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An Interactive Approach for Copolymer Design: Web-based Simulation and Analysis of Reactivity Ratios

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Abstract: In this study, three different methods, Mayo-Lewis, Fineman-Ross, and Kelen-Tüdös, were used together to determine monomer reactivity ratios in the copolymerization process. While the Mayo-Lewis method offers precise results with its optimization-based structure, the Fineman-Ross method draws attention with its simple and fast applicability. On the other hand, the Kelen-Tüdös method provides more stable and reliable estimates in large data sets. In addition, the Runge-Kutta 4th-order numerical solution method was applied to model the time-dependent change of monomer concentrations. The developed web-based platform can work with both synthetic and real experimental data, providing comprehensive analysis and visualization to the user. In this way, copolymerization kinetics and reactivity ratios are better understood, and reliable estimates are obtained by comparing the results of different methods. In addition, this tool can be used as important teaching material in polymer physics and chemistry education, helping students better understand copolymerization kinetics and reactivity ratios. The web application used in the study was developed with HTML, CSS, and JavaScript. Open-source libraries such as PapaParse, Numeric.js, and Plotly.js were used for data processing and graphical visualization. In this way, a user-friendly and interactive environment was created.

Keywords: Copolymerization, Reactivity Ratios, Mayo-Lewis Method, Kinetic Simulation, Runge-Kutta Method

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1. Introduction

Copolymerization is a type of reaction in which different types of monomers form polymer chains together and is of great importance in the fields of materials science and chemical engineering. In this process, reactivity ratios, which determine the chemical interactions of monomers with each other, are a critical factor. Reactivity ratios are influenced by various factors such as the molecular structures of monomers, the position of their active groups, and steric effects. For example, the double bond structure of a monomer can lead to reactivity uncertainties that can affect the desired properties of the polymer, which in turn play an important role in the mechanical strength or heat resistance of the polymer (Dube et al., 2013; Lundberg et al., 2024; Autzen et al., 2024).

In engineering and industrial applications of copolymerization, precise determination of monomer reactivity ratios is of great importance. Accurate determination of these ratios enables more effective control of the polymerization process and contributes to the desired properties of the resulting polymers. Both experimental methods and computational simulation techniques are used to determine reactivity ratios. Experimental studies are usually based on kinetic analyses, while computational approaches are supported by advanced methods such as molecular dynamics. This combination allows researchers and engineers to more accurately predict polymer properties and develop innovative solutions in new material designs (Nesvadba, 2012; Takahashi, 2024; van Herk and Klumperman, 2024).

In summary, monomer reactivity ratios play a critical role in understanding the fundamental mechanisms of copolymerization. The detailed study of data on the selection of monomers and their interactions enables the design of innovative and high-performance materials in polymer engineering. Therefore, the determination and evaluation of reactivity ratios is not only an academic field of study, but also an important guide for strategic decisions in industrial processes (Akyüz et al., 2006; Haque et al. 2022).

The precise and reliable determination of reactivity ratios is of great importance for the development and synthesis of new polymer materials. Various methods have been developed in the literature for this purpose. The Mayo-Lewis equation is considered a classical model that mathematically expresses the kinetic properties of monomers (Zapata-Gonzales et al., 2025). Furthermore, the Fineman-Ross and Kelen-Tüdös (1980) methods are linear regression-based techniques widely used to predict reactivity rates from experimental data (Pojnar et al., 2024). However, the application of these methods often requires complex calculations, data preprocessing, and rigorous analysis. Furthermore, there may be discrepancies between the results obtained from different methods, leading to difficulties in interpretation (Lynd et al., 2019; Autzen et al., 2024; Jackson and Savoie, 2025).

Recent increases in computing capacity and advances in web technologies have enabled the emergence of easily accessible, interactive, and visually rich analysis tools in the field of polymer chemistry. Such platforms allow researchers to quickly evaluate their experimental data, compare various methods, and visually inspect the results. However, a comprehensive and user-friendly platform that combines multiple reactivity ratio estimation methods, kinetic simulation, and failure surface analysis is scarce in the literature.

