

Kinetic Predictions Concerning the Long-Term Stability of TKX-50 and Other Common Explosives Using the NETZSCH Kinetics Neo Software

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Abstract: Explosives are used in both military and civilian applications all over the world. Sufficient longevity and good thermal stability are therefore essential for safe handling and safe storage of energetic materials. In this work, five well-known compounds, TKX-50, RDX, HMX, CL-20 and PETN, were investigated by means of different kinetic models, in order to make predictions about their long-term stability. For this purpose, the compounds were synthesized

according to literature-known procedures and thermogravimetric (TG) measurements were performed. The TG plots were analyzed using the Ozawa-Flynn-Wall, Friedman and ASTM E698 kinetic models with the NETZSCH Kinetics Neo software and the activation energy and isothermal long-term stability were determined. Moreover, various climatic predictions of different countries were made.

Keywords: Activation Energy · Energetic Materials · Kinetic Studies · Long-term Stability · Storage Safety

1 Introduction

In order to be used in an industrial scale an energetic compound has to meet certain criteria [1,2], some of them are shown in Figure 1.

Of course, economic aspects like price and yield play a major role during the development of energetic materials. The synthesis should follow a simple route, with a minimal amount of reaction steps, and should ideally start from cheap chemicals, which are potentially recyclable. In addition, the yield of the product should be as high as possible and both reactants and products, should be neither toxic nor harmful to the environment [3].

In addition, the initiation properties and the compatibility [4] of energetic compounds are of high importance, since they are commonly used in mixtures or compositions. Those mixtures usually contain common secondary explosives such as hexogen (RDX), octogen (HMX) or pentaerythritol tetranitrate (PETN) [5–8].

In terms of safe handling the sensitivities of high explosives towards impact, friction and electrostatic discharge (ESD) are important parameters [9]. Those can easily be determined accurately by standardized measurements according to BAM [10]. However, energetic compounds are not only sensitive towards the previously named stimuli but also towards thermal influences. Most energetic compounds are potentially able to undergo self-accelerated decomposition, when exposed to higher temperatures [11]. This process also takes place at room temperature, if the compound is stored for very long periods of time. In order to guarantee safe long-term storage, the explosive compounds must be stable at low and especially at high tem-

peratures. This longevity is important to prevent catastrophic accidents, such as the ammonium nitrate detonation, which recently occurred in Beirut [12].

In order to better forecast the long-term stability, in this work, kinetic predictions were performed using the example of the widely used secondary explosives TKX-50, RDX, HMX, CL-20 and PETN. The structures of these compounds are shown in Figure 2. Since energetic materials are used all over the world and for a wide variety of applications, this work also investigates the stability of named compounds in regard to different climatic profiles like Munich, Washington D.C. and Cairo.

In the following, the long-term stability predictions and calculations for TKX-50 are discussed in detail, and compared to the other commonly known energetic materials. The in-depth results of the other compounds can be found in the Supplementary Information.

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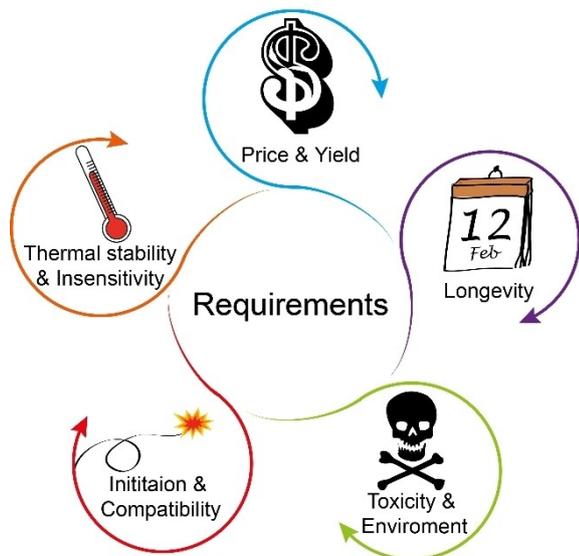


Figure 1. Main requirements of a commercial explosive like TKX-50.

