INVESTIGATION OF FACTORS AFFECTING COKE STRENGTH AFTER REACTION (CSR) AND DEVELOPING A STATISTICAL MODEL FOR CSR PREDICTION

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ABSTRACT

INVESTIGATION OF FACTORS AFFECTING COKE STRENGTH AFTER REACTION (CSR) AND DEVELOPING A STATISTICAL MODEL FOR CSR PREDICTION

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This study was aimed at investigating the coke strength after reaction (CSR) prediction before coke production by regression modelling. Initially, quality parameters of studied coals, namely Australian, American and Canadian coals, were categorized to understand fluctuation in the parameters. Parameters studied consist of proximate analysis, physical properties, rheological properties, ash chemistry, petrographical analysis and coke quality parameters of the coals. After understanding remarkable difference in coal quality parameters relative to origin, regression analysis was performed for the coals under study. Highly correlated parameters were detected by correlation analysis, performed via Excel and Minitab, considering both Pearson Correlation Coefficient and p - values. Devore states that two variables show strong relationship when correlation coefficient of them is above 0.8. Absolute values of correlation coefficients above 0.8 evaluated as highly correlated. Absolute values of correlation coefficients between 0.6 and 0.8 and p – values below 0.05 also evaluated as highly correlated. Then, best subset analysis was carried out by Minitab to indicate best alternative regression model. Decision of which parameters are included into model was given by evaluating R – square, R – square (adj) and R – square (pred) of best subset analysis model alternatives. For studied Australian, American and Canadian coals, CSR prediction models were developed individually. Categorization and origin base CSR prediction model development studies created the base of CSR prediction model for coal blends. Precision of the models controlled by mean hypothesis and whether residues of model are equal to zero or not was checked. 1 – sample t test, 2 – sample t test and one-way ANOVA test were used for mean hypothesis. In addition, Origin base CSR prediction models were comprised with formulas retrieved from literature. At the end of study, CSR prediction models were developed with 96.5 %, 93.41 %, 86.21 % and 80.99 % R – square for Australian, American, Canadian coals and coal blends respectively.

Keywords: Coke Strength after Reaction, Coal Quality, Coke Quality, Model Development, CSR Prediction, Blend Design

REAKSİYON SONRASI KOK MUKAVEMETİNİ (CSR) ETKİLİYEN FAKTÖRLER VE CSR'Yİ TAHMİN ETMEK İÇİN İSTATİSTİKSEL MODEL GELİŞTİRİLMESİ

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Bu çalışmada reaksiyon sonrası kok mukavemetinin üretim öncesinde regresyon modeli ile tahmin edilmesi amaçlanmıştır. Başlangıçta çalışılan Avustralya, Amerika ve Kanada kömürlerinin kalite parametrelerinin nasıl değişkenlik gösterdiğinin anlaşılması için sınıflandırma çalışması yapılmıştır. Çalışılan parametreler kömürün kısa analizi, fiziksel, reolojik, kimyasal, petrografik ve kok kalite analizlerinden oluşmaktadır. Kömür orijinine göre göze çarpan farklılıklar anlaşıldıktan sonra çalışılan kömürler için regresyon analizi yapılmıştır. Excel ve Minitab ile gerçekleştirilen korelasyon analizleri sayesinde, Pearson korelasyon katsayısı ve p değerleri göz önüne alınarak yüksek ilişkili parametreler tespit edilmiştir..Korelasyon katsayısı mutlak değeri 0.8 ve üzerinde olan parametreler yüksek ilişkili olarak değerlendirilmiştir. Korelasyon katsayısı mutlak değeri 0.6 ile 0.8 arasında olan ve p değerleri 0.05 den küçük olan parametreler de yüksek ilişkili olarak değerlendirilmiştir. Sonrasında en iyi model alternatifini belirlemek için Minitab ile en iyi alt küme analizi gerçekleştirilmiştir. Hangi parametrelerin regresyon modelinde yer alacağı en iyi alt küme model alternatiflerinin R², R² (adj) ve R² (pred) değerlerine bakılarak karar verilmiştir. CSR tahmin modelleri çalışılan Avusralya, Amerika ve Kanada kömürleri için ayrı ayrı geliştirilmiştir. Kategorizasyon ve orijin bazlı CSR tahmin model çalışmaları kömür harmanı için CSR tahmin modelinin temelini oluşturmuştur. Model tahmin artıklarının sıfıra eşit olup olmadığına bakmak için ortalama hipotezleri kurulmuş ve model tahmin hassasiyeti kontrol edilmiştir. Ortalama hipotezleri için 1 – sample t test, 2 – sample t test and one-way ANOVA testleri kullanılmıştır. Ek olarak, Orijin bazlı CSR tahmin modelleri literatürden bulunan formüller ile kıyaslanmıştır. Çalışmanın sonunda Avustralya, Amerika, Kanada ve Kömür harmanları için CSR tahmin modelleri sırasıyla % 96.5, % 93.41, %86.21 ve % 80.99 R² ile modellenmiştir.

Anahtar Kelimeler: Reaksiyon sonrası kok mukavemeti, Kömür kalitesi, kok kalitesi, istatistiksel model, CSR tahmini, Harman dizaynı.

To The Harmony of Theory and Practice

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CHAPTER 1

INTRODUCTION

Iron and steel production is one of the world's most important and biggest industry. Main usage areas of steel are construction, transportation, energy, packaging and industrial supplies. These are basis of modern life; that is why, progress of steel industry is an indication of country's economic progress. Because of the fact that steel is new cement of current civilization, world steel production rate is increasing year by year.

According to World Steel Association (WSA), steel production increased 30 % in last 10 years. In 2006, 1,250,098 thousand tonnes steel was produced in world while 1,620,408 thousand tonnes of steel was produced in 2015 (World Steel Association Economics Committee, 2016). 83 % of steel is being produced in top 10 steel producer countries. On the other hand, China is the world's biggest steel producer and 50 % of steel is being produced there. It means nearly 33 % of steel is being produced in the remaining 9 countries including Turkey. Top 10 steel producing countries are listed in Table 1-1 in accordance with data provided by WSA (World Steel Association, 2017). Turkey ranks eighth in the list out of 66 WSA-member countries. Turkey's steel production is nearly 33 million tonnes, which makes up 2 % of total steel production in the world. In a similar manner to world increasing steel production rate, Turkey's production also increased 42 % in last 10 years.

Table 1.1 WSA 2016 Country Basis Steel Production Rates

Rank	Country	Production (million tonnes)
1	China	808.4
2	Japan	104.8
3	India	95.6
4	United States	78.5
5	Russia	70.8
6	South Korea	68.6
7	Germany	42.1
8	Turkey	33.2
9	Brazil	31.3
10	Ukraine	24.2
	Top 10 Total	1357.5
	World Total	1629.6

There are two main steel production processes:

- 1. Integrated Steel Plants (Oxygen process)
- 2. Electrical Arc Furnaces (Electrical process)

In an integrated steel plant, iron ore is melted with coke in blast furnace. Iron ore may be in the form of lump ore, sinter or pellet. Coke is a residue of coal pyrolysis process, which is called carbonization. However, in an electrical arc furnace, scrap is used to produce molten iron. In the world, 74.4 % of steel is produced from iron ore by basic oxygen furnaces (BOF) in an integrated steel plant. 25.1 % of steel is produced from scrap by electric in electrical arc furnaces. In contrast to the world, 35 % of steel is produced by blast furnace and 65 % of steel is produced by electrical arc furnace in Turkey (World Steel Association, 2017).

In Turkey, there are three integrated steel plants.

- 1. İskenderun Iron and Steel Company (İSDEMİR)
- 2. Ereğli Iron and Steel Company (ERDEMİR)
- 3. Karabük Iron and Steel Company (KARDEMİR)

Crude steel capacities of İSDEMİR, ERDEMİR and KARDEMİR are 5.3, 3.85 and 1.5 million tonnes, respectively (TC Kalkınma Bakanlığı, 2014)

In an integrated steel plant, iron ore is melted with a unique carbon fuel, that is coke, in blast furnaces. Coke used in blast furnace must have four basic properties.

- 1. It must be a heat provider,
- 2. It must be a reducing agent,
- 3. It must have enough strength to allow smooth descend of burden,
- 4. It must allow gas and molten product transfer.

Coke is produced by subjecting coking coals to heat in coke oven batteries in the absence of air. While coking, volatile matter of coal is extracted as coke oven gas (COG). COG is used as energy source in both heating of coke oven batteries and other units of an integrated iron and steel plant. The solid residue of coal carbonization, which is coke, has unique properties for blast furnace process that satisfy above necessities. Coke is a carbon rich fuel. The exothermic reactions below between coke and oxygen provides the heat needed to melt iron.

$$2 C + O_2 \rightarrow 2 CO + heat$$

The product of the chemical reaction above, carbon monoxide, reduces iron oxide.

$$FeO + CO \rightarrow Fe + CO_2$$

Carbon dioxide also reacts with carbon and regenerates reducing agent, carbon monoxide.

$$CO_2 + C \rightarrow 2 CO$$

After carbonization, coke gains enough strength, which is expressed as coke stability factor and coke strength after reaction (CSR). It enables to support burden in blast furnace. In addition to these, manageable size distribution of coke allows both gas permeability and the flow of molten products in the blast furnace. For these reasons, coke is inevitable for an integrated iron and steel plant.

According to International Energy Agency (IEA) 1,072 billion tonnes of coking coal was produced in 2015. From 2001 to 2015, world coking coal production increased 131 %. China consumes nearly 60 % of coking coal produced. However, biggest coking coal exporter of world is Australia. In 2015, 299.2 million tonnes of coking coal was exported and Australia's share was 187.7 million. It means Australia exported more coking coal than rest of world in 2015. World coking coal export data retrieved from Key Coal Trend Report 2016, which is summarized in Table 1-2 (International Energy Agency, 2016).

Table 1.2 International Energy Agency Major Coking Coal Exporters in 2013 to 2015

Country	2013	2014	2015
Australia	154,2	180,5	187,7
United States	59,6	54,5	41,7
Canada	35,0	31,1	28,0
Russia	21,5	21,1	18,3
Mongolia	7,7	6,0	7,7
Other	16,7	17,5	15,6
World	294,9	310,7	299,2

Even if increasing steel production rates increased coking coal production, it should be noted that increase in both steel and coking coals production in China affects these number critically. In addition, unstable coking coal price prevents long term purchasing contracts and finding stable quality coking coals. Since 2007, coking coal price fluctuated between 80 and 340 \$ per tonne. For this reason, contract terms decreases to 3 months from 12 months (Lüngen, 2016). These challenges make sustaining coke quality more difficult and predicting the coke quality before production more important.

There are four main parameters, which are standardized by ASTM, in evaluating coke quality. These are listed below with their ASTM standards and common targets.

- 1. Coke Stability (ASTM D3402) (> 60 %)
- 2. Coke Hardness (ASTM D3402) (> 70 %)
- 3. Coke Reactivity Index (ASTM D5341) (< 25 %)
- 4. Coke Strength After Reaction (ASTM D5341) (> 65 %)

There are also some coke quality parameters such as sulphur, ash, alkali content ($Na_2O + K_2O$) in ash etc., however, they are controlled by raw material selection and blend design. That is why these four parameters are more important.

The most important coke quality criteria is the strength. Coke strength is divided into two parts as cold and hot strength, which are coke stability and coke strength after reaction, respectively. Shrinkage of coke destroys the size distribution and it prevents uniform gas permeability and molten material flow in a blast furnace. Fortunately, before charging of coke into blast furnace, generally a final sieving is performed. Fine coke, generally – 25 mm, is separated from the coke to be charged into the furnace. Furthermore, coke must have also enough strength against to degradation in blast furnace's hot and abrasive environment. It is represented by coke strength after reaction (CSR) or coke hot strength.

For stability and hardness, 10 kg coke sample in a size range of -75 +50 mm is taken. Sample is subjected to 1400 rotations at 24 rpm in a tumbler, which is standardized by ASTM. After 1400 revolution, sample is sieved using 25 mm and 6.3 mm. Weight percent of above 25 mm portion represents the coke stability and above 6.3 mm represents the coke hardness (ASTM, 2008). Basically, coke stability is resistance to

shrinkage and coke hardness is resistance to abrasion. Coke stability is also known as coke cold strength.

Nippon Steel Cooperation first designed CSR test and later ASTM standardized it by following Nippon Steel procedure. It has been realized that coke stability or coke cold strength is not enough to represent coke behavior in blast furnace, a new indication was researched. When coke lumps descend in the blast furnace, they are subjected to two stresses. First, is chemical reaction with reverse current CO₂, and second is physical stress due to abrasion caused by rubbing of cokes and the walls of blast furnace. These simultaneous processes physically weaken and chemically react with coke lumps. Therefore, excess of fines is produced and burden permeability decreases. These phenomena result in increased coke rates and lost hot metal production. Nippon Steel's coke strength after reaction (CSR) test method was designed to measure coke behavior in the blast furnace indirectly.

CSR test procedure begins with coke reactivity index (CRI) test. Coke reactivity index is an indication of reaction rate between coke and CO₂. 200 g coke sample in a size range of -22.4 + 19 mm is subjected to CO₂ for 2 hours at 1100 °C. Percent of mass loss represents coke reactivity index. After reaction, coke residue is subjected to 600 revolutions with 20 rpm in a tumbler, which is standardized by ASTM too. Then coke sample is sieved at 9.5 mm sieve. Percent of mass above 9.5 mm represents coke strength after reaction (ASTM, 2014).

Predicting the coke quality before production is inevitable to optimize the production cost while providing best coal blend. Especially for tough economic conditions, it becomes more important. For example, coking coal prices fluctuated from 80 to 330 \$ per ton in 2016. In addition to that, main portion of steel production cost is raw material cost, specifically coking coal and iron ore in form of sinter, pellet or lump ore cost in an integrated steel plant. Furthermore, coking coal is more expensive than iron ore.

Coke quality prediction research can be divided into three stages. First is based on stability prediction created by Shapiro and Gray (Cordova *et al.*, 2016). Then, CSR is developed by Nippon Steel and it was understood that CSR is a better test method to predict coke behavior in a blast furnace. Second stage was based on theoretical formulas to predict CSR. While working with one-region coals, these formulas gives relatively accurate results. Unfortunately, prediction accuracies are not satisfactory for a blend, which includes different region's coals. Therefore, third stage prediction attempts were based on statistical modelling.

Attempts of predicting coke quality are focusing on possible usage of particular regions' coals rather than developing a statistical model for quality prediction from coals all around the world. Because, each coking coal customer or integrated iron and steel plants purchase coals from specific countries due to geographic and economic circumstances. Consequently, there is no reason to develop coke quality prediction model applicable for coals from all over the world. From this point of view, in order to develop an accurate coke quality prediction model, first factors affecting coke strength after reaction should be determined. Prediction model should be based on these factors rather than only statistical studies. Then how much these factors affect CSR individually should be determined. In addition to this, examined coals should be classified regarding their origin and coals' positive or negative effects on coke quality should be determined based on their origin. Finally, a statistical model to predict coke quality based on coal quality would be developed.

CHAPTER 2

THEORY AND LITERATURE REVIEW

Coke as a blast furnace fuel first used in England at the beginning of 18th century (Kobus, 2015). In last 300 years, technology, machinery and even coke making processes changed. However, the inevitability of coke production for blast furnace in integrated steel plants have not changed. Through the developing a statistical model for coke strength after reaction (CSR) prediction, a brief of coke making history and modern coke making process is explained. Then, coal formation is investigated. After classification of coals, metallurgical coal quality is examined. In order to create the basis of prediction model, coal to coke transformation should be understood. That is why, theory of carbonization will be searched. Then coke quality and CSR is explained. At that point, factors affecting CSR is investigated. Theoretical CSR prediction formulas is also explained. Finally, a statistical prediction model for CSR is developed with the help of literature review.

2.1 Definition and History of Coking

Coking is thermochemical decomposition of coal in absence of air. When a pyrolysis process residue is carbon rich, it is called carbonization. Therefore, coking is coal carbonization process to produce coke, which has more carbon, low volatile matter and mechanical strength. This process has been applied over 300 years for metallurgical purposes. Coking in piles is first technique to produce coke. Then it evolved to coking in beehive ovens. The third and ongoing process is coking in byproduct type coke ovens (retort ovens).

Coking in piles is a similar process with charcoal production from wood. In this method, coal pile was ignited from middle of pile's bottom. Piles were covered with

wet leaves, dirt or breeze in order to reduce air contact. Despite this precaution, it could not prevent coal burning. In addition, some of coal was consumed to provide heat. Therefore, coke yield varied between 33 to 50 %, which is very low (Kobus, 2015). Another problem was that extracted gas released to the atmosphere. This caused both environmental pollution and energy waste.

Extracted volatile matter of coal can be used as heat source instead of coal, if coking is performed in a close area. In beehive oven process, coking begins with remaining heat of oven due to previous coking period. Because of heating raw coke gas is extracted from coal. The coke oven gas is ignited and burnt by supplied external air. Delivered air is controlled and is not enough to burn all coke oven gas. Unburnt gas is driven off to the atmosphere. Due to controlled combustion by air, coal do not burn in the oven. However, released coke oven gas is still an emission source. Beehive ovens was a distinctive design relative to coking in pile method, nevertheless, there were still unsolved problems. These are,

- It was still labor intensive process,
- Operation condition was not suitable for human nature due to dust, dirt and heat,
- Unburnt/surplus gas was wasted in terms of both environment and energy,
- Heating system could not be controlled to sustain uniform coking.

In order to solve these problems, new designs were developed. The Welsh drag oven and Thomas oven reduced labor intense. Excess gas was burnt in bottom of oven rather than releasing to atmosphere in Ramsey oven design. Lowe oven was first energy conversing oven design. Here, surplus gas was used to produce steam. Moreover, Newton-Chamber ovens was first attempt to recover by-products in coke oven gas, which are tar, light oils and ammonia (Kobus, 2015).

These progresses brought the coke making from coking in the pile to by-product (slot) type coke oven batteries. In this design, extracted gas is sent to the by-product plant by continuous pipeline in order to recover tar, ammonia and light oils. After that, clean

gas is used for heating both coke oven batteries and other units of an integrated iron and steel plant. Gas is burnt in flues, which is separated from coking chambers by silica bricks. Air and gas can be controlled for each flue. This provides uniform heating and coking. Beside better quality coke production, design enables energy saving and ensures minimum emission. Thanks to technological advancement, coke oven machineries also reduce labor intensive production. That is why; by-product type coke oven batteries are preferred in the world today.

In chronological order, progress in coke oven technology summarized as follows.

- Stauf developed gas recovery battery. In this design, the aim was producing
 coke oven gas as city gas rather than coke. In other words, coke was by-product
 and coke oven gas was product.
- Carl Knab developed first by product type battery and an exhauster was used to collect extracted gas.
- Simon introduce battery regenerator. Regenerator was heated with combusted gas waste heat. Then supplied air and gas introduced to the battery via this regenerator and they heated up. Help of the design has reached the battery higher temperatures by using same amount of gas supply.
- Evence Coppee introduced 28-flue design and Gustave Hilgenstock created under jet heating.
- Koppers developed cross regenerative heating and gas gun. They ensured proper air gas distribution for each gas flue.
- Otto designed twin flue heating walls. After taller coke oven batteries were discussed,
- Carl Still introduced multi stage air supply for heating flues to sustain homogenous temperature distribution for them.

Beehive ovens have advantages such as low construction cost, simple refractory configuration, no restriction for restart after shut down. However, energy inefficiency, environmental problems and lower coke rate are disadvantages. Slot ovens allows

recovering by-products, energy efficient and environmental friendly production. Nevertheless, refractory works of slots ovens is highly expensive, technical and skilled workers are necessary. Another drawback is that a slot oven cannot be restarted after shut down of heating. Heating must continue 24 hours of day, 7 days of week.

All in all, by-product type coke oven batteries give better coke quality and decrease production cost by valuable by-products gained. Therefore, it is preferred rather than other designs.

2.2 Coal Formation

Coal is combustible, sedimentary organic rock, composed primarily of carbon, hydrogen, oxygen, formed from vegetation, which has been consolidated between other rock strata to form coal seam and altered by combined effects of both microbial action and pressure – heat over considerable time period. (Saad, 2016)

Rodovic and Schobert carbon cycle is illustrated in Figure 2.1. Carbon dioxide in atmosphere exchanges with carbon dioxide in water and rocks. Plants convert CO₂ to O₂ by photosynthesis. However, animals convert O₂ to CO₂ again by breathing. Fatality of both animals and plants produces CO₂ because of decaying. This is the brief explanation of carbon cycle.

Carbon cycle may be interrupted by geological events such as floods, earthquakes, volcanic eruptions, mountain formation. Then, these events cause decaying of plants and animals to be buried under sediments (Arnold, 2013). It is the beginning of coalification.

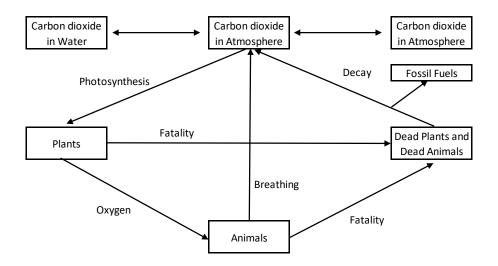


Figure 2.1 Rodovic and Schobert Carbon Cycle

There are two basic types of coals depending on their originating vegetation and decaying conditions. They are sapropelic (non-banded) coals and humic (banded) coals. Sapropelic coals originate from algae or spore, which are called boghead or cannel coals, respectively (Price, 2015). They decay under anaerobic conditions (Saad, 2016). They are rich in hydrocarbon and valuable for synthetic fuel production. During 19th century, sapropelic coals were used in illuminating gas production (Kopp, 2017). Humic coals were formed mainly from cellulosic (woody stalks and roots) and suberized materials (leaves, barks) (Price, 2015). They decay under anaerobic conditions (Saad, 2016). Coking coals are bituminous coals, which are humic.

In humic coals, there are different organic fragments that is called macerals. They are vitrinite, exinite, inertinite and they have different characters because they consist of different parts of vegetation. Exinite (or liptinite) is derived from algae, spore, pollen and resin. It is the most fluid maceral in coking process. Exinite have quasi-crystalline structure that is why, it resists biological degradation during peat formation (Price, 2015). Vitrinite originates from cellulosic materials such as stems, trunks, roots. Vitrinite is subjected to humification and gelification during peat formation. When vitrinite heated, their aliphatic chains breakdown, then aromatic carbon structure

softens, swells and agglomerates other macerals (Falcon, 2013). Due to this technological property, vitrinite is most important and desired maceral for coking process. Inertinite also originates from cellulosic material. However, they burnt or are subjected to excess oxidation before burial. Therefore, inertinite is inert during coking while vitrinite is reactive.

After carbon cycle interruption during decaying of vegetation, peat formation starts. Peat is partially decomposed vegetation remains. While decaying and peat formation easily disintegrated or degraded compounds are extracted as carbon dioxide, ammonia, methane, and water in gas form. Lignin, tannin and resin are converted to humic acid by oxidation, which is called humification. Humic acid is soluble in alkali solutions. Fungi destroys cellulosic woody tissues of vegetation and aerobic bacteria activity converts these tissues to humic acids. Humins are formed because of repolymerisation and polycondensation of humic acids. This humification process is then subjected to gelification. Here, humin forms a plastic gel phase called huminite. Lipids, which are spore, pollen, exine and fat, are resistant to degradation. They do not undergo humification as well as gelification (Price, 2015).

Thus far, carbon cycle interruption by geological events causes vegetation decaying. Then fungal and bacterial activity converts cellulosic tissues to humic acids. Humin forms because of repolymerisation and polycondensation of humic acids. After that, huminite formation occurs due to gelification of humins. This first step of coalification, which is till lignite formation, is called diagenesis and it includes decaying of vegetation and peat formation. The second part of coalification continues with sinking or subsidence of vegetation remains. This forms deposits. Then metamorphism of organic material begins because depth, temperature and pressure increases. This second stage is called catagenesis (Loison *et al.*, 1989).

In Figure 2.2, coalification steps and their related chemical reactions are expressed (Price, 2015). After peat formation decarboxylation, which is carbon dioxide extraction from carboxyl groups (-COOH), dehydration, which is elimination of water,

dealkylation, which is elimination of methyl group (-CH₃) in form of methane (CH₄) and gelification, which is explained above, alter peat to lignite (70 % carbon, daf). Lignite metamorphose to bituminous coal (84-90 % carbon, daf) by decarboxylation and hydrogen disproportioning, which is elimination of hydrogen from naphthenic groups (- CH₂ -) with transformation of hydro aromatic rings into aromatic rings. Bituminous coals are altered to semi anthracite (>90 % carbon, daf) by condensation of small aromatic ring system. When these small aromatic rings transform into larger aromatic rings, anthracite (95 % carbon) forms. Meta anthracite (>97 % carbon, daf) is a complete carbonification product, occurred by graphitization. Low rank coals have more hydrogen bonding due to their hydroxyl (-OH), carboxyl (R-OH) and methoxyl (CH₃O-) groups content. As the rank of coal increases, these are eliminated and aromatization is increasing. However, increasing aromatization in coal gets structural intermolecular forces stronger. Then the intermolecular forces become sufficiently strong to cause insolubility in solvents and more importantly infusibility during carbonization (Loison et al., 1989). As explained above, aromatization starts with formation semi-anthracite and decarboxylation, dehydration, hydrogen disproportioning is completed with bituminous coal formation. It is the reason that coking coals are bituminous coals.

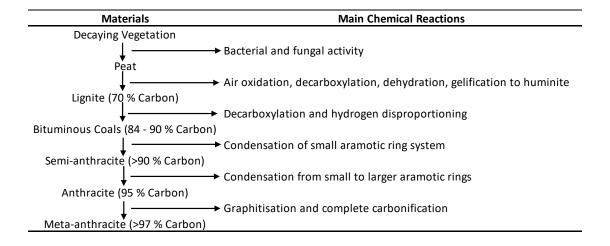


Figure 2.2 Coalification Steps and their Chemical Reactions

During peat formation, type of deposition, depositional medium, peat temperature, pH of medium and depth of peat are the effects of biological degradation. In-situ depositions creates thick coal seams while transported vegetation depositions creates thin ones. Depositional medium such as land, seawater and swamp affect directly coal ash composition. Bacteria flourish in neutral to weakly alkaline environment; nevertheless, they die in acidic conditions. In addition, bacterial population decreases with depth (Atalay, 2016). After biological degradation, coals are altered by geological factors and time. Pressure and temperature increase with depth. Coal, which are subjected to more pressure and temperature, will be more mature. However, time is third factor. If there are two coals, which were subjected to same geological conditions, older one is more mature. Hilt state that across the coal deposit, an upper seam has lower rank than the lower seam. In same depth, the quality of coals as well as degree of coalification are identical (Stiskala, 2016). This explanation is only valid for comparisons of coals in limited areas. It is known that some younger coals have more degree of alteration than older coals. It is contact type alteration, which occurs due to direct contact of heat provided by igneous rocks. Therefore, degree of coalification is a function of pressure and temperature due to geological activity and time. All in all, there are several factors affecting coal formation and there are no two identical coals because of this diversity.

2.3 Coke Making Process Flowsheet

In a coke making plant, domestic or internationally supplied coals are stocked in open or close coal storage yard. Instead of using only one coal, a coal blend must be prepared for various reasons:

- Limited availability of ideal coals
- Compensation need for lack of properties of single coals
- The aim of reducing production cost
- To prevent from possible logistic problems

There are two blending methods. First, each coal is discharged on top of previous discharged coal. Therefore, coal layers create a blend heap. In second method each coal is discharged into coal yard separately, in other words, each coal heap consists of one coal. Then individual coals are transported to coal bins by conveyor belts. By dosing scales, coal blend is prepared.

Blended coal is transported to coke oven battery coal tower by conveyor belts. Charging car is loaded under the coal tower and charges empty or pushed oven. Coal is coked during coking time. Coking time changes depending on coke chamber capacity and coking rate. It generally varies from 18 to 22 hours. While coking volatile matters are driven off from coal and they are sent directly to by-product plant by continuous pipeline. Exhausters create pipeline vacuum, which is necessary for uniform gas flow. After the end of coking time, pusher machine pushes coke in the chamber. Coke moves through coke guide car and falls into quenching car wagon. Coking is performed in absence of air, however, coke starts burning after pushing because of open air. Quenching car transfers coke from in front of the pushed oven to quenching tower. Here, coke is quenched with water. Then quenched coke is fallen into coke wharf by quenching car. Coke is kept for a while in the wharf to decrease moister content by its own heat.

After wharf, coke is transferred to coke crushing and screening unit by conveyor belts. Size intervals vary up to blast furnace demand. Generally, they are -60 + 25 mm (metallurgical coke), -25 +10 mm (nut coke) and -10 mm (coke breeze). In coke production, the aim is producing metallurgical coke and it is sent to blast furnace. Nut coke may be sent to blast furnace or it is possible to sell it, if there is a demand. Coke breeze is used for agglomeration in sinter.

Illustration of coke making flowsheet is given in Figure 2.3.

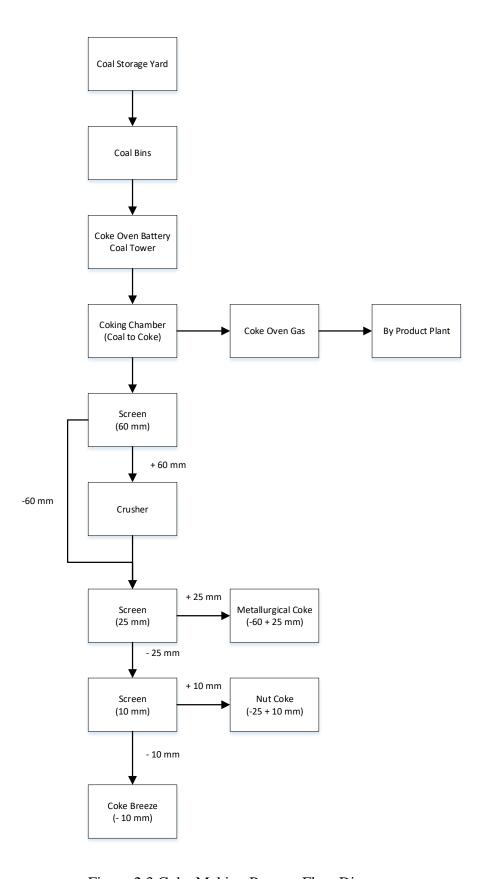


Figure 2.3 Coke Making Process Flow Diagram

2.4 Coal Quality

Coal quality is examined by four main groups of test, which are proximate analysis, ultimate analysis, physical properties, and carbonization properties. Details in coal quality test are listed in Figure 2.4. Proximate analysis consists of moisture, ash, volatile matter, fixed carbon and calorific value. Moisture is determined by mass loss between original and dried coal sample. Ash content is the residue remaining after total combustion of coal sample. When coal is heated, gasses or vapors are driven off. Those products excluding moisture is volatile matter of coal sample. Fixed carbon is calculated by difference between 100 % and sum of moisture, ash and volatile matter as percentage. Calorific value is determined by bomb calorimeter.

Ultimate analysis consists of carbon, hydrogen, sulphur, nitrogen and oxygen content. Carbon and hydrogen is determined by burning of coal sample at 1350 °C. All carbon is converted to carbon dioxide and all hydrogen is converted to water. Then, suitable reagents absorb the products. Sulphur is determined by gravimetric method. Amount of nitrogen is determined by Kjeldahl method. Oxygen is calculated by difference between 100 % and sum of carbon, hydrogen, sulfur, nitrogen and ash contents as percentage.

Physical tests include Hard Grove Index, reflectance of light, bulk density and sieve analysis. Hard Grove is an index of the relative ease with which a coal may be pulverized in comparison with coals chosen as standards. Coal sample is subjected to constant grinding energy by a ball mill at constant revolution. Then, product is sieved and undersized fraction is used to calculate HGI. Bulk density is the mass an assembly of coal particles in a container divided by the volume of container. It depends true density, particle size distribution, particle shape, surface moisture, degree of compaction (Price, 2015).