In this study, we developed a web-based analysis platform that integrates Mayo-Lewis, Fineman-Ross, and Kelen-Tüdös methods, works well with both synthetic and real experimental data, and provides dynamic visualizations. In addition, a Runge-Kutta-based kinetic simulation module, which simulates the change of monomer concentrations over time and provides a better understanding of the copolymerization process, is also included in the platform. The designed system aims to serve as a valuable tool for polymer scientists and engineers in both education and research fields.

2. Theoretical Background

Reactivity ratios refer to the tendency of a monomer to join to the chain end formed from its own species or other monomer species. These ratios are usually denoted by r_1 and r_2 and are defined as follows (Araujo et al., 2002; Beckingham et al., 2015).

$$r_1 = k_{11}/k_{12}, r_2 = k_{22}/k_{21} \tag{1}$$

Here, k11 and k22 are the rate constants for the addition of monomer 1 of its own species and monomer 2 of its own species to the chain end, respectively. k12 and k21 are the rate constants for the addition of monomers of other species to the chain ends. The copolymer composition is a function of the feed rates f1 and f2 and the reactivity ratios. The instantaneous copolymer composition F1 (mole fraction of monomer 1 in the copolymer) is expressed by the following Mayo-Lewis equation (Zapata-Gonzales et al., 2025).

$$F_1 = \frac{r_1 {f_1}^2 + f_1 f_2}{r_1 {f_1}^2 + 2 f_1 f_2 + r_2 {f_2}^2} \tag{2}$$

This equation shows how the copolymer composition changes depending on monomer feed rates and reactivity ratios (Odian, 2004; Hasirci et al., 2011).

Predicting reactivity ratios from experimental data is a critical step in copolymerization studies. Various methods have been developed for this purpose.

The Mayo-Mayo-Lewis equation mathematically describes the relationship between copolymer composition and feed rates. The reactivity ratios r1 and r2 are estimated using optimization algorithms that minimize the difference between the experimentally measured copolymer composition and the theoretical composition. In this study, the following error function was minimized using the Levenberg-Marquardt algorithm (Fienen et al., 2025):

$$Error = \sum_{i=1}^{n}(F_{1,exp,\,i} - F_{1,calc,i})^2 \tag{3}$$

Where $F_{1,exp,i}$ is the experimentally measured mole fraction of monomer 1 in the copolymer for the i^{th} data point, and $F_{1,\,calc,i}$ is the corresponding mole fraction calculated using the Mayo-Lewis equation.

The Fineman-Ross Method is based on linear regression. Using equation (4), where F is the copolymer composition and f is the feed ratio, f (F-1) / f and f_2/F values are calculated, the graph is plotted, and r_1 and r_2 are estimated from the intersections with the slope.

$$\frac{f(F-1)}{F} = r_1\frac{f^2}{F} - r_2 \tag{4}$$

The Kelen-Tüdös method is similar to the Fineman-Ross method, but the parameter α is defined to give more reliable results. Using the values in expression (5), where H = f2/F, reactivity ratios are estimated from the linear relationship in equation (6).

$$\alpha = \sqrt{H_{\min}.H_{\max}},\ \eta = \frac{f(F-1)}{F(\alpha+H)},\ \xi = \frac{f^2}{F(\alpha+H)} \tag{5}$$

$$\eta = r_1\xi - \frac{r_2}{\alpha} \tag{6}$$

In the copolymerization process, the concentration of monomers varies with time. The differential equations of the kinetic model for this variation are given in (7) and (8), where $[M_1]$ and $[M_2]$ are monomer concentrations and $[M_1^*]$, $[M_2^*]$ are active chain end concentrations. Various numerical methods solve these equations. In this study, we modeled the time-dependent variation using the 4th-order Runge-Kutta method. The 4th order Runge-Kutta method is a widely used technique for obtaining numerical solutions of differential equations (Ahmed et al., 2015). The basic idea of this method is to calculate the slope at multiple intermediate points to represent the curve of a function more accurately. First, the starting point of the solution is determined. Then, the step size of the solution is chosen.

