# Innovative insights into heat transport mechanisms during coal-biomass co-pyrolysis: a hybrid experimental and physics-informed artificial intelligence modelling approach

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## Introduction

Coal continues to serve as one of the foremost energy resources globally [1]. Yet increasingly stringent environmental legislation calls for partial replacement with alternative energy sources and greater utilization of residual energy from waste streams [2, 3]. This transition has heightened the focus on dedicated energy vegetation and residual biomass feedstocks. Biomass is commonly considered carbon-neutral and structurally analogous to coal; however, compositional differences result in distinct thermochemical behaviour. Within the Circular Economy paradigm, there is growing emphasis on characterizing the thermophysical properties of waste-derived materials. Fundamental properties (specific heat capacity, density, thermal diffusivity, and conductivity) are essential for optimising thermochemical processes (e.g., pyrolysis) and predicting fuel response under variable-temperature conditions, and play a crucial role in energy-recovery processes, material recycling, and the design of thermal waste treatment technologies [4].

The current research assesses the thermophysical characteristics of bituminous coal (WJ), agricultural biomass residues (BA), forest biomass waste (BL), and their blends (25%WJ/75%BA, 50%WJ/50%BA, 75%WJ/25%BA, 25%WJ/75%BL, 50%WJ/50%BL, 75%WJ/25%BL), in composite form.

Various research methodologies were used to conduct the studies. The selected materials exhibit structural heterogeneity, organic decomposition, and variable porosity, which govern their thermophysical response.

The literature indicates that the thermophysical properties of fuels/waste vary widely depending on moisture content, organic fraction, density, and mineral composition. The existing datasets focus on selected fuels/waste types and lack a consistent experimental framework. This highlights the need for comprehensive, cross-material measurements conducted under identical conditions, enabling reliable comparisons and supporting the development of practical classification approaches in the circular-economy context. This study offers a coherent, methodologically consistent assessment of the pyrolysis of coal, biomass waste, and their mixtures.

Accordingly, the present study provides a novel, consistent comparison of materials. A physics-informed artificial intelligence (AI) method, developed in the study and based on Gaussian Process Regression (GPR), enables mapping of continuous thermal conductivity for coal blends with forest and agricultural biomass.

## Research methodology

The fundamental aim of this investigation was to quantify variations in the thermal conductivity of the examined fuels during pyrolysis up to a peak temperature of 500°C. Determination of this parameter required the experimental evaluation of density (ρ), specific heat capacity ($c_p$) and thermal diffusivity (α), combined according to the fundamental relationship (1):

$$\lambda(T) = \rho(T) \cdot c_p(T) \cdot \alpha(T) \qquad (1)$$

The materials originated from a Polish power plant.

Before analysis, materials were comminuted, milled, and sieved to < 200 μm. Each material was weighed and uniaxially pressed in a hydraulic press to obtain cylindrical samples with a diameter of 5 mm (for TG/DTG/DSC tests), cylindrical samples with a diameter of 12.6 mm (for LFA tests), and cylindrical samples with a diameter of 10 mm (for DIL tests).

TG/DTG/DSC, helium pycnometry, DIL, LFA, WDXRF, and XRD measurements were performed at the Faculty of Materials Science and Ceramics, AGH University of Krakow.

