

Original paper

Numerical Modelling and Time-to-Threshold Prediction of Spontaneous Combustion in Post-Mining and Abandoned Deposits

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ABSTRACT

Spontaneous combustion remains a significant safety and environmental risk in abandoned stockpiles, spoil heaps, and post-mining deposits containing reactive carbonaceous materials. This study presents an integrated framework for the assessment and prediction of spontaneous combustion risk based on the combined use of long-term monitoring data, statistical trend analysis, and physically based numerical modelling, developed in line with the preventive principles of the FRAM concept.

A three-dimensional numerical model is employed to describe coupled heat and mass transfer in a porous reactive body, explicitly accounting for oxygen transport, low-temperature oxidation, and the influence of atmospheric boundary conditions, including wind-induced aeration. The model provides spatially resolved insight into temperature evolution, oxygen depletion, and the formation of localised hot spots associated with accelerated self-heating.

In parallel, trend-based predictors derived from monitoring time series are used to estimate the remaining time to reach critical thermal conditions. The results demonstrate that the combination of numerical modelling and data-driven prediction enables early identification of hazardous states and improves the reliability of risk assessment.

The proposed framework supports preventive fire-risk management by providing actionable information for targeted monitoring, prioritisation of mitigation measures, and decision-support in post-mining and abandoned storage environments.

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1. Introduction

Spontaneous combustion of coal remains one of the most serious safety and environmental hazards associated with the storage, handling, and long-term deposition of coal and coal-derived materials. Despite continuous improvements in operational practices and monitoring technologies, self-heating processes leading to smoldering and, in extreme cases, open fires still occur in coal stockpiles, waste dumps, and post-mining deposits worldwide (Taraba et al. 2006a; Taraba et al. 2006b; Taraba 2003). These events are associated with significant economic losses, increased greenhouse gas emissions, deterioration of air quality, and risks to both personnel and surrounding communities (Moni and Taraba 2013; Chen and Stott 1993).

The development of spontaneous combustion in coal deposits is governed by a complex interaction of physical, chemical, and environmental factors. Low-temperature oxidation of coal, controlled by coal rank, particle size, moisture content, porosity, permeability, and oxygen availability, leads to gradual heat accumulation within the deposit (Dobal et al. 1983; Akgün and Arisoy 1994; Michalec et al. 2013). If heat dissipation is insufficient, a critical state may be reached,

resulting in accelerated oxidation, rapid temperature increase, and the onset of self-heating. External influences such as atmospheric conditions, wind-induced aeration, solar radiation, and precipitation further complicate the evolution of these processes, making reliable predictions particularly challenging (Moni 2014; Taraba et al. 2014).

Traditional approaches to the assessment of spontaneous combustion risk have relied primarily on empirical indicators, simplified criteria, or qualitative expert judgement (Taraba et al. 2006a; Taraba et al. 2006b). While such methods are valuable for operational decision-making, they often lack the ability to capture the dynamic nature of self-heating processes and their sensitivity to changing boundary conditions. In recent years, increasing attention has therefore been directed towards the use of advanced numerical and statistical methods, which allow integration of long-term monitoring data with physically based models of heat transfer, mass transport, and chemical reactions within coal deposits (Taraba et al. 2011; Zhang et al. 2016; Wang et al. 2003).

Within this context, numerical modelling techniques, including computational fluid dynamics (CFD) and coupled heat- and mass-

transfer models, provide a powerful framework for analyzing the internal behavior of coal stockpiles and waste dumps. By explicitly considering oxygen diffusion, convective transport, heat generation due to oxidation, and the influence of meteorological conditions, these models enable a more realistic description of the evolution of temperature fields and gas concentrations inside coal bodies (Taraba et al. 2014; Nordon et al. 1989). When combined with statistical evaluation of long-term field measurements, numerical models offer the potential not only to interpret observed phenomena, but also to predict the time to reach critical conditions associated with irreversible self-heating (Moni 2014; Zhang et al. 2016).

The importance of predictive approaches has been further highlighted in the framework of the FRAM project (Fire Risk Assessment and Management of European Coal Heaps), which aims to develop comprehensive methodologies for assessing and managing fire risks in coal spoil heaps and post-mining deposits across Europe (Zhang et al. 2022). A key objective of FRAM is the transition from reactive measures towards preventive risk management, based on early identification of hazardous conditions and timely implementation of mitigation measures. Reliable prediction of spontaneous combustion therefore represents a cornerstone of effective fire-risk management strategies (Chen and Stott 1993; Zhang et al. 2022).

This paper addresses the assessment and prediction of spontaneous combustion risk in coal stockpiles through the application of modern numerical and statistical methods. The study builds on an extensive database of long-term field measurements, including temperature monitoring and gas analyses, complemented by laboratory investigations of coal oxidation behavior (Taraba 2003; Dobal et al. 1983). By integrating statistical trend analysis with physically based numerical modelling, a comprehensive framework is developed for evaluating the thermal state of coal deposits and estimating the time to reach critical self-heating conditions (Taraba et al. 2011; Nordon et al. 1989).

The main objective of this work is to demonstrate how combined statistical evaluation of monitoring data and advanced numerical modelling can improve the reliability of spontaneous combustion risk assessment in coal stockpiles and waste deposits. The presented approach contributes to the development of predictive tools that support early warning, targeted monitoring, and timely preventive interventions, in line with the broader goals of the FRAM project and contemporary fire-risk management in post-mining environments (Zhang et al. 2016; Zhang et al. 2022).

2. Methodology and numerical modelling framework

2.1 Overview of the methodological approach

The project methodology is built on an interdisciplinary integration of geotechnical, hydrogeological, hydraulic, and material research. This methodological framework adopted in this study combines long-term field monitoring, laboratory investigations, statistical data evaluation, and physically based numerical modelling. This integrated approach reflects the inherently multi-factorial nature of spontaneous combustion processes in coal stockpiles, where thermal behavior is controlled by the interaction of coal properties, gas transport, heat transfer, and external environmental conditions (Taraba et al. 2006a; Dobal et al. 1983; Moni 2014).

The primary objective of the methodology is not only to describe the current thermal state of a coal deposit, but also to predict the temporal evolution of self-heating processes and to estimate the time required to reach critical conditions associated with irreversible spontaneous combustion. To achieve this, the workflow was structured into four mutually linked components:

1. long-term in-situ monitoring of temperature and gas composition,
2. laboratory characterisation of coal oxidation behaviour,
3. statistical trend analysis of monitored parameters,
4. numerical modelling of coupled heat and mass transfer processes.

This structure ensures that numerical simulations are continuously constrained and validated by experimental and field data, thereby increasing the robustness and practical applicability of the results (Taraba et al. 2011; Zhang et al. 2016; Wang et al. 2003).