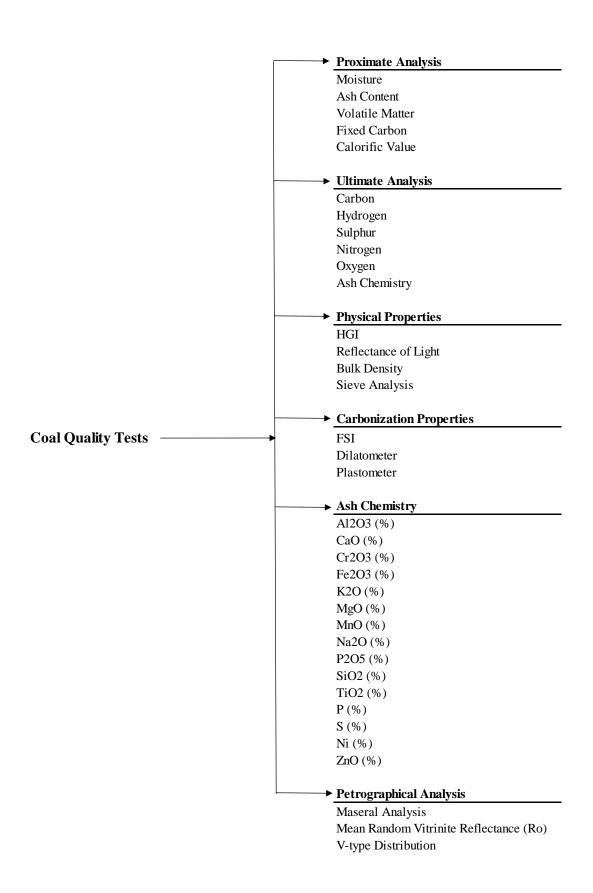


Figure 2.4 Coal Quality Tests

Carbonization tests consist of FSI, dilatometer and plastometer. Free swelling is an index, which is determined by swelled coal shape comparison. Ground coal sample is placed in a silica crucible. Temperature is raised to 820 °C and the sample is kept at that temperature for 2,5 minutes. Swelled coal profile is compared with 17 standard shapes, which were determined by ASTM. Dilatometer test is an indicator of coal swelling properties measured by volumetric method. Coal is compressed into a coal pencil of which the volumetric changes are recorded using a piston resting on the top of the pencil in the course of uniform heating at the rate of 3 °C/min. Contraction, dilatation, softening temperature, maximum contraction temperature and maximum dilatation temperature are outputs of the test. In plastometer, coal fluidity is measured as the rates of stirrer movement placed in a crucible, filled by coal. Temperature is increased by 3 °C/min and stirrer movement is recorded as ddpm. Fluidity, softening temperature, maximum fluidity temperature, solidification temperature and fluid range are outputs of the test (Stiskala, 2016). Fluidity is one of main indicator for coal blend design for coke production. It is important that the temperature intervals of the plastic state for coals constituting a blend should overlap. The longer the overlapping of maximum activity intervals of two particles, the more the number of chemical bonds formed in the contact area (Hardarshan, 2015).

Ash chemistry is determined by XRF. Reflectance is a percentage of the incident light reflected from polished coal tablet. Macerals have different reflectance and vitrinite phase are filtered out to determine the V-type distribution. (Stiskala, 2016).

2.5 Coal Classification

Non-banded coals are rich in inertinite or liptinite, whereas, banded coals are composed mainly of cellulosic materials and they are rich in vitrinite. Calorific value, volatile matter and agglomerating character are basis of coal classification. These properties vary systematically in vitrinite rich coals; however, inertinite and liptinite rich coals shows diversely relative to coal alteration or coalification. That is the reason

behind the fact that vitrinite rich coals or banded coals can be classified while inertinite - liptinite rich coals or non-banded coals cannot.

ASTM Standard Classification of Coals by Rank (D388-17) is commonly used and well accepted coal classification standard. Because of explanation above, the standard is applicable to banded coals and it is based on coal rank. Fixed carbon, volatile matter and calorific value are used as an indication of coal rank or coalification. In addition to coal rank, agglomeration character is also used for coal classification. In the standard, there are four main coal groups, which are lignite, subbituminous, bituminous and anthracite.

Below 69 % fixed carbon, calorific value, moisture and mineral matter free (dmmf) basis, is only indication. According to the standard, coals, which have less than 19.3 Mj/kg calorific value (dmmf) is called Lignite. Coals, have calorific value (dmmf) between 14.7 and 19.3 Mj/kg, is Lignite A. Coals, have calorific value (dmmf) less than 14.7 Mj/kg, is Lignite B.

When the calorific value is between 26.7 and 19.3 Mj/kg, it is called Subbituminous coals. Between 19.3 and 22.1 Mj/kg, it is called Subbituminous C; between 22.1 and 24.4 Mj/kg, it is called Subbituminous B and between 24.4 and 26.7 Mj/kg, it is called Subbituminous A.

Classification continues by calorific value until coals reach 69 % fixed carbon. High volatile coals have less than 69 % fixed carbon and their calorific value is greater than 24.4 Mj/kg. If calorific value is between 24.4 and 26.7 Mj/kg, normally it is called Subbituminous A. Here the difference is agglomerating character. Subbituminous A is not agglomerating.

Bituminous coals, which have a calorific value between 24.4 and 26.7, Mj/kg is agglomerating. As indicated in the standard, there may be some exceptions; however, bituminous coals are expected as agglomerating coals. Between 26.7 and 30.2 Mj/kg, coals are named by High Volatile C. When calorific value is between 30.2 and 32.6 Mj/kg, it is called High Volatile B. If a coal has 69 % fixed carbon (dmmf), less than 31 % volatile matter (dmmf) and greater than 32.6 Mj/kg calorific value (dmmf), it is

named by High Volatile A. After that, coals are classified by fixed carbon and volatile matter content. Medium volatile bituminous coals have fixed carbon in the range of 69 % to 78 % (dmmf) and volatile matter in the range of 22 % to 31 % (dmmf). Low volatile bituminous coals have fixed carbon in the range of 78 % to 86 % (dmmf) and volatile matter in the range of 14 % to 22 % (dmmf).

While passing to semi-anthracite from low volatile bituminous, condensation of small aromatic ring system occurs. This causes the loss of agglomerating character. That is why anthracite group coals is not agglomerating while bituminous coal group is. Semi-anthracite coals have fixed carbon in the range of 86 % to 92 % (dmmf) and volatile matter in the range of 8 % to 14 % (dmmf). Anthracite coals have fixed carbon in the range of 92 % to 98 % (dmmf) and volatile matter in the range of 2 % to 8 % (dmmf). Meta-anthracite is at the top of coalification. These coals have fixed carbon above 98 % (dmmf) and volatile matter below 2 % (dmmf) (ASTM, 2017). Coal classification table is given in Appendix A.

Coals used for coking must have agglomerating character. Otherwise, fusion of coal particles will not occur and coke formation does not exist. Therefore, bituminous coals are used for coke production. One particular coal cannot be used for industrial applications because of both technical and economic reasons. Optimum inert – reactive ratio, plasticity, coal blend cost requirements are satisfied by coal blending. All subgroups of bituminous coals – low, medium and high volatile coals, are used for coal blending for coke production.

2.6 Coal Carbonization at Coke Oven Batteries

Blended coal is charged into coke oven batteries by a machine called charging or larry car in order to produce porous, strong, stable coke lumps from fine coal grains. There are heating walls at each side of coking chamber. This means that coal is heated from two sides in absence of air. This process is special type of pyrolysis. As solid residue of the process is carbon rich, process is called by carbonization instead of pyrolysis. Figure 2.5 is retrieved from Readyhough's presentation at Mc Master University in

2015 (Readyhough and Todoschuk, 2015). It expresses carbonization steps relative to temperature and time.

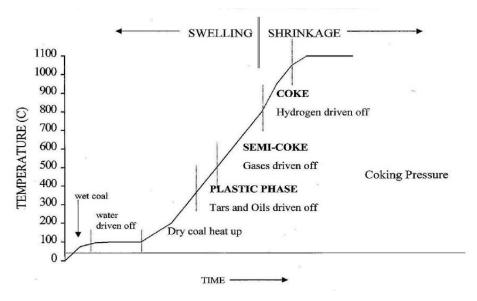


Figure 2.5 Coal to Coke Transformation (Todoschuk, 2015)

After charging, coal is heated up. Water content of coal is driven off at 100 °C. Heating continues as temperature rises, which follows dehydration. At about 350 °C, coals starts to soften. As explained in section 2.4 Coal Classification, not all coal is softening but coking coals are. This feature is represented in ASTM coal classification system by agglomerating character. Between 350 to 500 °C, coal is in plastic phase. It is the most important part of carbonization in terms of both theoretically and technologically. There are three phases in plastic state of coal. First one is solid phase. They are minerals or ash and non-fusible organic content of coal, which is inertinite. Second is plastic phase and they are reactive or fusible organic portion of coal such as vitrinite. Last one is gaseous phase. It is the volatile matter content of coal, which is extracted due to carbonization. After temperature reaches softening temperature of coal, tar and light oils are extracted. These are in the form of aliphatic chains and molecular phase. In addition to that, coal particles agglutinate because of plastic layer fusibility. Fluidity, which can be measured by plastometer, is increasing while temperature is increasing. When maximum fluidity temperature is reached, it starts to decrease until solidification, which occurs at 480 - 500 °C generally. Solidification causes

repolymerisation and carbon bridges arise. This phenomenon gives coke stronger strength than original coking coal. At solidification temperature, semi coke forms however, it contains nearly 12 – 16 % of volatile matter. The difference between volatile matter content of plastic phase and semi coke is composition. In both intervals, molecular phase volatiles are extracted. Hydrocarbons in aliphatic chains are driven off in plastic state and light hydrocarbons are driven off in semi coke state. The reason of relatively high volatile content of semi coke is the gases in semi coke pore structure and it is mainly hydrogen. From 500 °C to 800 °C semi coke is heated and volatile matter content decreases. After 800 °C coke forms. Hydrogen extraction continues till 1000 °C (Isler, 2016). Volatile matter of end coke is below 1 %. That is why end coke temperature, which means the temperature of coke before pushing, is an important operational parameter.

From carbonization of 1000 kg dry coal, nearly 750 kg dry coke, 30 kg tar, 7 kg benzol, and 30 kg water are produced. The rest is coke oven gas and it is used for both heating of coke oven batteries and other units of an integrated iron and steel plant such as hot mill ovens. Coke oven gas' calorific value is about 4200 kcal/m³. Because of high calorific value, which is nearly half of LPG, it is desirable for suitable heating operations.

2.7 Coke Quality

Valia stated that a high quality coke should be able to support smooth descent of the burden with as little degradation as possible while providing the lowest amount of impurities, highest thermal energy, highest metal reduction and optimum permeability for flowage of gaseous and molten products (Valia, 2015). This is the summary of coke quality requirements for blast furnace operations.

In upper cold part of blast furnace, coke should be suitable for gas flowage and able to support burden in the furnace. At that part size distribution, cold strength (stability), and moisture are important quality factors. In middle part of furnace, iron starts to

melt. Therefore, coke should drain melt iron and slag. Coke is also a source of reducing agent carbon monoxide. Carbon dioxide is reacted with coke, which is carbon source to produce carbon monoxide. Gas flowage and need for supporting upper burden is also necessary for this middle part. For these reasons, size distribution, stability and abrasion resistance (hardness) are critical. At bottom part of furnace or dead man region, coke act as a heat source while producing reducing gas and providing enough strength to support burden. Here, coke hot strength, reactivity and coke chemistry are vital quality parameters for cast iron production.

Stiskala created a brief table to express coke quality requirements in North America and Europe in Coke Making Seminar in 2016, given in Table 2.1.

Table 2.1 Coke Quality Requirements in North America and Europe (Stiskala, 2016)

Parameter	North America	Europe
Mean Size	> 50	50 - 55
+60 mm, %		33
+50 mm, %	> 50	
- 25 mm, %	< 3	< 3
Stability, %	> 61	
Moisture, %	< 5	< 4
Sulfur, %	< 0.75	< 0.90
Alkalis, %	< 0.25	< 0.20
Phosphorus, %	< 0.02	< 0.02
CSR, %	> 62	> 65

Coke chemistry in terms of sulfur, alkalis (Na₂O and K₂O) and phosphorus, is directly related with coal blending. These are additive values. It means that coals, which consist of the blend, give their impurities proportional to their percentages in the blend.

Moisture is related with the coke quenching operation. Old design, slow quenching operation results in around 8 % moisture. Faster next quenching design results in 3.5 to 4 % moisture. Newest technology about coke quenching is Coke Stabilizing

Quenching (CSQ), which is developed by Thyssen Krupp. Designer claims that coke quenched by CSQ have a moisture near 2 %.

Size distribution also highly depends on operational factors such as crushing and sieving. Desired size intervals also differ plant to plant. For this reason, coke chemistry, moisture and size distribution will not be investigated further.

Cold coke mechanical strength is represented by coke stability and coke hardness. Stability is coke's resistance to crushing and hardness is coke's resistance to abrasion. ASTM (D 3402 Standard Test Method for Tumbler Test for Coke) standardizes both quality parameters. Tumbler has dimensions 50 mm height, 457 mm width and 914 mm length. 10 kg coke sample with a size range between 2 to 3 inches, which moisture content is below 1 % and sized in a square mesh sieve, is subjected to 1400 revolution in the tumbler with 24 ± 1 rpm. Then, the product of tumbler is sieved by 1 and $\frac{1}{4}$ inches sieves. Mass percentages of + $\frac{1}{4}$ inch portion represents stability factor and mass percentages of + $\frac{1}{4}$ inch portion represents hardness factor.

Last and most important quality parameters are coke reactivity index (CRI) and coke strength after reaction (CSR). The reaction that gives name to two test is take place between carbon (coke) and carbon dioxide. It is the same reaction occurs in blast furnace dead man region to produce reducing agent carbon monoxide. Similar with coke cold strength test, there are two steps. First, coke reacts with carbon dioxide and percent of mass loss in solid coke is represented by coke reactivity index. Second, reacted coke is subjected to a tumbler test. Product of tumbler is sieved and mass percentage of above 3/8 inches is represented by coke strength after reaction. After understanding that coke cold mechanical properties are not enough for blast furnace coke quality representation, Nippon Steel developed CRI and CSR tests for better understanding of coke behavior under high temperature. Then ASTM standardized the tests by the procedure of D 5341 Measuring Coke Reactivity Index (CRI) and Coke Strength After Reaction (CSR). Details about the test is given in Section 2.7.1.

2.7.1 Coke Strength after Reaction Test Procedure

This test was developed by Nippon Steel Cooperation and standardized by ASTM. It determines lump coke reactivity with carbon dioxide and coke strength after the reaction between coke and carbon dioxide. Mass loss of coke as percentage is coke reactivity index. After the reaction, there is a tumbling test. Reacted coke is subjected to the tumbler test and + 9.5 mm portion of tumbler product as percentage is represented by coke strength after reaction.

Coke should handle chemical and mechanical stresses in a blast furnace. Chemical stress is caused by the reaction between countercurrent flow of carbon dioxide and coke. Mechanical stress is caused by abrasion, which is due to coke's rubbing both together and against the furnace walls. Coke Reactivity Index is designed to predict coke chemical stress resistance and Coke Strength after Reaction is designed to predict coke mechanical stress by taking account of chemical reaction between coke and CO₂.

In the test, there are 7 apparatus, which are electric furnace, reaction vessel, flowmeters, thermocouple, sieves and CSR tumbler. Minimum 57 kg sample should be collected. Below 25 mm sample is separated by sieving. Coarser part of the sample is crushed and again sieved to obtain the size fraction between 19 mm and 22.4 mm. crushing continue until all plus 25 mm sample become below 22.4 mm. From this portion three 250 g test sample are prepared by using riffle splitter. Two of them are used for duplicated test procedure and third is spared in case of above 10 g loss between duplicated tests.

First 200 ± 2.0 g samples are prepared. Before reaction vessel placed into the furnace, it should be heated up such that coke must reach 1100 ± 5 0 C in 30 minutes. After coke reached desired temperature, it soaks 10 minutes more at same temperature. Then CO_2 is fed for 120 minutes at again same temperature, 1100 ± 5 0 C. CO_2 is purged by N_2 and reaction vessel is removed from the furnace to cool the coke to 100 0 C. Reacted coke is weighed. Then, it is placed into the tumble for 600 revolutions in 30 minutes

at 20 ± 1 rpm. After tumbler test, product is sieved to 9.5 mm. Both undersize and oversize are weighed. There are three weighing in one test and the test is duplicated. If there is an above 10 g difference between weighting of duplicated tests, third test should be conducted. Weight ratio between reacted coke and test sample is Coke Reactivity Index (CRI). Weight ratio between oversize of tumble product and reacted coke is Coke Strength after Reaction (CSR). Mean values of CRI and CSR calculated from two or three tests are reported as result. ASTM CSR test procedure is illustrated in Figure 2.6.

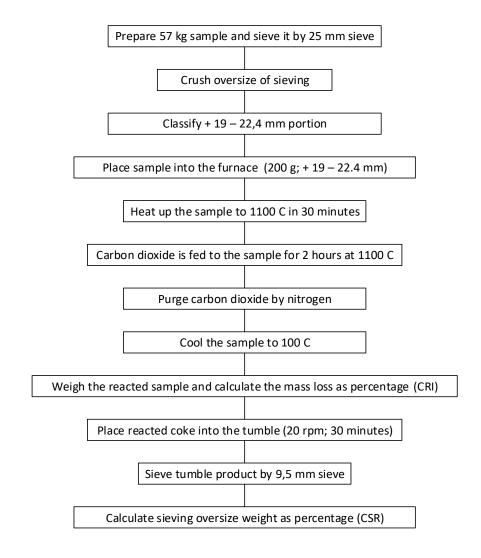


Figure 2.6 ASTM CSR Test Procedure (ASTM, 2014)

2.7.2 Factors Affecting Coke Strength after Reaction (CSR)

Factors affecting Coke Strength after Reaction was determined by literature review and are listed in Figure 2.7. (Loison et al., 1989) (Price, 2015) (Stiskala, 2016) (Isler, 2016). CSR is affected by three main factors, which are coke surface area, coke chemistry and coke carbon forms. Coke, which have smaller size distribution, cause greater surface area. Coke surface area changes with oven bulk density, quenching practice and dilatation. Greater oven bulk density or coal bulk density results compact and higher strength coke. Oven bulk density affected by coal moisture, coal grain size, density modifiers and charging practice. Coal moisture and density modifiers increase coal bulk density. While density modifiers increase production rate, high moisture content decreases production. Finer size distribution for coal cause lesser bulk density. On the other hand, coarser size distribution is the reason of fusion problems in plastic state of coking and lesser coke strength. Optimum charging practice is filling the oven up to leveling bar space uniformly at minimum time. Bad charging practice prevents uniform heating and cause smaller coke size distribution. Quenching is the first change to eliminate cokes which have internal cracks. It is called coke stabilization. High dilatation values cause internal cracks and lower coke strength.

Coke chemistry consist of coal blend ash analysis, coal sulphur, coal blend ash content and additives. Higher basicity indexes decrease CSR. Basicity index is explained in Section 2.8.1. Coal sulphur disturb coke carbon structure. It weakens coke and decreases CSR. Higher ash contents decrease CSR.

Coke carbon form is affected by coal blend rheology, coal macerals, coal V – type distribution, pyrolytic carbon, additives and width of plastic zone. Coal blend rheology, macerals and coal V – types is explained in Section 2.4. increase in width of plastic zone increase CSR. Working with lower coking rates and wider blend fluid range increase width of plastic zone.

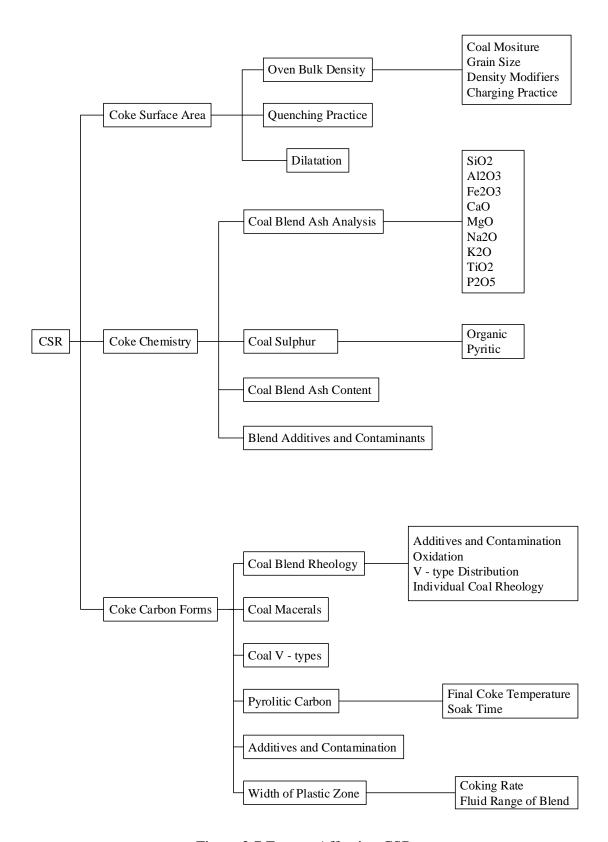


Figure 2.7 Factors Affecting CSR

2.8 Developing a Statistical Model for CSR Prediction

Coke quality prediction research can be divided into three stages. First is based on stability prediction created by Shapiro and Gray (Shapiro et al., 1961). It was based on ash chemistry and coal petrography. They defined two parameters, which are composition balance index (CBI) and Strength Index (SI). Then they developed the stability prediction curve, which predicts estimated coke stability by using calculated composition balance index and strength index. Then, CSR was developed by Nippon Steel and it was understood that CSR is a better test method to predict coke behavior in blast furnace because coke stability test result gives information about only coke cold behavior. On the other hand, CSR test is done after coke is reacted with CO₂ at 1100 °C. Second stage was based on theoretical formulas to predict CSR. While working with one-region coals, these formulas gives relatively accurate results. Unfortunately, prediction accuracies are not satisfactory for a blend, which includes different region's coals. Below Table 2.2, parameters of early attempt CSR prediction formulas developed by steel companies are listed chronologically. In addition to that, 8 most famous theoretical formulas are given in Section 2.8.1. They will also be used to comprise developed statistical prediction formula, which is the aim of this study.

After 1980s international coal trade have grown due to both low cost and high quality coke production. It accompanied a challenge for coke makers, coke quality prediction for coal blends, containing international coals. Therefore, third stage prediction attempts were based on statistical modelling.

Table 2.2 Theoretical CSR Prediction Equations' Parameters developed by Steel Companies

Company	Coal Petrography	Coal Rheology	Ash	Others	Year
British Steel	Vitrinite Reflectance		Coke ash content		1977
NKK				Coke petrography	1978
Nippon Steel	Inertinite %, Maximum medium reflectance	Maximum fludity	Coal ash alkali index		1980
BCRA	Inertinite %	Maximum fludity	Coal alkali content	Coal Oxygen and Carbon content; pores/cm2 coke	1982
Kobe Steel	Maximum medium reflectance	Maximum fludity	Coal ash alkali index		1985
CANMET	Maximum medium reflectance		Coal ash modified basicity index	Total dilatation	1988
ВНР	Inert Content	Maximum fludity	Coal ash basicity	Volatile matter	1989
Indland Steel		Plastic temperature range	Coal ash alkali index	Coal Sulphur	1989
ISCOR	Vitrinites maximum reflectance; organic inerts %	Maximum fludity	Coal ash basic oxides		1990

2.8.1 Theoretical CSR Prediction Equations

There are several theoretical CSR prediction formulas in literature. In general, they were developed to research particular region coal's availability of use in coal blends for coke making. Some of them are given in sub-titles of Section 2.8.1.

Formulas explained in further sub-sections are retrieved from literature as follows.

- Coke Quality Seminar by Victor Stiskala,
- Coal for metallurgical coke production: prediction of coke quality and future requirements for coke making by Diez, Alvarez and Barriocanal,
- Influence of Geology on CSR by Pearson
- Review on Modeling of Coal Blends for Prediction of Coke Quality by Cordova, Madias and Barreiro

In titles, formulas represented by origin country names because there is no terminology for them.

2.8.1.1 Canadian Formula 1

$$CSR = 84.376 - 18.909 \times A \times BI$$

 $BI = (CaO + MgO + Na_2O + K_2O + Fe_2O_3) \div (SiO_2 + Al_2O_3)$

Where A is ash,

BI is basicity index.

This formula was retrieved from Ted Todoschuk study. (Todoschuk et al., 2018)

2.8.1.2 Canadian Formula 2

$$CSR = 83.217 - 167.801 \times BI + 147.816 \times BI^{2}$$

 $BI = (CaO + MgO + Na_{2}O + K_{2}O + Fe_{2}O_{3}) \div (SiO_{2} + Al_{2}O_{3})$

Where BI is basicity index.

This formula was retrieved from Stiskala's Coke Quality Seminar. (Stiskala, 2016)

2.8.1.3 American Formula 1

$$\begin{split} CSR &= 28.91 + 0.63 \times FR - 9.64 \times Al - 14.04 \times S \\ Al &= Ash \ (\%) \times (CaO + MgO + Na_2O + K_2O + Fe_2O_3) \div (SiO_2 + Al_2O_3) \end{split}$$

Where FR is fluid range,

Al is alkali index,

S is sulfur.

This formula is retrieved from Diez, Alvarez and Barriocanal's "Coal for metallurgical coke production: prediction of coke quality and future requirements for cokemaking" study. (Diez *et al.*, 2001)

2.8.1.4 American Formula 2

$$CSR = 66.89 \times MMR + 7.8 \times log (F) - 89 \times BAR - 32$$

 $BAR = (CaO + MgO + Na2O + K2O + Fe2O3) ÷ (SiO2 + Al2O3 + TiO2)$

Where MMR is mean maximum reflectance of vitrinite,

F is maximum fluidity,

BAR is basic to acidic ratio.

This formula was retrieved from Stiskala's Coke Quality Seminar. (Stiskala, 2016)

2.8.1.5 Australian Formula 1

$$\begin{split} &CSR = 94.2 - 1.275 \times (13.4 + 9.35 \times MBI) - 0.45 \times MBI^2 \\ &MBI = 100 \times ash \times (CaO + MgO + Na_2O + K_2O + Fe_2O_3) \div ((100 - VM) \times (SiO_2 + Al_2O_3)) \end{split}$$

Where MBI is modified basicity index,

VM is volatile matter content (%).

This formula was retrieved from Stiskala's Coke Quality Seminar. (Stiskala, 2016)

2.8.1.6 Australian Formula 2

$$CSR = 133.8 - 15.56 \times BI - 3.1 \times VM + 8.5 \times log (F) + 0.22 \times Inerts (\%)$$

$$BI = (CaO + Na2O + K2O + Fe2) \div (SiO2 + Al2O3)$$

Where BI is basicity index,

VM is volatile matter content (%),

F is maximum fluidity,

Inerts (%) is inert content (%).

This formula was retrieved from Pearson's "Influence of Geology on CSR" study. (Pearson, 2016)

2.8.1.7 Japanese Formula

$$CSR = 70.9 \times MMR + 7.8 \times log (F) - 89 \times BAR - 42$$

 $BAR = (CaO + Na2O + K2O + Fe2O3) ÷ (SiO2 + Al2O3)$

Where MMR is mean maximum reflectance of vitrinite,

F is maximum fluidity,

BAR is basic to acidic ratio.

This formula was retrieved from Pearson's "Influence of Geology on CSR" study. (Pearson, 2016)

CHAPTER 3

STATEMENT OF THE PROBLEM

The objective of this study is to develop a statistical model to predict coke strength after reaction (CSR) based on coal quality test results. CSR is one of coke quality parameter and it is the most important one. Generally, high quality coking coal definition is used for coals, which have high CSR values in metallurgical coal trade. There are several factors affecting CSR. In addition to these factors, different coals from different regions show characteristic coking properties. Moreover, coking coal cost is the biggest cost in steel production. Economic crises and uncertainties fluctuate coking coal prices. Because of this diversity in quality parameters and challenges in feasible coke production make coke quality prediction critical. CSR as most important coke quality criteria must be predicted before industrial coke production. Theoretical formulas were developed as an attempt to predict CSR, however, they are not giving accurate predictions relative to actual test results. Current industrial trend and solution is developing statistical models based on plant's own imported coking coals. Therefore, the primary goal in this study is to obtain an accurate CSR prediction model relative to both theoretical formulas developed before and actual laboratory coke quality test results. In this manner, this study consists of four main phases. These are:

- 1. Determining factors affecting coke strength after reaction (CSR)
- 2. Determining how much these factors affect CSR, which are most critical
- 3. Classification of studied coals regarding to their origin and positive or negative effects
- 4. Developing an accurate CSR prediction model

CHAPTER 4

MATERIALS AND METHODS

4.1 Coking Coal Samples

In this study, 49 coking coals are examined. 22 of them are Australian coals, 20 of them are American coals and 7 of them are Canadian coals. There are 192 set of analysis for these 49 coals. These analyses have already been carried out before the start of the study. Performing analyses is not a part of this study. Each analysis set have 115 parameters. They are listed in Appendix C, Table C.1. These coals are already used for industrial application, coke making. In order to keep operational know-how and technological information confidential, coal names, supplier company names and consumer company name will not be given. Coals are named according to their origin, for example, "Australian coal # 16".

4.2 Coal Sample Quality Characterization Studies

In this part, coals are classified according to laboratory analysis. There are three phases in analysis. After coal is supplied, first, individual coal analyses are done. Then, coke analysis performed by individual coals. Finally, coke quality tests are made by coal blend for industrial production. In this study, coals are classified according to coal and coke quality parameters, which are explained in sections 2.4 and 2.7 respectively. In addition to these, origin of coal is considered as a factor. It means that general characteristics of coals according to their origin is also examined. Therefore, outstanding coals', which are American, Canadian and Australian, reason of popularity is explained. This part of the study is done to understand usual and unusual changes by classification before developing a statistical model for CSR prediction.

In coal characterization, 5 main analyses groups will be investigated.

- Proximate analysis
- Physical properties
- Rheological properties
- Ash chemistry
- Petrographical analysis

Proximate analysis consists of moisture, volatile matter, ash, fixed carbon and calorific value. Physical analysis includes hard grove index, reflectance of light, bulk density and sieve analysis. Rheological analyses include free swelling index (FSI), plastometer and dilatometer test results. Coal ash mineral analysis consists of Al₂O₃, CaO, Cr₂O₃, Fe₂O₃, K₂O, MgO, MnO, Na₂O, P₂O₅, SiO₂, TiO₂, P, S, ZnO. In addition to these, total sulfur and total phosphor analysis are also done. Investigated petrographic analysis of coal samples includes mean random vitrinite reflectance (Ro), V – type distribution and maceral analysis, which are vitrinite, liptinite, semi-fusinite and inertinite contents.

Analysis of coals samples are given in Appendix B. In section 5.1, each parameter of analysis is examined and basic statistic table is given with a box plot graph in order to understand distribution of data relative to coal origin. Average origin base proximate, physical, rheological, chemical and petrographic analysis of coal samples are given in Table 4.1, Table 4.2, Table 4.3, Table 4.4, Table 4.5 relatively.