After this step, four different intermediate slopes are calculated. The first slope is the value of the function at the starting point. The second slope is obtained by increasing the current values by half a step. The third slope is calculated using the updated values, again by half a step. Finally, the fourth slope is calculated with values incremented by a full step. The new value is determined using the average of these four intermediate slopes. Then, the x value is increased by the step size. This process is repeated until the desired solution range is reached. The 4th order Runge-Kutta method is frequently preferred in engineering and scientific research due to its high accuracy and wide range of applications (Jerbi et al., 2025).

$$\frac{d[M_1]}{dt} = -k_{11}[M_1^*][M_1] - k_{21}[M_2^*][M_1] \tag{7}$$

$$\frac{d[M_2]}{dt} = -k_{22}[M_2^*][M_2] - k_{21}[M_1^*][M_2] \tag{8}$$

2. Material And Method

3.1. Software Development

The developed copolymer analysis tool was created as a web-based application using HTML, CSS, and JavaScript. The user interface was designed to allow researchers to easily enter experimental data, select analysis methods, and visualize results.

3.2. Technologies Used

HTML, CSS, JavaScript: They form the basis of the web interface. HTML structures the content, while CSS provides visual design and organization. JavaScript manages user interaction and dynamic features.

Plotly.js: Used for the creation of dynamic and interactive graphics. Various visualizations, such as error surface plots, kinetic simulations, and linear regression plots, are provided with this library.

Numeric.js: Used for mathematical calculations such as matrix operations and optimization algorithms.

PapaParse: Used for parsing CSV files and easy import of data sets.

3.3. User Interface

The user interface includes input fields for entering experimental data, buttons to start analysis, and dynamic graphs to visualize results. The graphics are interactive, allowing users to examine the data closely, zoom in, and see detailed information.

3.4. Data Entry and Processing

The copolymer analysis tool supports both synthetic and experimental data entry.

3.4.1. Synthetic Data Generation:

Synthetic data is generated using an algorithm that simulates copolymerization experiments according to user-defined reactivity ratios and noise levels. This feature allows users to test the tool and explore the effects of different parameters on the analysis results. Here, a synthetic data-generating function was first defined. The values $r_1 = 0.46$ and $r_2 = 0.52$ were chosen for use in this function. These are the actual parameters used to generate the synthetic data. The function calculates the theoretical copolymer fractions for the specified actual reactivity ratios and feed fractions. It then adds small random noise to these fractions, generating a synthetic data set similar to the actual experimental data. This synthetic data is reflected in the table in the user interface.

3.4.2. CSV File Upload and Data Editing:

Experimental data can be imported into the tool by uploading in CSV (Comma Separated Values) format. The CSV file needs to be in a specific format, which includes columns for monomer feed rates and copolymer compositions. Once the CSV file is uploaded, the data is validated and cleaned to ensure consistency. The data is then displayed in tabular form so that users can review and edit the data before starting the analysis.

3.5. Analysis Methods

The copolymer analysis tool applies the following methods to estimate reactivity ratios:

3.5.1. Mayo-Lewis Method

Initially, values of 1.0 are assigned for r_1 and r_2. In each iteration, the estimated F_1 is calculated for each data point according to the Mayo-Lewis model, and the difference (residual) with the experimental $F_{1,exp}$ is found. The derivatives of these residual values with respect to r_1 and r_2 are approximated numerically to form the Jacobian matrix (J). Within the scope of the Levenberg-Marquardt algorithm, the product of the transpose of the Jacobian matrix (J^T)and the Jacobian and the product of the Jacobian and the residual vector are calculated; the stability of the algorithm is increased by applying a damping factor (1 + λ) to the diagonal elements of the matrix (Equation (9)). In Equation (9) Δp is the parameter update (r_1 and r_2 are updated by Δ).

$$(J^T J + \lambda I)\Delta p = J^T(ycalc_{exp}) \qquad (9)$$

Then, by solving the system of linear equations, the parameter update amounts are found and r_1 and r_2 are updated with these delta values. When the update amounts fall below the specified tolerance, the iteration is terminated and the estimated r_1 and r_2 values are displayed on the screen. Then, with the plotContour() function, equally spaced values between 0.1 and 2.0 are set for the parameters r_1 and r_2 and the total squared error is calculated using the experimental data for each pair of parameters. These error values are stored in a matrix to represent the z-axis and contour plotted using the Plotly library; in the plot, the x and y axes show the values of r_1 and r_2, respectively, while the true values are marked with a red star and the predicted values with a white cross. Readability and aesthetics are improved by editing the graph title, axis names, and fonts. Thus, the Levenberg-Marquardt algorithm determines the optimal reactivity ratios by minimizing the sum of squared errors between the experimental data and the predictions of the Mayo-Lewis model. These results are visually presented on the error surface.