2.2 Long-term field monitoring data

The numerical and statistical analyses presented in this study are based on an extensive database of long-term measurements obtained from coal stockpiles and waste dumps operated by selected coal-mining companies. The monitoring programme included continuous or repeated measurements of internal temperatures and concentrations of desorbed gases commonly associated with spontaneous combustion processes, such as carbon monoxide, carbon dioxide, methane, and oxygen (Taraba 2003; Moni 2014).

Temperature monitoring was performed using embedded sensors installed at different depths within the coal body, allowing the spatial and temporal evolution of the thermal field to be assessed. Gas samples were collected both in situ and under laboratory conditions, enabling comparison between field observations and controlled oxidation experiments. In addition to internal parameters, relevant atmospheric data, including air temperature, wind speed and direction, precipitation, solar radiation, and barometric pressure, were recorded and incorporated into subsequent analyses (Moni 2014; Taraba et al. 2014).

The long-term nature of the monitoring programme is particularly important for spontaneous combustion studies, as self-heating processes typically develop over extended time scales. This data set therefore provides a solid basis for identifying trends, correlations, and early indicators of critical thermal behavior (Taraba et al. 2006a; Taraba et al. 2006b).

2.3 Statistical evaluation and trend analysis

Statistical methods were employed as a first step in the assessment of spontaneous combustion risk, serving both descriptive and predictive purposes. Time series of temperature and gas concentrations were analyzed to identify systematic trends indicative of increasing oxidation intensity and heat accumulation (Taraba et al. 2011).

Linear and non-linear regression techniques were applied to evaluate the rate of change of selected indicators and to estimate the time required to reach predefined threshold values associated with critical self-heating conditions. This approach enables a preliminary prediction of the time to spontaneous combustion based solely on monitoring data, providing a valuable early-warning tool for operational decision-making (Moni 2014; Zhang et al. 2016).

However, purely statistical prediction has inherent limitations, particularly when boundary conditions change or when multiple interacting processes influence system behavior. For this reason, statistical trend analysis was not used as a standalone tool, but rather as an input and validation component for the physically based numerical modelling described in the following sections. The exact formulations of the linear and quadratic time-to-threshold predictors, including special-case handling (non-increasing trend, negative discriminant), are summarized in **Appendix B**.

2.4 Numerical modelling concept

To capture the physical mechanisms governing self-heating in coal stockpiles, a numerical modelling framework was developed based on coupled heat and mass transfer with chemical reaction terms. The model explicitly considers oxygen transport within the porous coal body, heat generation due to low-temperature oxidation, and heat dissipation to the surrounding environment (Taraba et al. 2014; Nordon et al. 1989).

The coal stockpile is represented as a porous medium, characterized by effective properties such as porosity, permeability, thermal conductivity, and specific heat capacity, derived from laboratory measurements and literature data (Dobal et al. 1983; Akgün and Arisoy 1994; Michalec et al. 2013). Gas flow within the pile is described by diffusion-dominated transport with possible convective contributions induced by pressure gradients and buoyancy effects. The surrounding atmosphere is modelled to account for wind-induced aeration and external heat exchange. The numerical simulations were implemented using a three-dimensional computational framework, allowing spatially resolved analysis of temperature fields, gas concentrations, and oxidation rates. This approach makes it possible to identify localized zones of increased self-heating intensity and to assess the influence of external factors such as wind and atmospheric conditions on the internal behavior of the coal body (Taraba et al. 2014).

2.5 Integration with FRAM risk-assessment objectives

The developed methodological framework is fully aligned with the objectives of the FRAM project, which emphasizes preventive fire-risk management based on early detection and prediction rather than reactive mitigation (Zhang et al. 2022). By combining statistical evaluation of monitoring data with physically based numerical modelling, the approach enables a more comprehensive assessment of spontaneous combustion risk than traditional empirical methods alone.

Importantly, the methodology supports the identification of critical transition points, at which self-heating processes shift from a reversible to an irreversible regime. Estimation of the time remaining until such a transition provides essential information for planning targeted interventions, optimizing monitoring strategies, and prioritizing risk-mitigation measures at coal stockpiles and post-mining deposits.

3. Numerical model description

This section describes the physically based numerical model developed to analyze self-heating and spontaneous-combustion precursors in coal stockpiles. The model follows the established concept of coupling reactive heat generation with oxygen transport in a porous coal body, while explicitly accounting for wind-driven aeration around the pile and its influence on boundary fluxes (Taraba 2003; Michalec et al. 2013; Taraba et al. 2014; Zhang et al. 2016).

3.1 Model concept and computational domains

A three-dimensional CFD framework was adopted with two interacting domains (Michalec et al. 2013; Taraba et al. 2014; Zhang et al. 2016):

- Coal pile domain (porous medium) — represents the stockpile as a permeable, reactive porous body where oxygen transport, heat conduction, and oxidation occur (Taraba 2003; Dobal et al. 1983; Wang et al. 2003; Nordon et al. 1989).

- Atmospheric (wind) domain — represents turbulent flow around the pile and sets the external convective heat and mass transfer conditions at the pile surface (Taraba et al. 2014; Zhang et al. 2016).

This two-domain approach enables a consistent treatment of wind effects that are known to modify oxygen supply, moisture and heat exchange, and the spatial pattern of hot-spot development in coal piles (Michalec et al. 2013; Moni 2014; Taraba et al. 2014; Zhang et al. 2016).

3.2 Geometry and material parameterisation

3.2.1 Stockpile geometry

The coal stockpile was idealized as a right circular cone with a diameter of 14.00 m, a height of 5.87 m, and a side-slope angle of 40°. This simplified geometry reflects typical operational coal stockpiles and has been commonly used in numerical studies investigating self-heating and spontaneous combustion phenomena (Michalec et al. 2013; Taraba et al. 2014; Taraba et al. 2011).

3.2.2 Coal properties (porous-medium inputs)

The porous coal domain was defined by effective properties derived from operational and laboratory characterization, including moisture content, ash, volatile matter, fixed carbon, porosity, permeability, and representative particle size (Moni and Taraba 2013; Chen and Stott 1993; Dobal et al. 1983; Akgün and Arisoy 1994). The selected parameters correspond to highly reactive brown coal, consistent with laboratory oxidation tests and previous modelling studies (Taraba 2003; Dobal et al. 1983; Wang et al. 2003).