## Experimental results

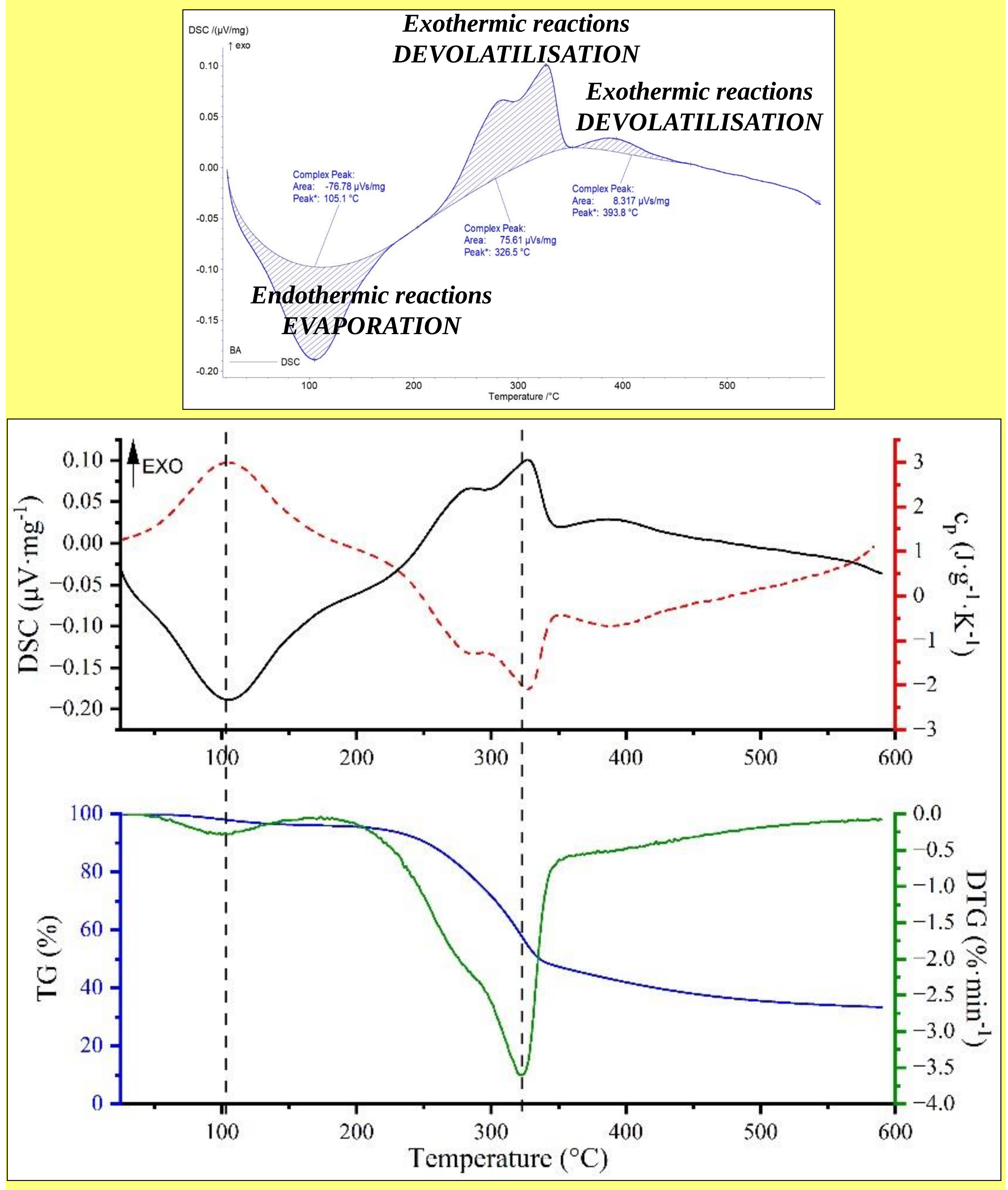

**Fig.1.** Example of measurements results for BA

Characteristic endothermic and exothermic peaks observed on DSC curves reflect the heat effects of chemical reactions within specific temperature ranges. Biomass exhibits a higher rate of mass loss during degassing than coal, with BA showing the highest reactivity ($DTG_{max}$: BA=3.62%·$min^{-1}$, BL=1.56%·$min^{-1}$, WJ=0.56%·$min^{-1}$). Increasing biomass content in fuel also enhances fuel reactivity.