Table 4.1 Average Origin base Proximate Analysis of Coal Samples

Coal Origin	Moisture (%)	Volatile Matter (%) (db)	Ash (%) (db)	Fixed Carbon (%) (db)	Calorific Value (db) (kcal/kg)
American	8.29	25.96	8.34	65.71	7690
Australian	9.50	24.70	9.27	66.03	7482
Canadian	8.93	24.16	9.07	66.77	7565

db: dry base

Table 4.2 Average Origin base Physical Analysis of Coal Samples

Coal Origin	HGI	Reflectance of Light (%)	Bulk Density (gr/cm3)	+6,30 mm (%)	-0,425 mm (%)
American	76.38	90.56	0.77	22.38	23.81
Australian	74.81	94.16	0.82	36.16	19.40
Canadian	83.32	92.40	0.71	16.75	34.93

Table 4.3 Average Origin base Rheological Analysis of Coal Samples

Coal Origin / Parameter	American	Australian	Canadian
FSI	8.14	7.24	7.39
Maximum Fluidity (ddpm)	5272	1333	104
Softening Temp. (Plastometer) (°C)	403	400	412
Maximum Fluidity Temperature (°C)	448	435	444
Solidification Temperature (°C)	487	464	472
Fluid Range (°C)	71	61	60
LGF (Logarithmic Fluidity)	2.55	2.11	1.80
Maximum Dilatation (%)	147.47	70.13	45.28
Maximum Contraction (%)	-1.02	-11.10	-20.53
Softening Temp. (Dilatometer) (°C)	390	404	404
Dilatation Starting Temperature (°C)	425	442	445
Dilatation Finishing Temperature (°C)	480	449	475

ddpm: dual division per minute

Table 4.4 Average Origin base Chemical Analysis of Coal Samples

Coal Origin / Parameter	American	Australian	Canadian
Total Sulphur (%) (db)	0.848	0.515	0.442
Total Phosphor (%) (db)	0.021	0.039	0.071
Total Alkalis in ash (%)	2.740	1.164	0.910
Basicity Index (BI)	0.201	0.124	0.094
Basic to Acid Ratio (BAR)	0.197	0.121	0.092
Modified Basicity Index (MBI)	2.207	1.488	1.129

Chemical analyses were performed by dry basis (db) sample.

Table 4.5 Average Origin base Petrographical Analysis of Coal Samples

Coal Name	(Ro)	Vitrinite	Liptinite	Semifusinite	Inertinite
American	1.04	66.45	7.94	8.50	21.40
Australian	1.08	67.72	5.20	14.57	24.57
Canadian	1.06	70.14	3.29	11.75	24.18

4.3 Coke Sample Quality Characterization Studies

There are 6 examined coke quality parameters.

- Coke stability factor,
- Coke hardness factor,
- Maximum gas pressure of coking,
- Maximum wall pressure of coking,
- Coke reactivity index and
- Coke strength after reaction,

Coke quality characterization parameters are listed in Appendix B, Table B.6. In section 5.2 basic statistics about coke quality parameters is also given. In addition, box plot representation will be used to help understanding both particular origin base and between fluctuations in origins. Average origin base coke quality analysis of coal samples are given in Table 4.6.

Table 4.6 Average Origin base Coke Quality Analysis of Coal Samples

Coal Origin	Stability (%)	Hardness (%)	CRI (%)	CSR (%)	Max Gas Pressure (kPa)	Max Wall Pressure (kPa)
American	57.53	64.48	28.73	54.24	9.44	5.18
Australian	57.02	63.60	28.90	57.68	4.68	4.70
Canadian	59.13	65.10	22.56	66.23	2.01	2.89

4.4 Developing Multiple Linear Regression Model for Origin based CSR Prediction

A model is an adequate representation of a real process system, and modeling is the act of model development. There are two types of model, physical and mathematical. Physical models are full scale or scaled-down replica of the real systems. They allow direct experiment without assumptions. Mathematical models represent process or some aspects of a process quantitatively by set of equations. Mathematical models consist of fundamental models, empirical models and phenomenological models. Fundamental models explain transport phenomena and chemical rates in a process. Empirical models based on dependent or independent operational variables to predict a process response. Phenomenological models combines both fundamental and empirical approach to understand of a process (Hoşten, 2014).

First order multiple linear regression model is represented below (Devore, 2012).

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_k x_k + \epsilon = \sum_{j=1}^k \beta_j x_j + \epsilon$$

where "y" is response,

"x" is regressor variable

"E" is unobservable random error,

"β" is regression coefficient.

Hoşten states the steps of empirical model representation for a continuous process, which is listed below.

- 1. Define purpose of model
- 2. Select response and factors
- 3. Select forms for model (functional relationship between the response and factors)
- 4. Devise a data acquisition plan and obtain raw data

- 5. Adjust raw data statistically
- 6. Fit models to adjusted data
- 7. Test adequacy of fitted equations.

The purpose of this study is predicting CSR. Therefore, response is CSR and parameters are coal and coke analysis. 218 set of analysis about both coal and coke were collected and categorized in an excel file for statistical use.

In this study, steps listed below were followed as parts of regression analysis.

- 1. Classification of raw coal and coke analysis data.
- 2. Elimination of parameters that shows similar behavior.
- 3. Best subset analysis to decide regression parameters.
- 4. Regression model development.
- 5. Testing fitted linear model.

Before regression model development, correlation analysis was performed to decrease number of parameter from 115 to below 30. Pearson correlation coefficient and p-value are considered in correlation analysis. The Pearson correlation coefficient is a statistical tool to evaluate the linear relationship between two continuous variables. It is a value between "- 1" and 1. Through "- 1" negative relation between two variable increases. Likewise, positive relation between two variable increases through "1". "0" represent there is no relation. By excel correlation tool, correlation analysis was performed for 115 parameters. It is considered that parameters that have over 0.8 and below – 0.8 Pearson correlation coefficient are highly correlated and one of two should be eliminated (Devore, 2012).

This elimination was not enough to decrease number of parameters below 30. For this reason, second stage correlation was performed by using both Excel and Minitab correlation tools. After determination of the parameters that have above 0.6 or below -0.6 correlation by Excel correlation tool, p-values of correlated parameters were

controlled by Minitab correlation tool. Thus, parameters, which have correlation coefficient between 0.6 (- 0.6) and 0.8 (- 0.8) and below 0.05 p-values were eliminated.

Rest of parameters created regression database after elimination of correlated parameters. In order to decide which parameters will be used in regression model, best subset analysis was performed in Minitab. Best subset analysis gives a table including R – square, R – square adjusted, R – square predicted, Mallows' Cp, error standard deviation and the components of possible regression models. R² is called the coefficient of determination. It is used to judge regression model adequacy. Higher Rsquare values represent higher adequacy of regression model. However, adding parameter to regression model also increase R-square value. R – square (adj) is a modified version of R - square that has been adjusted for the number of predictors in the model. Predicted R - square indicates how well the model predicts responses for new observations. Mallows' Cp is another statistic for assessing how well the model fits the data. Mallows' Cp should be close to the number of predictors contained in the model plus the constant. Using Mallows' Cp to compare regression models is only valid when you start with the same set of variables. "s" is the error standard deviation. A good model should have a high R, high adjusted R, high predicted R, small s, and Mallows' Cp close to the number of predictors plus the constant contained in the model. (Minitab Software, 2018). From best subset analysis, parameters used in up to 10 variable model alternatives are selected for regression analysis.

First regression analysis is performed to evaluate variables again by ANOVA table of regression. Contribution of parameters are evaluated by p – values. Parameters, which have $0.05\ p$ – value or above, are considered unnecessary or insignificant. After this last step parameter or variable elimination, second regression model is developed to predict response, which is CSR.

In regression model, there are some assumptions listed below (Hosten, 2014).

- 1. The error term ε in the model is normally distributed with an expected value of zero and an unknown variance,
- 2. The ε are uncorrelated random variables,
- 3. The variance of model error equals the variance of measurement.

Because of these assumptions, fitted linear model should be tested. Testing is done by residuals usually. If scatter plot of residuals and predicted responses is homogenous or randomly scattered, it means that the variance is constant. Normality test is also shows the distribution's type. Thanks to Minitab, all these can be seen by graphical representation.

Expectations from developed models are listed below.

- 1. R square should be over 85 %
- 2. Residues of predicted response should be distributed normally.
- 3. Residues of predicted response should be distributed homogenously.
- 4. Developed model should predict CSR more precisely than theoretical formulas given in Section 2.8.1.

4.5 Comparison of Origin base CSR Prediction Models with Theoretical Formulas

The aim of linear multiple variable regression model is predicting response values exactly. It means that difference between actual value and predicted response value should be zero. Comparison of models and formulas retrieved from literature bases on this assumption.

First residues, which means the difference between actual values and predicted values, will be calculated. Then, hypothesis will be created based on residues means and suitable test will be performed. Three hypothesis tests will be used in this study.

- 1. 1 sample t test,
- 2. 2 sample t test,
- 3. One way ANOVA test.

Residue populations should distribute normally. In addition to that, variances of populations should be equal.

In 1 – sample t test, a population mean's equality to zero is investigated. Original hypothesis is mean of population is equal to zero. Alternative hypothesis is the mean is not equal to zero. If p – value of the 1 – sample t test is greater than confidence level, original hypothesis is true or vice versa. Confidence level is expected 5 % in this study. Representation of 1 – sample t test is explained below.

```
Ho: \mu (model) = 0 if p – value > \alpha, Ho is true
Ha: \mu (model) \neq 0 if p – value < \alpha, Ha is true
\alpha = 0.05
```

In 2 – sample t test, means of two populations' equality is investigated. Original hypothesis is mean of first population is equal to mean of second population. Alternative hypothesis is mean of first population is not equal to mean of second population. If p – value of the 2 – sample t test is greater than confidence level, original hypothesis is true or vice versa. Confidence level is expected 5 % again. Representation of 2 – sample t test is explained below.

```
Ho: \mu (model) = \mu (formula 1) if p-value>\alpha, Ho is true Ha: \mu (model) \neq \mu (formula 1) if p-value<\alpha, Ha is true \alpha=0.05
```

In one – way ANOVA test, means of more than two populations' equality is investigated. Original hypothesis is population means are equal to each other. Alternative hypothesis is at least one of population has different mean. If p – value of the one – way ANOVA test is greater than confidence level, original hypothesis is true or vice versa. Confidence level is expected 5 % again. Representation of one – way ANOVA test is explained below.

```
Ho: \mu (model) = \mu (formula 1) = \mu (formula 2) if p – value > \alpha, Ho is true Ha: at least one is different if p – value < \alpha, Ha is true \alpha = 0.05
```

In conclusion, residues of population(s) will be investigated in terms of mean(s). If single model or formula is examined, 1 – sample t test will be used. If developed model is comprised with a formula, 2 – sample t test will be used. In order to comprise developed model with more than one formulas, one – way ANOVA test will be used if population variances are equal. If they are not equal to each other, paired populations will be examined by 2 – sample t test.

4.6 Developing a CSR Prediction Model for Coal Blends

Procedure for developing a model for coal blend CSR prediction is almost the same as

for developing a model for origin base coals. The difference is that parameters of origin

base model will be determined by correlation and best subset analysis. However,

parameters of blend model will be determined by considering literature,

characterization studies and origin base model development. Then regression analysis

will be performed.

Normality and homogeneity of model residues is an indication of model fitness. In

addition to that 1 – sample t test will be performed to check the model precision. In

theory, if model predict responses exactly, residues of the model must be zero, so as

mean of residues. By performing 1 – sample t test, whether the mean of model residues

is equal to zero will be controlled.

Representation of 1 – sample t test is explained below.

Ho: μ (model) = 0

if p – value > α , Ho is true

Ha: μ (model) $\neq 0$

if p – value $< \alpha$, Ha is true

 $\alpha = 0.05$

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CHAPTER 5

RESULTS AND DISCUSSION

5.1 Coal Quality Characterization Studies

Coal quality consist of 5 test groups, which are proximate analysis, physical analysis, carbonization properties, ash chemistry and petrographic analysis.

5.1.1 Proximate Analysis of Coal Samples

Statistical data about coal sample's proximate analysis are listed in Table 5.1.

Proximate analysis includes moisture, volatile matter, ash, fixed carbon and calorific value. The analyses of coal samples are listed in Appendix B, Table B.1. Australian coals have higher moisture relative to others. American coals have lesser moisture content. In average; Australian coals have 9,50 %, American coals have 8,29 % and Canadian coals have 8,93 % moisture content.

American coals have higher volatile matter relative to others. In average; Australian coals have 24,70 %, American coals have 25,96 % and Canadian coals have 24,16 % volatile matter content. Canadian coals have lowest volatile matter content. The reason is higher degree of coalification because of temperature and geological activity rather than age.

Australian coals have higher ash relative to others. In average; Australian coals have 9,27 %, American coals have 8,34 % and Canadian coals have 9,07 % ash content. American coals have lowest ash content. It is known that ash content and composition is related with peat formation environments, which is explained in section 2.3.

Table 5.1 Descriptive Statistics of Coal Samples' Proximate Analysis

Analysis	Statistic	Australian	American	Canadian
	Minimum	7.05	6.64	8.44
Maiatrona	Median	9.46	8.07	8.80
Moisture	Average	9.50	8.29	8.93
	Maximum	11.70	10.69	9.76
	Minimum	19.12	17.03	20.75
Volatile	Median	23.48	25.66	23.86
Matter	Average	24.70	25.96	24.16
	Maximum	35.04	32.11	27.03
	Minimum	7.24	6.09	8.31
Ash	Median	9.55	8.23	9.02
ASII	Average	9.27	8.34	9.07
	Maximum	10.58	11.57	9.94
	Minimum	56.45	60.75	64.66
Fixed Carbon	Median	66.88	65.89	66.83
rixeu Carbon	Average	66.03	65.71	66.77
	Maximum	71.16	76.07	70.07
	Minimum	6865	7446	7477
Calorific	Median	7552	7683	7588
Value	Average	7482	7690	7565
	Maximum	7744	8004	7621

Australian, Canadian and American coals have similar fixed carbon values. In average; Australian coals have 66,03 %, American coals have 65,71 % and Canadian coals have 66,77 % fixed carbon content.

All coal samples have similar gross calorific values, which are between 7400 and 7600 kcal/kg. In average; Australian coals have 7482 kcal/kg, American coals have 7690 kcal/kg and Canadian coals have 7565 kcal/kg calorific value. All coal samples' gross calorific value are between 7400 and 7600 kcal/kg generally because all coals are belong to bituminous coal class. That is why calorific values are close to each other.

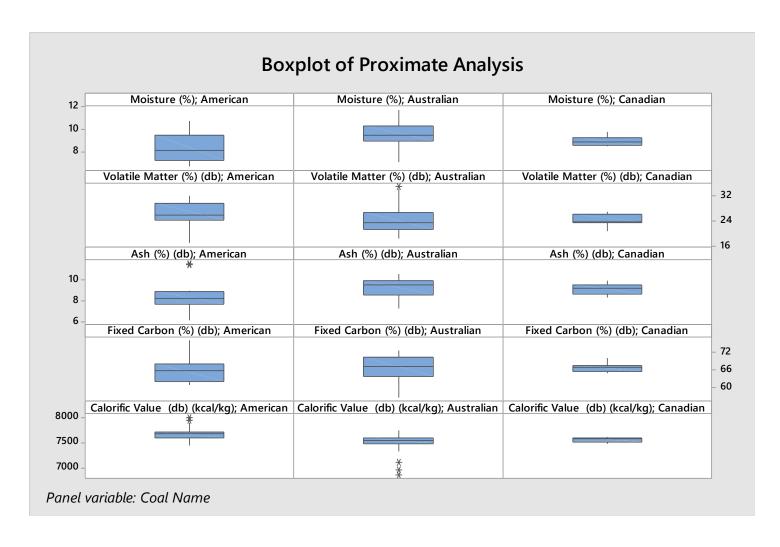


Figure 5.1 Box Plot of Proximate Analysis of Coal Samples

In order to understand fluctuations in proximate analysis according to different origins and samples from same origin, box plot representation is given in Figure 5.1.

5.1.2 Physical Properties of Coal Samples

Descriptive statistics of coal sample's physical properties are listed in Table 5.2.

Table 5.2 Descriptive Statistics of Coal Samples' Physical Properties

Variables	Statistic	Australian	American	Canadian
	Minimum	47.70	58.74	80.87
пот	Median	78.69	78.15	83.00
HGI	Average	74.81	76.38	83.32
	Maximum	88.15	95.40	86.93
	Minimum	90.21	67.14	91.38
Reflectance	Median	94.66	92.00	92.28
of Light	Average	94.16	90.56	92.40
	Maximum	98.29	97.11	93.96
4	Minimum	0.75	0.67	0.68
Bulk	Median	0.82	0.76	0.72
Density	Average	0.82	0.77	0.71
	Maximum	0.88	0.85	0.75
	Minimum	27.33	9.36	10.14
+ 6.3 mm	Median	33.70	20.68	17.17
+ 0.3 11111	Average	36.16	22.38	16.75
	Maximum	49.98	38.65	20.00
	Minimum	9.73	12.99	27.81
0.425	Median	19.80	23.67	34.48
- 0.425 mm	Average	19.40	23.81	34.93
	Maximum	25.09	30.94	44.43

Physical tests of coal samples consist of hard grove index, reflectance of light, bulk density and sieve analysis. 50, 25, 12.5, 6.3, 3.15 and 0.425 mm sieves are used to determine size distribution. In coke making, plus 6.3 mm portion can be considered as coarse and minus 0,425 mm portion can be considered as fine. For this reason, plus

6.3 mm and minus 0.425 mm portions of sieve analysis are used in this study. Physical properties of coal samples are listed in Appendix B, Table B.2.

Canadian coals have higher hard grove index than other coals. American coals are similar with Australian coals In average; Australian coals have 74,81 %, American coals have 76,38 % and Canadian coals have 83,32 % HGI. Grindability of Canadian coals are easier than other coals. The reason is that Canadian coals coalification is high. However, geological activity and temperature gradient played more important role in this coalification rather than age. Therefore, Canadian coals have been subjected to geological and temperature stresses and it cause fine particle size distribution.

Australian, American and Canadian coals have similar light reflectance, which are over 90 %. In average; Australian coals have 94,16 %, American coals have 90,56 % and Canadian coals have 92,40 % reflectance of light. All coals' reflectance of light is over 90 % generally. Reflectance of light is an indication of coal oxidation. When coal is stored several months, it starts to oxidize. Oxygen bonds decrease coke strengths. For this reason, lesser stock time or oxygen bonds in carbon structure is desired in coke making. Over 90 % reflectance of light represents not awaited or newly-mined coal.

Australian and Canadian coals have higher bulk densities than Canadian coals. Canadian coals have lowest bulk density although they have finer size distribution, which will be explained next item. In average; Australian coals have 0,823 g/cm³, American coals have 0,767 g/cm³ and Canadian coals have 0,711 g/cm³ bulk densities.

Australian coals have higher + 6,3 mm size particles than other coals. Canadian coals have lowest coarse particle. In average; Australian coals have 36,16 %, American coals have 22,38 % and Canadian coals have 16,75 % + 6,3 mm size portion.

Canadian coals have higher -0.425 mm size particles than other coals. In average; Australian coals have 19,40 %, American coals have 23,81 % and Canadian coals have 34,93 % - 0,425 mm size portion.

In order to understand fluctuations in physical properties according to different origins and samples from same origin, box plot representation is given in Figure 5.2.

In order to understand fluctuations in physical analysis according to different origins and samples from same origin, box plot representation is given in Figure 5.2.

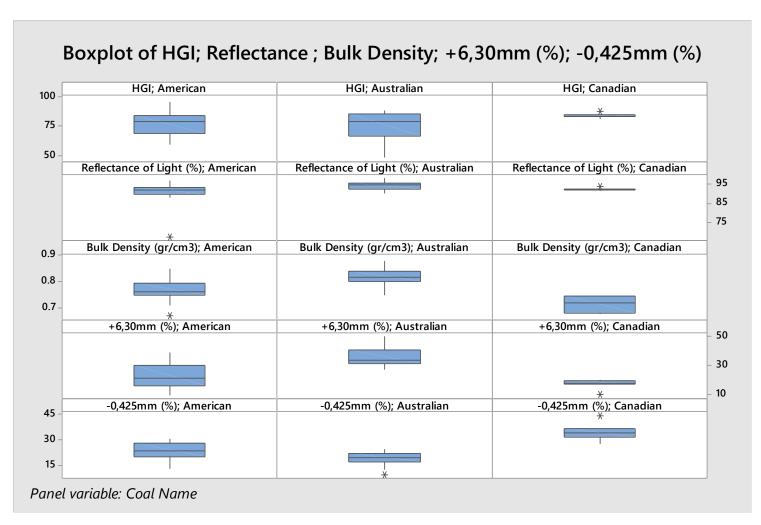


Figure 5.2 Box Plot of Physical Analysis of Coal Sample

5.1.3 Rheology and Free Swelling Index of Coal Samples

Rheological properties of coal include plastometer and dilatometer test.

Output of plastometer tests are:

- Maximum fluidity,
- Softening temperature,
- Maximum fluidity temperature,
- Solidification temperature,
- Fluid range (difference between maximum fluidity temperature and solidification temperature),
- LGF (is logarithmic maximum fluidity)

Output of dilatometer test are:

- Maximum dilatation,
- Maximum contraction,
- Softening temperature,
- Dilatation starting temperature,
- Dilatation finishing temperature

Descriptive statistics of coal sample's rheology and FSI are listed in Table 5.3.

Free swelling index (FSI) is also considered in this section although it is agglomeration characteristic rather than rheological parameter. Rheological Properties of coal samples are listen in Appendix B, Table B.3.

American coals have higher free swelling index relative to others. Canadian have lesser FSI. In average, Australian coals have 8.0, American coals have 8.0 and Canadian coals have 7.5 FSI. It should be note that nearly all coals are coking coals. That is why all have over 7.0 FSI generally.

Table 5.3 Descriptive Statistics of Coal Samples' Rheology and FSI

 Variables	Statistic	Australian	American	Canadian
	Minimum	2.5	7.0	7.0
	Median	8.0	8.0	7.5
FSI	Average	7.2	8.1	7.4
	Maximum	8.5	9.0	8.0
	Minimum	2	72	18
Maximum	Median	140	1518	71
Fluidity	Average	1333	5272	104
	Maximum	18969	23799	233
	Minimum	201	314	374
Plastometer	Median	419	409	422
Softening Temperature	Average	400	403	412
1 cmpci ature	Maximum	459	448	432
Plastometer	Minimum	217	350	403
Maximum	Median	459	455	458
Fluidity	Average	435	448	444
Temperature	Maximum	480	482	463
	Minimum	229	380	425
Plastometer	Median	492	495	488
Solidification	Average	464	487	472
Temperature	Maximum	504	511	492
	Minimum	29	63	46
Eluid Danas	Median	Iedian 65		62
Fluid Range	Average	64	84	60
	Maximum	87	104	68
	Minimum	-8.00	18.00	13.00
Maximum	Median	63.14	137.10	39.80
Dilatation	Average	70.13	147.47	45.28
	Maximum	164.00	260.75	91.00
	Minimum	-26.00	-26.00	-26.14
Maximum	Median	-21.00	-22.00	-22.50
Contraction	Average	-18.85	-19.45	-20.53
	Maximum	-4.29	-3.76	-7.07
D31-4-42	Minimum	414	410	436
Dilatation Starting	Median	442	424	446
Temperature	Average	442	425	445
	Maximum	471	460	458

American coals have higher maximum fluidity relative to others. Canadian coals have lowest maximum fluidity. In average; Australian coals have 1333, American coals have 5272 and Canadian coals have 104 ddpm maximum fluidity. It should be note that fluidity is key parameter in plastic phase of coking. Due to fluidity's necessity, American coals is inevitable in coal blend design for coke making.

Australian, American and Canadian coals have similar plastometer softening temperatures (0 C). In average, softening temperatures are 400 0 C, 403 0 C and 412 0 C for Australian, American and Canadian coals respectively.

Australian, American and Canadian coals have similar maximum fluidity temperatures (0 C). In average, maximum fluidity temperatures are 435 0 C, 448 0 C and 444 0 C for Australian, American and Canadian coals respectively.

Australian, American and Canadian coals have similar solidification temperatures (0 C). In average, solidification temperatures are 464 0 C, 487 0 C and 472 0 C for Australian, American and Canadian coals respectively.

Fluid range is difference of solidification temperature and softening temperature. American coals' fluid range is much more than others. Canadian coals have lowest fluid range. In average, fluid ranges are 63.5, 83.97 and 60.16 for Australian, American and Canadian coals respectively.

Dilatation is volume expand of coal when heated. American coals' maximum dilatation is much more than others. Canadian coals have lowest dilatation. In average, maximum dilatations are 70.13, 147.47 and 45.28 for Australian, American and Canadian coals respectively.

Contraction is volume decrease of coal when heated. Canadian coals' maximum contraction is much more than others. In average, maximum contractions are -18.85, -19.45 and -20.53 for Australian, American and Canadian coals respectively.

Australian, American and Canadian coals have similar dilatation softening temperatures. In average, softening temperatures are 404 0 C, 390 0 C and 404 0 C for Australian, American and Canadian coals respectively.

Australian and Canadian coals have higher dilatation starting temperatures. In average, dilatation-starting temperatures are 442 0 C, 425 0 C and 445 0 C for Australian, American and Canadian coals respectively.

Australian, American and Canadian coals have similar dilatation finishing temperatures. In average, dilatation-finishing temperatures are 449 0 C, 480 0 C and 475 0 C for Australian, American and Canadian coals respectively.

In order to understand fluctuations in rheological analysis according to different origins and samples from same origin, box plot representation is given in Figure 5.3 and Figure 5.4.

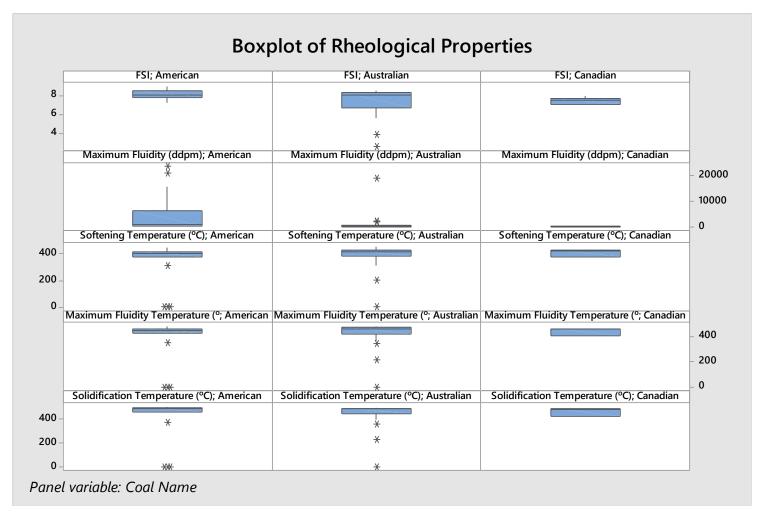


Figure 5.3 Box Plot of Rheological Analysis of Coal Samples

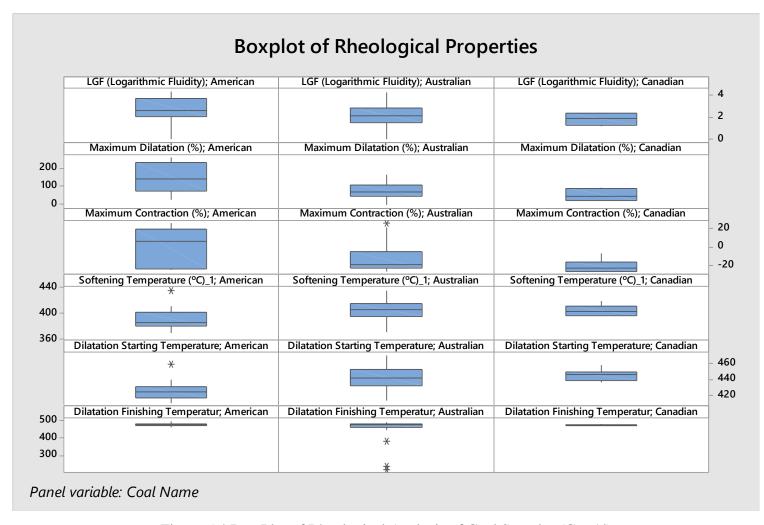


Figure 5.4 Box Plot of Rheological Analysis of Coal Samples (Cont'd)

5.1.4 Ash Chemistry, Sulphur and Phosphor in Coal Samples

Descriptive statistics of coal sample's chemical analysis are listed in Table 5.4.

Table 5.4 Descriptive Statistics about Coal Samples' Chemical Analysis

Variable	Statistic	Australian	American	Canadian		
-	Minimum	0.28	0.50	0.34		
Total S	Median	0.52	0.88	0.44		
in Coal	Average	0.51	0.85	0.44		
	Maximum	1.02	1.14	0.56		
	Minimum	0.01	0.00	0.05		
Total F	Median	0.04	0.02	0.06		
in Coal	Average	0.04	0.02	0.07		
	Maximum	0.10	0.05	0.10		
Total	Minimum	0.62	0.72	0.64		
Alkalis	Median	1.20	2.84	0.83		
in Coal	Average	1.16	2.74	0.91		
Ash	Maximum	1.90	3.50	1.25		
	Minimum	3.25	5.41	3.24		
Fe ₂ O ₃	Median	5.70	7.68	3.55		
Fe ₂ O ₃	Average	5.87	8.65	3.71		
	Maximum	10.68	17.76	4.47		
	Minimum	0.08	0.14	0.09		
Basicity	Median	0.12	0.17	0.10		
Index	Average	0.12	0.20	0.09		
	Maximum	0.24	0.53	0.10		
Basic to	Minimum	0.07	0.14	0.09		
Acidic	Median	0.11	0.17	0.09		
Ratio	Average	0.12	0.20	0.09		
	Maximum	0.23	0.52	0.10		
Madie - 1	Minimum	0.84	1.14	1.01		
Modified Basicity	Median	1.43	2.05	1.11		
Index	Average	1.49	2.21	1.13		
	Maximum	2.71	5.35	1.25		

Coal ash mineral analysis consists of Al₂O₃, CaO, Cr₂O₃, Fe₂O₃, K₂O, MgO, MnO, Na₂O, P₂O₅, SiO₂, TiO₂, P, S, ZnO. In addition to these, total sulfur and total phosphor analysis are also done. In this section, not all ash minerals will be investigated separately. Total sulfur in coal, total phosphor in coal, total alkali in ash (Na₂O + K₂O), Fe₂O₃, basicity index (BI), basic to acidic ratio (BAR) and material balance index (MBI) will be studied. Formulas for BI, BAR and MBI are mentioned in section 2.8.1 Theoretical CSR Prediction Equations and given again below. Coal Chemistry parameters are listed in Appendix B, Table B.4.

$$\begin{split} BI &= (CaO + Na_2O + K_2O + Fe_2) \div (SiO_2 + Al_2O_3) \\ BAR &= (CaO + MgO + Na_2O + K_2O + Fe_2O_3) \div (SiO_2 + Al_2O_3 + TiO_2) \\ MBI &= 100 \times ash \times (CaO + MgO + Na_2O + K_2O + Fe_2O_3) \div ((100 - VM) \times (SiO_2 + Al_2O_3)) \end{split}$$

American coals sulfur content is higher than others. Canadian coals have lowest sulfur impurity. In average, total sulfur contents of coals are 0.51 %, 0.85 % and 0.44 % for Australian, American and Canadian coals respectively.

Canadian coals phosphor content is higher than other coals. American coals have lowest phosphor impurity. In average, total phosphor contents of coals are 0.039 %, 0.021 % and 0.071 % for Australian, American and Canadian coals respectively.

American coals total alkali in ash is higher than other coals. Canadian coals have lowest alkali impurities. In average, total alkalis of coals' ash are 1.16 %, 2.74 % and 0.91 % for Australian, American and Canadian coals respectively.

American coals' Fe₂O₃ contents in ash are higher than other coals. Canadian coals have lowest Fe₂O₃ content in ash. In average, Fe₂O₃ content of coals' ash are 5.87 %, 8.65 % and 3.71 % Australian, American and Canadian coals respectively. Due to the nature of analysis, pyritic sulfur is also measured as iron oxide. The reason of high iron oxide content of American coals may be high pyritic sulfur and it may be cause of high sulfur content.

American coals basicity indexes are higher than others. Canadian coals have lowest basicity index. In average, basicity indexes of coals are 0.124, 0.201 and 0.094 for Australian, American and Canadian coals respectively.

American coals basic to acidic ratios are higher than others. Canadian coals have lowest basic to acidic ratios. In average, basic to acidic ratios of coals are 0.121, 0.197 and 0.092 for Australian, American and Canadian coals respectively.