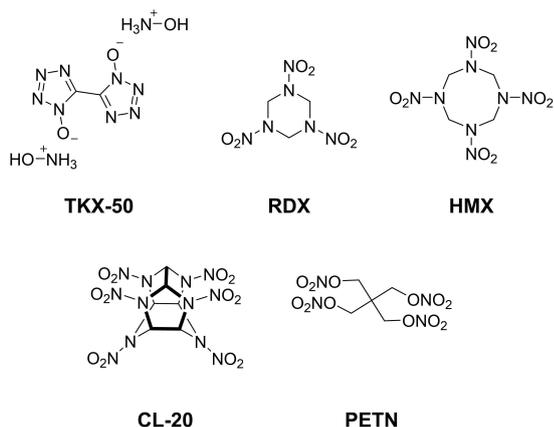


Figure 2. Molecular structures of TKX-50, RDX, HMX, CL-20 and PETN.

2 Experimental Section

All compounds were prepared according to literature-known syntheses [13,14]. They were checked for purity by NMR and elemental analysis.

To evaluate the samples with the NETZSCH Kinetics Neo software [15], thermal gravimetric analysis (TGA) measurements with a PerkinElmer TGA4000 were performed. In order to provide a consistent set of measurements, the samples were dried and sieved to keep them solvent free and within a uniform range of particle size. The measurements were performed at heating rates of 1 Kmin⁻¹ (m = 2.071 mg), 2 Kmin⁻¹ (m = 1.879 mg), 5 Kmin⁻¹ (m = 2.285 mg) and 10 Kmin⁻¹ (m = 2.105 mg) within a temperature range of 303 K to 673 K.

The sample weights of the verification experiment can be found in the SI.

3 Results and Discussion

3.1 Theoretical Background

In order to do predictions of the long-term stabilities, the kinetics of the decomposition processes have to be studied. Based on the data provided by the TGA measurements at different heating rates, kinetic models can be developed to accurately describe the decomposition process [11,16]. Different established theoretical methods like ASTM E698, Ozawa-Flynn-Wall and Friedman have been investigated, to find the model, which best fits the experimental data. All three of those methods are model free approaches, which allow to determine the necessary parameters like activation energies and pre-exponential factors, without assumption of the reaction type. Therefore, a set of several TGA measurements is required [17].

The ASTM method is based on first-order kinetics, determining the activation energy using peak maxima points of the temperature T_p [18]. With the assumption that the extent of the reaction rate at T_p is constant, a set of heating rates β is used to plot $\ln(\beta)$ against $1/T_p$, resulting in a straight line. The slope of this line is proportional to the activation energy. Since decomposition reactions are usually multistep and not first-order reactions, in most cases this approach is not suitable for a decent description of the kinetic behavior of decomposing energetic materials.

Therefore, the Ozawa-Flynn-Wall and Friedman approaches, which are both isoconversional methods and suitable for multiple-step reactions, were investigated [16]. To apply those methods, two assumptions are made. The first assumption of model-free analysis is that the reaction can always be described by eq. 1. It is based on the dependence of the activation energy E_a and the pre-exponential factor A on the reaction progress α .

$$\frac{d\alpha}{dt} = A(\alpha)f(\alpha) \exp\left(-\frac{E(\alpha)}{RT}\right) \quad (1)$$

Secondly it is assumed that the reaction rate at a constant conversion value can be described as a function, which is only dependent on the temperature.

The Ozawa-Flynn-Wall method is an integral isoconversional approach, solving eq. 1 by integration, which results in eq. 2 [19].

$$g(\alpha) = \int_0^1 \frac{d\alpha}{f(\alpha)} = \frac{A(\alpha)}{\beta} \int_{T_0}^T \exp\left(-\frac{E(\alpha)}{RT}\right) dT \quad (2)$$

This equation is transformed into eq. 3 by the approximation according to Doyle [20].

$$\log(\beta) = \log\left(\frac{AE_a}{R}\right) - 2.315 - 0.4567 \frac{Ea}{RT} \quad (3)$$

The graphic logarithm of the heating rate is applied to the inverse temperatures of the points with the same conversion for different heating rates, resulting in straight lines connecting points of same conversion. From the slope of these lines the activation energy and the preexponential factor can be determined [21].