Example parameter set used in the model:

- Moisture: 1.7 wt%
- Ash: 3.0 wt%
- Volatiles: 33.5 wt%
- Fixed carbon: 63.5 wt%
- Permeability: $\kappa = 8.23 \times 10^{-10} \text{ m}^2$
- Porosity: $\epsilon \approx 10\%$
- Representative particle size: 10–20 mm
- Reactivity class: Category I (highly reactive; $q_{30} > 7.5 \text{ J}\cdot\text{g}^{-1}$)

3.3 Governing equations (porous reactive flow + external wind)

The model is based on conservation equations of mass, momentum, species, and energy, formulated for a reactive porous medium in the coal domain and for turbulent flow in the wind domain (Michalec et al. 2013; Taraba et al. 2014; Zhang et al. 2016; Nordon et al. 1989).

In the coal pile, the governing equations describe mass balance in the pore space, momentum transport with permeability controlled resistance, species transport for key indicator gases (O_2 , CO , CO_2 , CH_4), and energy conservation including heat generation due to low temperature oxidation (Taraba 2003; Dobal et al. 1983; Taraba et al. 2011; Wang et al. 2003).

To maintain readability of the main text, the full mathematical formulation of the governing equations and source terms is provided in Appendix A.

3.4 Oxidation kinetics and heat-source formulation

3.4.1 Arrhenius-type oxidation rate

Low-temperature coal oxidation was represented using an Arrhenius-type formulation, where the oxidation rate depends on temperature and oxygen availability (Taraba 2003; Chen and Stott

1993; Taraba et al. 2011; Wang et al. 2003). A representative form used in the model:

$$r_{\text{ox}} = A C_{\text{O}_2} \exp\left(-\frac{E}{RT}\right) \quad (1)$$

with example parameter values:

$A = 13500 \text{ [s}^{-1}\text{]}$ (pre-exponential factor)

$E = 50.5 \text{ [kJ.mol}^{-1}\text{]}$ (activation energy)

$R = 8.3145 \text{ [J.mol}^{-1}\text{.K}^{-1}\text{]}$

T in K (example evaluation at $T=373 \text{ K}$)

3.4.2 Reaction pathways and threshold behaviour

Two simplified reaction regimes were considered, separated by a threshold temperature T_{th} , reflecting the observed acceleration of oxidation above a critical thermal state (Taraba 2003; Dobal et al. 1983; Wang et al. 2003).

- For $T < T_{\text{th}}$: oxidation produces CO_2 , H_2O , and oxidised coal in a „slow“ regime. For $T > T_{\text{th}}$: oxidation yields increased CO_2 and a small CO fraction, representing a „faster“ regime.

3.4.3 Coupling to species and energy source terms

Oxygen consumption was introduced as a sink term in the O_2 transport equation, while heat generation was directly linked to oxygen consumption via a stoichiometric coupling. This ensures consistency between chemical reactions, gas evolution, and temperature rise within the coal pile (Dobal et al. 1983; Taraba et al. 2011; Wang et al. 2003).

3.5 Boundary and initial conditions

3.5.1 Wind inflow profile and meteorological forcing

Meteorological forcing was applied through a standard vertically varying inflow profile and site-based time series where available. The detailed profile definition and parameter values used in the simulations are provided in Appendix A.

3.5.2 Interface conditions at the pile surface

At the interface between the wind domain and the coal domain, continuity of fluxes was enforced:

- convective heat exchange and radiative/solar forcing (if considered) affect surface temperature,
- mass transfer controls oxygen availability at the surface and thus oxidation intensity in near-surface layers.

3.6 Discretisation, mesh and time stepping

The mesh was refined near the pile surface to resolve steep gradients in temperature and oxygen concentration; time-dependent simulations were performed with standard convergence criteria. Full numerical settings (mesh statistics, time-step strategy, solver settings) are reported in Appendix A.

(If solar radiation and precipitation are included later, they can be introduced as additional boundary flux terms rather than altering the core PDE set. (Taraba et al. 2014; Zhang et al. 2016))

3.7 Model outputs and validation strategy

The model provides spatially and temporally resolved outputs including:

- 3D temperature fields $T(x, y, z, t)$,
- oxygen concentration and depletion zones,
- predicted locations of accelerated oxidation (incipient hot spots),
- evolution of indicator gases (CO , CO_2 , CH_4) where reaction coupling is enabled.

Validation is performed by comparing simulated temperature patterns and trend behaviour with long-term monitoring data (temperature probes, gas sampling) and with thermal imaging where available. This comparison is essential to ensure the model can support predictive decision-making (e.g., time-to-threshold estimation) rather than only qualitative interpretation (Moni 2014; Taraba et al. 2014; Zhang et al. 2016).

4. Model outputs and validation strategy

4.1 Overview of simulated thermal and gas-transport behaviour

Numerical simulations provided a detailed spatial and temporal description of temperature fields, oxygen distribution, and indicator gas evolution within the coal stockpile. The results confirm that self heating is a strongly localized process governed by the interaction between internal oxidation kinetics and external boundary conditions, particularly wind induced aeration, which is consistent with previous experimental observations and numerical studies (Taraba 2003; Michalec et al. 2013; Taraba et al. 2014; Zhang et al. 2016).

For all simulated scenarios, temperature increase initiated in near surface or shallow subsurface zones where oxygen availability was highest. Similar localization of early hot spot formation has been reported in both laboratory and field based investigations of coal stockpiles (Taraba 2003; Moni 2014; Wang et al. 2003).

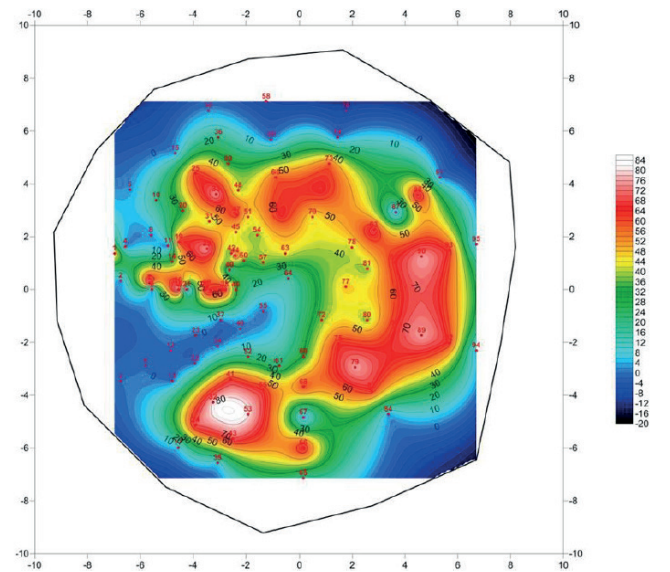


Fig. 1. Spatial distribution of internal temperatures in a horizontal cross-section 1 m above the ground surface, derived from a dense network of monitoring points inside the test pile. The map highlights pronounced thermal heterogeneity and the formation of localised hot spots associated with intensified self-heating.