American coals' modified basicity indexes are higher than others. Canadian coals have lowest modified basicity indexes. In average, modified basicity indexes of coals are 1.488, 2.207 and 1.129 for Australian, American and Canadian coals respectively.

In order to understand fluctuations in chemical analysis according to different origins and samples from same origin, box plot representation is given in Figure 5.5.

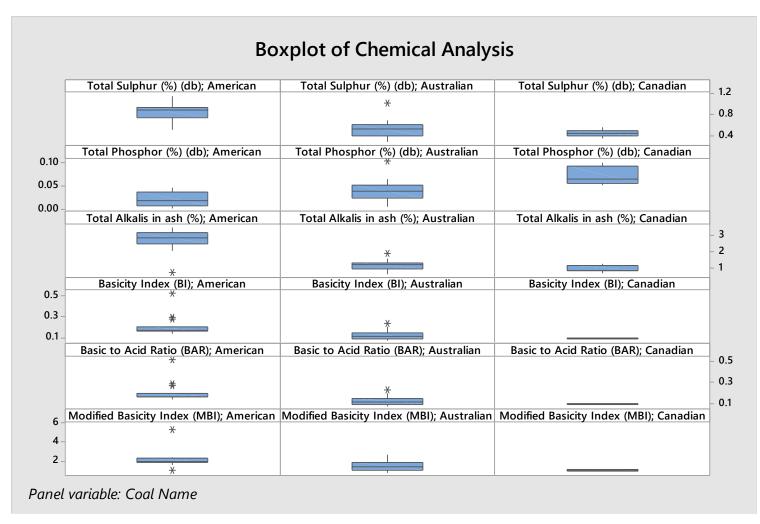


Figure 5.5 Box Plot of Chemical Analysis of Coal Samples

5.1.5 Petrographic Analysis of Coal Samples

Descriptive statistics of coal sample's petrographical analysis are listed in Table 5.5.

Table 5.5 Descriptive Statistics of Coal Samples' Petrographical Analysis

Variable	Statistic	Australian	American	Canadian
	Minimum	0.75	0.71	0.97
Ro	Median	1.07	1.15	1.08
NO	Average	1.08	1.09	1.06
	Maximum	1.50	1.39	1.11
	Minimum	52.58	56.34	55.00
Vitrinito	Median	66.91	65.94	72.89
Vitrinite	Average	67.72	66.45	70.14
	Maximum	81.40	79.50	79.80
	Minimum	0.00	3.30	0.50
Lintinita	Median	5.67	8.20	3.08
Liptinite	Average	5.20	7.94	3.29
	Maximum	12.00	12.67	6.51
	Minimum	5.20	4.00	7.10
Semi	Median	12.77	9.05	11.29
fusinite	Average	14.57	8.50	11.75
	Maximum	31.33	12.33	17.33
	Minimum	16.30	14.90	16.65
T	Median	24.19	22.23	21.03
Inertinite	Average	24.57	21.40	24.18
	Maximum	36.33	26.66	38.00

Investigated petrographic analysis of coal samples consist of mean random vitrinite reflectance (Ro), V – type distribution and maceral analysis, which are vitrinite, liptinite, semi-fusinite and inertinite contents. Ro is an indication of coalification. Higher Ro values represents more matured coals. V-type distribution gives an idea about coal volatile matter such that V 7 to V 10 considers as high volatile, V 11 to V 14 considers as medium volatile and V 15 to V 18 considers as low volatiles. Macerals are smallest carbon structure of coals. They are similar concept of minerals.

Petrographic properties of coal samples are listed in Appendix B, Table B.5.

Australian, American and Canadian coals' mean random vitrinite reflectance (Ro) are similar. It means coalification degrees of these coals are similar. In average, mean random vitrinite reflectance of coals are 1.08, 1.09 and 1.06 for Australian, American and Canadian coals respectively.

Vitrinite content of Canadian coals are higher than other coals. Vitrinite is technologically desired for coke making. In average, vitrinite content of coals are 67.72, 66.45 and 70.14% for Australian, American and Canadian coals respectively.

Liptinite content of American coals are higher than others. Canadian coals have lowest liptinite content. In average, liptinite content of coals are 5.20, 7.94 and 3.29 % for Australian, American and Canadian coals respectively.

Semi-fusinite content of Australian coals are higher than others. American coals have lowest semi-fusinite content. In average, semi-fusinite content of coals are 14.57, 8.50 and 11.75 % for Australian, American and Canadian coals respectively.

Inertinite content of Australian and Canadian coals are higher than American coals. In average, inertinite content of coals are 24.57, 21.40 and 24.18 % for Australian, American and Canadian coals respectively.

American and Australian coals' peak in average V – type distribution is between V 7 to V 14, which are high volatile to medium volatile. Canadian coals' peak is between V 9 to V 12, which is in medium volatile range. It should be note that if there is one peak in V type distribution, investigated coals is one particular coal. If there are two or more peak, that means investigated coal is a blended coal, which includes two or more different coals.

In order to understand fluctuations in chemical analysis according to different origins and samples from same origin, box plot representation is given in Figure 5.6.

Graphical representation of coal samples average V – type distribution relative to their origin is given Figure 5.7.

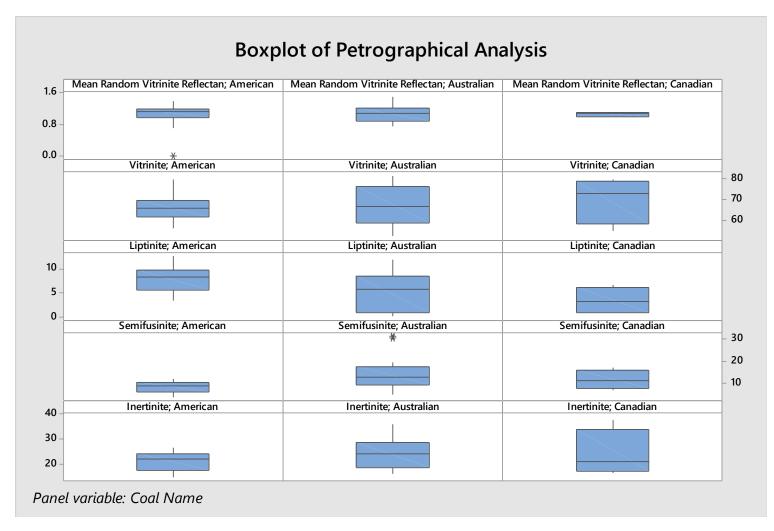


Figure 5.6 Box Plot of Petrographical Analysis of Coal Samples

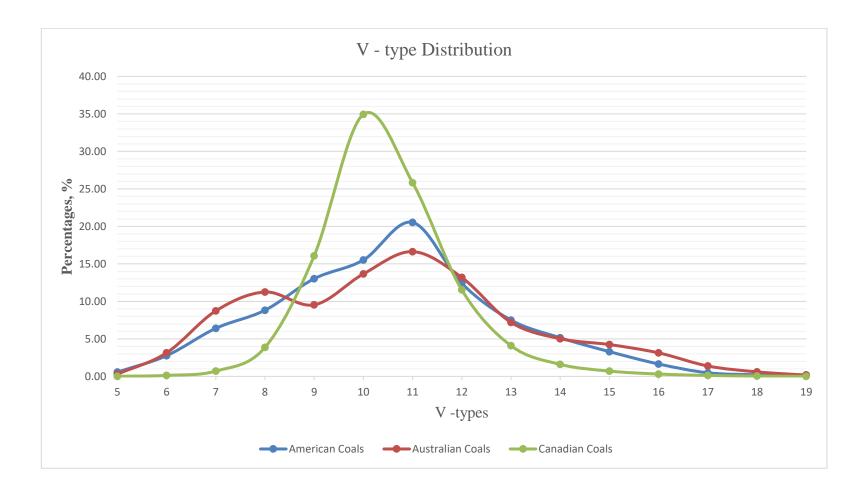


Figure 5.7 Coal Samples' V - type Distribution

5.2 Coke Quality Characterization Studies

For each coal sample coking test also performed. In this section, the following parameters were analyzed for coke quality.

- Coke stability factor,
- Coke hardness factor,
- Maximum gas pressure of coking,
- Maximum wall pressure of coking
- Coke reactivity index and
- Coke strength after reaction,

Coke quality characterization parameters are listed in Appendix B, Table B.6.

Descriptive statistics of coke quality categorization is given in Table 5.6.

Stability indexes of Australian, American and Canadian coals are similar. In average, stability indexes of coals are 57.02, 57.53 and 59.13 % for Australian, American and Canadian coals respectively.

Hardness indexes of Australian, American and Canadian coals are similar. In average, Hardness indexes of coals are 63.60, 64.48 and 65.10 % for Australian, American and Canadian coals respectively.

While American coals have maximum gas pressure, Canadian coals have lowest. In average, maximum gas pressures of coals are 4.68, 9.44 and 2.01kPa for Australian, American and Canadian coals respectively.

While American coals have maximum wall pressure, Canadian coals have lowest. In average, maximum wall pressures of coals are 4.70, 5.18 and 2.89 kPa for Australian, American and Canadian coals respectively.

Table 5.6 Descriptive Statistics of Coke Quality Categorization

Variable	Statistic	Australian	American	Canadian
	Minimum	25.70	46.60	56.80
Coke	Median	59.37	58.33	58.00
Stability	Average	57.02	57.53	59.13
	Maximum	64.10	64.08	61.66
	Minimum	49.40	59.10	62.16
Coke	Median	65.23	65.14	64.45
Hardness	Average	63.60	64.48	65.10
	Maximum	68.45	68.28	67.40
	Minimum	18.01	16.81	19.80
CRI	Median	25.79	26.92	21.79
CKI	Average	28.90	28.73	22.56
	Maximum	48.40	47.41	28.35
	Minimum	18.12	24.46	59.12
CSR	Median	62.30	56.26	66.19
CSK	Average	57.68	54.24	66.23
	Maximum	71.65	72.31	71.59
74	Minimum	0.26	0.75	0.96
Gas	Median	1.63	4.31	1.80
Pressure	Average	4.68	9.44	2.01
	Maximum	48.31	36.66	3.66
	Minimum	0.55	0.58	0.35
Wall	Median	4.32	4.45	3.45
Pressure	Average	4.70	5.18	2.89
	Maximum	19.73	12.86	4.46

Canadian coals have lowest coke reactivity indexes. In average, CRI of coals are 28.90, 28.73 and 22.56 % for Australian, American and Canadian coals respectively.

Canadian have higher coke strength after reaction indexes, on the other hand, American coals have lowest CSR. In average, CSR of coals are 57.68, 54.27 and 66.23 % for Australian, American and Canadian coals respectively.

Box plot representation of coke quality parameters is given in Figure 5.8.

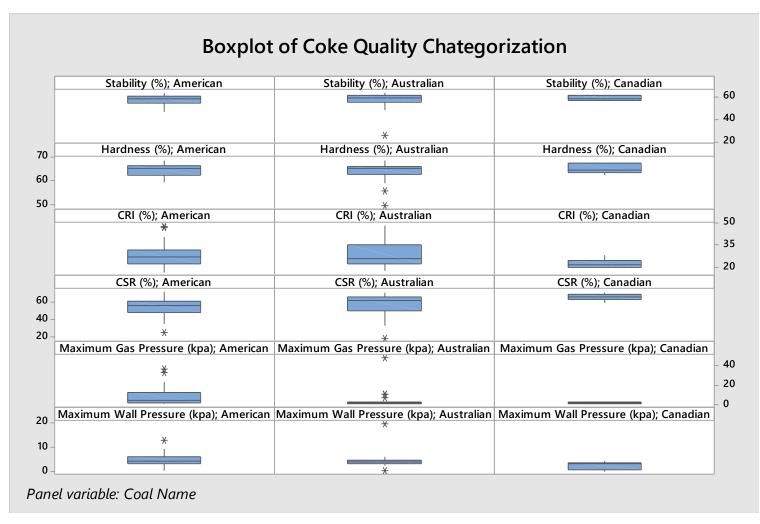


Figure 5.8 Box Plot of Coke Quality Analysis of Coal Samples

5.3 Developing Origin Base CSR Prediction Model

5.3.1 Developing a CSR Prediction Model for Australian Coals

In this study, 22 different Australian coals are investigated. These coals have 69 analysis set, which have 115 parameters for each.

First correlation analysis was performed by excel. 50 parameters, which have over \pm 0.8 Pearson correlation coefficient, were eliminated. Correlated parameters and the eliminated ones are listed in Appendix D in Table D.1. Second correlation analysis was performed by Minitab. 28 parameters, which have over \pm 0.6 Pearson correlation coefficient and below 0.05 p – value, were eliminated. They are listed in Appendix D Table D.2. Number of non-eliminated parameter is 28 and it is enough for best subset analysis by Minitab. Analyzed parameters are listen in Table 5.7.

Table 5.7 Rest of Parameters after Correlation Analysis for Australian Coals

#	Parameter Name	#	Parameter Name
1	Volatile Matter (%) (db)	15	Dilatation Finishing Temperature (°C)
2	Ash (%) (db)	16	CRI (%)
3	Sulphur (%) (db)	17	Stability (%)
4	Phosphor (%) (db)	18	Porosity (%)
5	Calorific Value (db) (kcal/kg)	19	Charged Coal Moisture (%)
6	Reflectance of Light (%) (T17)	20	Bulk Density (kg/m3) (db)
7	Total Alkalis in ash (%)	21	Maximum Gas Pressure (kPa)
8	Na2O (%)	22	Mean Rand. Vit. Reflectance (Ro)
9	TiO2 (%)	23	V9 - V11 (%)
10	Basicity Index (BI)	24	V12 - V14 (%)
11	Maximum Fluidity (ddpm)	25	V15 - V18 (%)
12	Maximum Fluidity Temperature (°C)	26	Vitrinite
13	Maximum Dilatation (%)	27	Fusinite
14	Maximum Contraction (%)	28	Semifusinite

Table 5.8 Best Subset Analysis of Australian Coals

_	⁄ars	R-Sq	_	R-Sq (pred)	Mallows Cp	S	Volatile Matter (%) (db)	Sulph ur (%) (db) (coal)	Total Alkalis in ash (%)	Na2O (%) (in ash)		Max Dilatation (%)	Maximum Contraction (%)		CRI (%)	Stability (%)	Max Gas Pressure (kpa)		V9 - V11 (%)	V12 - V14 (%)	V15 - V18 (%)
	1	82.0	81.7	80.6	223.1	2.47									x						
	1	67.6	66.9	64.5	441.1	3.32										x					
	2	93.5	93.2	92.3	52.2	1.50									Х	x					
		91.7	91.4	90.1	79.2	1.69									х						
		95.9	95.6	94.9	18.1	1.21						X			х	Х					
	3	95.7	95.5	94.7	20.3	1.23	X								х	Х					
	4	96.6	96.3	95.8	9.2	1.107				X		X			Х	X					
	4	96.6	96.3	95.6	9.6	1.111		x			Х				Х	X					
		97.0	96.6	96.0	5.6	1.056		x			Х				Х	Х		x			
		96.9	96.5	96.0	7.4	1.076				х		X			Х	x		X			
_1		97.3	96.9	96.3	2.9	1.011		x		х	Х				Х	x		x			
77		97.3	96.9	96.0	3.0	1.012		x			Х				Х	x	X	x			
		97.5	97.1	96.2	1.2	0.975		x		х	Х				Х	x	X	x			
		97.4	97.0	96.0	3.2	1.001		x			Х		x		Х	x	X	x			
		97.6	97.2	83.7	1.6	0.965		x		х	Х			x	Х	Х	X	x			
		97.6	97.2	96.2	1.8	0.967		x		х	х				X	х	X	X			
	9	97.8	97.3	96.2	1.9	0.953		x		х	х			X	X	х	X	X			
	9		97.3	96.4	2.0	0.953		x		х	х				X	х	X		X	X	X
		97.9	97.3	96.6	2.3	0.941		x	X		х			X	X	х	X		X	X	X
	10	97.9	97.3	95.5	2.4	0.942		X		X	х			x	x	x	x		Х	Х	x

Best subset analysis of the rest 28 parameters are listen in Table 5.8. CRI is most contributed parameter for CSR prediction of Australian Coals with an 82.0 % R – square. Stability follows CRI with a 67.6 % R – square. Other parameters are volatile matter of coal (%), sulfur of coal (%), total alkali in ash (%), Na₂O (%), maximum fluidity (ddpm), maximum dilatation (%), maximum contraction (%), dilatation finishing temperature (0 C), maximum gas pressure (kPa) and mean random vitrinite reflectance (Ro, %), V9 – V11 (%), V12 – V14 (%) and V15 – V18 (%).

With most contributor parameters for CSR prediction Regression analysis was performed. It is given in Figure 5.9.

Analysis of Variance					
Source	DF	Adj SS	Adj MS	F-Value	P-Value
Regression	15	1749.40	116.627	110.58	0.000
Volatile Matter (%) (db)	1	0.01	0.014	0.01	0.909
Sulphur (%) (db) (coal)	1	5.29	5.289	5.02	0.031
Total Alkalis in ash (%)	1	0.04	0.044	0.04	0.840
Na2O (%)(in ash)	1	3.00	2.996	2.84	0.100
Maximum Fluidity (ddpm)	1	3.36	3.363	3.19	0.082
Maximum Dilatation (%)	1	0.74	0.739	0.70	0.408
Maximum Contraction (%)	1	0.10	0.098	0.09	0.762
Dilatation Finishing Temperatur	1	0.76	0.757	0.72	0.402
CRI (%)	1	332.61	332.613	315.37	0.000
Stability (%)	1	46.72	46.723	44.30	0.000
Maximum Gas Pressure (kpa)	1	1.81	1.811	1.72	0.198
Mean Random Vitrinite Reflectan	1	0.14	0.139	0.13	0.718
V9 - V11 (%)	1	2.63	2.628	2.49	0.123
V12 - V14 (%)	1	2.38	2.379	2.26	0.141
V15 - V18 (%)	1	1.58	1.577	1.50	0.229
Error	38	40.08	1.055		
Total	53	1789.48			
Model Summary					
S R-sq R-sq(adj) R-sq(p 1.02698 97.76% 96.88% 95	red)				

Figure 5.9 Screen of Minitab Analysis of Variance Table for Australian Coal Regression

The analysis of variance table shows the amount of variation in the response data explained by the predictors and the amount of variation left explained (Minitab Software, 2018). Here, one of most important parameter is p – value to evaluate

parameter contribution to prediction. Parameters, which have near or greater 0.05 p – values can be considered unnecessary for model. Except sulphur, stability and CRI and maximum fluidity, all parameters' p – values are above 0.1. After elimination of unnecessary or insignificant parameters, regression analysis was performed again. Final regression analysis' ANOVA table and variable descriptions is given in Figure 5.10.

Analysis of Variance									
Source	DF	_		_				P-Val	
Regression	4			431.7					
Sulphur ($%$) (db)(coal)		23	.24	23.2	44	18.	19	0.0	00
Maximum Fluidity (ddpm)	1	37	.56	37.5	60	29.	39	0.0	00
CRI (%)	1	512	.69	512.6	89	401.	13	0.0	00
Stability (%)	1	72	.44	72.4	37	56.	67	0.0	00
Error	49	62	.63	1.2	78				
Total	53	1789	.48						
Model Summary S R-sq R-sq(adj) 1.13054 96.50% 96.219									
Coefficients									
Term		Coef	SE	Coef	T-	Value	P-	Value	VIF
Constant	5	6.85		6.00		9.47		0.000	
Sulphur (%) (db)(coal)	-1	2.04		2.82		-4.26		0.000	1.84
Maximum Fluidity (ddpm) -	-0.00	1442	0.0	00266		-5.42		0.000	1.68
CRI (%)				.0478				0.000	2.19
Stability (%)				.0830				0.000	
200222201 (0)	•	0210							

Figure 5.10 Screen of Minitab Regression Analysis for Australian Coals

Regression analysis of Minitab is given in Figure 5.10 and equation for Australian coals CSR prediction is given in Formula 1.

$$CSR = 56.85 - 12.04 \text{ Sulphur (\%)} - 0.001442 \text{ Max Fluidity (ddpm)}$$

- 0.9570 CRI (\%) + 0.6248 Stability (\%) (1)

Residual plots of Australian coals CSR prediction model is given in Figure 5.11. Residuals are distributed normally (p – value = 0.956 > 0.05) which is represented upper left side of Figure 5.43. In addition, residuals distributed homogeneously. It is also represented upper right side. R – square is 96.50 %. It can be concluded that fitness of the model is good.

Scatter plots of model variables and CSR is given in Figure 5.12. It is clear that coal content (%), maximum fluidity (ddpm), CRI (%) and stability (%) are highly related with CSR (%).

Increase in sulphur (%), maximum fluidity (ddpm), CRI (%), decreases CSR according to the regression model. On the other, increase in stability shows positive effect for CSR.

Database variation range is a criterion for a regression analysis. Predictor values, is out of database range, can cause meaningless response predictions. For this reason, basic statistics of response and variables of Australian coals CSR prediction model is given in Table 5.9.

Table 5.9 Basic Statistics of Response and Variables of Australian CSR Prediction Model

<u>Variable</u> Statistic	CSR (%)	Sulphur (%)	Maximum Fluidity (ddpm)	CRI (%)	Stability (%)
Mean	65.01	0.53	539	23.56	60.54
Std Dev	5.81	0.07	757	4.81	2.90
Minimum	47.85	0.34	0	17.30	52.90
Quarter 1	61.85	0.50	38	19.75	59.81
Median	66.24	0.53	149	22.55	61.25
Quarter 3	69.77	0.58	771	25.71	62.33
Maximum	72.66	0.67	3364	38.35	64.80
Range	24.81	0.33	3364	21.05	11.90

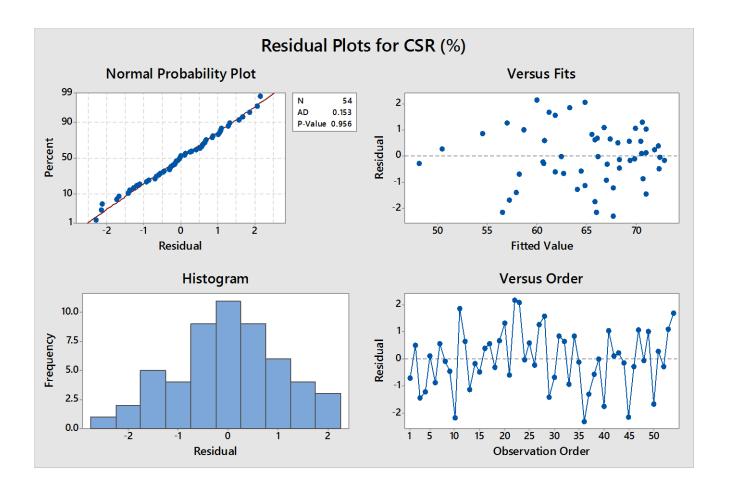


Figure 5.11 Minitab Screen of Residual Plots of Australian CSR Prediction Model

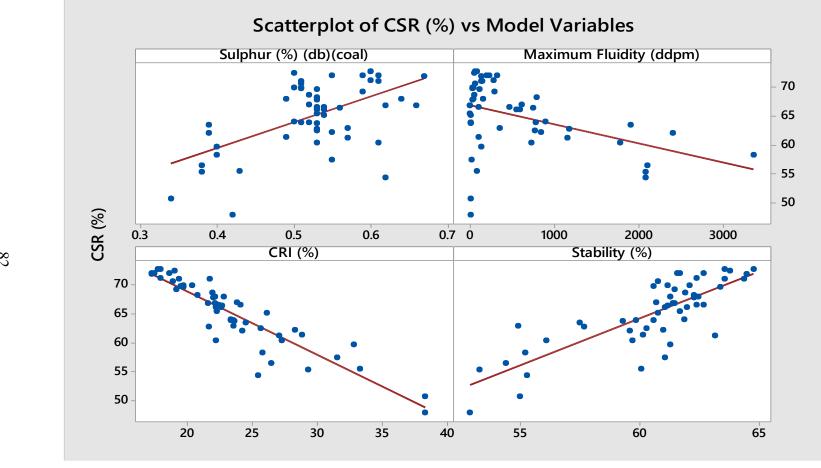


Figure 5.12 Scatter Plots of Regression Model Variables and CSR for Australian Coals

5.3.2 Developing a CSR Prediction Model for American Coals

In this study, 20 different American coals are investigated. These coals have 89 analysis set, which have 115 parameters for each.

First correlation analysis was performed by excel. 56 parameters, which have over \pm 0.8 Pearson correlation coefficient, were eliminated. Correlated parameters and the eliminated ones are listed in Appendix D in Table D.4. Second correlation analysis was performed by Minitab. 19 parameters, which have over \pm 0.6 Pearson correlation coefficient and below 0.05 p – value, were eliminated. They are listed in Appendix D Table D.5. Number of non-eliminated parameter is 25 and it is enough for best subset analysis by Minitab. Analyzed parameters are listen in Table 5.10.

Table 5.10 Rest of Parameters after Correlation Analysis for American Coals

#	Parameter Name	#	Parameter Name
1	Volatile Matter (%) (db)	14	Stability (%)
2	Ash (%) (db)	15	Porosity (%)
3	Sulphur (%) (db)	16	Charged Coal Moisture (%)
4	ZnO (%)	17	V7 and less
5	Basicity Index (BI)	18	V9 - V11 (%)
6	-6,30 +3,15mm (%)	19	V12 (%)
7	Maximum Fluidity (ddpm)	20	V17 (%)
8	Maximum Fluidity Temperature (°C)	21	Vitrinite
9	Fluid Range (°C)	22	Liptinite
10	Maximum Dilatation (%)	23	Semifusinite
11	Maximum Contraction (%)	24	Micrinite
12	Volatile Matter (%) (db)	25	İnertinite
13	CRI (%)		

Table 5.11 Best Subset Analysis of American Coals

V	ars	R-Sq	_	R-Sq (pred)	Mallows Cp	S	Volatile Matter (%) (db)	Ash (%) (db) (coal)	Sulphur (%) (db) (coal)	Basicity Index (BI)		CRI	Stability (%)	Porosity (%)	V		V17 (%)	Liptinite	Semi- fusinite	Micrinite
	1	88.00	87.80	87.00	68.6	3.12						X								
	1	39.50	38.60	35.90	614.9	7.01				X										
	2	92.00	91.80	90.70	24.8	2.56						X	X							
	2	90.20	89.90	88.90	45.5	2.84	X					X								
	3	92.80	92.50	91.30	17.8	2.45		X				X	X							
	3	92.60	92.20	91.10	20.6	2.49						X	X					X		
)	4	93.40	93.00	91.90	12.9	2.36		X				X	X					X		
•	4	93.20	92.80	91.60	15.8	2.40		X				X	X				X			
	5	93.80	93.30	92.10	11.0	2.31		X				X	X					X		X
	5	93.70	93.20	92.00	12.4	2.34		X				X	X				X	X		
	6	94.20	93.60	90.60	8.8	2.26		X		X		X	X					X		X
	6	94.00	93.40	92.20	10.9	2.30		X				X	X		X			X		X
	7	94.50	93.90	91.30	6.9	2.21	X	X		X		X	X					X		X
	7	94.40	93.80	91.00	8.0	2.23		X		X		X	X			X		X		X
	8	94.70	94.10	91.80	6.3	2.18		X		X		X	X			X	X	X		X
	8	94.60	94.00	91.60	7.3	2.20	X	X		X		X	X				X	X		X
	9	94.90	94.10	91.30	7.0	2.17	X	X		X		X	X	X			X	X		X
	9	94.80	94.10	91.80	7.0	2.17		X		X	X	X	X			X	X	X		X
	10	95.00	94.10	91.70	7.8	2.17		X		X	X	X	X			X	X	X	X	X
	10	95.00	94.10	91.40	7.8	2.17	X	X	X	X		X	X	X			X	X		X

ó

Best subset analysis of the rest 25 parameters are listen in Table 5.11. CRI is most contributed parameter for CSR prediction of American Coals with an 88.0 % R – square. Basicity Index follows CRI with a 39.5 % R – square. Other parameters are volatile matter of coal (%), ash (%), sulfur of coal (%), - 6,3 + 3,15 mm portion of coal, stability (%), porosity (%), V9 – V11 (%), V12 (%), V17 (%), liptinite (%), semifusinite (%) and micrinite (%).

With most contributor parameters for CSR prediction Regression analysis is performed. It is given in Figure 5.13.

Analysis of Variance					
Source	DF	Adj SS	Adj MS	F-Value	P-Value
Regression	14	5325.81	380.415	79.75	0.000
Volatile Matter (%) (db)	1	2.52	2.517	0.53	0.471
Ash (%) (db)(coal)	1	36.77	36.771	7.71	0.007
Sulphur (%) (db)(coal)	1	4.93	4.926	1.03	0.314
Basicity Index (BI)	1	31.06	31.059	6.51	0.013
-6,30 +3,15mm (%)	1	7.75	7.745	1.62	0.208
CRI (%)	1	771.13	771.133	161.66	0.000
Stability (%)	1	49.77	49.766	10.43	0.002
Porosity (%)	1	7.08	7.075	1.48	0.228
V9 - V11 (%)	1	0.16	0.158	0.03	0.856
V12 (%)	1	3.79	3.793	0.80	0.376
V17 (%)	1	17.21	17.205	3.61	0.063
Liptinite	1	16.34	16.342	3.43	0.069
Semifusinite	1	6.46	6.456	1.35	0.250
Micrinite	1	29.26	29.257	6.13	0.016
Error	56	267.12	4.770		
Total	70	5592.93			
Model Summary					
S R-sq R-sq(adj)	R-s	q(pred)			
2.18405 95.22% 94.03%		90.97%			

Figure 5.13 Screen of Minitab Analysis of Variance Table for American Coal Regression

As explained before, parameters, which have near or greater 0.05 p – values can be considered unnecessary for model. P – value of volatile matter is 0.471, sulphur is 0.314, -6.3 + 3.15 mm portion of coal is 0.208, porosity is 0.228, V9 – V11 is 0.856, V12 is 0.376, V17 is 0.063, liptinite is 0.069, these are considered unnecessary or

insignificant parameters based on ANOVA analysis. Parameters, which will be used in regression model, are ash (%), basicity index, stability (%), CRI (%) and micrinite (%). Final regression analysis' ANOVA table and variable descriptions is given in Figure 5.14.

Analysis of Variance						
Ash (%) (db)(coal) Basicity Index (BI) CRI (%) Stability (%) Micrinite Error	5 1 1 1 1 1 65	5224.44 41.47 20.72 1216.18 240.51 21.52	1044.89 41.47 20.72 1216.18 240.51 21.52 5.67	3.65 214.53 42.43 3.80	0.000 0.009 0.060 0.000	
10041	, 0	0032.30				
Model Summary						
S R-sq R-sq(adj) R-sq(pred) 2.38098 93.41% 92.90% 89.29%						
Coefficients						
	78.4 -0.99 -16.7	40 5. 96 0.3 72 8. 37 0.08	.24 14. 368 -2. .75 -1. 329 -14.	91 0.0 65 0.0	00 09 1.08 60 2.54 00 2.92	

Figure 5.14 Screen of Minitab Regression Analysis for American Coals

Regression equation for American coals CSR prediction is given in Formula 2.

$$CSR = 78.40 - 0.996 \text{ Ash (\%)} - 16.72 \text{ Basicity Index} - 1.2137 \text{ CRI}$$

(\%) + 0.3997 Stability (\%) - 0.431 Micrinite (2)

Residual plots of American coals CSR prediction model is given in Figure 5.47. Residuals are distributed normally (p – value = 0.956 > 0.05) which is represented upper left side of Figure 5.47. In addition, residuals distributed homogeneously. It is also represented upper right side. R – square is 93.41 %. It can be concluded that fitness of the model is good.

Scatter plots of model variables and CSR is given in Figure 5.15. It is clear that coal ash content (%), basicity index, CRI (%) and stability (%) are highly related with CSR (%). However, there is no meaningful relationship between micrinite and CSR. It may be due to correlated other parameter(s) with micrinite.