The Friedman approach relies on a differential solution of eq. 1, resulting in eq. 4, where R is the universal gas constant and T is the temperature [22]. The activation energy and the preexponential factor are determined analog to the previous method, by the slope and intersect of the straight lines, connecting points of same conversion when plotting the logarithm of the conversion rate against the inverse temperatures [23].

$$\ln\left(\frac{d\alpha}{dt}\right) = \ln(A f(\alpha)) - \frac{Ea}{RT} \quad (4)$$

In addition to these model-free methods, a model-based approach was investigated for TKX-50. Therefore, again several assumptions were made. The reaction has to consist of a number of reaction steps, and for each of these steps the reaction rate can be described by the kinetic equation 5, depending on the concentration of the initial reactant e_j , the concentration of the product p_j , the preexponential factor A_j and the activation energy E_j . This equation is specific for the reaction step j and the reaction type of each step can be described by the function f_j [24].

$$\alpha = A_j f_j(e_j, p_j) \exp\left[\frac{-E_j}{RT}\right] \quad (5)$$

The second assumption is that the relevant factors including activation energy, preexponential factor, order of reaction and reaction type for each step are considered constant. Lastly, it is assumed that the thermoanalytical signal equals the sum of the signals of the single reaction steps, while the effect of each step is calculated by multiplying the reaction rate with the mass loss of this step.

In case of TKX-50, a three-step decomposition process was observed from the TGA measurements. The best fit to the analytical data was achieved by assuming the first step to be an auto-catalytic reaction of first order and the following two steps reactions of n^{th} order. All investigated models were compared in terms of their fit to the measured data and the results are summarized in Table 1 for the example of TKX-50.

The best fit was achieved using the Friedman method, with an excellent R^2 value of 0.99971. The model-based approach was only slightly lower with an R^2 of 0.99964. In order to calculate long term stabilities, the R^2 value should be around 0.999 to give decent predictions. Therefore, the

Table 1. Comparison of the kinetic models in regard to their fit to the measured data of TKX-50.

Method	R^2 [a]	Sum of dev. squares	Mean Residual
OzawaFlynnWall	0.98085	99829	2.758
ASTM E698	0.98200	93910	4.117
Model based	0.99964	1913	0.607
Friedman	0.99971	1543	0.493

[a] Correlation coefficient.

Friedman method was chosen for all investigated compounds, since it provided the best fit values over all.

3.2 Method Evaluation

In order to obtain a solid set of data, TGA measurements were performed at four different heating rates, shown in Figure 3, for the example of TKX-50. A three-step decomposition process with a sudden mass loss between 180 and 220 °C, depending on the heating rate, can be observed. During the first step a mass loss of about 50% takes place, followed by a slightly flattened second step, which leads to a mass loss of over 80%. The third step is much slower in comparison to the first two, resulting in an overall mass loss of about 90%, when heating to 400 °C.

Following the same method, the remaining four compounds were analyzed. RDX starts decomposing between 160 and 180 °C in a much more unsteady manner compared to TKX-50. This can be explained by partial melting and decomposition showing a mass loss of about 20%. A second step can be observed between 200 and 250 °C, showing a clean decomposition leading to a mass loss of over 95%. In case of HMX the TGA measurements show a one-step decomposition process starting between 230 and

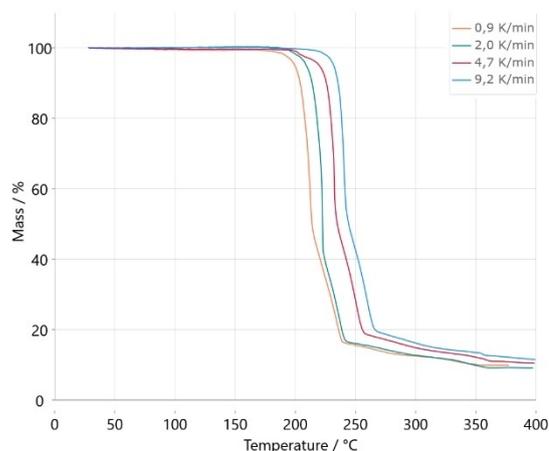


Figure 3. TGA measurements of TKX-50.

260 °C and ending at 260 to 280 °C with a mass loss of 95%. CL-20 has a first decomposition step starting at 200–240 °C and leading to a mass loss of about 90%. A second very slow step takes place between 250 and 400 °C with an additional minor mass loss of 5%. When looking at the measurement of PETN a mass loss of 95–98%, starting at 140–170 °C, depending on the heating rate, can be observed.