**Table 1.** Characteristic peaks on the TG/DTG and $c_p$ curves

| Material/ parameter | $T_{DTG\ peak}$ (◦C) | DTG $_{peak}$ (%·min.$^{-1}$) | $c_p$ at $T_{DTG\ peak}$ (J·g$^{-1}$·K$^{-1}$) | TG - change mass (%) | Total enthalpy ΔH (J·g$^{-1}$) |
|---|---|---|---|---|---|
| Biomass BA | 101<br>321 | 0.31<br>3.62 | 2.98 (endothermic stage)<br>2.09 (exothermic stage) | 27-170 ◦C (3.97%) (endothermic stage)<br>170-350 ◦C (48.69%) (exothermic stage)<br>350-582 ◦C (13.99%) (exothermic stage) | 248 (27-582 ◦C) residual mass: 33.35% |
| Biomass BL | 97<br>327 | 0.43<br>1.56 | 3.59 (endothermic stage)<br>0.56 (exothermic stage) | 27-180 ◦C (6.55%) (endothermic stage)<br>180-358 ◦C (29.08%) (exothermic stage)<br>358-582 ◦C (14.93%) (exothermic stage) | 586 (27-582 ◦C) residual mass: 49.45% |
| Coal WJ | 101<br>426 | 0.20<br>0.56 | 2.41 (endothermic stage)<br>1.32 (exothermic stage) | 27-168 ◦C (3.27%) (endothermic stage)<br>168-317 ◦C (2.76%) (exothermic stage)<br>317-515 ◦C (13.93%) (exothermic stage)<br>515-582 ◦C (3.95%) (endothermic stage) | 959 (27-582 ◦C) residual mass: 76.09% |
| 25WJ/75BA | 105<br>325 | 0.30<br>2.80 | 2.75 (endothermic stage)<br>1.27 (exothermic stage) | 27-175 ◦C (3.86%) (endothermic stage)<br>175-350 ◦C (37.98%) (exothermic stage)<br>350-582 ◦C (15.00%) (exothermic stage) | 328 (27-582◦C) residual mass: 43.16% |
| 50WJ/50BA | 92<br>326<br>432 | 0.30<br>1.96<br>0.49 | 2.74 (endothermic stage)<br>0.29 (exothermic stage)<br>0.38 (exothermic stage) | 27-175 ◦C (3.97%) (endothermic stage)<br>175-357 ◦C (27.42%) (exothermic stage)<br>357-500 ◦C (11.45%) (exothermic stage)<br>500-582 ◦C (3.54%) (exothermic stage) | 516 (27-582◦C) residual mass: 53.62% |
| 75WJ/25BA | 105<br>326<br>430 | 0.25<br>0.97<br>0.52 | 2.65 (endothermic stage)<br>0.56 (exothermic stage)<br>0.91 (exothermic stage) | 27-175 ◦C (3.82%) (endothermic stage)<br>175-358 ◦C (15.36%) (exothermic stage)<br>358-513 ◦C (12.35%) (exothermic stage)<br>513-582 ◦C (3.49%) (endothermic stage) | 734 (27-582◦C) residual mass: 64.98% |
| 25WJ/75BL | 106<br>327 | 0.45<br>1.24 | 3.61 (endothermic stage)<br>0.15 (exothermic stage) | 27-180 ◦C (6.11%) (endothermic stage)<br>180-365 ◦C (23.48%) (exothermic stage)<br>365-495 ◦C (11.11%) (exothermic stage)<br>495-582 ◦C (3.54%) | 796 (27-582◦C) residual mass: 55.76% |
| 50WJ/50BL | 100<br>335<br>435 | 0.36<br>0.91<br>0.54 | 4.47 (endothermic stage)<br>1.12 (exothermic stage)<br>1.64 (exothermic stage) | 27-180 ◦C (5.82%) (endothermic stage)<br>180-365 ◦C (16.73%) (exothermic stage)<br>365-495 ◦C (11.12%) (exothermic stage)<br>495-582 ◦C (4.23%) (endothermic stage) | 1100 (27-582◦C) residual mass: 62.10% |
| 75WJ/25BL | 106<br>336<br>440 | 0.33<br>0.45<br>0.45 | 3.86 (endothermic stage)<br>1.52 (exothermic stage)<br>1.60 (exothermic stage) | 27-180 ◦C (4.94%) (endothermic stage)<br>180-360 ◦C (10.19%) (exothermic stage)<br>360-582 ◦C (16.09%) (exothermic stage) | 1104 (27-582◦C) residual mass: 68.4% |