3.5.2. Fineman-Ross Method

This method uses linear regression to estimate reactivity ratios from experimental data.In the Fineman-Ross method, the G and H values for each experimental data point are calculated using the relevant formulas. Then, the best linear fit, i.e. slope and y-intercept, is found by taking the H values as the independent variable and the G values as the dependent variable through the function linearRegression(x, y). As a result of this regression, the slope is assigned as r_1 and the y-intercept as $-r_2$. The function returns the calculated r_1 and r_2 values, as well as the G and H data, as output. In summary, the Fineman-Ross method estimates reactivity ratios by linear regression on G and H values derived from experimental data, and this process is explicitly and directly implemented in the code in the calculateFinemanRoss() function.

3.5.3. Kelen-Tüdös Method

The model uses linear regression to predict reactivity rates from experimental data.

The Kelen-Tüdös method is a linearization method for estimating reactivity ratios similar to the Fineman-Ross method, but it provides more stable and reliable results. In this study, this method was implemented by calculating the values of G and H for each experimental data point, where G and H are found by the formulas $G = f(F-1)/F$ and $H= f^2/FH$, respectively. Then the parameter α, the geometric mean of the smallest and the largest of the H values, is calculated. The values of ξ and η for each data point are determined from equation (6). Linear regression is performed on these ξ and η values to find the slope and y-intercept. Finally, using the reactivity ratios r_1 and r_2, slope and y-intercept, r1=slope + intercept and r_2 = -intercept.α. Thus, the Kelen-Tudös method estimates reactivity ratios, including the parameter α, from the values of G and H derived from experimental data. This process is implemented systematically and explicitly in the code within the calculate KelenTudos() function.

3.6. Kinetic Simulations

Kinetic simulations were performed using the Runge-Kutta 4th order method to solve ordinary differential equations (ODEs) describing dynamic changes in monomer concentrations during copolymerization, and the simulation parameters (such as initial monomer concentrations and reaction rate constants) can be set by the user. In this study, the Runge-Kutta method was implemented as a classical 4th order algorithm in the rungeKutta4() function, with the parameters initial time, initial state, step size, and total number of steps. At each iteration, four intermediate slopes are calculated using the function defining the differential equations. The new state value is determined by taking the weighted average of these slopes. The time is advanced by one step, and this process is repeated for all steps. The time and state values are then recorded. In the runSimulation() function, the initial concentrations and time interval are determined, and the Runge-Kutta function is called. The differential equations describing the variation of monomer concentrations with time are contained in the odes() function. As a result, the polymerization kinetics is solved numerically by the Runge-Kutta method, and the obtained time-concentration data are visualized graphically.

4. Results And Discussion

The web-based copolymer analysis tool developed in this study can analyze both synthetic and experimental data by integrating different reactivity ratio estimation methods. In addition, with the kinetic simulation module, the time-dependent change of monomer can be observed. The buttons at the top of Figure 1 and their functions can be summarized as follows. Upload CSV File: Allows users to upload a CSV file containing their pre-prepared experimental data. The uploaded file is read with the PapaParse library and the data is imported into the table. Generate Synthetic Data:Generates a synthetic experimental data set using the actual reactivity ratios defined in the script ($r_1 = 0.46$, $r_2 = 0.52$) and specific f_1 values, with small random noise added. This is used for analysis and testing purposes.Estimate r_1 and r_2 (Mayo-Lewis): Estimates reactivity ratios with the Levenberg-Marquardt algorithm using the Mayo-Lewis model on the current data set and displays the results on the screen. Run Simulation: Simulates the time-dependent change of monomer concentrations using the Runge-Kutta method and generates a kinetic graph. Analyze All Methods: Runs Mayo-Lewis prediction, Fineman-Ross and Kelen-Tüdös analyses sequentially and presents all results with graphs.