Here it has to be mentioned, that in order to improve the accuracy of determining the stability it might be necessary to take the individual characteristics like melting point, vapor pressure and exact decomposition reactions into account. In order to not overcomplicate the analysis and comparison we decided to not take these variables into account.

The measured datasets were now evaluated with the Netsch kinetics Neo software. In order to make long term

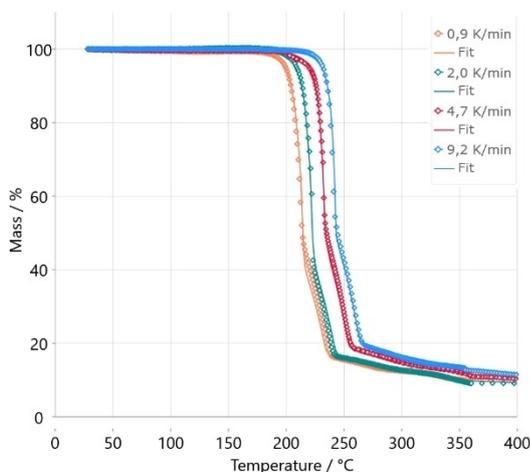


Figure 4. Friedman conversion-fit of TKX-50.

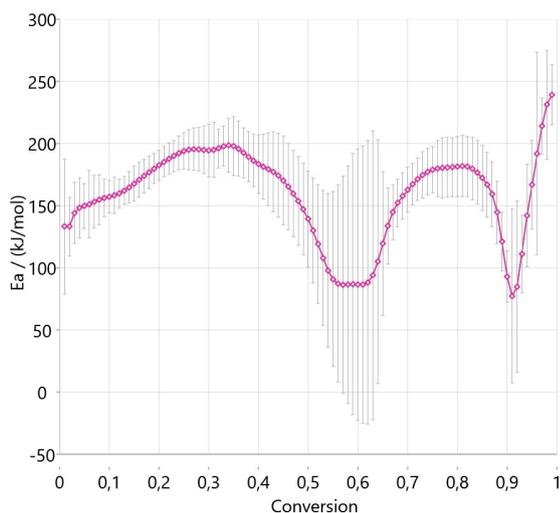


Figure 5. Activation energy applied against the conversion for the decomposition of TKX-50 determined by the Friedman method.

stability predictions the previously established Friedman method was used to describe the decomposition process of all five compounds. These fits of the calculated values compared to the measured data are shown on Figure 4 for the example of TKX-50.

In case of TKX-50, RDX and PETN the Friedman method produced a fit with excellent R^2 values of above 0.999. Due to their very sudden decomposition, HMX and CL-20 showed slightly lower R^2 values of 0.99768 (HMX) and 0.99776 (CL-20), but in order to get a good comparison and full dataset the samples were evaluated even though they did not reach the ideal R^2 value.

3.3 Activation Energy

With the analysis by the Friedman method, the activation energy throughout the decomposition process was determined and depicted against the conversion in Figure 5 for the example of TKX-50 [25,26].

The determined activation energy accurately describes the three-step decomposition process of TKX-50 with three peak maxima. It starts at 133 kJ mol^{-1} and reaches a maximum of 198 kJ mol^{-1} during the first decomposition step which ends with a minimum of 86 kJ mol^{-1} at a conversion of 50%. Afterwards, it rises to a local maximum of 181 kJ mol^{-1} during the second step, followed by a minimum of 77 kJ mol^{-1} . The last decomposition step is characterized by a sudden increase to a peak maximum of 239 kJ mol^{-1} . According to literature the activation energy of TKX-50 was already determined using different methods. Values between 112 kJ mol^{-1} and 176 kJ mol^{-1} were reported, so our predicted value of 133 kJ mol^{-1} fits well to previous calculations [25].