Increase in ash (%), basicity index, CRI (%) and micrinite (%) decreases CSR according to the regression model. On the other, increase in stability shows positive effect for CSR. Scatter plot of variables and CSR is given in Figure 5.16.

Database variation range is a criterion for a regression analysis. Predictor values, is out of database range, can cause meaningless response predictions. For this reason, basic statistics of response and variables of Australian coals CSR prediction model is given in Table 5.12.

Table 5.12 Basic Statistics of Response and Variables of American CSR Prediction Model

Variable Statistic	CSR (%)	Ash (%)	Basicity Index	CRI (%)	Stability (%)	Micrinite
Mean	58.34	8.4181	0.18504	26.008	57.906	0.355
Std Dev	8.94	0.8017	0.05182	5.868	5.301	1.392
Minimum	24.46	6.76	0.13667	16.81	45.6	0
Quarter 1	53.29	8.01	0.16109	22.13	53.8	0
Median	59.36	8.48	0.17424	24.81	58.1	0
Quarter 3	63.72	8.79	0.19608	28.9	62.8	0
Maximum	73.01	11.57	0.52869	46.79	65.5	10.8
Range	48.55	4.81	0.39202	29.98	19.9	10.8

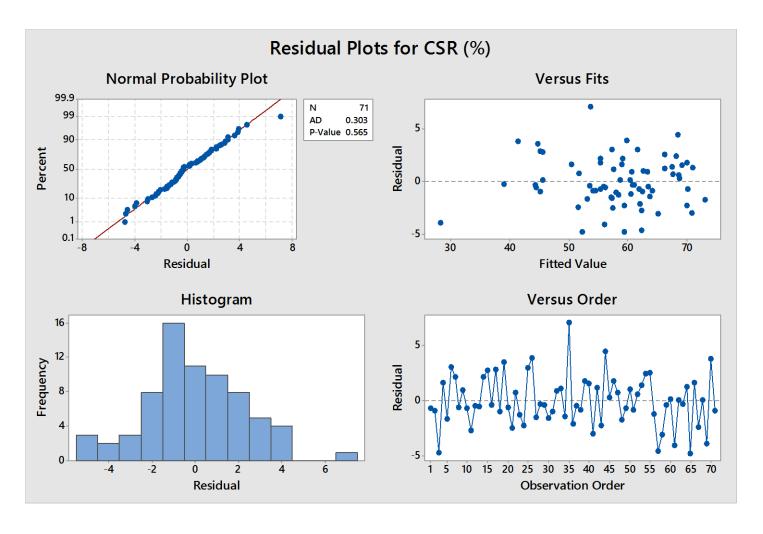


Figure 5.15 Minitab Screen of Residual Plots of Australian CSR Prediction Model

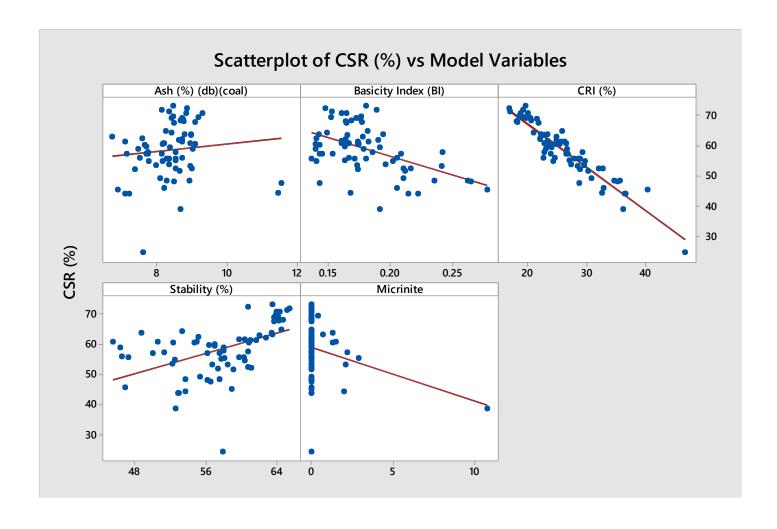


Figure 5.16 Scatter Plots of Regression Model Variables and CSR for American Coals

5.3.3 Developing a CSR Prediction Model for Canadian Coals

In this study, 7 different Canadian coals are investigated. These coals have 34 analysis set, which have 115 parameters for each.

First correlation analysis was performed by excel. 64 parameters, which have over \pm 0.8 Pearson correlation coefficient, were eliminated. Correlated parameters and the eliminated ones are listed in Appendix D in Table D.6. number of parameter after elimination is 24. Thus there is no need for second correlation by Minitab. Analyzed parameters are listen in Table 5.13.

Table 5.13 Rest of Parameters after Correlation Analysis for Canadian Coals

#	Parameter Name	#	Parameter Name
1	Volatile Matter (%) (db)	13	Basicity Index (BI)
2	Ash (%) (db)	14	Maximum Fluidity Temperature (°C)
3	HGI	15	Dilatation Finishing Temperature (°C)
4	Calorific Value (db) (kcal/kg)	16	CRI (%)
5	Reflectance of Light (%) (T17)	17	Stability (%)
6	Bulk Density (gr/cm3)	18	Charged Coal Moisture (%)
7	Al2O3 (%)	19	Bulk Density (kg/m3) (db)
8	Cr2O3 (%)	20	Maximum Gas Pressure (kpa)
9	Fe2O3 (%)	21	Maximum Wall Pressure (kpa)
10	MnO (%)	22	Coke Rate (%) (db)
11	Na2O (%)	23	Mean Rand Vitrinite Reflectance (Ro)
12	TiO2 (%)	24	Vitrinite

Best subset analysis of the rest 24 parameters is listen in Table 5.14. Stability (%) is most contributed parameter for CSR prediction of Canadian Coals with an 88.0 % R – square. Volatile matter (%) follows stability with a 38.6 % R – square.

Table 5.14 Best Subset Analysis of Canadian Coals

							Ash	Calorific	Ref of									Bulk	Max	Coke		
Va	rs R-Sq		R-Sq (pred)	Mallows Cp	S	VM (%) (db)	(%) (db) (coal)	Value (db) (kcal/kg)	Light (%) (T17)	Bulk Density (gr/cm3)	Cr2O3 (%)	Fe2O3 (%)	MnO (%)	Na2O (%)	Dilatation Finishing Temp (ºC)	CRI (%)	Stability (%)	Density (kg/m3) (db)	Wall Pressure (kpa)	Rate (%) (db)	Mean Rand Vit Ref (Ro)	Vitrinite
1	88.00	87.80	87.00	68.6	3.12	()	((,,	(/	(9-77	(,-,	(,-,	1/-/	(/-/		(,,,	X	(5)	(()	,	
1	39.50	38.60	35.90	614.9	7.01	X																
2	92.00	91.80	90.70	24.8	2.56	X										X						
2	90.20	89.90	88.90	45.5	2.84											X	X					
3	92.80	92.50	91.30	17.8	2.45	X										X		X				
3	92.60	92.20	91.10	20.6	2.49	X						X				X						
4	93.40	93.00	91.90	12.9	2.36	X									X	X					X	
4	93.20	92.80	91.60	15.8	2.40	X						X			X	X						
5	93.80	93.30	92.10	11.0	2.31	X						X			X	X					X	
5	93.70	93.20	92.00	12.4	2.34	X						X			X	X		X				
6	94.20	93.60	90.60	8.8	2.26		X	X			X		X	X		X						
6	94.00	93.40	92.20	10.9	2.30	X	X				X		X	X		X						
7	94.50	93.90	91.30	6.9	2.21		X			X	X		X	X		X					X	
7	94.40	93.80	91.00	8.0	2.23		X	X		X	X		X	X		X						
8	94.70	94.10	91.80	6.3	2.18	X	X			X	X		X	X	X	X						
8	94.60	94.00	91.60	7.3	2.20		X	X		X	X		X	X		X					X	
9	94.90	94.10	91.30	7.0	2.17		X	X		X	X		X	X		X					X	X
9	94.80	94.10	91.80	7.0	2.17		X	X		X	X		X	X	X	X				X		
10	95.00	94.10	91.70	7.8	2.17		X	X	X	X	X		X	X	X	X				X		
10	95.00	94.10	91.40	7.8	2.17		X	X		X	X		X	X		X			X		X	X

Other parameters are ash (%), calorific value (kcal/kg), reflectance of light (%), bulk density of coal (g/cm³), Cr₂O₃ (%), Fe₂O₃ (%), MnO (%), Na₂O (%), dilatation finishing temperature (0 C), CRI (%), bulk density of coke (kg/m³), maximum wall pressure (kPa), coke rate (%), mean random vitrinite reflectance (%) and vitrinite (%).

Because of number of parameter is so much for 10 variable regression model alternatives, parameter used in 5 variables regression model alternatives are used for first modelling. These parameters are volatile matter (%), Fe₂O₃ (%), dilatation finishing temperature (0 C), CRI (%), stability (%), bulk density of coke (kg/m³) and mean random vitrinite reflectance (%). With these 7 parameters regression analysis was performed. It is given in Figure 5.17.

```
Analysis of Variance
                                         Adj MS F-Value P-Value
                              DF
                                 Adj SS
Source
                               7 370.493
                                 370.493 52.928 23.26
43.189 43.189 18.98
                                                         0.000
Regression
 Volatile Matter (%) (db)
                                                          0.000
                                                  1.46
                                  3.332 3.332
 Fe2O3 (%)
                                                           0.237
 0.020
                                                   6.18
                                                  64.99
                                                           0.000
                              1
 Stability (%)
                                  0.105
                                          0.105
                                                   0.05
                                                           0.832
 Bulk Density Coke (kg/m3) (db)
                                  7.892
                                          7.892
                                                   3.47
                                                           0.074
                             1 3.1.
26 59.162
                                          3.160
                                   3.160
 Mean Random Vitrinite Reflectan
                                                   1.39
                                                           0.249
                                           2.275
Error
                              33 429.655
Total
Model Summary
         R-sq R-sq(adj) R-sq(pred)
1.50846 86.23% 82.52%
                           40.07%
```

Figure 5.17 Screen of Minitab Analysis of Variance Table for Canadian Coal Regression

As explained before, parameters, which have near or greater 0.05 p – values can be considered unnecessary for model. P – value of Fe₂O₃ (%) is 0.237, stability is 0.832, bulk density is 0.074 and Ro is 0249. Considering all these parameters insignificant and getting them out of model decreases R – square up to 80 %. For this reason, only stability is considered unnecessary based on ANOVA analysis. Parameters, which will be used in regression model, are volatile matter (%), Fe₂O₃ (%), dilatation finishing

temperature (0 C), CRI (%), bulk density of coke (kg/m 3) and mean random vitrinite reflectance (%). Final regression analysis' ANOVA table and variable descriptions is given in Figure 5.18.

```
Analysis of Variance
                                 DF Adj SS
                                               Adj MS F-Value P-Value
Source
  Volatile Matter (%) (db) 1 87 361 07 06
                                                               0.000
Regression
                                  1 87.361 87.361
1 15.127 15.127
                                                        39.80
                                                                 0.000
  Dilatation Finishing Temperatur
                                                         6.89
                                                                 0.014
                                  1 216.813 216.813 98.77
                                                                 0.000
  CRT (%)
  Bulk Density Coke (kg/m3) (db) 1
                                      8.858 8.858 4.04 0.055
                                  1 4.196 4.196 1.91
1 3.960 3.960 1.80
                                                                 0.178
  Fe203 (%)
  Mean Random Vitrinite Reflectan
                                                                 0.190
                                27 59.266 2.195
Error
                                 33 429.655
Total
Model Summary
     S R-sq R-sq(adj) R-sq(pred)
1.48157 86.21% 83.14% 57.32%
Coefficients
                                  Coef SE Coef T-Value P-Value
Term
                                                                    VIF
Constant
                                 214.7 44.8 4.79 0.000
Volatile Matter (%) (db)
                                         0.252 -6.31 0.000 4.44
                                -1.589
Dilatation Finishing Temperatur -0.2056 0.0783 -2.63 0.014 2.79 CRI (%) -1.244 0.125 -9.94 0.000 1.23 Bulk Density Coke (kg/m3) (db) 0.0212 0.0106 2.01 0.055 1.98
                                0.574 0.415
                                                   1.38 0.178 1.33
Fe203 (%)
                                          1.62 -1.34 0.190 1.81
Mean Random Vitrinite Reflectan -2.18
```

Figure 5.18 Screen of Minitab Regression Analysis for Canadian Coals

Regression equation for Canadian coals CSR prediction is given in Formula 3.

CSR =
$$214.7 - 1.589$$
 Volatile Matter (%) $- 0.2056$ Dilatation
Finishing Temperature (0 C) $- 1.244$ CRI (%) $+ 0.0212$ Coke Bulk
Density (kg/m 3) $+ 0.574$ Fe₂O₃ (%) $- 2.18$ Mean Random Vitrinite (3)
Reflectance (Ro)

Residual plots of Canadian coals CSR prediction model is given in Figure 5.19. Residuals are distributed normally (p - value = 0.600 > 0.05) which is represented

upper left side of Figure 5.51. In addition, residuals distributed homogeneously. It is also represented upper right side. R – square is 86.21 %. It can be concluded that fitness of the model is good.

Scatter plots of model variables and CSR is given in Figure 5.20. It is clear that volatile matter content (%), dilatation finishing temperature (0 C), CRI (%) and mean random vitrinite reflectance (%) are highly related with CSR (%). Fe₂O₃ (%) and bulk density of coke (kg/m³) do not show meaningful linear relationship with CSR (%). It may be due to other correlated parameters with them or nonlinear relationship.

Increase in volatile matter (%), dilatation finishing temperature (0 C), CRI (%) and mean random vitrinite reflectance (%) decreases CSR according to the regression model. On the other, increase in Fe₂O₃ (%) and bulk density of coke (kg/m³) shows positive effect for CSR. Database variation range is a criterion for a regression analysis. Predictor values, is out of database range, can cause meaningless response predictions. For this reason, basic statistics of response and variables of Canadian coals CSR prediction model is given in Table 5.15.

Table 5.15 Basic Statistics of Response and Variables of Canadian CSR Prediction Model

<u>Variable</u> Statistic	CSR (%)	Volatile Matter (%) (db)	Fe2O3 (%)	Dilatation Finishing Temp (°C)	CRI (%)	Bulk Density (kg/m3) (db)	Mean Rand Vit Ref (Ro)
Mean	67.089	23.686	3.816	476.29	21.913	728.91	1.113
Std Dev	3.608	2.158	0.717	5.5	2.283	22.5	0.1019
Minimum	59.12	20.4	2.357	468	17.92	683.14	0.93
Quarter 1	64.45	22.567	3.282	472.75	20.19	707.61	1.025
Median	67.445	23.455	3.681	475	21.965	734.05	1.1
Quarter 3	69.582	25.152	4.404	478.25	22.828	746.34	1.225
Maximum	73.29	27.88	5.191	490	28.35	764.21	1.3
Range	14.17	7.48	2.834	22	10.43	81.07	0.37

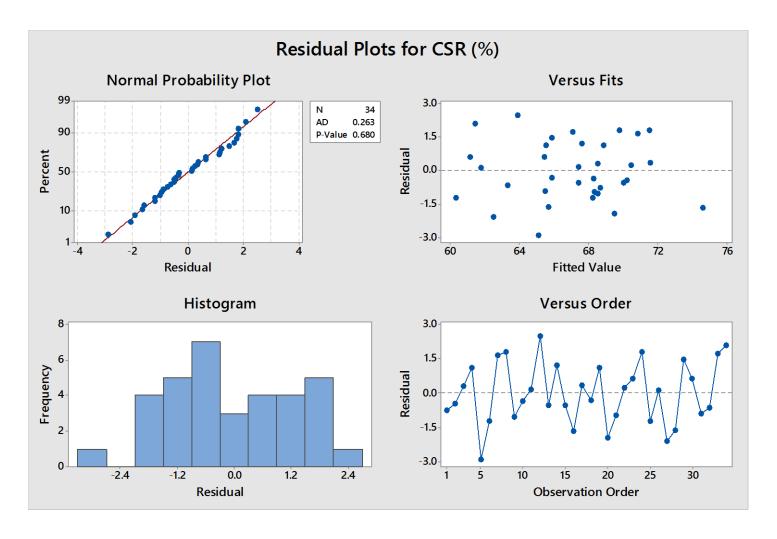


Figure 5.19 Minitab Screen of Residual Plots of Australian CSR Prediction Model

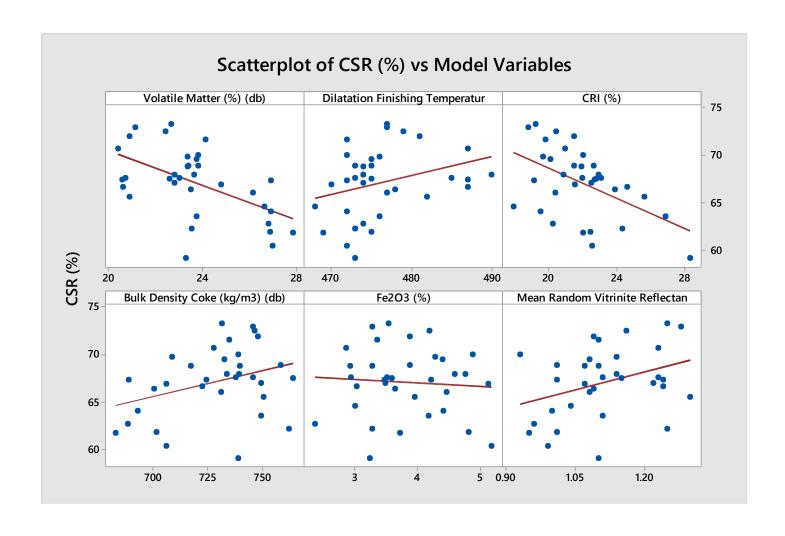


Figure 5.20 Scatter Plots of Regression Model Variables and CSR for Canadian Coals

5.4 Comparison of Origin base CSR Prediction Models with Theoretical Formulas

In this section, developed linear regression model for origin base coals' CSR prediction will compare theoretical formulas, which is discussed in section 2.8.1, in terms of accuracy.

5.4.1 Comparison of Australian Coals CSR Prediction Model and Theoretical Formulas

There are three formulations for Australian coals CSR prediction. One is developed model and the other two are formulas retrieved from literature, which is discussed in Section 2.8.1.

Developed regression equation 1 is,

Australian Formula 1 is,

$$\begin{split} &CSR = 94.2 - 1.275 \times (13.4 + 9.35 \times MBI) - 0.45 \times MBI^2 \\ &MBI = 100 \times ash \times (CaO + MgO + Na_2O + K_2O + Fe_2O_3) \div ((100 - VM) \times (SiO_2 + Al_2O_3)) \end{split}$$

Where MBI is modified basicity index,

VM is volatile matter content (%).

Australian Formula 2 is,

$$CSR = 133.8 - 15.56 \times BI - 3.1 \times VM + 8.5 \times log (F) + 0.22 \times Inerts (\%)$$

$$BI = (CaO + Na2O + K2O + Fe2) \div (SiO2 + Al2O3)$$

Where BI is basicity index,

VM is volatile matter content (%),

F is maximum fluidity,

Inerts (%) is inert content (%).

In order to compare these three equations, first, responses are produced for all three. Then, residues are calculated by subtracting lab results from equations' results. Three residue populations are produced. Theoretically, residues should be distributed normally and means of residues should be zero when formulas predict lab results exactly. Probability plot of model residues is given in Figure 5.11. It is distributed normally (p-value = 0.956 > 0.05) with a mean of -0.005 and standard deviation of 1.087. Probability plot of formula 1 residues is given in Figure 5.21. It is distributed normally (p-value = 0.075 > 0.05) with a mean of 4.199 and standard deviation of Probability plot of formula 2 residues is given in Figure 5.22. It is not 6.375. distributed normally (p-value < 0.05) and its mean is -18.99 and standard deviation is10.12. Formula 2 is clearly different and worse than model and formula 1. Model residue mean is significantly smaller than formula 1's residue mean. In order to prove this again statistically 2 sample t test is designed. Original hypothesis is model residue mean is equal to formula 1 residue mean. Alternative hypothesis is model residue mean is not equal to formula 1 residue mean. Confidence level is expected 5 %. It means that if p-value of the test is smaller than 5 %, alternative hypothesis is true.

Ho: μ (model) = μ (formula 1)

Ha: μ (model) $\neq \mu$ (formula 1)

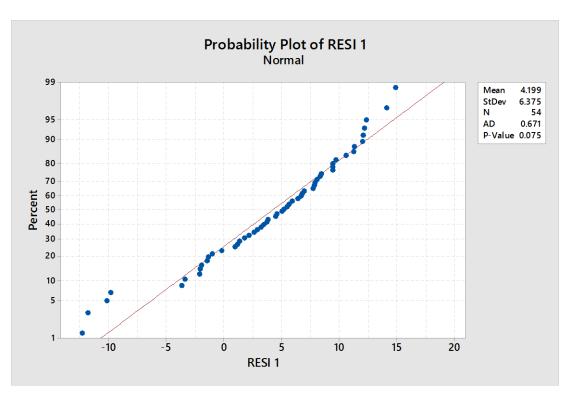


Figure 5.21 Probability Plot of Australian Formula 1

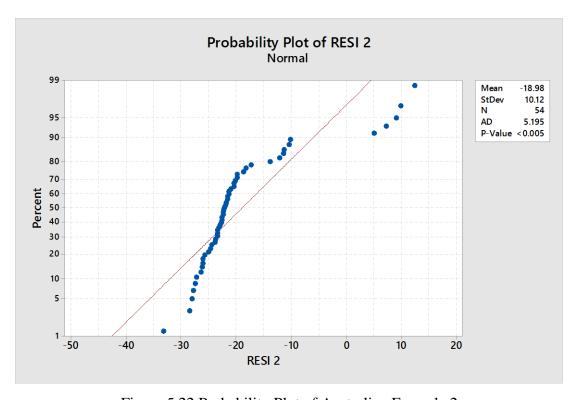


Figure 5.22 Probability Plot of Australian Formula 2

Minitab 2 sample t test result is given in Figure 5.23.

Figure 5.23 Minitab 2 sample t test Result for Model Residues and Australian Formula 1 Residues

Alternative hypothesis, which is means of the two population are different, is true because p – value of the test is 0. Model mean is 0 and standard deviation is 1.09, on the other hand, formula 1 mean is 4.20 and standard deviation is 6.37. It is clear that model predicts Australian coals CSR values more precisely than formula 1. In addition, box plot representation of model and formula 1 residues is given in Figure 5.24.

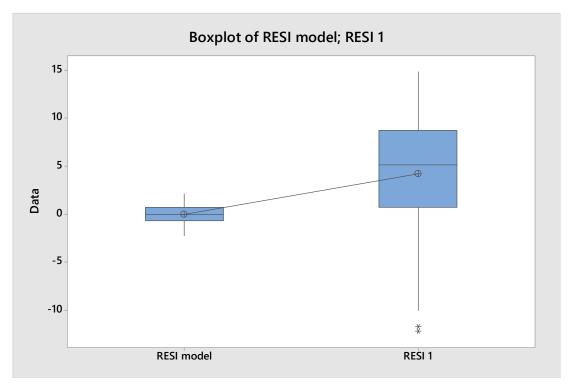


Figure 5.24 Box Plot of Australian Coal Model and Formula 1 Residues

5.4.2 Comparison of American Coals CSR Prediction Model and Theoretical Formulas

There are three formulation for American coals CSR prediction. One is developed model and the other two are formulas retrieved from literature, which is discussed in Section 2.8.1.

Developed regression equation 2 is,

$$CSR = 78.40 - 0.996 \text{ Ash } (\%) - 16.72 \text{ Basicity Index} - 1.2137 \text{ CRI } (\%) + 0.3997 \text{ Stability } (\%) - 0.431 \text{ Micrinite}$$

American Formula 1 is,

$$CSR = 28.91 + 0.63 \times FR - 9.64 \times Al - 14.04 \times S$$

 $Al = Ash (\%) \times (CaO + MgO + Na2O + K2O + Fe2O3) ÷ (SiO2 + Al2O3)$

Where FR is fluid range,

Al is alkali index,

S is sulfur.

American Formula 2 is,

$$CSR = 66.89 \times MMR + 7.8 \times log (F) - 89 \times BAR - 32$$

$$BAR = (CaO + MgO + Na2O + K2O + Fe2O3) \div (SiO2 + Al2O3 + TiO2)$$

Where MMR is mean maximum reflectance of vitrinite,

F is maximum fluidity,

BAR is basic to acidic ratio.

In order to compare these three equations, same procedure is followed with previous comparison. Residues are calculated by subtracting lab results from equations' results. Three residue populations are produced. Probability plot of model residues is given in Figure 5.15. It is distributed normally (p-value = 0.565 > 0.05) with a mean of -0.006 and standard deviation of 2.294. Probability plot of formula 1 residues is given in Figure 5.26. It is not distributed normally (p-value < 0.05) with a mean of 2.212 and standard deviation of 11.55. Probability plot of formula 2 residues is given in Figure 5.27. It is not distributed normally (p-value < 0.05). Its mean is 8.769 and standard deviation is 15.34. Formula 1 and 2 are clearly different and worse than model. Model residue mean is significantly smaller than formula 1 and 2's residue means. In order to prove that model is predicting CSR precisely, 1 sample t test is designed. Original hypothesis is model residue mean is equal to 0. Alternative hypothesis is model residue mean is not equal to 0. Confidence level is expected 5 %. It means that if p-value of the test is smaller than 5 %, alternative hypothesis is true.

```
Ho: \mu (model) = 0
Ha: \mu (model) \neq 0
```

Minitab 1 sample t test result is given in Figure 5.25.

One-Sample T: RESImodel

Figure 5.25 Minitab 1 sample t test Result for American Prediction Model Residues

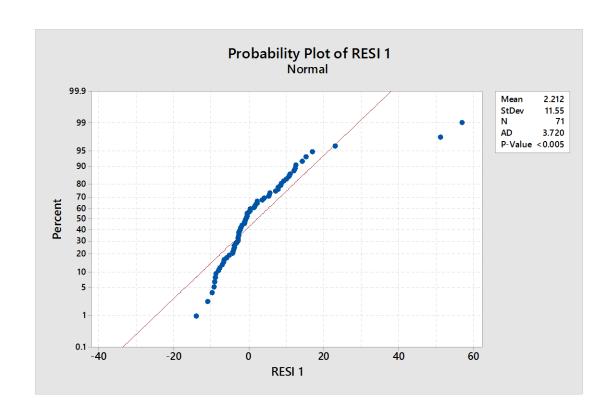


Figure 5.26 Probability Plot of American Formula 1

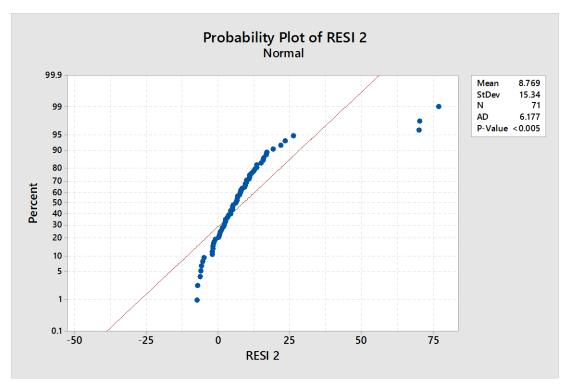


Figure 5.27 Probability Plot of American Formula 2

Original hypothesis, which is mean of the model residue is 0, is true because p – value of the test is 0.938. Model mean is – 0.006 and standard deviation is 2.294. It is clear that model predicts American coals CSR values more precisely than formula 1 and 2. In addition, box plot representation of model residues is given in Figure 5.28.

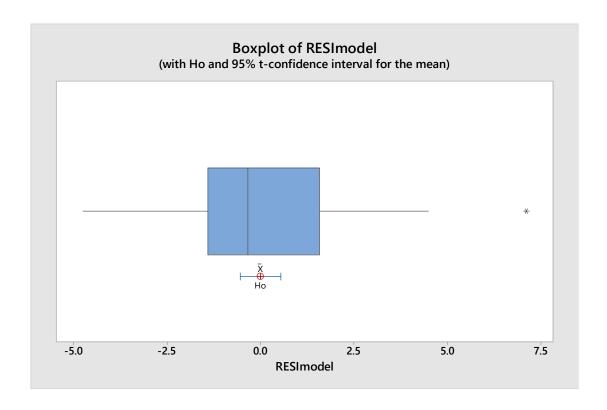


Figure 5.28 Box Plot of American CSR Prediction Model Residues

5.4.3 Comparison of Canadian Coals CSR Prediction Model and Theoretical Formulas

There are three formulations for Canadian coals CSR prediction. One is developed model and the other two are formulas retrieved from literature, which is discussed in Section 2.8.1.

Developed regression equation 3 is,

 $CSR = 214.7 - 1.589 \ Volatile \ Matter (\%) - 0.2056 \ Dilatation \ Finishing \ Temperature$ $(^{0}C) - 1.244 \ CRI \ (\%) + 0.0212 \ Coke \ Bulk \ Density \ (kg/m^{3}) + 0.574 \ Fe_{2}O_{3} \ (\%) - 2.18$ Mean Random Vitrinite Reflectance (Ro)

Canadian Formula 1 is,

$$CSR = 84.376 - 18.909 \times A \times BI$$

 $BI = (CaO + MgO + Na_2O + K_2O + Fe_2O_3) \div (SiO_2 + Al_2O_3)$

Where A is ash,

BI is basicity index.

Canadian Formula 2 is,

$$CSR = 83.217 - 167.801 \times BI + 147.816 \times BI^{2}$$

 $BI = (CaO + MgO + Na_{2}O + K_{2}O + Fe_{2}O_{3}) \div (SiO_{2} + Al_{2}O_{3})$

Where BI is basicity index.

In order to compare these three equations, first, responses are produced for all three. Then, residues are calculated by subtracting lab results from equations' results. Three residue populations are produced. Theoretically, residues should be distributed normally and means of residues should be zero when formulas predict lab results exactly. Probability plot of model residues is given in Figure 5.19. It is distributed normally (p-value = 0.680 > 0.05) with a mean of -1.39 and standard deviation of 3.57. Probability plot of formula 1 residues is given in Figure 5.29. It is distributed normally (p-value = 0.642 > 0.05) with a mean of -1.371 and standard deviation of 3.778. Probability plot of formula 2 residues is given in Figure 5.30. It is also distributed normally (p-value = 0.624 > 0.05). Its mean is -1.742 and standard deviation is 3.488. All three equations gives close precise results. In order to understand which one is most precise, one way ANOVA test or 2-sample t test can be performed. In addition to normal distribution requirement, ANOVA test needs that populations have equal variances. If they have equal variances, it is possible to test all three in one test by ANOVA. Otherwise, three 2-sample t test are required.