4.2 Temperature field evolution and hot-spot development

Figure-based analyses of simulated temperature fields (not shown here) demonstrate a gradual transition from a quasi-uniform initial temperature distribution to highly heterogeneous thermal patterns. The onset of accelerated self-heating was marked by the emergence of discrete hot spots, characterized by a rapid local temperature increase once a critical thermal state was exceeded.

The depth and intensity of these hot spots were found to be sensitive to coal permeability and porosity. Higher permeability values facilitated deeper oxygen penetration, resulting in hot spots forming at greater depths below the pile surface. Conversely, lower permeability constrained oxidation to shallow layers, where heat losses to the atmosphere partially mitigated temperature growth. Temporal analysis indicates that the transition from slow oxidation to accelerated self-heating occurs over a relatively short time interval once critical conditions are reached. This non-linear behavior highlights the importance of early detection and predictive assessment, as the window for effective preventive intervention may be limited (Taraba 2003; Wang et al. 2003).

4.3 Oxygen depletion and indicator gas production

Simulated oxygen concentration fields reveal progressive oxygen depletion in regions of intensified oxidation. The spatial correlation

between oxygen consumption and temperature rise confirms the strong coupling between chemical reaction rates and the thermal field.

Increased production of indicator gases, particularly CO and CO₂, was predicted in zones undergoing accelerated self heating. This behavior corresponds well with established interpretations of gas evolution during low temperature coal oxidation and spontaneous combustion processes (Taraba 2003; Chen and Stott 1993; Moni 2014; Wang et al. 2003).

Importantly, the simulations indicate that changes in gas concentrations may precede significant temperature increases at certain locations, supporting the use of gas based indicators as early warning signals (Moni 2014; Taraba et al. 2011).

4.4 Influence of wind and atmospheric boundary conditions

Parametric simulations demonstrate that atmospheric conditions, especially wind velocity, exert a pronounced influence on self heating dynamics. Increased wind speed enhances oxygen supply to the pile, while simultaneously affecting convective heat transfer at the surface.

This dual effect leads to a non monotonic response of temperature evolution to wind intensity, which has also been identified in previous CFD studies of coal stockpiles (Taraba et al. 2014; Zhang et al. 2016). The results confirm that neglecting wind effects may result in underestimation of both the rate and spatial variability of self heating.

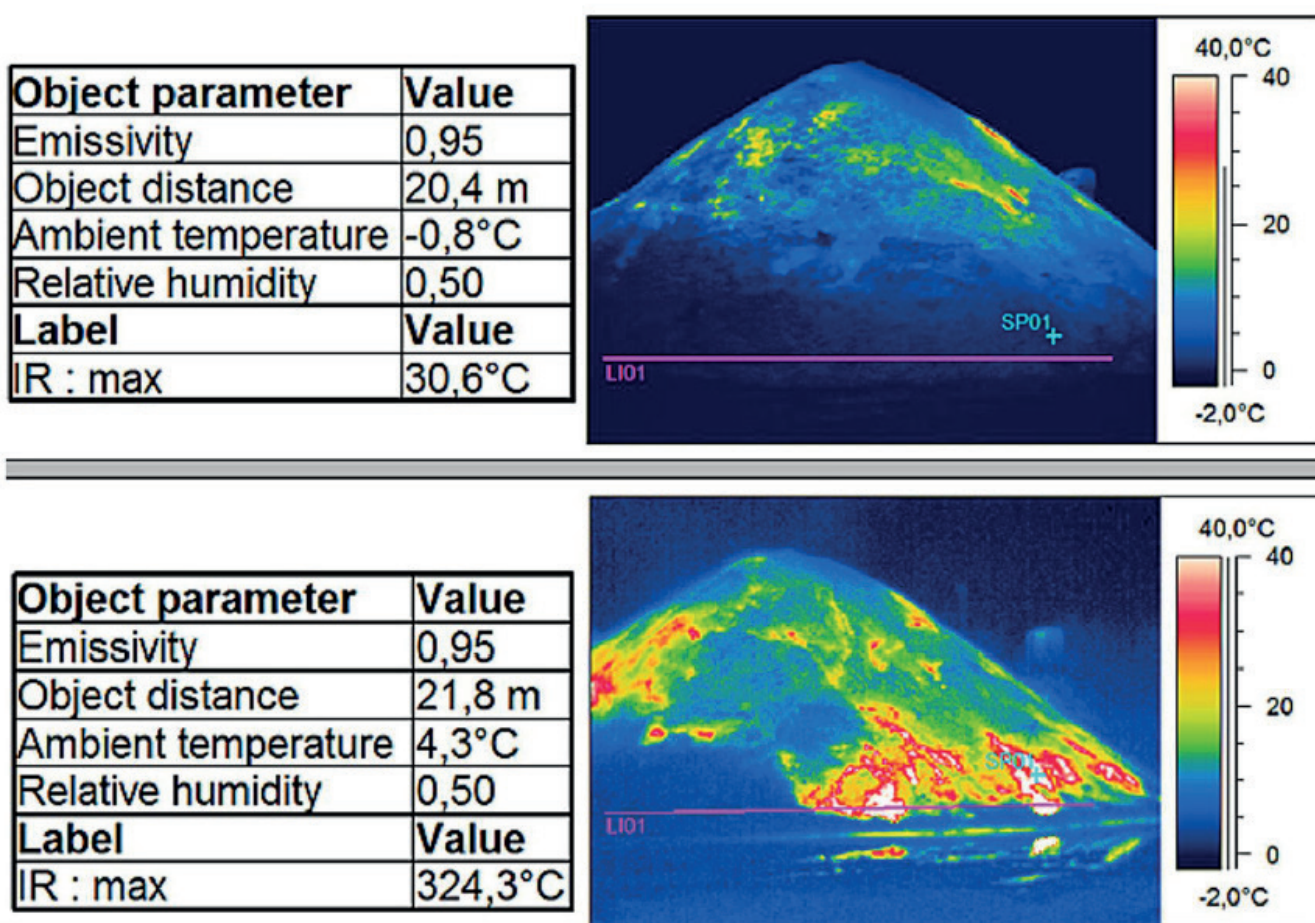


Fig. 2. Infrared thermogram showing surface temperature distribution on the test pile during field monitoring. Elevated surface temperatures correspond to zones of intensified internal self-heating predicted by numerical modelling. The comparison illustrates the temporal evolution of surface heating, with maximum surface temperatures reaching up to 324 °C in the final thermogram.

4.5 Performance of time-to-threshold predictors

Time-to-threshold prediction was evaluated using the linear and quadratic predictors defined in Appendix B.

The linear and quadratic trend predictors were applied to simulated and measured time series of temperature and indicator gas concentrations. Both predictors successfully identified increasing trends associated with developing self heating.

The linear predictor provided robust and conservative estimates of the remaining time to reach critical threshold values, particularly during the early stages of self-heating. Its simplicity and stability make it suitable for routine operational use, especially when monitoring data are limited or noisy.