The activation energy plot of RDX also meets the expectations, starting at 170 kJ mol^{-1} . Followed by the first unsteady decomposition step, which is represented by a peak maximum of 238 kJ mol^{-1} : After that a sharp drop to 60 kJ mol^{-1} at a conversion of around 15% could be seen. With the start of the second decomposition step the activation energy rises to 213 kJ mol^{-1} at 30% conversion and then steadily drops down to 40 kJ mol^{-1} at the end of the reaction. In case of HMX the activation energy starts at 95 kJ mol^{-1} and increases to 387 kJ mol^{-1} at a conversion of 20%. From that point it rises slowly to an overall maximum of 428 kJ mol^{-1} at a conversion of about 70% followed by a minor drop to 360 kJ mol^{-1} at the end of the decomposition. The plot for CL-20 shows an initial activation energy of 163 kJ mol^{-1} , which increases to 383 kJ mol^{-1} at a conversion value of about 0.1. The energy value then slowly decreases to 230 kJ mol^{-1} until 85% of the reaction has taken place, where it drops suddenly to 3 kJ mol^{-1} , rises to 143 kJ mol^{-1} and finally decreases again to -354 kJ mol^{-1} , indicating a barrier-free reaction during the final part of the decomposition process. The reaction of PETN starts at an activation energy of 132 kJ mol^{-1} and immediately drops to

44 kJ mol⁻¹ at a conversion of 10%. It then slowly increases to a maximum value of 83 kJ mol⁻¹ at a conversion of 90%, followed by a final sharp drop to -31 kJ mol⁻¹.

3.4 Isothermal Predictions and Long-Term Stability

In order to evaluate all compounds in regard to their long-term stability, isothermal predictions at different temperatures were calculated over a time period of 10 years. Starting at 0 °C we calculated mass loss in 20 °C steps, up to 100 °C, which gives a comprehensive insight into the thermal stabilities of the investigated compounds, ranging from a frozen storage to high-temperature stress. The isothermal prediction for TKX-50 is depicted in Figure 6.

TKX-50 shows excellent thermal stabilities between 0 °C and 40 °C, with no notable mass loss over the predicted time period. Even when stored at 60 °C, which has been measured as a maximum temperature for sea shipping container, the predicted mass loss of TKX-50 is below 2% over 10 years [27]. If TKX-50 is exposed to high-temperature stress of 100 °C the prediction shows a steep mass loss of about 20% during the first 3 years, and a total mass loss of 27% over the entire 10 years.

RDX performs quite similar to TKX-50, with no notable mass loss between 0 °C and 40 °C, but it shows a slightly higher mass loss of about 35% when stored under 100 °C. When looking at HMX, a surprisingly low mass loss of only 5% can be observed, when stored at 100 °C over 10 years, with the majority taking place during the first year. In addition, HMX already has a notable mass loss of 1.5% at 40 °C, which makes it less stable than RDX and TKX-50 at lower temperatures. CL-20 possesses the best overall stability at all measured temperatures. No notable mass loss can be detected up to 60 °C and even at 100 °C the mass loss over ten years barely reaches the 4% mark. In contrast to this,

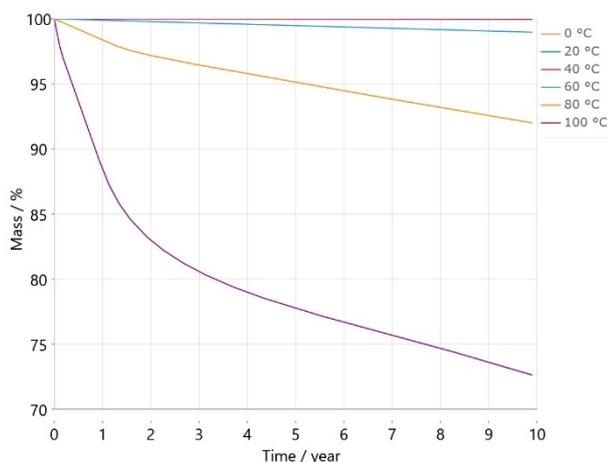


Figure 6. Isothermal predictions of TKX-50 at different temperatures for 10 years.

PETN exhibits the lowest long-term stability of the tested compounds. In this case the prediction does not reflect the actual behavior of PETN in storage, since PETN has a low melting point and an overall higher vapor pressure, which leads to a slight, but constant mass loss up to the decomposition during the TGA measurement. This mass loss process is interpreted by the software as a decomposition and therefore the prediction shows a lower stability than PETN exhibits in reality. Nonetheless the overall trend fits the expectations of PETN being the least stable of the investigated compound. According to the prediction it is stable without mass loss between 0 °C and 20 °C, but already decomposes entirely after 3 years, when stored at 40 °C. Above 60 °C the decomposition takes place in under 3 months.