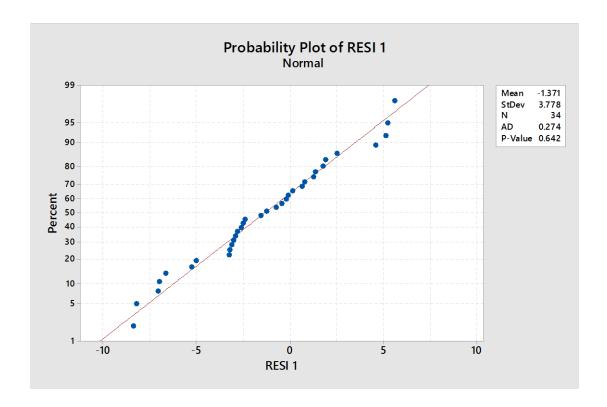


Figure 5.29 Probability Plot of Canadian Formula 1

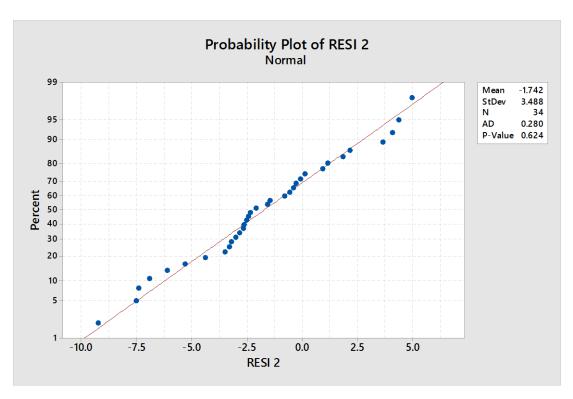


Figure 5.30 Probability Plot of Canadian Formula 2

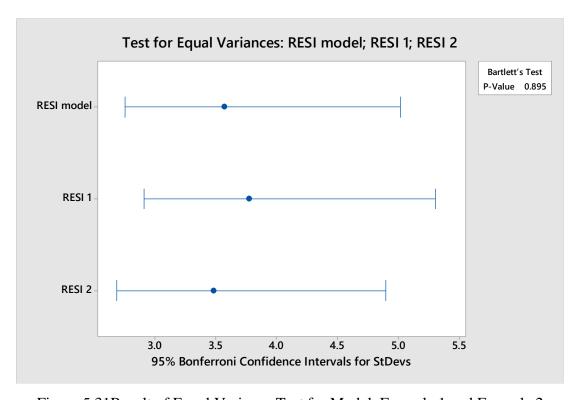


Figure 5.31Result of Equal Variance Test for Model, Formula 1 and Formula 2

By Minitab, variance equality test is performed. It is given in Figure 5.31. Model, Formula 1 and Formula 2 have equal variances because test statistic, p – value is 0.895, which is greater than 0.05 confidence level. Normality and equal variance requirements of one-way ANOVA test are satisfied. Then, the test is performed. Original hypothesis is model, formula 1 and formula 2 residuals have equal variances. Alternative hypothesis is at least one is different. Confidence level is expected 5 %. It means that if p-value of the test is smaller than 5 %, alternative hypothesis is true.

```
Ho: \mu (model) = \mu (formula 1) =\mu (formula 2)
Ha: at least one is different
```

Minitab one-way ANOVA test result is given in Figure 5.32.

One-way ANOVA: RESI model; RESI 1; RESI 2

```
Method

Null hypothesis All means are equal Alternative hypothesis At least one mean is different Significance level α = 0.05

Equal variances were assumed for the analysis.

Factor Information

Factor Levels Values Factor 3 RESI model; RESI 1; RESI 2

Analysis of Variance

Source DF Adj SS Adj MS F-Value P-Value Factor 2 2.97 1.486 0.11 0.893

Error 99 1293.65 13.067

Total 101 1296.62

Model Summary

S R-sq R-sq(adj) R-sq(pred) 3.61485 0.23% 0.00% 0.00%
```

Figure 5.32 Minitab One-Way ANOVA Test Result for Canadian Model, Formula 1 and Formula 2 Residues

Original hypothesis, which is all means are equal, is true because p – value of the test is 0.893. It means that all three equations predict CSR with similar precision. Tukey comparison for paired populations is given Figure 5.33. As expected, there is no significant difference between means of model, formula 1 and formula 2 because all paired mean differences lines includes zero.

In conclusion, Canadian model, formula 1 and formula 2 produce same precision for CSR prediction statistically.

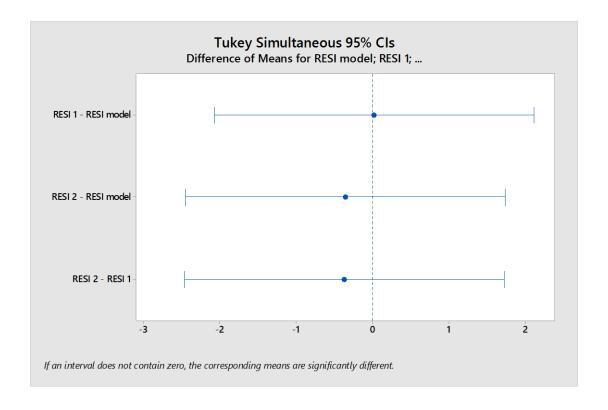


Figure 5.33 Difference of Means of Canadian Model, Formula 1 and Formula 2

5.5 Developing a CSR Prediction Model for Coal Blends

In this study, 46 different coal blends, which consist of Australian, Canadian and American coals, are investigated. Individual coal analysis of blends exists. Parameters to create regression model are chosen from developed Australian, American, Canadian CSR prediction models and literature.

In Section 5.3.1 Australian model was developed. Parameters of the model are sulfur in coal (%), maximum dilatation (ddpm), CRI (%) and stability (%). In Section 5.3.2 American model was developed. Parameters of the model are ash in coal (%), basicity index, CRI (%), stability (%) and micrinite (%). In Section 5.3.3 Canadian model was developed. Parameters of the model are volatile matter of coal (%), dilatation finishing temperature (0 C), CRI (%), coke bulk density (kg/m 3), Fe₂O₃ in ash (%) and Ro (%). In addition, it was proven that there is no difference between developed model and theoretical models, which consist ash and basicity index as variable, in terms of precision.

It is important that the temperature intervals of the plastic state for coals constituting a blend should overlap. The longer the overlapping of maximum activity intervals of two particles, the more the number of chemical bonds formed in the contact area (Hardarshan, 2015). In order to consider this information fluid range is calculated by subtracting minimum solidification temperature and maximum softening temperature of blend coals. As discussed in Section 2.3, coal behavior highly depended on its formation process, especially vegetation type. Petrographic analysis is an indication of coal formation. Finally, "Ash (%) x Basicity Index" is used as a parameter, because basicity index is a ratio of ash compounds regardless of mass. In order to consider both basicity and mass of ash compounds, it is also included into parameters.

Parameters chosen from models and literature are listed in Table 5.16.

Table 5.16 Parameters used in CSR Prediction for Coal Blends

#	Parameter Name	#	Parameter Name
1	S (% in coal)	12	Fe2O3 (%)
2	Maximum Fluidity (ddpm)	13	Mean Rand Vitrinite Reflectance (Ro)
3	Coal CSR (%)	14	Ash (%) x Basicity Index
4	Coal CRI (%)	15	Fluid Overlapping Range of Coals
5	Coal Stability (%)	16	Softening Temperature (°C)
6	Ash (%) (db)	17	Solidification Temperature (°C)
7	Basicity Index (BI)	18	Vitrinite (%)
8	Micrinite (%)	19	Liptinite (%)
9	Volatile Matter (%) (db)	20	Semifusinite (%)
10	Dilatation Finishing Temp (°C)	21	Inertinite (%)
11	Coke Bulk Density (kg/m3) (db)		

For the parameters except fluid range and dilatation finishing temperature, weighted average is calculated for blend value. Weighting is done according to coal percent of use in coal blend. Blend dilatation finishing temperature expect as maximum dilatation finishing temperature of coals. Fluid overlapping range of blend is considered the range which all coals are fluid. That is why, it is calculated by subtracting maximum softening temperature and minimum solidification temperature of blended coals.

Best subset analysis of 21 parameters are listen in Table 5.17. Coals CRI (%) average is most contributed parameter for CSR prediction of coal blends with a 45.0 % R – square. Average logarithmic maximum fluidity follows CRI with a 25.0 % R – square.

Table 5.17 Best Subset Analysis of Coal Blend CSR Prediction

Var	s R-Sq	R - Sq (adj)	R - Sq ! (pred)	Mallows Cp	s	Volatile Matter (%) (db)	Ash (%) (db)	Sulphur (%) (db) (coal)	Fe2O3 (%)	Basicity Index (BI)	AxBI	Fluidity	Softening Temperat ure (°C)		Fluid Range (°C)	LGF (Log Fluidity	DFT (°C)	CSR	CRI (%)	Stability (%)	(kg/m3) (db)	Mean Random Vitrinite Reflecta nce (Ro)	Vitrinite	Liptinit e	Semifusi nite	i Micrinit e	Înertinit e
1	45	43.6	40.4	31.1	1.8489														Х								
1	25.6	23.6	18	54.8	2.1513											x											
2	54.7		48.3	21.2	1.7002					X									X								
2	54.5	52.1	45.2	21.5	1.7043							x							X								
3	60.4	57.1	51.3	16.3	1.6113	X								X					X								
3	60.4	57.1	50.3	16.3	1.6127			X											X								X
4	65.3	61.3	54.5	12.4	1.5315	X			X						X				X								
4	65	61	54.3	12.7	1.5365														X						X	X	X
5	75	71.3	65.2	2.5	1.319	X					X														X	X	X
5	74.3		65.5	2.7	1.3226	X				X															X	X	X
6	76.8			2.3	1.2884	X					X		X												X	X	X
6	76.5			2.7	1.2973	X				X			X												X	X	X
7	78.5			2.2	1.2595	X					X												X	X	X	X	X
7	78.2		64.8	2.6	1.2682					X													X	X	X	X	X
8	79.6		66.9	2.9	1.246				X	X			X			X									X	X	X
<u>5 </u>	79.6		62.7	2.9	1.2474	X					X									X			X	X	X	X	X
9	81		68.7	3.2	1.2237	X			X	X			X							X			X		X	X	X
9	80.8			3.5	1.2309	X			X	X			X			X	X								X	X	X
10	81.7		65.2	4.3	1.2201	X			X	X			X							X			X	X	X	X	X
10	81.7		64.5	4.4	1.2225	Х		X	X	X			X			Х	X								X	X	X
11	81.7			5.1	1.2084	Х	X		X	X	Х		X										X	X	X	X	X
11	81.7			5.1	1.209	Х	X			X	Х								X	X			X	X	X	X	X
12	84.4			5		Х	X			X	Х		X						X	X			X	X	X	X	X
12	83.4			6.2	1.2051	Х	X		X	X	Х		X							X			X	X	X	X	X
13	84.7			6.7	1.1793		Х			X	X		X			X			X	X			X	X	X	X	X
13	84.7		60.5	6.7	1.1805		Х			X	X		X	X					X	X			X	X	X	X	X
14	85.1			8.1	1.1856		Х			X	X		X	X		X			X	X			X	X	X	X	X
14	85			8.3	1.1906	X	Х			X	X		X		X	X			X	X			X	X	X	X	X
15	85.7	76.7	57	9.5	1.1881		х			X	X		X	X		х	X	X	X	X			х	X	X	X	X
15	85.6	76.6	56.7	9.6	1.191	X	X			X	Х		X	X	X	X			X	X			X	X	X	X	X

Minitab explain R – square as proportion of variation in the response data explained by the predictors in the model. Adjusted R – square is a modified version of R – square that has been adjusted for the number of predictors in the model. Predicted R – square indicates how well the model predicts responses for new observations. R – square increase with addition of variable into model. For this reason, adjusted R – square and predicted R – square are more important. Maximum R – square (adj) is 77.5 % with 12 variable and 62.5 % R – square (adj). Maximum R – square (pred) is 68.7 % with 9 variable and 75.3 % R – square (adj). due to relatively small differences in R – square (adj), 9 variables model is chosen. Variables are volatile matter of coal (%), Fe₂O₃ in ash (%), basicity index, softening temperature (0 C), stability (%), vitrinite (%), semifusinite (%), micrinite (%) and inertinite (%). It should be note that these parameters are weighted averages of blend coals' parameters according to their mass percentages in the blend.

Analysis of variance table screen of Minitab is given in Figure 5.34.

```
Analysis of Variance
                             DF Adj SS Adj MS F-Value P-Value
Source
 egression 9 191.342 21.260 14.20 0.000

Volatile Matter (%) (db) 1 42.696 42.696 28.51 0.000
Regression
 Fe203 (%) 1 5.894 5.894
Basicity Index (BI) 1 14.768 14.768
                                                    3.94
9.86
                                                              0.056
                                                              0.004
  Softening Temperature (°C) 1
                                   7.619 7.619
                                                      5.09
                                                              0.032
  Stability (%)
                              1 3.485 3.485
                                                     2.33
                                                              0.138
                                  6.260 6.260 4.18
60.606 60.606 40.47
56.155 56.155 37.50
  Vitrinite.
                              1
                                                              0.050
  Semifusinite
                                                               0.000
                              1
 Micrinite
                                                    37.50
                                                              0.000
                              1 22.329 22.329 14.91
  İnertinite
                                                              0.001
Error
                              30 44.923
                                           1.497
                              39 236.265
Total
Model Summary
          R-sq R-sq(adj) R-sq(pred)
1.22369 80.99%
                75.28% 68.66%
```

Figure 5.34 Screen of Minitab Analysis of Variance Table for Coal Blend Regression Finally, regression analysis' variable descriptions is given in Figure 5.35.

Coefficients

Term	Coef	SE Coef	T-Value	P-Value	VIF
Constant	-133.4	60.6	-2.20	0.036	
Volatile Matter (%) (db)	2.003	0.375	5.34	0.000	2.82
Fe2O3 (%)	2.26	1.14	1.98	0.056	25.54
Basicity Index (BI)	-127.4	40.6	-3.14	0.004	14.83
Softening Temperature (°C)	0.238	0.106	2.26	0.032	3.28
Stability (%)	0.381	0.250	1.53	0.138	2.09
Vitrinite	0.348	0.170	2.04	0.050	10.53
Semifusinite	-0.658	0.103	-6.36	0.000	2.60
Micrinite	-0.5176	0.0845	-6.12	0.000	2.00
İnertinite	0.800	0.207	3.86	0.001	11.49

Figure 5.35 Screen of Minitab Regression Analysis for Canadian Coals

Regression equation for coal blend CSR prediction is given in Formula 4.

$$CSR = -133.4 + 2.003 \text{ Volatile Matter (\%) (db)} + 2.26 \text{ Fe2O3 (\%)} - 127.4 \text{ Basicity Index} + 0.238 \text{ Softening Temperature (}^{0}\text{C)} + 0.381$$

$$Stability (\%) + 0.348 \text{ Vitrinite (\%)} - 0.658 \text{ Semi-fusinite (\%)} - 0.5176 \qquad (4)$$

$$Micrinite (\%) + 0.800 \text{ Inertinite (\%)}$$

Residual plots of coal blend CSR prediction model is given in Figure 5.36. Residuals are distributed normally (p – value = 0.183 > 0.05) which is represented upper left side of Figure 5.36. In addition, residuals distributed homogeneously. It is also represented upper right side. R – square is 80.99 %. It can be concluded that fitness of the model is good.

Increase in Basicity Index, Semi-fusinite (%) and Micrinite (%) decreases CSR according to the regression model. On the other hand, increase in Volatile Matter (%), Fe₂O₃ (%), Softening Temperature (⁰C), Stability (%), Vitrinite (%) and Inertinite (%) shows positive effect for CSR.

R – sq of blend model is less than origin based models since contribution of some common variables in origin based models are greater than that of blend model. For

example, contribution of *stability* (%) to adequacy (R - sq) of Australian model is 2.7 %, however, it is only 1.8 % in R - sq of blend model.

Database variation range is a criterion for a regression analysis. Predictor values, is out of database range, can cause meaningless response predictions. For this reason, basic statistics of response and variables of coal blend CSR prediction model is given in Table 5.18.

Table 5.18 Basic Statistics of Response and Variables of Canadian CSR Prediction Model

Variable	Mean	Std Dev	Min	Q1	Median	Q3	Max	Range
Blend CSR (%)	67.55	2.32	62.38	65.61	67.82	69.31	71.76	9.38
VM (%)	25.40	1.02	21.98	24.88	25.37	26.08	27.13	5.15
Fe ₂ O ₃ (%)	6.63	1.00	4.33	6.09	6.44	7.27	8.56	4.23
Basicity Index	0.150	0.021	0.096	0.136	0.150	0.158	0.194	0.098
Soft. Temp (⁰ C)	414	11	367	413	416	418	436	69
Stability (%)	58.70	1.83	52.30	57.90	59.31	59.94	60.79	8.49
Vitrinite (%)	64.8	3.8	60.0	62.0	64.2	66.8	79.8	19.8
Semifusinite (%)	12.9	3.0	7.4	10.6	12.9	14.6	19.8	12.4
Micrinite (%)	1.3	3.2	0.0	0.0	0.0	0.0	13.0	13.0
Inertinite (%)	23.5	3.2	16.3	21.6	23.3	25.7	30.5	14.2

Theoretically, residue of the model, which is difference of actual and predicted response, should be zero in case of exact prediction. Residues of the model are calculated. In order to prove that model predicts blend CSR precisely, 1 sample t test is designed. Original hypothesis is model residue mean is equal to 0. Alternative hypothesis is model residue mean is not equal to 0. Confidence level is expected 5 %. It means that if p-value of the test is smaller than 5 %, alternative hypothesis is true or vice versa.

Ho: μ (model) = 0

Ha: μ (model) $\neq 0$

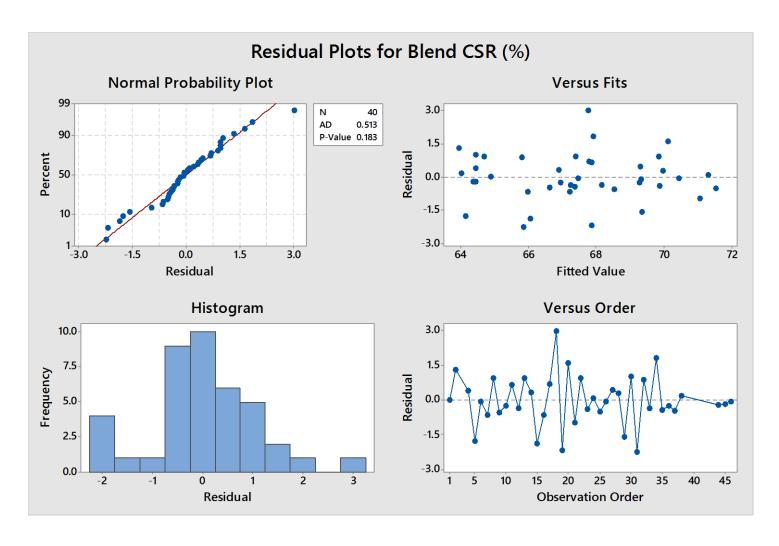


Figure 5.36 Minitab Screen of Residual Plots of Coal Blend CSR Prediction Model

Minitab 1 sample t test result is given in Figure 5.37.

One-Sample T: RESI

```
Test of \mu = 0 vs \neq 0   
Variable N Mean StDev SE Mean 95% CI T P RESI 40 0.159 1.073 0.170 (-0.185; 0.502) 0.93 0.356
```

Figure 5.37 Minitab 1 sample t test Result for American Prediction Model Residues

P – value of the test is 0.356, which is greater than confidence level, 0.05. For this reason, original hypothesis is true. Mean of model residues is equal to zero statistically.

Box plot representation of the residues is illustrated in Figure 5.38.

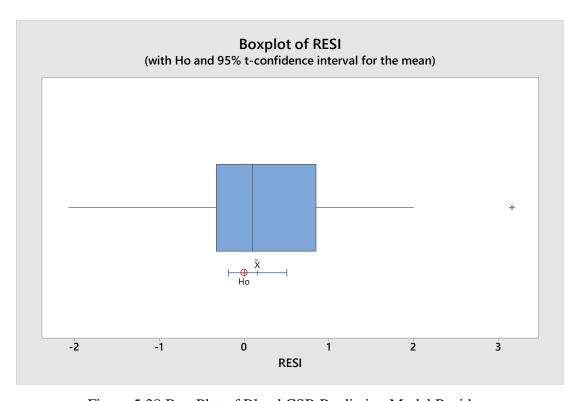


Figure 5.38 Box Plot of Blend CSR Prediction Model Residues

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

Coke strength after reaction (CSR) is a key parameter used in coal blend design for coke making. Due to its ability to represent coke's behavior in hot and reducing environment as blast furnace, CSR is a worldwide index to evaluate coke quality. Bad quality coke in terms of CSR causes high coke rates, heating problems and prevents smooth descent of burden in blast furnace operations. These drawbacks also increase cost of raw liquid iron production coast. Coke, which have 60 - 65 % CSR values expected as good quality cokes. In addition to operational point of view, CSR is also an evaluation index for coking coal and coke trade. Higher CSR values for both coal and produced coke increase the price of product.

Because of both economic and technological reasons, predicting coke CSR before production is necessary that only solution is developing a precise CSR prediction model

Literature search has been done in Section 2. Studied coals categorized in section 5.1 and 5.2. Basic statistics such as maximum, minimum, mean and average were used to detect remarkable differences. Box plot graphs were also used to understand fluctuations in variables. In a regression model, variables should be independent. For this reason, highly correlated parameters should be eliminated. Correlation analysis was performed by Excel and Minitab. One of two parameters that have greater than 0.8 correlation coefficient was eliminated. For parameters that have a correlation coefficient between 0.6 and 0.8, Minitab correlation analysis was performed to check p-values. One of two parameters that have correlation coefficient between 0.6 and 0.8 and less than 0.05 p - value was also eliminated. Then, best subset analysis was

performed with rest of parameters to examine alternative regression models. R – square, R – square (adj) and R – square (pred) were used to evaluate model alternatives. After indicating best regression model alternative, regression analysis was performed to develop the model. For an exact prediction, model fit values should be equal to response value. In other words, residue of the prediction should be zero. Precision of developed models were controlled by hypothesis tests for residue means.

Australian coals' CSR values were modelled with 96.5 % R – square by sulphur (%), maximum fluidity (ddpm), CRI (%) and stability (%). Regression equation is given in Formula 1 in Section 5.3.1.

American coals' CSR values were modelled with 93.41 % R – square by Ash (%), Basicity Index, CRI (%), Stability (%) and Micrinite. Regression equation is given in Formula 2 in Section 5.3.2.

Canadian coals' CSR values were modelled with 86.21 % R – square by Dilatation Finishing Temperature (0 C), CRI (%), Coke Bulk Density (kg/m 3), Fe₂O₃ (%) and Mean Random Vitrinite Reflectance (Ro). Regression equation is given in Formula 3 in Section 5.3.3.

In conclusion, this study shows that a regression model for both individual coals and coal blends can predict CSR with greater than 80 % R – square. It should be noted that this study established the CSR prediction of 49 coals from Australia, America and Canada. Therefore, the following are suggested for future work to improve model precision and predict other coal's CSR:

 Regression models work within the range of parameters' values in their database. That is why, an out of range parameter may cause unexpected response prediction. For new coals or even same coal's different analysis set, database should be updated. It should not be forgotten that model development in not a formula and it is an ongoing process.

- 2. In order to increase precision of models and ease of adding new coals to the model database, regression model may be developed a piecewise function for key parameters such as volatile matter content, sulfur, basicity index, coke reactivity index, fluidity, vitrinite, semi-fusinite and inertinite. This type of categorization provides studying narrower variable value range; therefore, more precise models can be developed.
- 3. It is clear that coke reactivity index is highly associated with coke strength after reaction. All three origin based CSR prediction models use CSR as a variable. For this reason, model of CRI before coal blend CSR modelling may be developed. Then, variables of CRI prediction model can be used for coal blend CSR prediction best subset analysis.
- 4. In this study, only linear relationship between variables and CSR was investigated. However, some variables' quadratic or cubic relations with CSR may explain CSR better. For example, Canadian Formula 2 uses square of basicity index. Although this formula uses only basicity index as variable to explain CSR, its residues are zero and similar with developed model, which have 6 variables, statistically. Thus, parameters' quadratic and cubic correlations may be studied before regression analysis in order to add these as a new parameter into regression analysis. In addition to that, multiple linear regression followed by correlation analysis was used in this study. However, other methods such as forward selection, backward elimination and stepwise selection, could be better for variable selection and predicting adequacy of models.

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APPENDICES

APPENDIX A

A. ASTM D388 – 17 STANDARD CLASSIFICATION OF COALS BY RANK

Table A.1 ASTM D388 – 17 Standard Classification Coal Classification

Class/Group	Fixed C Limits (dry mi matter basis)	(%) ineral	(%) (dry r	er Limits mineral er free	MJ/kg)	Btu/lb / (moist * I matter	Agglomerating Character
	= or >	<	=	= or <	= or >	<	
Anthracite Meta- anthracite	98	-	-	2	-	-	Non- agglomerating
Anthracite Semi anthracite	92 86	98 92	2	8 14	-	-	Non- agglomerating Non- agglomerating

Table A.1 Cont'd

Class/Group Bituminous Low volatile Medium volatile High volatile A High volatile B	Fixed Carbon Li (dry mineral ma basis)			e Matter Limits (%) neral matter free	Calorific Value Lir MJ/kg) (moist * i free basis)	Agglomerating Character		
	= or >	<	=	= or <	= or >	<	- 	
Bituminous								
Low volatile	78	86	14	22	-	-	Commonly agglomerating	
Medium volatil	e 69	78	22	31	-	-	Commonly agglomerating	
High volatile A	-	69	31	-	14000**/32.6	-	Commonly agglomerating	
High volatile B	-	-	-	-	13000**/30.2	14000/32.6	Commonly agglomerating	
High volatile C	-	-	-	-	11500/26.7	13000/30.2	Commonly agglomerating	

Table A.1 Cont'd

Class/Group	Fixed Carbon Li (dry mineral ma basis)			atile Matter Limits (%) mineral matter free is)	Calorific Value MJ/kg) (moist free basis)	Agglomerating Character		
	= or >	<	=	= or <	= or >	<	-	
Subbituminous								
Subbituminous A	-	-	-	-	10500/24.4	11500/26.7	Non-agglomerating	
Subbituminous B	-	-	-	-	9500/22.1	10500/24.4	Non-agglomerating	
Subbituminous C	-	-	-	-	8300/19.3	9500/22.1	Non-agglomerating	
Lignitic					6000/11-	0000/100		
Lignite A	-	-	-	-	6300/14.7	8300/19.3	Non-agglomerating	
Lignite B	-	-	-	-	-	6300/14.7	Non-agglomerating	

APPENDIX B

B. QUALITY OF COAL SAMPLES

Table B.1 Proximate Analysis of Coal Samples

Coal Name	Moisture (%)	Volatile Matter (%) (db)	Ash (%) (db)	Fixed Carbon (%) (db)	Calorific Value (db) (kcal/kg)
American Coal #1	8.25	27.92	8.24	63.84	7722
American Coal #2	7.50	31.10	8.15	60.75	7657
American Coal #3	9.08	21.10	8.70	70.20	7657
American Coal #4	9.47	24.25	8.94	66.82	7544
American Coal #5	9.64	29.97	8.57	61.46	7623
American Coal #6	6.93	26.59	7.81	65.60	6162
American Coal #7	6.67	25.66	8.45	65.89	7713
American Coal #8	7.61	25.53	8.92	65.55	7692
American Coal #9	10.69	22.59	8.87	68.54	7723
American Coal #10	9.92	24.19	6.10	69.71	7958
American Coal #11	8.88	26.23	11.57	62.20	7513
American Coal #12	7.09	29.99	8.23	61.78	7673
American Coal #13	7.27	26.12	6.09	67.79	7893
American Coal #14	9.85	30.04	8.11	61.85	7585
American Coal #15	7.67	28.13	8.19	63.68	7646
American Coal #16	9.37	24.54	7.63	67.83	7724
American Coal #17	6.64	25.46	8.64	65.90	7596
American Coal #18	7.89	17.03	6.90	76.07	8004
American Coal #19	7.13	32.11	7.04	60.85	7733
American Coal #20	8.30	22.54	11.48	65.98	7446

Table B.1 Cont'd

Coal Name	Moisture (%)	Volatile Matter (%) (db)	Ash (%) (db)	Fixed Carbon (%) (db)	Calorific Value (db) (kcal/kg)
American Coal #14	9.85	30.04	8.11	61.85	7585
American Coal #15	7.67	28.13	8.19	63.68	7646
American Coal #16	9.37	24.54	7.63	67.83	7724
American Coal #17	6.64	25.46	8.64	65.90	7596
American Coal #18	7.89	17.03	6.90	76.07	8004
American Coal #19	7.13	32.11	7.04	60.85	7733
American Coal #20	8.30	22.54	11.48	65.98	7446
Australian Coal #1	9.53	18.31	9.01	72.69	7657
Australian Coal #2	10.26	19.70	10.06	70.24	6471
Australian Coal #3	10.02	23.57	8.96	67.47	6340
Australian Coal #4	7.93	28.51	8.99	62.50	7512
Australian Coal #5	8.61	23.30	9.89	66.81	7492
Australian Coal #6	9.71	23.48	9.64	66.88	7577
Australian Coal #7	10.65	24.59	9.11	66.31	5706
Australian Coal #8	9.40	21.27	10.48	68.25	7549
Australian Coal #9	8.64	35.04	7.24	57.73	7571
Australian Coal #10	9.79	20.00	9.55	70.46	7589
Australian Coal #11	10.26	22.13	7.69	70.18	7744
Australian Coal #12	9.02	19.12	9.73	71.16	7568
Australian Coal #13	9.02	33.27	10.29	56.45	7109
Australian Coal #14	9.37	21.96	9.44	68.60	7606
Australian Coal #15	10.40	22.29	8.36	69.35	6865
Australian Coal #16	10.68	20.80	8.21	70.99	7646
Australian Coal #17	7.05	27.68	10.58	61.74	6970
Australian Coal #18	9.02	23.26	10.22	66.52	7491
Australian Coal #19	11.70	26.30	9.88	63.82	7328
Australian Coal #20	7.51	34.12	7.95	57.93	7467
Australian Coal #21	11.55	24.23	8.61	67.16	7554
Australian Coal #22	8.99	24.19	9.74	66.07	7540

Table B.1 Cont'd

Coal Name	Moisture (%)	Volatile Matter (%) (db)	Ash (%) (db)	Fixed Carbon (%) (db)	Calorific Value (db) (kcal/kg)
Canadian Coal #1	8.72	23.34	9.15	67.51	7592
Canadian Coal #2	8.56	20.75	9.19	70.07	7621
Canadian Coal #3	9.23	27.03	8.31	64.66	7588
Canadian Coal #4	8.80	23.59	9.54	66.88	7522
Canadian Coal #5	8.44	26.18	8.61	65.21	7554
Canadian Coal #6	9.02	24.14	8.85	67.01	7602
Canadian Coal #7	9.76	23.29	9.94	66.77	7477
Russian Coal #1	8.70	33.08	8.49	58.43	7504
Russian Coal #2	9.26	33.41	9.89	56.70	7420
Colombian Coal #1	7.98	27.70	10.04	62.26	7468
Colombian Coal #2	7.77	31.71	9.00	59.29	7548
Colombian Coal #3	7.09	31.83	9.69	58.49	7473
Colombian Coal #4	7.02	30.90	9.96	59.14	7401

Table B. 2 Physical Properties of Coal Samples

Coal Name	HGI	Reflectance of Light (%)	Bulk Density (gr/cm3)	+6,30mm (%)	- 0,425mm (%)
American Coal #1	71.12	90.32	0.782	23.08	25.32
American Coal #2	61.35	92.02	0.804	30.47	23.20
American Coal #3	86.86	92.66	0.757	17.68	28.82
American Coal #4	82.62	92.00	0.760	15.64	29.22
American Coal #5	68.60	91.80	0.755	17.51	30.94
American Coal #6	67.84	90.07	0.798	32.22	18.59
American Coal #7	79.78	91.62	0.710	12.04	26.99
American Coal #8	77.58	92.41	0.670	14.15	25.16
American Coal #9	79.40	95.77	0.750	16.60	27.44
American Coal #10	84.05	88.07	0.770	9.36	30.73
American Coal #11	95.40	67.14	0.760	15.64	21.18
American Coal #12	67.26	92.49	0.780	27.41	22.06
American Coal #13	81.41	93.59	0.750	22.11	22.85
American Coal #14	69.20	88.30	0.840	37.55	12.99
American Coal #15	67.86	93.59	0.770	38.65	22.97
American Coal #16	90.00	97.11	0.750	12.02	24.15
American Coal #17	71.60	87.89	0.820	34.32	17.00
American Coal #18	88.20	90.77	0.750	20.68	28.64
American Coal #19	58.74	89.66	0.730	27.76	17.89
American Coal #20	78.71	93.65	0.850	23.45	20.09
Australian Coal #1	88.15	96.04	0.81	33.01	22.13
Australian Coal #2	86.93	93.18	0.84	28.98	25.09
Australian Coal #3	82.08	94.97	0.81	31.60	21.59
Australian Coal #4	60.87	91.23	0.83	43.15	18.42
Australian Coal #5	72.86	94.66	0.80	35.35	20.64
Australian Coal #6	83.34	91.71	0.81	33.70	19.83
Australian Coal #7	80.20	95.41	0.84	32.60	19.83
Australian Coal #8	85.48	95.60	0.82	32.99	19.77
Australian Coal #9	55.60	92.74	0.81	45.15	16.08
Australian Coal #10	86.73	95.92	0.79	29.03	23.86