The quadratic predictor proved more sensitive to acceleration in the monitored variables and yielded shorter predicted times to threshold during phases of rapidly increasing oxidation intensity. While this improves responsiveness, the quadratic predictor is more sensitive to measurement variability and should therefore be applied with caution and in conjunction with expert judgement.

Comparison between predictor outputs and numerical model results shows that trend-based predictions are consistent with physically based simulations when applied within their respective validity ranges. This confirms the suitability of combining statistical predictors with numerical modelling for early warning and risk assessment (Michalec et al. 2013; Taraba et al. 2011; Zhang et al. 2016).

4.6 Comparison with field observations

Quantitative validation of the proposed modelling and prediction framework was based on extensive long term field monitoring campaigns conducted at multiple coal stockpiles and post mining deposits, including sites at Vršany (Hrabák stockpile) and the Jiří open pit mine. The monitoring programmes were designed to capture the spatial and temporal evolution of self heating processes under realistic operational and environmental conditions.

Field measurements were carried out at tens to hundreds of monitoring locations per site, covering different depths and spatial positions within the coal body. Monitoring was performed across different seasons and repeated under varying climatic conditions. Each campaign lasted approximately two months and involved the simultaneous recording of several tens of thermal, gas composition, and environmental variables. As a result, the combined datasets

comprised millions of individual measured values. The complete monitoring programme was repeated seven times over multiple years, enabling observation of different stages of self heating development and providing a robust basis for validation of numerical and statistical approaches (Moni 2014).

For quantitative comparison, representative monitoring locations were selected from sites with continuous long term records and stable sensor operation. Both shallow and deeper probes were included in order to evaluate near surface behavior and internal thermal development. Simulated temperatures were extracted at identical spatial locations and matched time stamps corresponding to the field measurements.

Model performance with respect to temperature evolution was assessed using standard error metrics. The root mean square error (RMSE) and maximum absolute deviation were calculated as differences between simulated and measured temperatures over the evaluated monitoring period. These indicators provide a compact characterization of average predictive accuracy as well as localized discrepancies associated with transient boundary conditions, material heterogeneity, and uncertainty in model input parameters.

The performance of time to threshold prediction was evaluated by comparing predicted threshold crossing times with those inferred from monitoring data. Prediction errors were expressed as the time difference Δt between predicted and observed threshold crossings. Reported error ranges reflect variability observed across the analyzed monitoring scenarios and sensor locations rather than formal statistical confidence intervals.

Representative quantitative indicators derived from this comparison are summarized in Table 1. The reported values characterize typical model and predictor performance under practical field conditions and provide a quantitative basis for assessing the applicability of the proposed framework to early warning and fire risk assessment in coal stockpiles and post mining deposits.

The predictive performance of the linear and quadratic time to threshold approaches is quantitatively supported by comparison with field monitoring data, as summarized in Section 4.6 and Table 1.

5 Discussion

The presented results demonstrate that the combination of physically based numerical modelling and trend based prediction represents a robust approach for assessing spontaneous combustion

Table 1. Quantitative comparison between simulated and measured temperature evolution and time-to-threshold prediction at representative monitoring locations.

Monitoring location / data group	Metric	Value	Value
Shallow probes ($\approx 1-2$ m depth)	RMSE of temperature over monitoring period (K)	3.5–4.2	Agreement within the expected uncertainty range for heterogeneous porous media
Deep probes ($\approx 3-5$ m depth)	RMSE of temperature over monitoring period (K)	4.0–4.8	Stable reproduction of long-term internal thermal evolution
Combined shallow + deep probes	Maximum absolute temperature deviation (K)	≤ 6.5	Localised discrepancies during transient boundary conditions
Linear time-to-threshold predictor	Time-to-threshold prediction error, Δt (days)	8–12 (range across analysed scenarios)	Consistent with conservative early-warning behaviour
Quadratic time-to-threshold predictor	Time-to-threshold prediction error, Δt (days)	4–7 (range across analysed scenarios)	Increased sensitivity during accelerated self-heating phases

Note: Temperature errors are reported as differences between simulated and measured values and are expressed in kelvins; for temperature differences, numerical values in K and °C are equivalent. RMSE and maximum deviation were calculated using matched spatial locations and identical time stamps over the evaluated monitoring periods. Reported ranges of time-to-threshold prediction error reflect variability observed across multiple monitoring campaigns, sites, seasons, and sensor locations, rather than formal statistical confidence intervals.



Fig. 3. The fifth test pile in the Hrabák quarry.



risk in coal stockpiles. The numerical model captures the key mechanisms governing self heating, namely oxygen transport within the porous coal body, heat generation due to low temperature oxidation, and the influence of atmospheric boundary conditions, while statistical predictors provide a practical tool for estimating the time to reach critical states.

A key outcome of the study is the confirmation that spontaneous combustion is a highly localized and non linear process. Both simulations and field data indicate that once critical thermal conditions are exceeded, the transition from slow oxidation to accelerated self heating occurs rapidly, which is consistent with experimental observations and kinetic interpretations reported in the literature (Taraba 2003; Wang et al. 2003). This behavior explains why empirical indicators alone may fail to provide sufficient warning and highlights the importance of predictive methods capable of identifying early acceleration trends.

The explicit consideration of wind effects proved essential. The coupled wind–pile simulations show that external airflow can significantly alter oxygen availability and internal temperature distribution, leading to asymmetric hot spot development. This finding supports earlier CFD based studies demonstrating the promoting role of wind on spontaneous heating dynamics in coal stockpiles (Taraba et al. 2014; Zhang et al. 2016). From a practical perspective, this underscores the need to integrate meteorological data into risk assessment frameworks, particularly for exposed stockpiles and waste dumps.

The comparison of linear and quadratic trend predictors illustrates a trade off between robustness and sensitivity. The linear predictor provides conservative and stable estimates suitable for routine monitoring and early warning, whereas the quadratic predictor responds more rapidly to accelerating trends but is more sensitive to data variability. The results suggest that the greatest benefit is achieved when trend based predictors are not used in isolation but rather interpreted in conjunction with physically based model outputs and expert assessment, as also indicated in previous modelling and monitoring studies (Michalec et al. 2013; Taraba et al. 2011; Zhang et al. 2016).

Within the context of the FRAM project, the proposed framework supports the shift from reactive to preventive fire risk management. By linking long term monitoring data with numerical modelling and time to threshold prediction, the approach enables identification of critical transition points and estimation of the remaining time available for intervention.