In order to verify the calculated data, samples of the investigated compounds were placed in an oven at 100 °C for four weeks. The mass loss of each individual compound was measured after 4, 14 and 28 days, respectively and summarized in Table 2.

For a correct interpretation of the experimental values the samples were dried for 2 days in advance to eliminate unwanted mass loss due to moisture. When taking this into consideration, the experimental values certify the calculated stabilities exceptionally well. The mass loss of RDX and TKX-50 is comparable, with TKX-50 showing a slightly better performance when comparing the values of 4 to 28 days. The prediction of HMX showed a higher mass loss during the first months, which is also the case for the experimental data. As expected, CL-20 shows the lowest, and PETN the highest overall mass loss. To provide a better overview, the experimental results are visualized in Figure 7.

3.5 Climatic Predictions

In addition to isothermal temperature predictions, it was also possible to calculate long term stabilities in dependency of climatic data. Therefore the climatic data of different cities was averaged over the last 30 years and used to predict long-term stabilities for the investigated energetic materials, when stored under those conditions. The goal was to include a broad spectrum of different climatic conditions, while still using locations of high international importance. Our final selection included six cities on four different continents, including Munich, Moscow, Washington

Table 2. Mass loss of common explosives at 100 °C over 4 weeks.

Time ^[a] [d]	TKX-50 [mass%]	RDX [mass%]	HMX [mass%]	CL-20 [mass%]	PETN [mass%]
4	0.078	0.070	0.043	0.052	0.083
14	0.080	0.224	0.118	0.027	0.775
28	0.298	0.451	0.792	0.207	1.358

^[a] Time of storage at 100 °C in days.

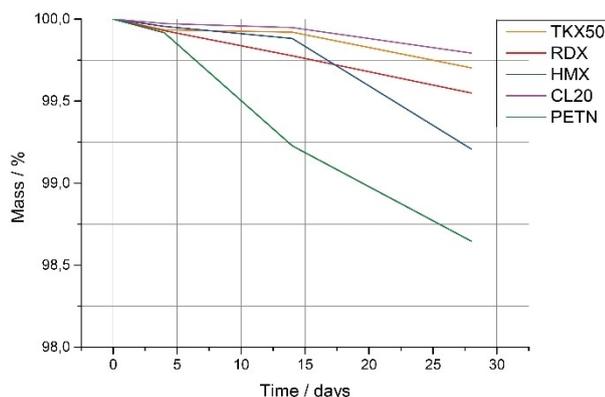


Figure 7. Mass loss of common explosives at 100 °C over 4 weeks.

D.C., Brasilia, Cairo and Beijing, representing Europe, North America, South America, Africa and Asia, respectively.

The climatic predictions for TKX-50 over 10 years are depicted in Figure 8. Similar to the isothermal predictions, TKX-50 shows excellent stabilities under all climatic conditions with a mass loss of below 0.01 mass % during the chosen time period. Even under harsh conditions like the

hot summers in Cairo and the tropical climate in Brasilia, TKX-50 only loses around 0.003% of its mass. But it has to be mentioned, that the humidity is not included in these predictions, as it is assumed that secondary explosives are stored under dry conditions. As expected the milder regions like Europe and North America show even better stabilities, with Moscow having the best values, due to its cold winters. For the other compounds, the observed trend for the isothermal predictions is validated by the climatic predictions. RDX has a comparable performance to TKX-50, while PETN shows the highest mass loss and CL-20 the overall best stability. HMX also fits the isothermal data well, showing a high mass loss at low temperatures in comparison to the other compounds.