Table B.2 Cont'd

Coal Name	HGI	Reflectance of Light (%)	Bulk Density (gr/cm3)	+6,30m m (%)	-0,425mm (%)
Australian Coal #11	82.98	92.26	0.83	39.93	23.98
Australian Coal #12	78.37	96.57	0.87	38.45	17.89
Australian Coal #13	47.70	93.71	0.84	49.17	9.73
Australian Coal #14	84.92	95.52	0.78	32.59	19.02
Australian Coal #15	86.00	98.29	0.84	35.57	18.61
Australian Coal #16	79.00	95.46	0.80	27.33	24.43
Australian Coal #17	67.40	95.67	0.86	33.27	16.66
Australian Coal #18	77.54	90.21	0.88	28.95	23.57
Australian Coal #19	60.36	93.63	0.87	47.51	13.47
Australian Coal #20	51.36	94.69	0.81	49.98	12.55
Australian Coal #21	71.40	92.73	0.75	28.76	22.11
Australian Coal #22	76.56	93.30	0.80	35.22	17.64
Canadian Coal #1	83.04	92.53	0.75	19.14	34.17
Canadian Coal #2	82.47	92.45	0.73	19.18	34.48
Canadian Coal #3	84.23	91.38	0.68	10.14	44.43
Canadian Coal #4	82.71	93.96	0.75	16.99	34.96
Canadian Coal #5	83.00	92.06	0.72	20.00	27.81
Canadian Coal #6	86.93	92.19	0.68	16.83	36.78
Canadian Coal #7	80.87	92.37	0.71	17.35	31.91
Russian Coal #1	63.47	90.90	0.78	25.93	18.29
Russian Coal #2	72.39	88.96	0.78	28.42	23.30
Colombian Coal #1	74.31	86.26	0.81	40.47	17.22
Colombian Coal #2	67.13	91.19	0.88	43.65	15.39
Colombian Coal #3	63.81	77.89	0.81	38.26	15.55
Colombian Coal #4	66.40	87.51	0.81	43.74	14.00

Table B. 3 Rheological Properties and FSI of Coal Samples

Coal Name	FSI	Maximum Fluidity (ddpm)	Softening Temperature (°C)	Maximum Fluidity Temperature (°C)	Solidification Temperature (°C)	Fluid Range (°C)	LGF (Logarithmic Fluidity)	Maximum Dilatation (%)	Maximum Contraction (%)	Softening Temperature (°C)	Dilatation Starting Temperature (°C)	Dilatation Finishing Temperature (°C)
American Coal #1	7.5	6900	389	431	475	86	3.33	133.79	12.96	383	421	474
American Coal #2	7.5	15686	378	423	466	88	3.92 174.76		3.76	370	413	471
American Coal #3	8.5	3323	423	472	508	85	2.95	138.20	8.93	406	434	489
American Coal #4	8.5	1518	314	350	380	66	2.39	170.75	10.50	399	425	485
American Coal #5	8.0	23799	399	446	496	97	4.33	260.75	14.00	369	412	483
American Coal #6	7.0	762	414	451	489	75	2.57	43.80	13.20	392	430	471
American Coal #7	8.0	6437	398	457	499	101	3.79	231.33	-23.67	381	416	485
American Coal #8	8.5	6194	393	455	497	104	3.79	233.00	-24.00	380	418	485
American Coal #9	8.0	442	426	471	511	85	2.65	136.00	26.00	402	430	479
American Coal #10	9.0							205.00	-24.00	389	427	486
American Coal #11	8.5	226	414	462	495	81	2.35	121.00	24.00	395	430	480
American Coal #12	8.0	20879	392	455	488	96	4.32	247.00	-25.00	369	412	481
American Coal #13	8.5							234.00	-21.00	380	416	485
American Coal #14	7.5	2034	413	445	493	80	3.31	124.00	25.00	381	419	472
American Coal #15	8.0	831	409	445	490	81	2.92	52.00	-23.00	383	422	466
American Coal #16	9.0	91	425	467	500	75	1.96	68.00	21.00	400	440	478
American Coal #17	7.5	248	409	448	487	78	2.39	18.00	-19.00	404	431	472
American Coal #18	8.0	72	448	482	511	63	1.86	73.00	25.00	436	460	498
American Coal #19	8.5							238.00	-24.00	373	410	477
American Coal #20	7.5	180	409	458	496	87	2.25	47.00	-21.00	411	435	476
Australian Coal #1	8.0	41	448	480	504	56	1.46	51.69	-18.23	436	461	495
Australian Coal #2	8.0	85	315	342	362	47	1.46	68.29	4.29	422	453	492
Australian Coal #3	8.0	670	417	462	498	82	2.73	99.33	-8.00	400	438	482
Australian Coal #4	6.5	2372	401	445	484	83	3.37	108.20	-13.00	376	422	471
Australian Coal #5	6.5	108	343	375	398	55	1.70	32.40	-21.20	409	447	386
Australian Coal #6	8.0	510	341	367	397	56	2.24	112.00	-13.20	399	436	480
Australian Coal #7	8.0	905	419	459	496	77	2.95	114.50	13.00	397	435	478
Australian Coal #8	8.0	279	425	472	501	76	2.44	90.25	-9.75	409	443	489

Table B.3 Cont'd

_	Coal Name	FSI	Maximum Fluidity (ddpm)	Softening Temperature (°C)	Maximum Fluidity Temperature (°C)	Solidification Temperature (°C)	Fluid Range (°C)	LGF (Logarithmic Fluidity)	Maximum Dilatation (%)	Maximum Contraction (%)	Softening Temperature (°C)	Dilatation Starting Temperature (°C)	Dilatation Finishing Temperature (°C)
A	australian Coal #9	8.5	18969	396	439	478	83	4.28	149.50	-26.00	371	414	463
I	australian Coal #10	8.5	97	430	475	497	68	1.94	52.50	-21.00	430	453	488
I	australian Coal #11	8.0	110	424	463	495	71	2.03	40.00	-24.00	414	448	480
I	australian Coal #12	6.0	8	442	472	493	51	0.85	-7.00	-18.00	429	471	242
I	australian Coal #13	4.0	8	201	217	229	29	0.59	-8.00	-23.00	392	432	223
I	australian Coal #14	8.5	254	432	465	497	65	2.37	87.00	-23.00	406	441	482
I	australian Coal #15	7.5	140	438	471	501	63	2.14	48.00	21.00	406	447	483
I	australian Coal #16	5.5	2	459	471	492	33	0.30	no dilatation	21.00	420	465	no dilatation
I	australian Coal #17	7.0	2062	405	447	492	87	3.31	164.00	26.00	379	421	478
I	australian Coal #18	8.0	438	415	457	493	78	2.64	85.00	-23.00	399	436	473
	australian Coal #19	2.5	8	422	450	468	46	0.92	no dilatation	-20.00	408	463	no dilatation
א א	australian Coal #20	8.0	849	402	438	472	70	2.93	58.00	-21.00	386	421	451
)\ _{	australian Coal #21	7.0	87	429	462	488	60	1.94	16.00	-23.00	407	448	470
I	australian Coal #22	7.5							41.00	-24.00	405	431	469
(Canadian Coal #1	7.5	68	374	403	428	54	1.62	39.80	-7.07	403	446	476
(Canadian Coal #2	7.0	18	380	404	425	46	1.13	13.14	-16.00	419	458	484
(Canadian Coal #3	8.0	233	422	456	488	66	2.35	84.00	-26.14	395	436	472
(Canadian Coal #4	7.0	71	423	460	491	68	1.85	28.00	-22.50	405	448	475
(Canadian Coal #5	7.5	207	422	458	488	66	2.32	91.00	-24.00	396	438	477
(Canadian Coal #6	7.5	116	428	463	490	62	2.06	48.00	-26.00	399	442	472
(Canadian Coal #7	7.0	18	432	462	492	60	1.26	13.00	-22.00	411	450	473
]	Russian Coal #1	8.0	4203	279	311	340	61	2.66	120.43	-24.43	376	415	464
]	Russian Coal #2	8.0	31215	379	442	487	108	4.49	331.00	-28.00	366	403	470
(Colombian Coal #1	7.0	895	400		483	83	2.94	78.67	-23.67	375	422	467
(Colombian Coal #2	7.5	3071	398		480	82	3.44	135.67	8.33	367	416	466
(Colombian Coal #3	8.0	1894	197	221	240	44	1.79	142.00	-25.50	366	414	466
(Colombian Coal #4	7.5	2955	394	442	481	87	3.47	129.00	-25.00	366	417	465

Table B. 4 Ash Chemistry, Sulfur and Phosphor in Coal Samples

_		Total	Total	Total	41202	G 0	G 202	F 403	TZAO	14.0	11.0	N. 40	DAO.	G:O3	Ti Oa			.	7.0
	Coal Name	Sulphur	Phosphor	Alkalis in				Fe2O3		_							S		ZnO
		(%) (db)	(%) (db)	ash (%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
A	merican Coal #1	0.89	0.01	2.62	27.62	3.69	0.03	8.74	2.19	1.22	0.05	0.43	0.28	51.04	1.60	0.12	1.03	0.02	0.03
A	merican Coal #2	0.89	0.01	2.71	28.47	2.04	0.03	7.53	2.33	0.95	0.03	0.37	0.25	53.99	1.65	0.11	0.42	0.01	0.03
A	merican Coal #3	0.74	0.04	2.58	30.87	2.79	0.04	7.34	2.10	1.08	0.03	0.48	0.97	49.99	1.72	0.43	0.71	0.02	0.03
A	merican Coal #4	0.80	0.04	2.60	29.90	2.62	0.03	7.37	2.17	1.10	0.04	0.43	0.91	50.28	1.65	0.40	0.68	0.02	0.03
A	merican Coal #5	0.75	0.04	3.18	29.80	2.70	0.04	7.05	2.41	1.46	0.04	0.77	1.16	51.22	1.58	0.51	0.50	0.02	0.04
A	merican Coal #6	0.94	0.01	3.02	29.28	2.27	0.03	9.16	2.56	1.19	0.03	0.46	0.22	51.32	1.57	0.09	0.53	0.02	0.04
A	merican Coal #7	0.74	0.02	2.07	28.85	3.87	0.03	7.69	1.90	1.03	0.03	0.17	0.56	50.23	1.68	0.25	1.09	0.00	0.04
A	merican Coal #8	0.80	0.02	2.07	28.67	2.95	0.04	7.67	1.84	1.08	0.03	0.22	0.49	52.25	1.73	0.21	0.76	0.00	0.04
A	merican Coal #9	0.50	0.02	2.34	32.75	3.37	0.04	5.41	2.00	1.20	0.04	0.33	0.49	50.63	1.95	0.22	0.58	0.03	0.03
A	merican Coal #10	0.88	0.00	3.50	22.95	2.38	0.03	12.90	3.36	1.44	0.03	0.15	0.10	46.13	0.97	0.04	0.50	0.00	0.03
A	merican Coal #11	1.14	0.05	0.72	26.26	1.98	0.00	8.77	0.45	0.66	0.00	0.27	0.10	58.44	1.41	0.05	0.56	0.02	0.01
A	merican Coal #12	0.63	0.04	2.47	32.14	3.07	0.05	6.30	2.08	1.45	0.03	0.39	1.15	47.53	1.70	0.50	0.99	0.00	0.03
A	merican Coal #13	0.88	0.02	2.97	31.46	1.19	0.04	6.35	2.74	0.77	0.01	0.23	0.75	50.10	1.22	0.33	0.05	0.00	0.03
A	merican Coal #14	0.90	0.01	3.29	28.31	3.21	0.05	8.87	2.67	1.40	0.08	0.61	0.27	51.31	1.35	0.12	0.87	0.02	0.04
A	merican Coal #15	0.92	0.03	3.43	28.78	2.32	0.03	7.49	2.65	0.96	0.02	0.78	0.96	52.43	1.30	0.42	0.44	0.00	0.05
A	merican Coal #16	0.95	0.02	3.20	21.22	8.13	0.05	17.76	2.16	2.67	0.23	1.05	0.62	38.89	0.86	0.27	2.68	0.01	0.03
A	merican Coal #17	0.92	0.01	3.31	27.47	1.48	0.03	7.03	2.87	1.41	0.06	0.44	0.18	54.92	1.41	0.08	0.33	0.01	0.06
A	merican Coal #18	0.73	0.00	2.49	25.85	3.42	0.05	13.39	1.91	1.54	0.06	0.58	0.15	49.09	1.54	0.07	1.12	0.02	0.04
A	merican Coal #19	0.98	0.00	3.18	26.20	1.24	0.03	8.21	2.83	0.88	0.02	0.35	0.09	53.62	1.42	0.04	0.16	0.00	0.01
A	merican Coal #20	0.99	0.04	3.09	27.36	1.74	0.03	7.94	2.75	0.88	0.03	0.34	0.78	53.74	1.42	0.34	0.17	0.00	0.02
A	australian Coal #1	0.52	0.06	1.59	32.43	3.42	0.02	5.98	1.09	0.85	0.05	0.50	1.63	50.58	1.72	0.71	0.47	0.01	0.04
A	australian Coal #2	0.62	0.02	1.53	28.57	1.53	0.03	3.84	1.06	0.64	0.04	0.48	0.56	59.33	1.59	0.25	0.30	0.02	0.03
A	australian Coal #3	0.53	0.04	0.97	32.58	1.84	0.01	6.49	0.59	0.96	0.03	0.36	0.98	52.79	1.68	0.43	0.21	0.01	0.03
A	australian Coal #4	0.39	0.05	1.30	29.51	4.25	0.02	5.71	1.15	1.05	0.06	0.15	1.23	51.05	1.44	0.54	1.09	0.01	0.03
A	australian Coal #5	0.36	0.05	1.19	35.68	2.52	0.03	5.04	1.10	1.16	0.04	0.15	1.41	49.83	2.16	0.62	0.37	0.00	0.03
A	australian Coal #6	0.54	0.03	1.16	22.59	1.98	0.01	4.14	0.97	0.56	0.05	0.19	0.79	64.22	1.39	0.35	0.34	0.01	0.04
A	australian Coal #7	0.52	0.02	1.20	31.95	0.89	0.01	4.63	0.80	0.61	0.04	0.40	0.51	57.06	1.80	0.22	0.09	0.02	0.03
A	australian Coal #8	0.60	0.03	1.22	24.16	1.32	0.01	3.56	0.97	0.58	0.06	0.25	0.64	64.76	1.39	0.28	0.16	0.01	0.04

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Table B.4 Cont'd

_		Total	Total	Total															
	Coal Name	Sulphur	Phosphor		Al2O3	CaO	Cr2O3	Fe2O3	K2O	MgO	MnO	Na2O	P2O5	SiO2	TiO2	P	\mathbf{S}	Ni	ZnO
	Coai Name	-	_		(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
_		(%) (db)	(%) (db)	ash (%)	20.72	1.04	0.01	2.25	0.60	0.60	0.00	0.22	0.00	50.20	2.12	0.40	0.15	0.02	0.00
	ustralian Coal #9	0.62	0.03	1.01	38.62	1.84	0.01	3.25	0.68	0.60	0.03	0.33	0.98	50.39					
	ustralian Coal #10	0.51	0.05	1.05	31.89	2.45	0.03	5.69	0.76	0.85	0.04	0.29	1.23	54.48					0.04
	ustralian Coal #11	0.42	0.04	0.87	27.83	4.63	0.04	9.37	0.74	0.85	0.06	0.14	1.22	49.42					,
	ustralian Coal #12	0.38	0.02	1.90	28.15	2.76	0.02	7.83	1.71	1.59	0.02	0.19	0.49	51.87	1.44				
A	ustralian Coal #13	0.55	0.03	1.23	21.69	1.62	0.02	4.55	0.89	0.84	0.02	0.35	0.58	61.86	1.10	0.25	0.57	0.00	0.02
A	ustralian Coal #14	0.61	0.02	1.15	24.36	0.88	0.02	3.93	0.94	0.62	0.04	0.21	0.39	63.06	1.61	0.17	0.15	0.00	0.01
A	ustralian Coal #15	0.51	0.05	1.38	34.62	2.95	0.02	5.94	0.65	0.89	0.05	0.74	1.50	50.27	1.81	0.66	0.34	0.01	0.03
A	ustralian Coal #16	0.28	0.04	0.69	33.91	4.43	0.02	8.71	0.37	1.17	0.04	0.33	1.12	46.10	1.85	0.49	1.22	0.02	0.03
A	ustralian Coal #17	1.02	0.02	1.28	27.79	1.08	0.00	6.37	1.04	0.30	0.00	0.24	0.36	59.61	1.81	0.15	0.17	0.03	0.03
A	ustralian Coal #18	0.52	0.04	0.83	20.23	2.58	0.02	3.89	0.61	0.35	0.04	0.22	0.93	63.70	1.92	0.41	0.56	0.00	0.01
	ustralian Coal #19	0.34	0.10	0.62	31.28	3.62	0.02	7.08	0.34	0.55	0.05	0.29	2.41	51.93	1.52	1.05	0.21	0.00	0.02
° A	ustralian Coal #20	0.69	0.01	1.31	36.01	0.72	0.02	7.69	1.07	0.53	0.02	0.24	0.19	50.18	1.63	0.08	0.16	0.01	0.08
A	ustralian Coal #21	0.39	0.06	0.79	29.18	5.18	0.03	10.68	0.67	1.26	0.12	0.12	1.62	45.92	1.59	0.72	1.36	0.01	0.02
A	ustralian Coal #22	0.44	0.04	1.33	30.83	1.47	0.02	4.70	1.22	0.62	0.04	0.11	0.91	56.20	1.89	0.40	0.17	0.00	0.02
C	anadian Coal #1	0.41	0.06	0.83	29.24	2.53	0.02	4.03	0.71	0.44	0.03	0.12	1.49	57.58	1.83	0.65	0.31	0.01	0.04
C	anadian Coal #2	0.34	0.05	0.64	28.51	3.27	0.01	3.34	0.54	0.50	0.03	0.10	1.29	57.57	1.76	0.57	0.73	0.00	0.02
C	anadian Coal #3	0.56	0.10	1.25	28.76	3.12	0.03	3.96	1.15	0.29	0.02	0.10	2.74	55.56	1.79	1.20	0.24	0.00	0.05
C	anadian Coal #4	0.44	0.06	0.81	28.87	3.59	0.02	3.55	0.69	0.51	0.03	0.13	1.54	56.68	1.90	0.68	0.83	0.00	0.03
C	anadian Coal #5	0.49	0.08	1.15	28.99	2.16	0.02	4.47	1.04	0.34	0.03	0.11	2.01	56.23	1.73	0.88	0.13	0.01	0.04
C	anadian Coal #6	0.46	0.09	0.86	28.39	3.01	0.01	3.35	0.72	0.35	0.03	0.14	2.38	58.67	1.70	1.04	0.08	0.00	0.04
C	anadian Coal #7	0.40	0.06	0.82	29.82	3.71	0.01	3.24	0.72	0.61	0.02	0.10	1.29	56.82	1.86	0.56	0.97	0.00	0.01
R	tussian Coal #1	0.72	0.06	1.94	22.06	7.64	0.02	10.48	1.41	2.25	0.06	0.53	1.63	44.36	1.00	0.72	2.45	0.00	0.03
R	tussian Coal #2	0.63	0.06	4.60	22.01	5.22	0.02	7.34	1.95	1.56	0.05	2.65	1.31	55.47	0.89	0.57	0.04	0.00	1.44
C	Colombian Coal #1	0.75	0.05	1.65	23.89	1.53	0.02	3.96	1.33	0.49	0.02	0.33	1.09	62.50	1.31	0.48	0.14	0.00	0.04
C	Colombian Coal #2	0.76	0.04	1.88	24.85	1.34	0.04	5.93	1.33	0.71	0.05	0.55	1.01	62.16	1.37	0.44	0.06	0.02	0.03
C	Colombian Coal #3	0.75	0.04	1.51	24.34	1.07	0.03	4.03	1.29	0.42	0.02	0.22	0.90	61.77	1.34	0.39	0.06	0.00	0.01
C	Colombian Coal #4	0.75	0.03	1.92	22.31	1.09	0.02	4.66	1.50	1.00	0.03	0.42	0.74	63.49	1.36	0.32	0.08	0.01	0.05

Table B. 5 Petrographical Analysis of Coal Samples

		Mean Random	¥75	N/C	V/9	¥70	¥70	¥/10	¥711	¥712	¥/12	X71.4	X/15	¥/1.6	¥71.7	¥710	¥710				
	Coal Name	Vitrinite Reflectance (Ro)	V5 (%)	V6 (%)	V7 (%)	V8 (%)	V9 (%)	V10 (%)	V11 (%)	V12 (%)	V13 (%)	V14 (%)	V15 (%)	V16 (%)	V17 (%)	V18 (%)	V19 (%)	Vitrinite	Liptinite	Inertinite	Semifusinite
	American Coal #1	1.00	0.72	1.81	5.06	12.20	19.49	17.90	13.98	7.90	5.43	3.80	3.01	1.55	1.38	0.82	0.54	46.85	9.17	8.08	7.89
	American Coal #2	0.85	1.30	4.95	13.50	23.16	22.45	15.88	10.45	4.46	1.64	1.16	0.65	0.30	0.10	0.00	0.00	44.31	9.52	9.26	7.46
	American Coal #3	1.30	0.00	0.02	0.07	0.38	1.39	9.39	19.52	19.96	21.90	15.10	6.00	3.25	2.07	0.58	0.27	61.85	8.03	10.04	7.24
	American Coal #4	1.20	0.25	2.00	4.92	9.09	9.92	20.36	18.55	5.88	4.47	5.89	5.80	4.09	3.26	3.01	2.42	50.82	5.80	7.71	7.71
	American Coal #5	0.71	0.42	1.75	5.00	14.42	33.67	16.00	2.58	1.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00	49.91	10.94	5.72	5.72
	American Coal #6	0.88	0.07	2.20	11.07	20.93	17.66	10.00	8.20	6.53	8.40	6.33	4.80	3.13	0.60	0.07	0.00	60.90	13.11	14.41	11.05
	American Coal #7	1.11	0.00	0.00	0.58	4.16	9.08	29.32	44.36	8.59	2.37	0.77	0.77	0.00	0.00	0.00	0.00				
	American Coal #8	1.18	0.00	0.00	1.67	2.50	6.67	18.34	25.84	21.67	14.96	6.67	1.68	0.00	0.00	0.00	0.00				
	American Coal #9	1.19	0.00	0.00	0.00	0.33	3.34	14.34	33.34	41.34	6.67	0.33	0.31	0.00	0.00	0.00	0.00	65.33	8.67	8.67	8.67
	American Coal #10	1.20	0.00	0.00	0.00	0.00	0.00	7.00	58.00	23.50	5.50	4.50	1.50	0.00	0.00	0.00	0.00				
	American Coal #11	0.96	0.00	1.00	5.33	20.66	43.67	20.33	6.00	2.34	0.33	0.33	0.00	0.00	0.00	0.00	0.66	60.59	15.32	23.82	10.00
20	American Coal #12	0.98	0.00	0.00	0.00	4.50	58.00	36.50	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	73.00	5.20	20.20	6.60
_	American Coal #13	1.15	0.00	0.00	0.00	0.00	0.00	20.00	64.00	15.50	0.50	0.00	0.00	0.00	0.00	0.00	0.00				
	American Coal #14	1.21	0.00	0.00	0.00	1.67	2.34	15.33	22.00	37.00	19.33	1.66	0.67	0.00	0.00	0.00	0.00	56.34	19.34	12.33	12.33
	American Coal #15	1.08	0.00	2.00	15.00	20.00	8.50	11.00	9.50	4.00	10.00	14.00	6.00	0.00	0.00	0.00	0.00	78.40	3.30	16.50	4.40
	American Coal #16	1.17	0.00	0.00	0.67	2.33	5.00	26.34	39.33	9.33	3.00	7.33	5.33	1.34	0.00	0.00	0.00	67.67	12.33	4.00	4.00
	American Coal #17	1.04	5.66	15.33	12.33	1.34	3.34	8.67	17.34	17.00	13.00	2.33	1.00	2.66	0.00	0.00	0.00				
	American Coal #18	1.39	0.00	0.00	0.67	2.00	3.33	5.33	6.33	14.34	13.34	15.00	21.00	16.66	2.00	0.00	0.00	62.67	9.34	6.66	6.66
	American Coal #19		3.00	23.00	42.50	25.50	4.50	0.00	0.50	0.50	0.00	0.00	0.00	0.00	0.00	100.00	0.00				
	American Coal #20	1.19	0.00	0.50	10.50	12.50	6.50	6.00	8.50	6.50	20.50	19.50	8.50	0.50	0.00	0.00	0.00	79.50	3.70	13.60	5.80
	Australian Coal #1	1.42	0.00	0.00	0.00	0.05	0.46	4.29	7.72	12.02	13.78	23.17	26.96	10.61	0.90	0.04	0.00	29.29	0.72	6.92	3.28
	Australian Coal #2	1.11	0.00	0.00	0.41	1.07	7.37	12.11	15.75	19.44	18.81	12.04	6.64	4.04	1.86	14.48	0.19	39.46	4.80	7.64	7.04
	Australian Coal #3	1.12	0.00	0.27	0.90	2.50	7.21	33.60	35.98	12.69	4.51	1.63	0.47	0.19	0.05	0.00	0.00	32.19	5.43	9.84	6.78
	Australian Coal #4	1.05	0.00	1.31	5.77	22.13	21.72	11.20	6.97	16.56	12.17	1.20	0.42	0.45	0.00	0.11	0.00	11.53	1.40	6.27	6.27
	Australian Coal #5	0.98	0.00	0.00	0.00	0.00	0.00	4.36	24.53	38.82	9.98	1.76	0.55	0.00	0.00	0.00	0.00				
	Australian Coal #6	0.75	0.00	0.00	1.80	11.07	8.61	10.81	18.76	9.82	4.73	4.47	4.67	3.20	1.60	20.40	0.06	12.84	1.68	3.94	3.94
	Australian Coal #7	1.06	0.00	0.17	0.17	5.25	23.84	40.67	22.50	6.66	0.67	0.08	0.00	0.00	0.00	0.00	0.00	48.91	9.01	15.60	13.60
	Australian Coal #8	1.44	0.00	0.00	0.00	0.17	0.42	0.34	4.33	11.25	26.54	22.50	18.33	11.09	2.96	1.42	0.67	17.92	3.25	3.17	3.17

Table B.5 Cont'd

Coal Name	Mean Random Vitrinite Reflectance (Ro)	V5 (%)	V6 (%)	V7 (%)	V8 (%)	V9 (%)	V10 (%)	V11 (%)	V12 (%)	V13 (%)	V14 (%)	V15 (%)	V16 (%)	V17 (%)	V18 (%)	V19 (%)	Vitrinite	Liptinite	Inertinite	Semifusinite
Australian Coal #9	0.80	0.83	12.80	44.11	28.13	11.81	2.34	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	34.30	6.00	12.50	5.10
Australian Coal #10	1.40	0.00	0.00	0.50	2.50	8.00	7.00	14.00	7.00	6.00	10.75	11.25	20.50	10.00	2.50	0.00	40.70	0.30	8.55	2.60
Australian Coal #11	1.16	0.00	0.00	0.00	0.00	1.00	16.75	55.50	25.75	0.50	0.50	0.00	0.00	0.00	0.00	0.00	39.80	0.00	9.80	4.00
Australian Coal #12	1.26	0.00	0.00	0.00	0.00	0.00	3.25	17.50	58.00	18.50	1.50	0.75	0.50	0.00	0.00	0.00	35.75	0.35	13.00	6.60
Australian Coal #13	0.78	5.00	13.25	26.25	38.25	1.75	1.00	0.50	2.75	3.75	2.25	0.25	1.00	1.50	1.75	0.75				
Australian Coal #14	1.20	0.00	0.00	0.00	0.00	0.75	16.25	39.75	30.75	9.00	1.75	1.25	0.50	0.00	0.00	0.00	38.35	0.35	10.50	4.70
Australian Coal #15	1.14	0.00	0.00	3.60	6.00	13.20	28.40	16.40	7.60	10.40	9.60	4.40	0.40	0.00	0.00	0.00	59.33	18.33	15.67	15.67
Australian Coal #16	1.50	0.00	0.00	0.40	0.40	2.00	2.80	7.20	6.00	13.60	14.80	16.40	16.00	11.60	6.80	2.00	52.58	20.97	30.65	30.65
Australian Coal #17	0.75	0.67	28.67	49.67	19.00	1.67	0.32	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	58.61	12.69	25.68	14.50
Australian Coal #18	1.08	0.00	0.00	0.00	1.50	22.00	43.00	25.50	3.50	2.00	1.50	0.50	0.50	0.00	0.00	0.00	77.20	0.80	20.60	10.50
Australian Coal #19	0.90	0.00	0.00	8.00	46.00	40.50	0.50	1.50	1.00	2.00	0.50	0.00	0.00	0.00	0.00	0.00				
Australian Coal #20	0.80	0.00	11.50	37.50	39.50	10.50	0.50	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00				
Australian Coal #21	1.06	0.00	0.00	0.00	1.50	21.50	49.00	17.50	9.50	1.00	0.00	0.00	0.00	0.00	0.00	0.00				
Australian Coal #22	1.02	0.00	1.00	13.00	22.50	5.50	12.00	33.50	11.00	0.50	0.50	0.50	0.00	0.00	0.00	0.00				
Canadian Coal #1	0.97	0.00	0.68	3.31	6.48	14.00	27.90	23.27	13.16	5.95	3.38	1.21	0.45	0.21	6.67	0.00	27.55	3.94	5.86	5.11
Canadian Coal #2	1.05	0.00	0.14	0.48	3.01	9.27	12.51	23.14	29.33	13.29	4.42	2.37	1.10	0.62	14.62	0.00	7.86	1.38	2.48	2.48
Canadian Coal #3	0.99	0.10	0.10	1.13	13.30	48.98	24.34	4.20	4.48	2.23	0.58	0.35	0.14	0.07	0.00	0.00	22.80	0.33	5.19	2.03
Canadian Coal #4	1.11	0.00	0.00	0.00	1.75	9.50	41.00	33.25	11.50	1.50	0.50	0.50	0.50	0.00	0.00	0.00	38.45	0.25	11.10	4.90
Canadian Coal #5	1.08	0.00	0.00	0.00	2.50	15.50	41.00	32.50	7.50	1.00	0.00	0.00	0.00	0.00	0.00	0.00				
Canadian Coal #6	1.10	0.00	0.00	0.00	0.00	7.34	49.33	34.00	5.33	2.67	1.33	0.00	0.00	0.00	0.00	0.00				
Canadian Coal #7	1.10	0.00	0.00	0.00	0.00	8.00	48.50	30.50	9.50	2.00	1.00	0.50	0.00	0.00	0.00	0.00				
Russian Coal #1	0.60	1.17	13.17	32.76	29.38	3.17	0.21	0.71	0.71	0.93	1.86	1.14	0.43	0.07	0.00	14.29	11.06	0.27	2.71	1.07
Russian Coal #2	0.81	0.50	1.50	33.00	56.00	7.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	80.10	1.10	17.50	5.40
Colombian Coal #1	1.03	0.67	3.30	17.01	22.77	16.91	7.06	6.54	7.84	4.06	4.10	2.93	2.73	2.03	1.37	0.68				
Colombian Coal #2	0.99	0.33	5.78	18.67	19.44	23.11	10.11	5.45	4.33	3.11	2.11	1.56	1.22	1.55	2.00	0.89	30.54	6.64	12.13	12.13
Colombian Coal #3 Colombian Coal #4	0.45 0.82	7.25 6.81	25.25 13.26	21.50 20.43	17.00 28.68	20.00 26.53	3.50 3.94	1.75 0.35	0.75 0.00	0.75 0.00	0.00	0.25	1.00	0.00	50.00	0.00	37.50	1.90	9.60	2.95