$^{*}\Delta H_{T_1-T_2} = c_{pT_1}^{\ T_2} \cdot (T_2 - T_1)$

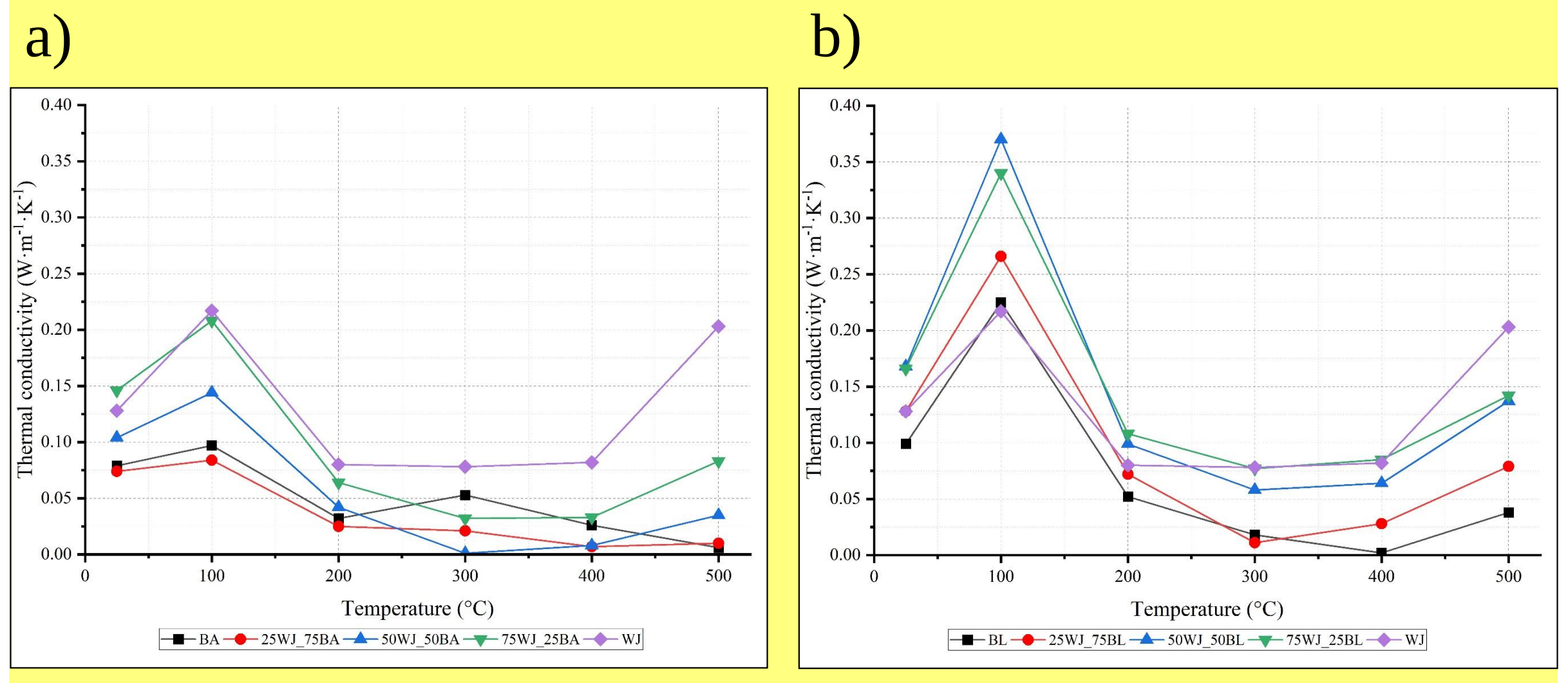

**Fig.2.** The thermal conductivity of fuels

Over the temperature range of 25–500°C, increasing the biomass content in WJ-biomass composites reduces thermal conductivity, although these values remain higher than those of pure biomass. In the 100–500°C range, WJ–BA composites exhibit lower thermal conductivity than coal, which is related to the relative density of the samples. In contrast, WJ–BL composites show higher conductivity than coal at 25–200°C, but lower values at higher temperatures.

## Gaussian Process Regression model

The 3D response maps shown in Fig. 3 depict interactions in the pyrolytic carbon matrix between 25 and 500°C. Both biomass types exhibit a peak in thermal conductivity near 100°C. The GPR model indicates a significant increase in this area for blends containing 25-50% biomass. It is likely the result of moisture and tight matter. A heat bottleneck appears during devolatilization between 300 and 400°C. The conductivity drops as low as 0.001 W·m-1·K-1 in BA blends. This significant decrease indicates pore-structure development, as volatiles escape and generate voids within the particles. The data show that agricultural biomass produces a deeper valley than Forest Biomass. This supports elemental and proximate analyses. High volatility and alkali content in BA lead to rapid structural changes, forming a complex interface between the char and pores.

