, M. C. S. Perera, P. J. Pomery, *Eur. Polym. J.* **1997**, *33*, 1353–1364.

Appendix A

Temperature integral can be derived from the Equation 2:

$g(x) = \int_0^\alpha \frac{d\alpha}{f(\alpha)}$ and can be approximated according to Senum and Yang[15] expression

in the form of:

$$\pi(x) = \frac{x^3 + 18x^2 + 88x + 96}{x^4 + 20x^3 + 120x^2 + 240x + 120} \quad \text{for } x > 20$$

Povzetek

Alilni polimeri predstavljajo pomembne materiale za izdelovanje optičnih leč izjemnih lastnosti in kakovosti namenjenih predvsem za korekturne leče (očesna optika). Najpomembnejši proces izdelave takšnih leč je še vedno kalupljenje z radikalsko polimerizacijo v masi. Kot značilen primer je bil uporabljen dialiltereftalat – DAT monomer z iniciatorjem cikloheksilperoksidikarbonatom – CHPC. Za analizo kinetike procesa polimerizacije je bila uporabljena izokonverzijska analiza brez predhodne določitve reakcijskega modela, $f(\alpha)$. Proces polimerizacije je bil izvajan pri izotermnih in neizotermnih pogojih v DSC aparaturi pri različnih hitrostih segrevanja β. Dobljeni kinetični parametri temeljijo na meritvah sproščene reakcijske toplote in jih je zato težko povezati zgolj z eno reakcijo, npr. izginevanjem C=C dvojnih vezi. Dobljene kinetične parametre tako označujemo kot navidezne (apparent). Rezultati kinetične analize izraženi v obliki kinetične "trojke" (Ea, A, $f(\alpha)$) se zelo spreminjajo glede na uporabljeno metodo računanja, glede na obseg reakcije, pri katerem so parametri izračunani in uporabljene procesne parametre, predvsem hitrosti segrevanja β. Takšno spreminjanje je znak večstopenjskega in kompleksnega reakcijskega mehanizma. Da bi bilo mogoče vsaj približno načrtovati reakcijski proces, je predlagana uporaba enostopenjskega reakcijskega modela $f(\alpha)$ v obliki $(1-\alpha)^n$ kot poenostavitev in dovolj dober približek resničnemu reakcijskemu mehanizmu. S pomočjo uporabe izokinetične enačbe imenovane "kompenzacijski učinek" (kompenzacija med Ea in A daje enake kinetične rezultate pri različnih Ea) v obliki enačbe premice $lnA_\alpha = aEa,app_\alpha + b$ je bilo odkrito, da premice za različne obsege reakcije α konvergirajo v skupno točko. Enako obnašanje izkazujejo tako rezultati dobljeni pri izotermnih kakor neizotermnih pogojih polimerizacije.

S pomočjo metode najboljšega prileganja podatkovnih matrik med seboj (r^2) je bila izbrana skupna točka NPI (kinetična "trojka"), ki jo je mogoče uporabiti za simulacijo polimerizacije tako pri izotermnih kakor neizotermnih pogojih. Opravljena je bila primerjava med načrtovanimi in dejanskimi podatki reakcijskega obsega α za polimerizacijski cikel, ki se uporablja v industrijskem procesu. Zelo dobro ujemanje rezultatov modela in preskusa kaže na možnost uporabe opisane metode modeliranja za nadaljnje optimiranje in spreminjanje polimerizacijskega procesa.

Izkazalo se je, da omejitve izokinetične analize DSC podatkov ne omogočajo globlje raziskati reakcijski mehanizem polimerizacije. Vzroki so predvsem v različnih možnih vzporednih reakcijskih poteh in difuzijskih omejitvah, ki omejujejo in s tem kontrolirajo potek procesa polimerizacije. Uporabljena metoda tako predstavlja le prvi korak v raziskavi in usmerja delo v uporabo še drugih metod kot npr. nelinearno regresijo in najboljše prileganje z modelom, sestavljenim iz več stopenj, z različnimi modeli posameznih reakcijskih poti.