Several limitations should be acknowledged. Model accuracy depends on the quality of input parameters, particularly permeability, porosity, and oxidation kinetics, which may vary spatially within real stockpiles. In addition, trend based predictors assume continuity of recent behavior and may be affected by sudden changes in boundary conditions. Nevertheless, these limitations do not undermine the overall applicability of the framework but rather point to the importance of continuous model calibration and integration with updated monitoring data.

6 Conclusions

This study presents an integrated framework for the assessment and prediction of spontaneous combustion risk in coal stockpiles, combining physically based numerical modelling with trend-based analysis of long-term monitoring data. The approach addresses key mechanisms governing self-heating, including oxygen transport in porous coal bodies, heat generation due to low-temperature oxidation, and the influence of atmospheric boundary conditions.

The numerical model provides a detailed description of temperature and gas-concentration fields and confirms that spontaneous combustion is a highly localized and non-linear process. Simulations demonstrate that external factors, particularly wind-induced aeration, play a critical role in controlling oxygen availability and the spatial development of hot spots. These effects cannot be reliably captured by simplified or purely empirical methods.

Trend-based predictors derived from monitoring data were shown to be effective tools for estimating the remaining time to reach critical self-heating conditions. Linear predictors offer robust and conservative early-warning capability, while quadratic predictors are more sensitive to accelerating trends and are suitable for advanced stages of self-heating. The results indicate that the greatest predictive reliability is achieved when statistical predictors are used in conjunction with physically based numerical modelling (Michalec et al. 2013; Taraba et al. 2011; Zhang et al. 2016)

The proposed framework directly supports preventive fire-risk management strategies promoted within the FRAM project. By enabling early identification of hazardous conditions and estimation of the available intervention time, the approach provides practical guidance for targeted monitoring, prioritization of mitigation measures, and reduction of spontaneous combustion risk in coal stockpiles and post-mining deposits.

Future work should focus on further calibration of model

parameters using site-specific data, extension of the framework to long-term climatic variability, and integration into operational decision-support systems. Nevertheless, the results presented here demonstrate that the combined use of numerical modelling and trend-based prediction represents a powerful and practical tool for managing spontaneous combustion risk in coal-handling and post-mining environments.

APPENDIX A. GOVERNING EQUATIONS AND SOURCE TERMS

A.1. Model domain and assumptions (coal pile / porous medium)

The coal stockpile is modelled as a reactive porous medium consisting of a solid coal matrix and a gas phase occupying the pore space. Gas transport within the pile is represented by advection–diffusion in porous media with permeability-controlled resistance, while heat transfer includes effective conduction and convective transport in pore gas. Chemical heat release is driven by low-temperature oxidation following an Arrhenius-type rate law.

A.2. Conservation equations (coal domain)

A.2.1 Continuity (mass conservation)

$$\frac{\partial(\varepsilon\rho)}{\partial t} + \nabla \cdot (\rho\mathbf{u}) = 0 \quad (A1)$$

where ε is porosity (–), ρ is gas mixture density [$\text{kg}\cdot\text{m}^{-3}$], and u is the superficial velocity vector [$\text{m}\cdot\text{s}^{-1}$].

A.2.2 Momentum (porous-medium flow with Darcy resistance)

A Darcy–Brinkman-type formulation is used to account for flow resistance through the pile:

$$\frac{\partial(\varepsilon\rho\mathbf{u})}{\partial t} + \nabla \cdot (\rho\mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot (\mu\nabla\mathbf{u}) + \rho\mathbf{f} - \frac{\mu}{\kappa}\mathbf{u} \quad (A2)$$

where p is pressure [Pa], μ is dynamic viscosity [$\text{Pa}\cdot\text{s}$], κ is permeability [m^2], and f denotes body forces (typically gravity) [$\text{m}\cdot\text{s}^{-2}$]. The last term represents permeability-controlled drag (Darcy resistance).

A.2.3 Species transport (O_2 , CO, CO_2 , CH_4)

For each gas species i in the mixture (e.g., O_2 , CO, CO_2 , CH_4):

$$\frac{\partial(\varepsilon\rho Y_i)}{\partial t} + \nabla \cdot (\rho\mathbf{u}Y_i) = -\nabla \cdot \mathbf{J}_i + R_i + S_i \quad (A3)$$

where Y_i is the mass fraction of species i (–), J_i is the diffusive mass flux [$\text{kg}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$], R_i is the net production/consumption rate due to chemical reactions [$\text{kg}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$], and S_i represents any additional sources (e.g., imposed injection; typically $S_i = 0$ here).

Diffusive flux (Fick’s law in porous medium):

$$\mathbf{J}_i = -\rho D_{i,\text{eff}} \nabla Y_i \quad (A4)$$

where $D_{i,\text{eff}}$ is the effective diffusion coefficient [$\text{m}^2\cdot\text{s}^{-1}$], treated as calibrated/experience-based in the legacy implementation.

A.2.4 Energy equation (heat transfer with reaction heat source)

The energy balance is written for a two-phase porous system (solid + pore gas):

$$\frac{\partial}{\partial t} [\varepsilon\rho_g c_{p,g} T + (1-\varepsilon)\rho_s c_{p,s} T] + \nabla \cdot (\rho\mathbf{u} c_{p,g} T) = \nabla \cdot (\lambda_{\text{eff}} \nabla T) - \sum_i \nabla \cdot (\mathbf{J}_i c_{p,i} T) + S_h \quad (A5)$$

where T is temperature [K], ρ_s , ρ_g are densities of solid and gas phase [$\text{kg}\cdot\text{m}^{-3}$], $c_{p,s}$, $c_{p,g}$ are specific heat capacities [$\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$], $c_{p,i}$ is the species-specific heat capacity, λ_{eff} is the effective thermal conductivity [$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$], and S_h his the volumetric heat source term [$\text{W}\cdot\text{m}^{-3}$].

A.3. Constitutive relations

A.3.1 Effective thermal conductivity

A commonly used mixing law:

$$\lambda_{\text{eff}} = \varepsilon\lambda_g + (1-\varepsilon)\lambda_s \quad (A6)$$

with λ_g and λ_s being thermal conductivities of gas and solid phase, respectively.

A.4. Oxidation kinetics and source terms

A.4.1 Arrhenius-type oxidation rate

Oxidation is represented by an Arrhenius-type rate depending on temperature and oxygen availability:

$$r_{\text{ox}} = A C_{\text{O}_2} \exp\left(-\frac{E}{RT}\right) \quad (A7)$$

where A is the pre-exponential factor [s^{-1}], E is activation energy [$\text{J}\cdot\text{mol}^{-1}$], R is the universal gas constant [$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$], and C_{O_2} denotes the oxygen fraction/availability term (dimensionless; implemented as molar or mass-fraction proxy). Representative parameter values (as used in the legacy model) include $A = 13500$ [s^{-1}] and $E = 50.5$ [$\text{kJ}\cdot\text{mol}^{-1}$].