These buttons allow users to easily perform basic operations such as data loading, data generation, parameter estimation and simulation.

The f_1 (Feed) and F_1_exp (Copolymer) values in the table in Figure 1 are generated by the generateSyntheticData() function defined in the code. This function uses $r_1 = 0.46$ and $r_2 = 0.52$ as the actual reactivity ratios and applies the Mayo-Lewis equation for five different predefined feed fractions f_1. For each f_1 value, the theoretical copolymer fraction is calculated and a small random noise is added to this value to generate F_1_exp values that appear to be experimental. These values are bounded between 0 and 1 and transferred to the table. Here f_1 is the initial mole fraction of monomer 1 entering the copolymerization reaction, i.e. its proportion in the mixture, while F_1_exp is the mole fraction of monomer 1 in the copolymer product, i.e. its proportion in the copolymer chain. These values may differ from f_1 depending on the copolymerization kinetics and reactivity rates. Thus, these synthetic data are used to test the accuracy of the model and analysis methods.

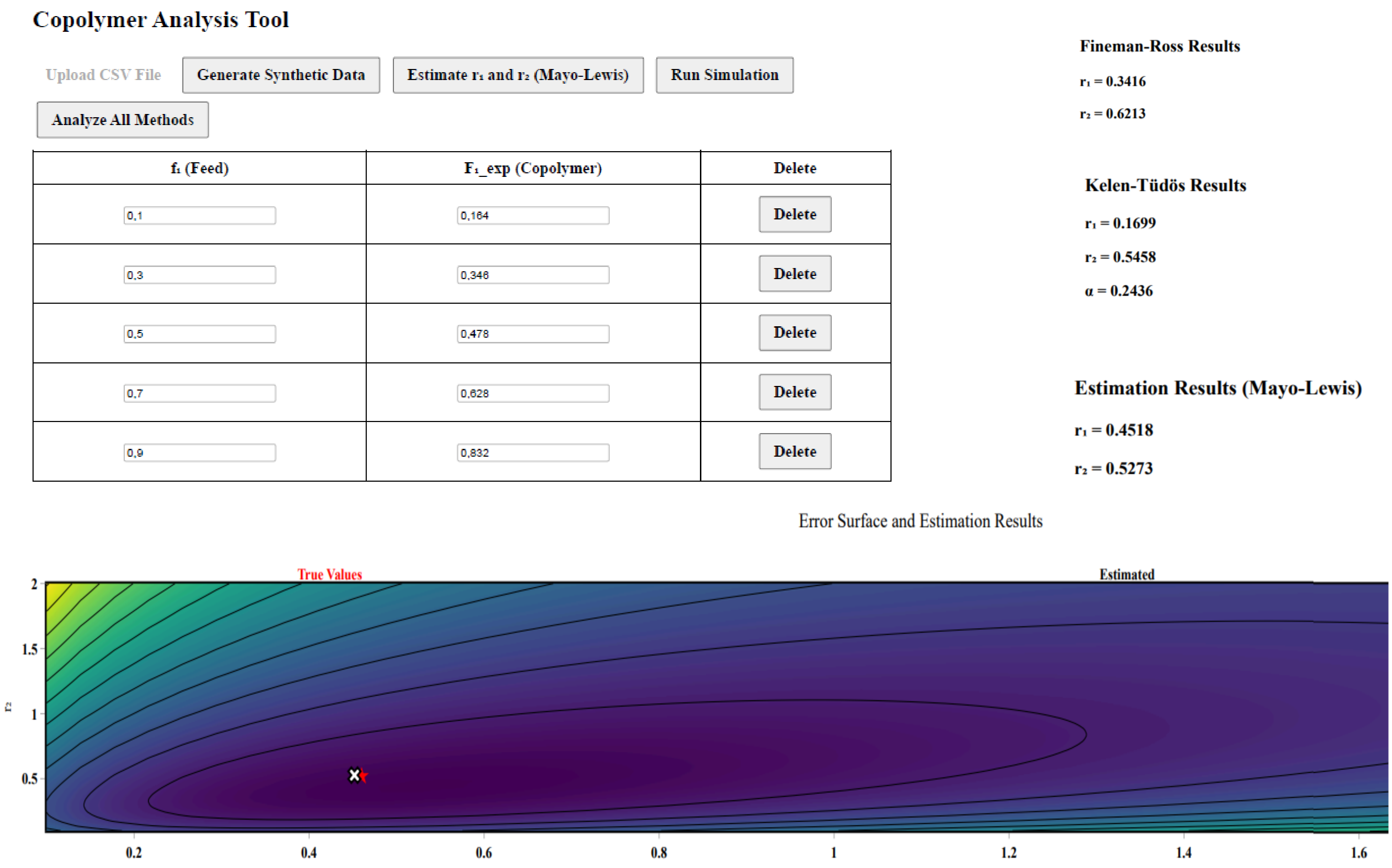
The "Error Surface and Estimation Results" graph in Figure 1 visually represents the error surface and parameter estimation results generated by the plotContour() function in your script. This plot consists of the total squared errors for the copolymerization reactivity ratios r_1 and r_2, calculated on a grid of 50 values equally spaced from 0.1 to 2.0, shown in a color scale. For each (r_1, r_2) pair, an estimated F_1 is calculated by the Mayo-Lewis equation using the values of f_1 and F_1_exp in the experimental data, and the total error is found by summing the squares of the differences between this estimate and the experimental value. This total error is expressed in color intensity as the z-axis on the graph, with darker colors indicating higher error and lighter colors indicating lower error. Thus, regions where the error surface is minimal represent areas of optimal reactivity ratios. In the graph, the red star symbol indicates the true reactivity ratios (e.g., r_1=0.46, r_2=0.52) used in the generateSyntheticData() function in the script. The white cross indicates the estimated values (e.g., r_1=0.4518, r_2=0.5273) calculated using the Levenberg-Marquardt algorithm with the estimateRR() function. These markings give a visual indication of how close the estimated parameters are to the true values. The axes and the title of the graph are arranged in Times New Roman font and bold font style, and the axis lines are designed in bold and black color. In addition, "True Values" and "Estimated" labels are placed on the chart with color and symbol descriptions. These arrangements enhance the readability and aesthetic appearance of the chart. As a result, this error surface plot provides the user with a comprehensive view of the accuracy of the parameter estimation and how the error structure of the model is distributed. Thus, the performance and reliability of the Mayo-Lewis model for predicting copolymerization reactivity rates are visually assessed.