4 Conclusion

In order to establish a reliable database about the long-term stability of energetic materials, five commonly known secondary explosives, TKX-50, RDX, HMX, CL-20 and PETN, were investigated in this work. Based on TGA measurements, three kinetic models, the Ozawa-Flynn-Wall method, the ASTM E698 and the Friedman method were evaluated

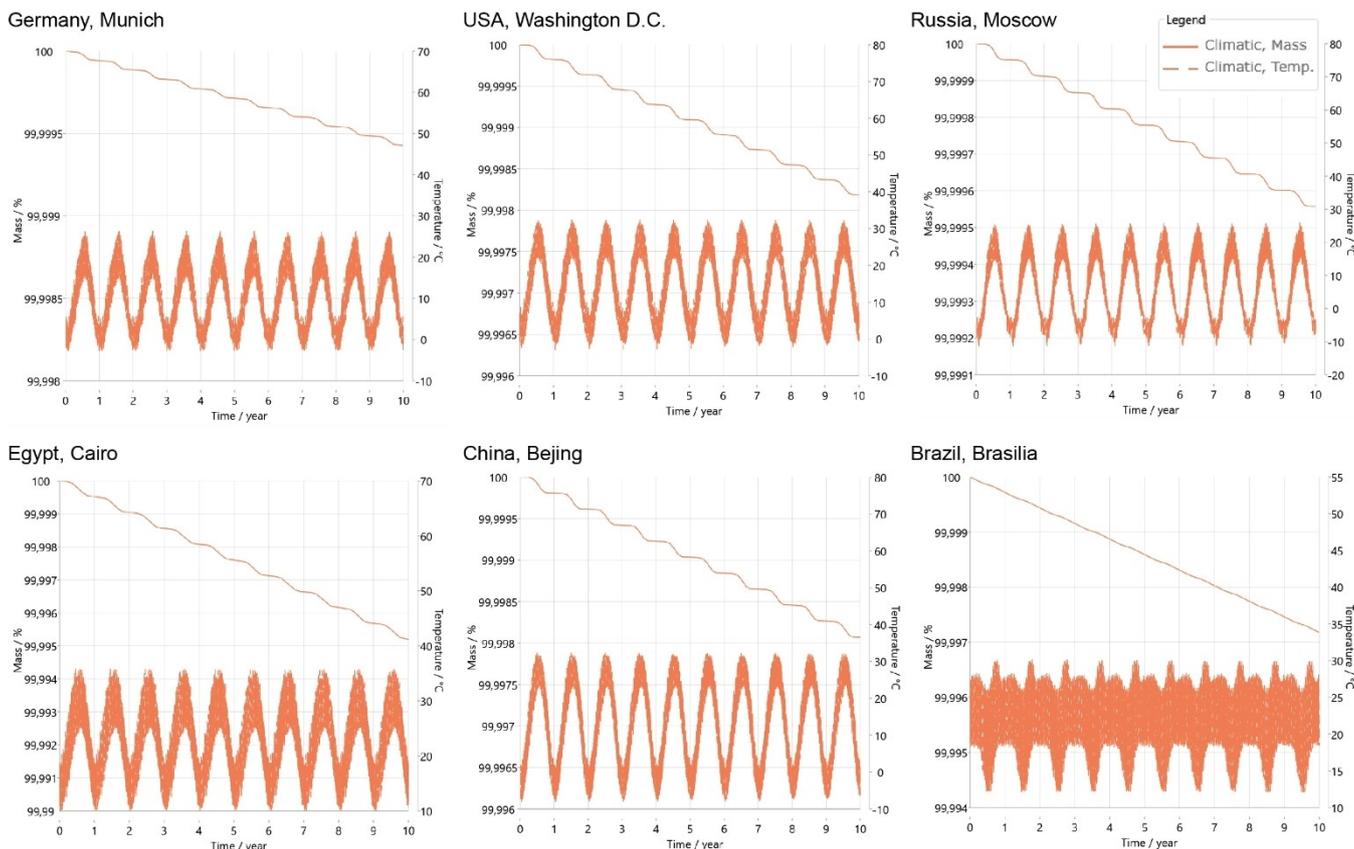


Figure 8. Climatic prediction of TKX-50 for 10 years using the average temperature data of the last 30 years in various different climate zones.

regarding their fit to the experimental data. In all cases, the best results were obtained with the Friedman method, which was used to predict long-term stabilities for the named compounds over 10 years. In summary, the highest long-term stability can be predicted for CL-20 and the lowest for PETN. TKX-50 shows excellent longevity, with a slightly better behavior than RDX. In addition, the long-term stability of TKX-50 was investigated in regard to various different climatic conditions.

In order to validate the calculated results, the five compounds were stored at 100 °C for 4 weeks and their mass loss was investigated during this time. The obtained data was consistent to the kinetic predictions.

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