A.4.2 Oxygen consumption source term

Oxygen consumption is introduced as a sink in the O_2 species equation. In the legacy formulation, the sink is proportional to the oxygen mass fraction and the Arrhenius term:

$$S_{\text{O}_2} = -\rho Y_{\text{O}_2} A \exp\left(-\frac{E}{RT}\right) \quad (A8)$$

with S_{O_2} in [$\text{kg}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$].

A.4.3 Heat-release source term

Heat generation is coupled to oxygen consumption via an effective enthalpy factor:

$$S_h = \Delta H_{\text{eff}} (-S_{\text{O}_2}) \quad (A9)$$

where ΔH_{eff} [$\text{J}\cdot\text{kg}^{-1}$ of consumed O_2] is either obtained from calibration or derived from an assumed reaction enthalpy and stoichiometry. The legacy document expresses this coupling through proportionality constants (e.g., “consth”).

A.4.4 Source terms for indicator gases (CO, CO₂, H₂O)

In the simplified stoichiometric coupling used in the legacy model, gas production terms are proportional to oxygen consumption:

$$S_{CO} = k_{CO} (-S_{O_2}), \quad S_{CO_2} = k_{CO_2} (-S_{O_2}), \quad S_{H_2O} = k_{H_2O} (-S_{O_2}) \quad (A10)$$

where κ_{CO} , κ_{CO_2} , κ_{H_2O} are yield factors (dimensionless mass-based coefficients). The legacy model defines these via ratios of mass fractions (e.g., $\kappa_{CO} = \frac{Y_{CO}}{Y_{O_2}}$, etc.).

A.4.5 Two-regime reaction behaviour (threshold temperature)

To reflect accelerated oxidation above a critical state, the legacy model considers two simplified reaction regimes separated by a threshold temperature T_{th} :

- for $T < T_{th}$: „slow“ oxidation with higher fraction of oxidised coal and lower CO yield,
- for $T > T_{th}$: „accelerated“ oxidation with increased CO₂ and a non-zero CO fraction.

$$k_{CO}(T), k_{CO_2}(T), k_{H_2O}(T) = \begin{cases} k_{\bullet}^{\leq}, & T < T_{th} \\ k_{\bullet}^{\geq}, & T \geq T_{th} \end{cases} \quad (A11)$$

where $k_{\bullet}^{\leq}$ and $k_{\bullet}^{\geq}$ are coefficients consistent with the two reaction pathways specified in the legacy description.

A.5. Boundary condition for heat transfer (Newton cooling)

At the pile surface, the legacy approach employs a Newton-type convective boundary condition for heat exchange with ambient air:

$$-\lambda_{eff} \nabla T \cdot \mathbf{n} = h (T - T_{\infty}) \quad (A12)$$

where h is the convective heat-transfer coefficient [$W \cdot m^{-2} \cdot K^{-1}$], T_{∞} is ambient air temperature [K], and $\mathbf{n}$ is the outward surface normal vector.

A.6. Wind inflow profile and atmospheric boundary conditions

Wind forcing in the atmospheric domain was prescribed using a vertically varying inflow velocity profile based on a standard power-law formulation:

$$v(z) = v_{10} \left(\frac{z}{10} \right)^{0.22} \quad (A13)$$

with an example reference wind speed $v_{10} = 4$ [$m \cdot s^{-1}$].

Where available, transient meteorological data (wind speed and direction, air temperature) from an on-site meteorological station were used to drive scenario-based simulations. The imposed inflow profile controls convective heat and mass exchange at the pile surface and directly influences oxygen supply to near-surface layers of the coal body.

A.7. Notes on practical implementation (recommended reporting items)

For reproducibility and peer-review clarity, the following should be reported (main text or Supplementary/Appendix):

- adopted values (or calibration strategy) for $D_{i,eff}$, h , and ΔH_{eff} ;
- mapping between monitoring-derived oxygen availability (mole vs. mass fraction) and the C_{O_2} term in (A7);
- threshold temperature T_{th} definition and how it is set (literature, calibration, or experimental basis).

APPENDIX B. TIME-TO-THRESHOLD PREDICTORS (LINEAR AND QUADRATIC TREND)

B.1. Purpose and definition of the prediction task

The aim of the predictor is to estimate the remaining time to reach a critical threshold associated with irreversible self-heating (incipient spontaneous combustion). The prediction is performed from the most recent monitoring data of selected state variables, such as internal temperature or indicator gas concentrations (e.g., T , CO, CO₂, CH₄, O₂).

Let $y(t)$ denote a monitored indicator and y_{lim} a predefined threshold value (e.g., y_{lim}). The objective is to estimate the crossing time t_{lim} such that:

$$y(t_{lim}) = y_{lim} \quad (B1)$$

The predicted remaining time from the most recent measurement at t_n is:

$$t_{pred} = t_{lim} - t_n \quad (B2)$$

The legacy procedure uses either a linear trend based on the last two measurements or a quadratic trend based on the last three measurements.

B.2. Linear trend predictor (two-point model)

B.2.1 Model form

Assume a linear relationship:

$$y(t) = kt + q \quad (B3)$$

with slope κ and intercept q .

B.2.2 Parameter estimation from the last two measurements

Using the two most recent observations (t_{n-1}, y_{n-1}) and (t_n, y_n) :

$$k = \frac{y_n - y_{n-1}}{t_n - t_{n-1}}, \quad q = y_n - kt_n \quad (B4)$$

This corresponds to the two-point linear update described in the legacy formulation.

B.2.3 Threshold crossing time and remaining time

Solving $y_{lim} = kt_{lim} + q_{gives}$:

$$t_{lim} = \frac{y_{lim} - q}{k} \quad (B5)$$

and therefore:

$$t_{pred} = \frac{y_{lim} - q}{k} - t_n \quad (B6)$$

This is equivalent to the original „linear trend“ predictor $t_{pred} = t_{lim} - t_n$.

B.2.4 Practical notes (linear case)

- If $k \leq 0$ (non-increasing trend), then the predictor indicates no imminent threshold crossing under the current trend assumption.
- If $t_{lim} \leq t_n$, then the threshold is already reached or the trend fit is inconsistent (measurement noise or regime change).

B.3. Quadratic trend predictor (three-point model)

B.3.1 Model form

Assume a quadratic trend:

$$y(t) = at^2 + bt + c \quad (B7)$$

as introduced in the legacy approach.

B.3.2 Coefficients from the last three measurements

Using the last three observations (t_{n-2}, y_{n-2}) , (t_{n-1}, y_{n-1}) , and (t_n, y_n) , the coefficients a , b , c can be obtained by solving the linear system:

$$\begin{bmatrix} t_{n-2}^2 & t_{n-2} & 1 \\ t_{n-1}^2 & t_{n-1} & 1 \\ t_n^2 & t_n & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} y_{n-2} \\ y_{n-1} \\ y_n \end{bmatrix} \quad (B8)$$

This is the most compact and reproducible expression of the „three-point quadratic regression“ described in the source text.