Below the Error Surface and Estimation Results graph is a graph showing the detailed time-dependent variation of the monomer concentrations in the kinetic simulation performed using the Runge-Kutta 4th order method. In this simulation, differential equations describing how the concentrations of monomer 1 (f_1) and monomer 2 (f_2) change during the polymerization process were determined with the odes() function. Initial concentrations of $f_1 = 0.5$ and $f_2 = 0.5$ were taken as initial concentrations. The rungeKutta4() function solves these differential equations numerically and calculates the values of f_1 and f_2 over a total of 200 steps between 0 and 10 time units, with a step size of 0.05. This time series data is visualized on a graph using the Plotly library via the runSimulation() function. In the graph, the concentration of monomer 1 is initially 0.5 and decreases over time to about 0.05, while the concentration of monomer 2 similarly starts at 0.5 and decreases over time. This decrease reflects the progress of the polymerization reaction and the incorporation of monomers into the copolymer chain. Thus, this graph provides an important tool for understanding the dynamic nature of copolymerization kinetics, studying reaction rates and evaluating the effects of different initial conditions. Through this simulation, users can make comparisons with experimental data and better understand the influence of kinetic parameters.

Figure 1 presents a detailed graph of the analysis results by the Fineman-Ross method under monomer concentration variation simulation, along with a visual representation of the numerical values. The graph presents the values of G and H on the axes, derived from the experimental data, where G = f(F-1)/F and H = f^2/F. These values are calculated from experimental data f_1 (feed fraction) and F_1_exp (copolymer fraction). The data points are marked on the graph as a scatter plot and the linear regression line for these points is drawn. The regression line represents the basic relationship used to predict reactivity rates in copolymerization kinetics. In the upper corner of the graph, the reactivity ratios $r_1 \approx 0.3416$ and $r_2 \approx 0.6213$ obtained from the regression are numerically indicated. The Fineman-Ross method is a classical method of choice for quickly and simply estimating reactivity ratios from copolymerization experiment data. In code, this analysis provides the user with a better understanding of the copolymerization process by presenting the kinetic parameters both numerically and visually. Thus, the user can reliably evaluate reactivity ratios in the light of experimental data and make comparisons with different methods.