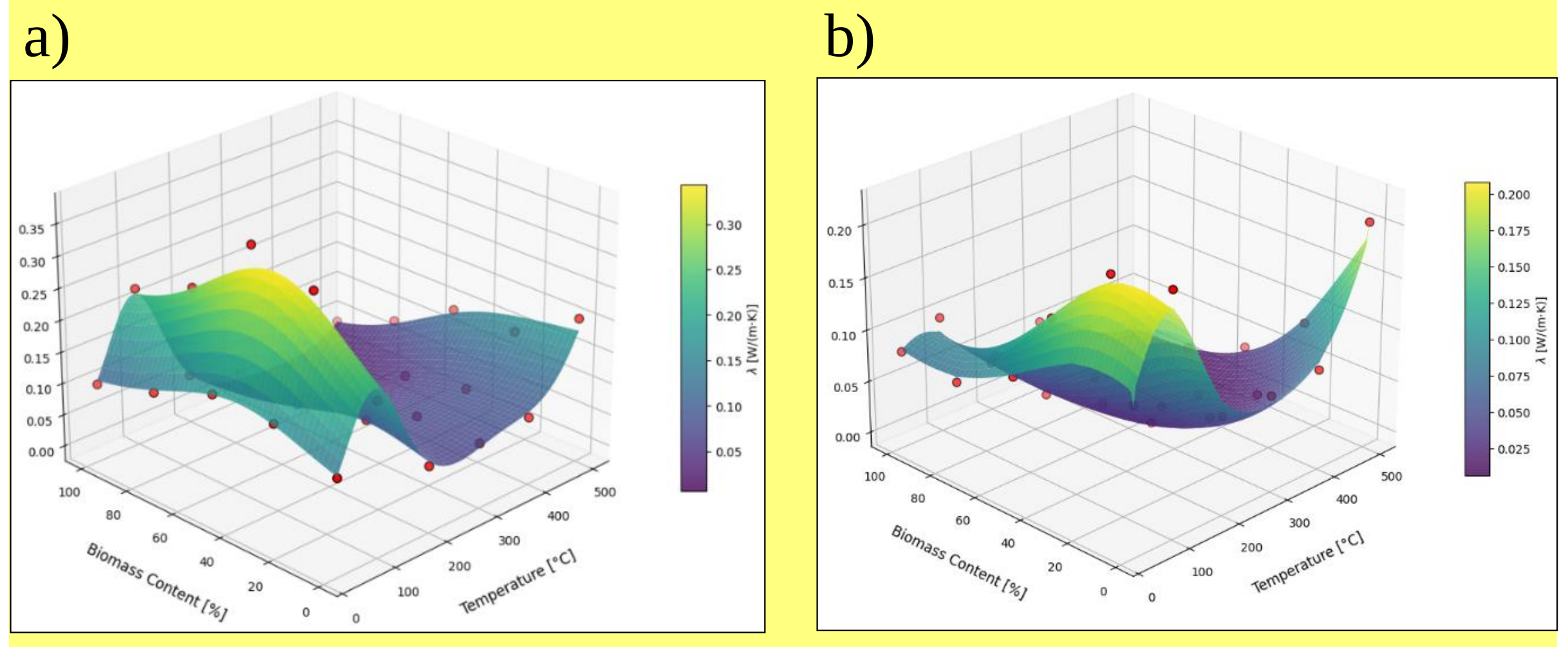

**Fig.3.** Thermal conductivity for: a) WJ, BL, and their mixtures, b) WJ, BA, and their mixtures (GPR model)

## Conclusions

1. XRD results show significant differences in mineralogical composition. Samples BA and BL are dominated by silica-based phases with varying structural order. In contrast, WJ exhibits a complex multi-mineral assemblage typical of clay-rich materials, including silicates and sulphates.
2. Biomass exhibits significantly higher devolatilization rates than coal. At 25°C, biomass shows higher specific heat capacity (1.265–1.277 J·g$^{-1}$·K$^{-1}$), while coal exhibits higher thermal diffusivity (0.090 mm$^2$·s$^{-1}$), reflecting the influence of coal content and density on heat transport.
3. Dilatometric analysis indicates that biomass undergoes greater dimensional changes during heating, whereas increasing coal content improves structural stability and reduces shrinkage.
4. Thermal conductivity increases with fixed-carbon content and bulk density, while higher volatile-matter content reduces heat-transfer efficiency. The highest conductivity at 25°C was observed for WJ–BL mixtures with >50% BL.
5. The physics-informed Gaussian process model accurately captures the non-linear relationship between biomass fraction and temperature, $R^2 = 0.916$ (BL-coal blends) and $R^2 = 0.761$ (BA-coal blends), enabling reliable prediction of thermal conductivity.

## References

[1] B. Ongar, et al. Optimization of the design and operating characteristics of a boiler based on three-dimensional mathematical modeling. *Bulgarian Chemical Communications* **55**, 153-159 (2023).

[2] A. Kijo-Kleczkowska. Analysis of cyclic combustion of the coal-water suspension. *Archives of Thermodynamics* **32(1),** 45–75 (2011).

[3] J. Taler, et al. Elektrociepłownia z silnikiem spalinowym zasilanym gazem drzewnym. *Rynek Energii* **4** (2013).

[4] A. Kijo-Kleczkowska, et al. Thermal properties of waste fuels for the circular economy. *Energy* **344**, 140077 (2026).

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