Implementation note: If the original regression subroutine is not available, the legacy document provides explicit expressions for a , b , c based on sums and auxiliary variables $z_1 \dots z_6$. Equation (B8) is mathematically equivalent and generally preferred for publication clarity.

B.3.3 Threshold crossing time

The crossing time t_{lim} is obtained by solving:

$$at_{lim}^2 + bt_{lim} + c = y_{lim} \quad (B9)$$

or:

$$at_{lim}^2 + bt_{lim} + (c - y_{lim}) = 0 \quad (B10)$$

The solutions are:

$$t_{lim} = \frac{-b \pm \sqrt{b^2 - 4a(c - y_{lim})}}{2a} \quad (B11)$$

where the discriminant:

$$D = b^2 - 4a(c - y_{lim}) \quad (B12)$$

must satisfy $D \geq 0$. This corresponds to the discriminant condition and root expression used in the legacy formulation.

B.3.4 Selecting the physically meaningful root and remaining time

From the two roots in (B11), select the smallest root that is greater than the current time t_n :

$$t_{lim} = \min\{t : y(t) = y_{lim}, t > t_n\} \quad (B13)$$

Then:

$$t_{pred} = t_{lim} - t_n \quad (B14)$$

This matches the original „quadratic trend“: interpretation $t_{pred} = t_{lim} - t_n$.

B.3.5 Practical notes (quadratic case)

- If $a \approx 0$, the quadratic model collapses to the linear case and should be handled using Appendix B.2.
- If $D < 0$, the quadratic fit does not reach y_{lim} (within the fitted curvature), indicating either insufficient upward trend or that the chosen threshold is not reachable under current dynamics.
- Because three-point quadratic fits can be sensitive to noise, it is recommended to apply the quadratic predictor only when the recent evolution shows consistent acceleration (e.g., increasing slope between $(n-2) \rightarrow (n-1)$ and $(n-1) \rightarrow n$).

B.4. Recommended usage and reporting in the manuscript

For each monitored indicator y (e.g., T , CO , CO_2 , CH_4 , O_2), the following should be reported:

1. The chosen threshold y_{lim} (and justification: operational limit, critical temperature concept, or empirical criterion).
2. The time window used (last 2 points for linear; last 3 points for quadratic).
3. Handling of special cases (negative slope, $D < 0$, $t_{lim} \leq t_n$).
4. Whether the predictor is applied to temperature only or also to indicator gases.

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References

- Taraba, B., Voráček, V., Král, V.: Analysis of coal self-ignition cases in OKR mines – Part I: A new method for assessing spontaneous combustion risk in longwall faces. *Uhlí, rudy, geologický průzkum*. 2006;13(11):34–37.
- Taraba, B., Pavelek, Z., Janek, J., Voráček, V., Král, V.: Analysis of coal self-ignition cases in OKR mines – Part II: Assessment of fire hazard and adequacy of suppression interventions. *Uhlí, rudy, geologický průzkum*. 2006;13(12):28–31.

Taraba, B.: Low-temperature oxidation and spontaneous combustion of coal matter. Ostrava: Ostravská univerzita; 2003. ISBN 80-7042-832-5.

Moni, V., Taraba, B.: Laboratory investigation of key parameters affecting oxidation of brown coals. *Zpravodaj Hnědé Uhlí*. 2013;(2):17–24.

Chen, X.D., Stott, J.B.: The effect of moisture content on the oxidation rate of coal during near-equilibrium drying and wetting at 50 °C. *Fuel*. 1993;72(6):787–792. [https://doi.org/10.1016/0016-2361\(93\)90081-C](https://doi.org/10.1016/0016-2361(93)90081-C).

Dobal, V., Sýkorová, I., Valeška, F., Hemelíková, B.: Methods for determining the oxygen reactivity of brown coals. Research report. Prague: ÚGG ČSAV; 1983.

Akgün, F., Arisoy, A.: Effect of particle size on the spontaneous heating of a coal stockpile. *Combustion and Flame*. 1994;99(1):137–146. [https://doi.org/10.1016/0010-2180\(94\)90085-X](https://doi.org/10.1016/0010-2180(94)90085-X)

Michalec, Z., Michalcová, V., Taraba, B.: Modelling the influence of coal stockpile parameters on the dynamics of spontaneous heating. *Zpravodaj Hnědé Uhlí*. 2013;(1):3–10.

Moni, V.: Evaluation of comprehensive long-term measurements on brown-coal stockpiles. *Zpravodaj Hnědé Uhlí*. 2014; (2): 27–35.

Taraba, B., Michalec, Z., Michalcová, V., Blejchař, T., Bojko, M., Kozubková, M.: CFD simulations of the effect of wind on the spontaneous heating of coal stockpiles. *Fuel*. 2014;118:107–112. <https://doi.org/10.1016/j.fuel.2013.10.064>

Taraba, B., Peter, R., Slovák, V.: Calorimetric investigation of chemical additives affecting oxidation of coal at low temperatures. *Fuel Processing Technology*. 2011;92(3):712–715. <https://doi.org/10.1016/j.fuproc.2010.12.003>

Zhang, J., Liang, Y., Ren, T.X., Wang, Z., Wang, G.: Transient CFD modelling of low-temperature spontaneous heating behaviour in multiple coal stockpiles with wind forced convection. *Fuel Processing Technology*. 2016;149:55–74. <https://doi.org/10.1016/j.fuproc.2016.04.011>

Wang, H., Dlugogorski, B.Z., Kennedy, E.M.: Coal oxidation at low temperatures: oxygen consumption, oxidation products, reaction mechanism and kinetic modelling. *Progress in Energy and Combustion Science*. 2003;29(6):487–513. [https://doi.org/10.1016/S0360-1285\(03\)00042-X](https://doi.org/10.1016/S0360-1285(03)00042-X)

Nordon, P., Bainbridge, N.W., Carras, J.N.: A numerical model of heat, water and oxygen interaction within a coal stockpile. In: *Extended Abstracts, Joint International Conference of the Australian/New Zealand and Japanese Sections of The Combustion Institute*; 24–27 Sep 1989; Sydney, Australia. pp. 208–210.

Zhang, H., Zhang, X., Wang, Y., Dong, W., Fan, J., Sasaki, K.: Application of aging effect model in numerical simulation for predicting spontaneous combustion of coal stockpiles. *Journal of Thermal Analysis and Calorimetry*. 2022;147(23):13847–13860. <https://doi.org/10.1007/s10973-022-11708-7>