The Kelen-Tudös plot in Figure1 is the output of the plotKelenTudos() function in your script and visually represents an advanced linearization method for the estimation of copolymerization reactivity ratios. The graph shows the values of ξ (xi) and η (eta) calculated from experimental data on the axes, where $\xi = H/(\alpha + H)$ and $\eta = G/(\alpha + H)$. The values of H and G are derived from the experimental f_1 and F_1_exp data, while the parameter α is calculated as the square root of the difference between the minimum and maximum of the H values, increasing the stability of the regression. On the graph, the data points are marked as a scatter plot and the linear regression line for these points is drawn. In the upper corner, the reactivity ratios $r_1 \approx 0.4681$, $r_2 \approx 0.5130$, and $\alpha \approx 0.2436$ are indicated numerically. This method gives more reliable and stable results than the Fineman-Ross method and is particularly robust to noise and measurement errors in experimental data. This analysis in the code provides the user with the necessary parameters for a more accurate understanding of copolymerization kinetics, both numerically and visually. Thus, the user can reliably evaluate kinetic parameters in the light of experimental data.

The three different reactivity ratio estimation methods used in the study have distinct advantages and limitations. While the Mayo-Lewis method provides more precise and flexible results due to its optimization-based structure, it takes longer to compute than other methods. The Fineman-Ross method stands out with its simplicity and rapid applicability, but should be used with caution as it is more sensitive to data quality. The Kelen-Tüdös method, on the other hand, provides more balanced and reliable results in large data ranges, but is a bit more complex in terms of calculation and interpretation. By integrating these methods, the developed tool provides a comprehensive analysis and allows the user to choose the appropriate method for different data sets. Furthermore, the kinetic simulation module enables a better understanding of the copolymerization process. In this way, it can be used as a powerful support tool for polymer design and optimization in both academic research and industrial applications



f₁ (Feed)	F₁_exp (Copolymer)	Delete
0,1	0,164	Delete
0,3	0,346	Delete
0,5	0,478	Delete
0,7	0,628	Delete
0,9	0,832	Delete

Fineman-Ross Results

$r_1 = 0.3416$

$r_2 = 0.6213$

Kelen-Tüdös Results

$r_1 = 0.1699$

$r_2 = 0.5458$

$\alpha = 0.2436$

Estimation Results (Mayo-Lewis)

