

## ABSTRACT

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Due to the decreasing availability of high-grade coking coals with simultaneously rising prices for these raw materials, steel-producing companies such as *ThyssenKrupp Steel Europe AG* have to intensify studies on quality assurance. In addition to the quality control, the identification of coking coals has to be included for the early detection of any incorrect deliveries and foreign admixtures directly at their delivery. Actually, current routine analysis is no longer purposeful for these issues. In different studies the pyrolysis gas chromatography mass spectrometry (Py-GC/MS) was applied for the investigation of complex substances such as coals. In this thesis, the Py-GC/MS was used to characterize coking coals, identify them clearly due to their chromatographic behavior and, based on these results, classify them.

Firstly, a method for the characterization of coking coals (MeKKDo) was developed, which then was used for the defined issues. After detailed investigation of the pyrolytic behavior of the coals, it was possible to prove by means of Euclidean distances that there are calculable differences between the chromatograms of different coking coals. Using two different methods of the multivariate data analysis, it was possible to develop two models for the identification of coking coals on the basis of their chromatograms. However, both the logistic regression and decision trees were not able to withstand a replication of the routine operation of the analyzer. Chromatographic effects such as shifts in retention times, led to unacceptable deviations in the identification.

Therefore, in cooperation with the company *Lablicate UG*, the mass spectrometric data were used. Since the data are independent of chromatographic variations with this database a valid system for the identification of coking coals have been established.

In context of this thesis, a method for the prediction of the volatile matter of coking coals due to their detected total mass signals could be developed and validated. In addition it was possible to place first cornerstones for the classification of coking coals, such as the separation of the studied coals according to their origin. A finer and technological meaningful separation of coals was not possible yet. Therefore, further investigations of the coals are necessary.

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