$r_1 = 0.4518$

$r_2 = 0.5273$

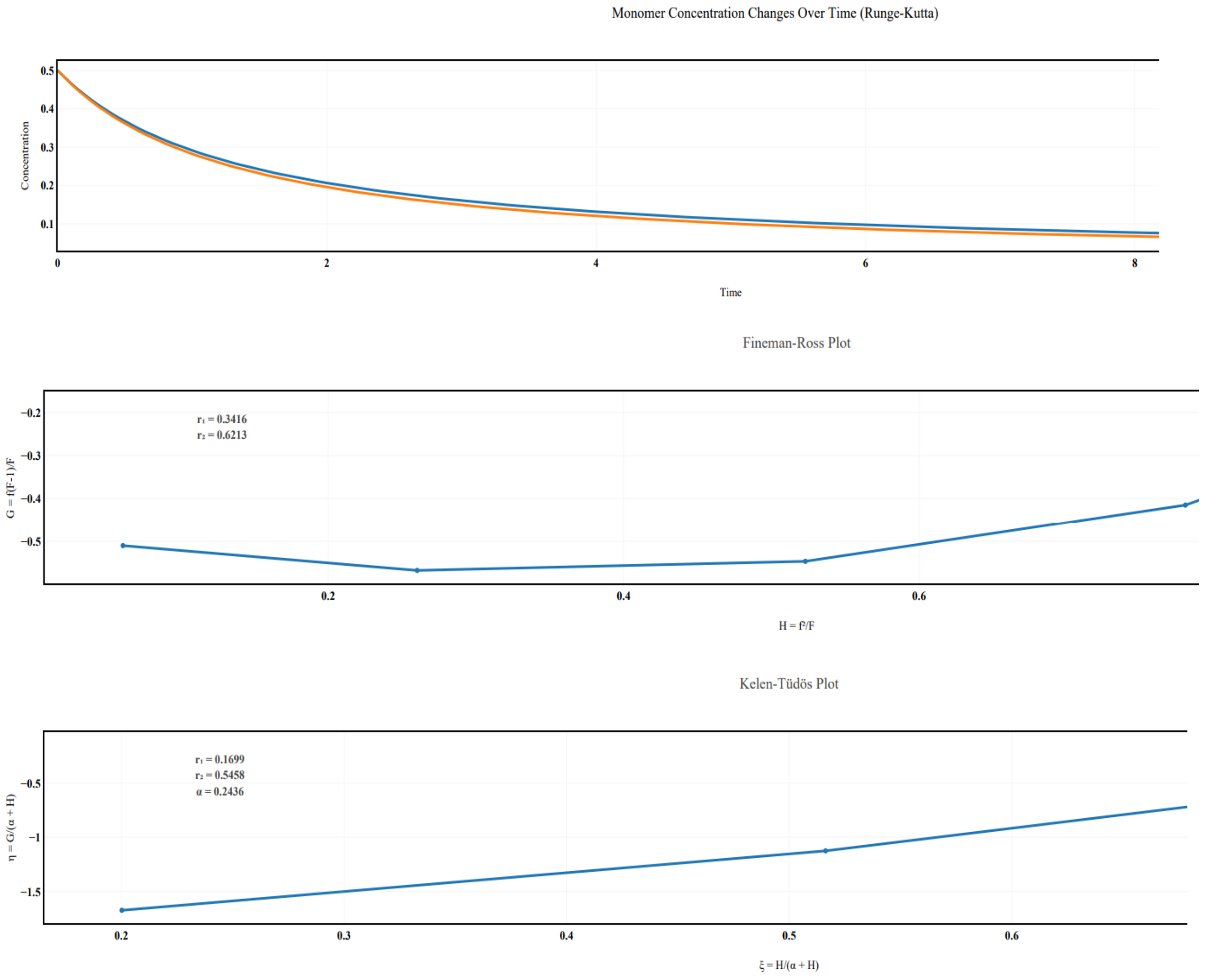


Figure 1. Screenshot of the website for the copolymerization process

5. Conclusions

Accurate and reliable determination of monomer reactivity ratios plays a critical role in effective control of the copolymerization process and achievement of targeted polymer properties. The analysis tool developed in this study integrates Mayo-Lewis, Fineman-Ross, and Kelen-Tüdös methods to provide a flexible and comprehensive evaluation tool that can adapt to different data sets. Furthermore, thanks to the Runge-Kutta-based kinetic simulation module, the time-dependent variation of monomer concentrations can be modeled numerically and compared with experimental data to understand the reaction dynamics better. This integrated approach provides powerful support for optimizing polymer design and production processes in both academic research and industrial applications. In addition, using the platform in polymer physics and chemistry education allows students to reinforce theoretical knowledge with practical applications, enriching the learning process. Thanks to the modern web technologies and open source libraries used, the tool is both accessible and user-friendly, which is a significant advantage for researchers and educators. In conclusion, the developed platform provides a comprehensive, reliable, and interactive solution for the analysis of copolymerization kinetics and reactivity rates, making valuable contributions to both research and educational activities in the field of polymer science.

The simulation is available on

https://aliakyuz12.github.io/copolymer/.

Ethics Committee Approval

N/A

Peer-review

Externally peer-reviewed.

Author Contributions

Conceptualization: A.A.; Investigation: K. K..; Material and Methodology: A.A., K.K.; Supervision: A.A..; Visualization: K.K..; Writing-Original Draft: A.A.; Writing-review & Editing: A.A.; Other: All authors have read and agreed to the published version of manuscript.

Conflict of Interest

The authors have no conflicts of interest to declare.

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