Table B. 6 Coke Quality Characterization

	Coal Name	Stability (%)	Hardness (%)	CRI (%)	CSR (%)	Porosity (%)	Maximum Gas Pressure (kpa)	Maximum Wall Pressure (kpa)	Coke Rate (%) (db)
	American Coal #1	58.71	66.14	29.46	54.63	49.75	4.12	4.87	73.85
	American Coal #2	52.20	62.43	25.30	57.89	49.51	1.28	4.56	72.15
	American Coal #3	64.08	68.18	19.86	68.66	48.72	17.82	7.92	79.67
	American Coal #4	63.85	68.28	21.35	68.31	49.54	23.22	8.37	77.77
	American Coal #5	59.61	65.39	22.61	61.31	48.76	3.16	3.85	72.46
	American Coal #6	53.64	64.98	32.28	47.84	48.85	4.50	4.41	73.66
141	American Coal #7	61.53	66.27	27.54	59.50	49.01	3.03	5.48	79.35
	American Coal #8	60.10	64.60	26.15	59.06	48.96	2.20	3.83	75.71
	American Coal #9	60.80	66.40	16.81	72.31	51.53	12.47	6.16	77.86
	American Coal #10	56.90	62.10	47.41	35.40	48.68	10.88	3.50	78.69
	American Coal #11	56.60	59.80	28.68	47.55	51.37	3.13	3.53	71.99
	American Coal #12	50.60	61.00	23.04	60.67	48.15	0.75	0.58	73.66
	American Coal #13	62.90	65.30	22.27	61.02	48.15	36.66	9.39	77.74
	American Coal #14	55.40	64.10	30.83	49.12	50.00	0.78	4.48	69.90
	American Coal #15	60.90	67.00	25.35	60.46	50.77	12.88	6.48	74.72
	American Coal #16	57.95	65.95	46.79	24.46	50.00	5.76	3.13	73.58
	American Coal #17	55.50	64.90	29.62	53.73	51.55	9.98	4.41	74.66
	American Coal #18	58.95	66.90	40.38	45.27	49.22	32.67	12.86	75.88
	American Coal #19	46.60	59.10	26.31	53.42	51.74	1.27	3.11	74.60

Table B.6 Cont'd

	Coal Name	Stability (%)	Hardness (%)	CRI (%)	CSR (%)	Porosity (%)	Maximum Gas Pressure (kpa)	Maximum Wall Pressure (kpa)	Coke Rate (%) (db)
	American Coal #20	53.80	60.80	32.64	44.27	48.15	2.29	2.71	79.47
	Australian Coal #1	61.37	65.33	22.52	66.99	45.36	48.31	19.73	80.96
	Australian Coal #2	63.01	67.03	19.29	70.51	49.56	7.52	4.63	80.39
	Australian Coal #3	60.98	65.27	26.36	63.02	50.25	1.87	3.45	77.01
	Australian Coal #4	56.00	64.08	26.11	59.09	48.17	0.56	4.68	72.50
_	Australian Coal #5	60.82	65.46	24.75	65.58	48.84	1.32	4.82	78.69
42	Australian Coal #6	61.98	66.04	22.44	66.51	49.07	1.66	3.12	77.14
	Australian Coal #7	59.94	64.25	23.55	63.30	49.21	1.38	4.29	75.43
	Australian Coal #8	62.05	65.75	18.01	71.10	49.64	10.45	3.41	81.24
	Australian Coal #9	55.70	66.60	23.88	57.40	46.60	2.04	6.16	67.07
	Australian Coal #10	64.10	68.45	20.42	71.65	48.52	11.02	4.50	81.70
	Australian Coal #11	60.70	64.85	33.11	57.61	24.28	2.17	3.72	75.73
	Australian Coal #12	53.95	59.05	38.34	49.28	50.00	0.26	4.55	76.35
	Australian Coal #13	25.70	49.40	48.40	18.12	49.07	0.32	3.05	68.82
	Australian Coal #14	58.70	62.25	22.86	65.39	49.34	2.98	2.65	78.03
	Australian Coal #15	61.30	67.00	25.48	67.71	50.75	2.42	3.46	75.12
	Australian Coal #16	58.20	63.80	39.56	52.61	50.26	1.59	3.95	75.61
	Australian Coal #17	58.20	65.70	26.27	50.54	51.02	0.69	4.34	76.78

Table B.6 Cont'd

	Coal Name	Stability (%)	Hardness (%)	CRI (%)	CSR (%)	Porosity (%)	Maximum Gas Pressure (kpa)	Maximum Wall Pressure (kpa)	Coke Rate (%) (db)
	Australian Coal #18	58.80	62.50	26.38	61.58	50.00	0.55	4.62	78.83
	Australian Coal #19	49.70	55.50	47.60	33.23	48.69	0.35	5.11	76.29
	Australian Coal #20	48.30	65.20	34.27	49.58	46.20	2.37	3.37	74.76
	Australian Coal #21	53.80	60.00	41.50	43.41	46.99	1.51	0.55	74.55
	Australian Coal #22	61.10	65.60	24.83	64.80	49.48	1.58	5.17	74.25
_	Canadian Coal #1	61.23	67.33	21.79	68.42	45.06	1.55	3.95	77.04
143	Canadian Coal #2	61.66	67.37	22.32	68.97	48.09	1.11	3.45	79.22
	Canadian Coal #3	56.81	62.16	20.55	63.26	41.26	1.80	3.34	77.73
	Canadian Coal #4	57.90	64.45	24.78	66.19	48.29	0.96	3.66	77.81
	Canadian Coal #5	58.00	63.80	20.36	66.06	48.19	2.92	4.46	76.75
	Canadian Coal #6	61.50	67.40	19.80	71.59	48.40	2.08	1.03	76.53
	Canadian Coal #7	56.80	63.20	28.35	59.12	47.06	3.66	0.35	79.41

APPENNDIX C

C. PARAMETERS USED IN REGRESSION ANALYSIS

Table C.1 Parameters used in Regression Analysis

#	Parameter Name	#	Parameter Name
1	Moisture (%)	33	-6,30 +3,15mm (%)
2	Volatile Matter (%) (db)	34	-3,15 +0,425mm (%)
3	Ash (%) (db)	35	-0,425mm (%)
4	Sulphur (%) (db) (coal)	36	Maximum Fluidity (ddpm)
5	Fixed Carbon (%) (db)	37	Softening Temperature (ºC)
6	Phosphor (%) (db)	38	Maximum Fluidity Temperature (ºC)
7	FSI	39	Solidification Temperature (°C)
8	HGI	40	Fluid Range (ºC)
9	Calorific Value (db) (kcal/kg)	41	LGF (Logarithmic Fluidity)
10	Calorific Value (kcal/kg)	42	Maximum Dilatation (%)
11	Reflectance of Light (%) (T17)	43	Maximum Contraction (%)
12	Bulk Density (gr/cm3)	44	Softening Temperature (°C)
13	Total Alkalis in ash (%)	45	Dilatation Starting Temperature (°C)
14	Al2O3 (%)	46	Dilatation Finishing Temperature (°C)
15	CaO (%)	47	Volatile Matter (%) (db)
16	Cr2O3 (%)	48	Ash (%) (db)
17	Fe2O3 (%)	49	Sulphur (%) (db)
18	K2O (%)	50	CRI (%)
19	MgO (%)	51	CSR (%)
20	MnO (%)	52	Stability (%)
21	Na2O (%)	53	Hardness (%)
22	P2O5 (%)	54	Porosity (%)
23	SiO2 (%)	55	Charged Coal Moisture (%)
24	TiO2 (%)	56	Charging Coal Weight (kg) (db)
25	P (%)	57	Bulk Density (kg/m3) (db) (coke)
26	S (%)	58	Soak Time (hr)
27	Ni (%)	59	Maximum Gas Pressure (kpa)
28	ZnO (%)	60	Maximum Wall Pressure (kpa)
29	+50,0mm (%)	61	Coke Rate (%) (db)
30	-50,0 +25,0mm (%)	62	Mean Random Vitrinite Reflectance (Ro)
31	-25,0 +12,5mm (%)	63	V5 (%)
32	-12,5 +6,30mm (%)	64	V6 (%)

Table C.1 Cont'd

#	Parameter Name	#	Parameter Name
65	V7 (%)	85	Sclerotinite (%)
66	V8 (%)	86	Inertodetrinite (%)
67	V9 (%)	87	Micrinite (%)
68	V10 (%)	88	Macrinite (%)
69	V11 (%)	89	inertinite (%)
70	V12 (%)	90	Mineral Matter (%)
71	V13 (%)	91	+3,35mm (%)
72	V14 (%)	92	-3,35 +1,70mm (%)
73	V15 (%)	93	-1,70 +0,50mm (%)
74	V16 (%)	94	-0,50 +0,25mm (%)
75	V17 (%)	95	-0,25 +0,125mm (%)
76	V18 (%)	96	-0,125mm (%)
77	V19 (%)	97	+75,00mm (%)
78	Vitrinite (%)	98	-75,00 +62,50mm (%)
79	Sporinite (%)	99	-62,50 +50,00mm (%)
80	Cutinite (%)	100	-50,00 +37,50mm (%)
81	Resinite (%)	101	-37,50 +25,00mm (%)
82	Liptinite (%)	102	-25,00 +6,30mm (%)
83	Fusinite (%)	103	-6,30mm (%)
84	Semifusinite (%)		

APPENDIX D

D. CORRELATION ANALYSIS FOR ORIGIN BASE COALS

Table D. 1 Elimination of Correlated Parameters FOR Australian Coals ($r > \pm 0.8$)

Factor 1	Factor 2	Correlation Coefficient	Elimination Decision
V15 - V18 (%)	V16 (%)	0.92	V16 (%)
Cutinite	Maximum Fluidity (ddpm)	0.99	Cutinite
Liptinite	Resinite	0.94	Resinite
Semifusinite	Liptinite	0.86	Liptinite
Inertodetrinite	Sulphur (%) (db)	0.80	Inertodetrinite
Micrinite	Maximum Fluidity (ddpm)	0.98	Micrinite
Macrinite	Fusinite	0.93	Macrinite
İnertinite	Resinite	0.87	İnertinite
Mineral Matter	Sulphur (%) (db) (coal)	0.82	Mineral Matter
+3,35mm (%)	Vitrinite	0.81	+3,35mm (%)
-3,35 +1,70mm (%)	Vitrinite	0.86	-3,35 +1,70mm (%)
-1,70 +0,50mm (%)	Vitrinite	0.82	-1,70 +0,50mm (%)
-0,50 +0,25mm (%)	Vitrinite	0.86	-0,50 +0,25mm (%)
-0,25 +0,125mm (%)	Vitrinite	0.83	-0,25 +0,125mm (%)
-0,125mm (%)	Vitrinite	0.82	-0,125mm (%)
-62,50 +50,00mm (%)	Vitrinite	0.83	-62,50 +50,00mm (%)
-50,00 +37,50mm (%)	Vitrinite	0.80	-50,00 +37,50mm (%)
-25,00 +6,30mm (%)	-37,50 +25,00mm (%)	0.97	-25,00 +6,30mm (%)
-6,30mm (%)	-50,0 +25,0mm (%)	-0.84	-6,30mm (%)

Table D.1 Cont'd

Factor 1	Factor 2	Correlation Coefficient	Elimination Decision
Fixed Carbon (%) (db)	Volatile Matter (%) (db)	-0.98	Fixed Carbon (%) (db)
HGI	Volatile Matter (%) (db)	-0.92	HGI
K2O (%)	Total Alkalis in ash (%)	0.88	K2O (%)
P2O5 (%)	Phosphor (%) (db)	0.98	P2O5 (%)
P (%)	Phosphor (%) (db)	0.98	P (%)
Basicity Index (BI)	CaO (%)	0.87	CaO (%)
Basicity Index (BI)	Fe2O3 (%)	0.93	Fe2O3 (%)
Basicity Index (BI)	Basic to Acid Ratio (BAR)	1.00	Basic to Acid Ratio (BAR)
Basicity Index (BI)	Material Balance Index (MBI)	0.95	Material Balance Index (MBI)
ZnO (%)	-50,0 +25,0mm (%)	0.82	-50,0 +25,0mm (%)
Volatile Matter (%) (db)	-3,15 +0,425mm (%)	-0.84	-3,15 +0,425mm (%)
-0,425mm (%)	-25,0 +12,5mm (%)	-0.86	-25,0 +12,5mm (%)

Table D.1 Cont'd

	Factor 1	Factor 2	Correlation Coefficient	Elimination Decision
	Maximum Fluidity Temperature (°C)	Softening Temperature (°C)	0.99	Softening Temperature (°C)
	Maximum Fluidity Temperature (°C)	Solidification Temperature (°C)	0.99	Solidification Temperature (°C)
	LGF (Logarithmic Fluidity)	Fluid Range (°C)	0.91	Fluid Range (°C)
	Maximum Dilatation (%)	LGF (Logarithmic Fluidity)	0.87	LGF (Logarithmic Fluidity)
	Ash (%) (db) (coal)	Ash (%) (db)(coke)	0.86	Ash (%) (db)(coke)
	Sulphur (%) (db) (coal)	Sulphur (%) (db) (coke)	0.99	Sulphur (%) (db) (coke)
	CRI (%)	FSI	-0.83	FSI
,	CRI (%)	Hardness (%)	-0.83	Hardness (%)
148	Porosity (%)	ZnO (%)	-0.98	ZnO (%)
	Maximum Gas Pressure (kpa)	Maximum Wall Pressure (kpa)	0.91	Maximum Wall Pressure (kpa)
	Coke Rate (%) (db)	Volatile Matter (%) (db)	-0.80	Coke Rate (%) (db)
	V7 (%)	Volatile Matter (%) (db)	0.81	V7 (%)
	V7 and less	V6 (%)	0.99	V6 (%)
	V8 (%)	Volatile Matter (%) (db)	0.83	V8 (%)
	V9 - V11 (%)	V10 (%)	0.92	V10 (%)
	V12 - V14 (%)	V13 (%)	0.89	V13 (%)
	V15 (%)	Maximum Gas Pressure (kpa)	0.81	V15 (%)
	V17 (%)	V16 (%)	0.90	V17 (%)
	V15 - V18 (%)	V14 (%)	0.84	V14 (%)

Table D. 2 Elimination of Correlated Parameters for Australian Coals (r $> \pm 0.6$)

Factor 1	Factor 2	Correlation Coefficient	p-value	Elimination Decision
Al2O3 (%)	<i>Ash</i> (%) (<i>db</i>)	-0.64	0.011	Ash (%) (db)
MgO (%)	Sulphur (%) (db)	-0.68	0.001	Sulphur (%) (db)
MnO (%)	Moisture (%)	0.64	0.042	Moisture (%)
SiO2 (%)	Al2O3 (%)	-0.77	0.000	Al2O3 (%)
SiO2 (%)	MgO (%)	-0.61	0.002	MgO (%)
Basicity Index (BI)	SiO2 (%)	-0.75	0.001	SiO2 (%)
Basicity Index (BI)	S (%)	0.77	0.001	S (%)
-12,5 +6,30mm (%)	Volatile Matter (%) (db)	0.72	0.026	Volatile Matter (%) (db)
-6,30 +3,15mm (%)	Cr2O3 (%)	-0.66	0.000	Cr2O3 (%)
-0,425mm (%)	-12,5 +6,30mm (%)	-0.74	0.008	-12,5 +6,30mm (%)
Maximum Dilatation (%)	Ni (%)	0.63	0.023	Ni (%)
Dilatation Starting Temperature (°C)	Maximum Dilatation (%)	-0.72	0.000	Maximum Dilatation (%)
Volatile Matter (%) (db) (coke)	Phosphor (%) (db)	0.67	0.006	Phosphor (%) (db)

Table D.2 Cont'd

-	Factor 1	Factor 2	Correlation Coefficient	p-value	Elimination Decision
•	CRI (%)	+50,0mm (%)	0.62	0.299	+50,0mm (%)
	Stability (%)	-0,425mm (%)	0.78	0.016	-0,425mm (%)
	Stability (%)	Maximum Fluidity Temperature (°C)	0.64	0.323	Maximum Fluidity Temperature (°C)
	Porosity (%)	-6,30 +3,15mm (%)	0.62	0.002	-6,30 +3,15mm (%)
	Mean Rand. Vit. Ref. (Ro)	Dilatation Starting Temperature (°C)	0.66	0.001	Dilatation Starting Temperature (°C)
	V5 (%)	Calorific Value (db) (kcal/kg)	-0.72	0.001	Calorific Value (db) (kcal/kg)
	V7 and less	Mean Rand. Vit. Ref. (Ro)	-0.66	0.011	Mean Rand. Vit. Ref. (Ro)
1.	V9 - V11 (%)	V11 (%)	0.69	0.001	V11 (%)
150	V12 - V14 (%)	V12 (%)	0.79	0.000	V12 (%)
	Semifusinite	V19 (%)	0.71	0.001	V19 (%)
	+75,00mm (%)	Na2O (%)	0.70	0.016	Na2O (%)
	V9 (%)	V9 - V11 (%)	0.48	0.016	V9 (%)
_	V18 (%)	V15 - V18 (%)	0.52	0.043	V18 (%)

Table D.3 Best Subset Analysis of Australian Coals

Vars	R-Sq		R-Sq (pred)	Mallows Cp	S	Volatile Matter (%) (db)	Ash (%) (db) (coal)	Total Alkalis in ash (%)	Na2O (%) (in ash)	+50,0 mm (%)	Max Fluidity (ddpm)	Max Fluidity Temp (°C)	Max Dilatation (%)	Dilatation Finishing Temp (°C)	<i>CRI</i> (%)	Stability (%)	Porosity (%)	Max Gas Pressure (kpa)	Mean Random Vitrinite Reflectan ce (Ro)
1	82.8	82.5	81.6	343.3	2.43										Х				
1	64.9	64.2	61.9	753.9	3.48											Х			
2	93.7	93.5	92.6	95.4	1.48										х	х			
2	91.4	91.1	90.0	147.9	1.73	х									Х				
3	95.8	95.6	94.9	49.3	1.22						Х				Х	x			
3	95.8	95.6	94.9	49.5	1.22								X		Х	Х			
4	96.7	96.4	95.8	31.5	1.098						Х		Х		Х	x			
4	96.6	96.3	95.8	33.5	1.113				Х				X		Х	Х			
5	97.2	96.9	96.4	21.5	1.017				Х		Х		X		Х	Х			
1 5	97.1	96.8	96.2	24.8	1.043					x	Х		Х		Х	х			
- 6		97.1	96.6	18.6	0.987				Х		Х		X		Х	Х			X
6		97.1	96.6	19.1	0.992				Х		Х	Х	Х		Х	х			
7	97.8	97.4	96.8	13.3	0.934				Х	x	Х	Х	Х		Х	х			
7	97.7	97.4	96.9	13.5	0.936				Х	х	Х		X		Х	Х			x
8	97.9	97.5	97.0	11.7	0.910				Х	х	Х	Х	X		Х	Х	Х		
8		97.5	95.9	12.4	0.917				х	x	Х	Х	X	Х	х	Х			
9	98.1	97.7	96.5	9.1	0.875				х	x	Х	Х	X	X	х	Х	Х		
9		97.7	96.2	9.3	0.877			X		X	Х	X	X	X	х	Х	Х		
10	98.3	97.9	97.2	7.4	0.847		x		Х	X	Х		X		х	Х	Х	Х	Х
10	98.2	97.8	97.1	8.4	0.857		х		Х	Х	Х	Х	X		х	х	х	х	

Table D.4 Elimination of Correlated Parameters FOR American Coals (r $> \pm 0.8$)

Factor 1	Factor 2	Correlation	Eliminated Parameter Selection
Fixed Carbon (%) (db)	Volatile Matter (%) (db)	-0.97	Fixed Carbon (%) (db)
HGI	Volatile Matter (%) (db)	-0.87	HGI
Fe2O3 (%)	Al2O3 (%)	-0.93	Fe2O3 (%)
K2O (%)	Total Alkalis in ash (%)	0.82	K2O (%)
MgO (%)	CaO (%)	0.94	MgO (%)
MnO (%)	Al2O3 (%)	-0.80	MnO (%)
P2O5 (%)	Phosphor (%) (db)	0.98	P2O5 (%)
SiO2 (%)	CaO (%)	-0.94	SiO2 (%)
TiO2 (%)	Al2O3 (%)	0.87	Al2O3 (%)
TiO2 (%)	Na2O (%)	-0.81	Na2O (%)
P (%)	Phosphor (%) (db)	0.98	P (%)
S (%)	CaO (%)	0.97	S (%)
Basicity Index (BI)	CaO (%)	0.93	CaO (%)
Basicity Index (BI)	TiO2 (%)	-0.80	TiO2 (%)
Basic to Acid Ratio (BAR)	Al2O3 (%)	-0.87	Basic to Acid Ratio (BAR)
Material Balance Index (MBI)	Al2O3 (%)	-0.86	Material Balance Index (MBI)
-12,5 +6,30mm (%)	-25,0 +12,5mm (%)	0.90	-25,0 +12,5mm (%)
-6,30 +3,15mm (%)	-50,0 +25,0mm (%)	-0.87	-50,0 +25,0mm (%)
-6,30 +3,15mm (%)	-12,5 +6,30mm (%)	0.86	-12,5 +6,30mm (%)

Table D.4 Cont'd

Factor 1	Factor 2	Correlation	Eliminated Parameter Selection
-0,425mm (%)	Bulk Density (gr/cm3)	-0.82	-0,425mm (%)
Maximum Fluidity Temperature (°C)	Softening Temperature (°C)	0.97	Softening Temperature (°C)
Solidification Temperature (°C)	Maximum Fluidity Temperature (°C)	0.98	Solidification Temperature (°C)
LGF (Logarithmic Fluidity)	Volatile Matter (%) (db)	0.80	LGF (Logarithmic Fluidity)
Dilatation Starting Temperature (°C)	Volatile Matter (%) (db)	-0.92	Dilatation Starting Temperature (°C)
Ash (%) (db) (coal)	Ash (%) (db)(coke)	0.85	Ash (%) (db)(coke)
Sulphur (%) (db) (coal)	Sulphur (%) (db) (coke)	0.88	Sulphur (%) (db) (coke)
Hardness (%)	Stability (%)	0.91	Hardness (%)
Maximum Wall Pressure (kpa)	Maximum Gas Pressure (kpa)	0.93	Maximum Wall Pressure (kpa)
V6 (%)	V5 (%)	0.84	V5 (%)
V7 (%)	Cr2O3 (%)	-0.84	Cr2O3 (%)
V7 and less	V6 (%)	0.87	V6 (%)
V7 and less	V7 (%)	0.98	V7 (%)
V8 (%)	V7 and less	0.97	V8 (%)
V9 (%)	Maximum Fluidity (ddpm)	0.86	V9 (%)
V9 - V11 (%)	V10 (%)	0.97	V10 (%)
V12 - V14 (%)	V13 (%)	0.90	V13 (%)
V15 (%)	Volatile Matter (%) (db)	-0.79	V15 (%)
V16 (%)	Fixed Carbon (%) (db)	0.81	V16 (%)

Table D.4 Cont'd

Factor 1	Factor 2	Correlation	Eliminated Parameter Selection
V18 (%)	Softening Temperature (°C)	-0.82	V18 (%)
V15 - V18 (%)	Softening Temperature (°C)	0.82	V15 - V18 (%)
V19 (%)	Softening Temperature (°C)	-0.83	V19 (%)
Liptinite	Resinite	0.83	Resinite
Fusinite	Ni (%)	-0.82	Ni (%)
Inertodetrinite	Fusinite	0.81	Inertodetrinite
Macrinite	Fusinite	0.86	Macrinite
Mineral Matter	Fusinite	-0.87	Mineral Matter
+3,35mm (%)	Ni (%)	0.92	+3,35mm (%)
-3,35 +1,70mm (%)	Ni (%)	0.90	-3,35 +1,70mm (%)
-1,70 +0,50mm (%)	Ni (%)	0.94	-1,70 +0,50mm (%)
-0,50 +0,25mm (%)	Ni (%)	0.94	-0,50 +0,25mm (%)
-0,25 +0,125mm (%)	Ni (%)	0.93	-0,25 +0,125mm (%)
-0,125mm (%)	Ni (%)	0.91	-0,125mm (%)
-75,00 +62,50mm (%)	Ni (%)	0.90	-75,00 +62,50mm (%)
-62,50 +50,00mm (%)	Ni (%)	0.92	-62,50 +50,00mm (%)
-50,00 +37,50mm (%)	Ni (%)	0.91	-50,00 +37,50mm (%)
-25,00 +6,30mm (%)	Phosphor (%) (db)	-0.79	-25,00 +6,30mm (%)

7.7

Table D.5 Elimination of Correlated Parameters for American Coals (r $> \pm 0.6$)

Factor 1	Factor 2	Correlation	p-value	Eliminated Parameter Selection
Calorific Value (db) (kcal/kg)	Ash (%) (db)	-0.78	0.001	Calorific Value (db) (kcal/kg)
Reflectance of Light (%) (T17)	FSI	0.60	0.030	FSI
Total Alkalis in ash (%)	Sulphur (%) (db)	0.71	0.006	Total Alkalis in ash (%)
+50,0mm (%)	Ash (%) (db)	0.66	0.015	+50,0mm (%)
-3,15 +0,425mm (%)	Volatile Matter (%) (db)	-0.62	0.022	-3,15 +0,425mm (%)
Maximum Fluidity (ddpm)	Volatile Matter (%) (db)	0.63	0.021	no elimination
Dilatation Finishing Temp (°C)	Volatile Matter (%) (db)	-0.70	0.008	Dilatation Finishing Temp (°C)
Stability (%)	Bulk Density (gr/cm3)	-0.63	0.021	Bulk Density (gr/cm3)
Maximum Gas Pressure (kpa)	Volatile Matter (%) (db)	-0.78	0.002	Maximum Gas Pressure (kpa)
Coke Rate (%) (db)	Volatile Matter (%) (db)	-0.75	0.003	Coke Rate (%) (db)
Mean Ran. Vit. Reflectance (Ro)	Maximum Fluidity (ddpm)	-0.73	0.004	Mean Ran. Vit. Reflectance (Ro)
V11 (%)	Porosity (%)	0.64	0.019	V11 (%)
V14 (%)	Maximum Dilatation (%)	-0.68	0.010	V14 (%)
V12 - V14 (%)	Maximum Fluidity (ddpm)	-0.71	0.007	V12 - V14 (%)
V15 - V18 (%)	Fluid Range (°C)	-0.76	0.003	V15 - V18 (%)
Fusinite	Vitrinite	0.65	0.016	Fusinite
Semifusinite	Reflectance of Light (%) (T17)	-0.68	0.011	Reflectance of Light (%) (T17)
İnertinite	Phosphor (%) (db)	-0.70	0.007	Phosphor (%) (db)
-37,50 +25,00mm (%)	Ash (%) (db)	-0.64	0.018	-37,50 +25,00mm (%)
-6,30mm (%)	V11 (%)	0.66	0.014	-6,30mm (%)

Table D. 6 Elimination of Correlated Parameters for Canadian Coals (r \geq ± 0.8)

Factor 1	Factor 2	Correlation	Eliminated Parameter Selection
Sulphur (%) (db)	Volatile Matter (%) (db)	0.97	Sulphur (%) (db)
Fixed Carbon (%) (db)	Volatile Matter (%) (db)	-0.97	Fixed Carbon (%) (db)
Phosphor (%) (db)	Volatile Matter (%) (db)	0.80	Phosphor (%) (db)
FSI	Ash (%) (db)	-0.87	FSI
Total Alkalis in ash (%)	Volatile Matter (%) (db)	0.98	Total Alkalis in ash (%)
Fe2O3 (%)	CaO (%)	-0.85	CaO (%)
K2O (%)	Volatile Matter (%) (db)	0.96	K2O (%)
MgO (%)	Ash (%) (db)	0.97	MgO (%)
P2O5 (%)	Ash (%) (db)	-0.84	P2O5 (%)
5 P(%)	Ash (%) (db)	-0.84	P (%)
S (%)	Ash (%) (db)	0.86	S (%)
ZnO (%)	Ash (%) (db)	-0.90	ZnO (%)
Ni (%)	Fe2O3 (%)	0.82	Ni (%)
Basicity Index (BI)	SiO2 (%)	-0.93	SiO2 (%)
Basicity Index (BI)	Modified Basicity Index (MBI)	0.81	Modified Basicity Index (MBI)
Basicity Index (BI)	Basic to Acid Ratio (BAR)	1.00	Basic to Acid Ratio (BAR)
-12,5 +6,30mm (%)	-25,0 +12,5mm (%)	0.98	-25,0 +12,5mm (%)
-6,30 +3,15mm (%)	-12,5 +6,30mm (%)	0.94	-6,30 +3,15mm (%)
-3,15 +0,425mm (%)	Calorific Value (db) (kcal/kg)	-0.80	-3,15 +0,425mm (%)
-12,5 +6,30mm (%)	-0,425mm (%)	-0.95	-0,425mm (%)
Volatile Matter (%) (db)	Maximum Fluidity (ddpm)	0.93	Maximum Fluidity (ddpm)
Softening Temperature (°C)	-50,0 +25,0mm (%)	-0.87	-50,0 +25,0mm (%)

Table D.6 Cont'd

Factor 1	Factor 2	Correlation	Eliminated Parameter Selection
Maximum Fluidity Temperature (°C)	Softening Temperature (°C)	0.99	Softening Temperature (°C)
Maximum Fluidity Temperature (°C)	Solidification Temperature (°C)	1.00	Solidification Temperature (°C)
Maximum Fluidity Temperature (°C)	Fluid Range (°C)	0.87	Fluid Range (°C)
LGF (Logarithmic Fluidity)	Volatile Matter (%) (db)	0.91	LGF (Logarithmic Fluidity)
Maximum Dilatation (%)	Volatile Matter (%) (db)	0.91	Maximum Dilatation (%)
Maximum Fluidity Temperature (°C)	Maximum Contraction (%)	-0.89	Maximum Contraction (%)
Softening Temperature (°C)	Volatile Matter (%) (db)	-0.93	Softening Temperature (°C)
Dilatation Starting Temperature (°C)	Volatile Matter (%) (db)	-0.97	Dilatation Starting Temperature (°C)
Ash (%) (db) (coke)	Ash (%) (db) (coal)	0.91	Ash (%) (db) (coke)
Sulphur (%) (db) (coke)	Volatile Matter (%) (db)	0.93	Sulphur (%) (db) (coke)
Hardness (%)	Stability (%)	0.98	Hardness (%)
-12,5 +6,30mm (%)	Porosity (%)	0.89	-12,5 +6,30mm (%)
+50,0mm (%)	Charged Coal Moisture (%)	-0.90	+50,0mm (%)
Bulk Density (kg/m3) (db)	Porosity (%)	0.89	Porosity (%)
Maximum Gas Pressure (kpa)	Volatile Matter (%) (db) (coke)	0.86	Volatile Matter (%) (db) (coke)
Bulk Density (kg/m3) (db)	V5 (%)	-0.98	V5 (%)
Mean Rand Vit Reflectance (Ro)	V6 (%)	-0.80	V6 (%)
Mean Rand Vit Reflectance (Ro)	V7 (%)	-0.89	V7 (%)
Mean Rand Vit Reflectance (Ro)	V7 and less	-0.89	V7 and less
Mean Rand Vit Reflectance (Ro)	V8 (%)	-0.84	V8 (%)
Bulk Density (kg/m3) (db)	V9 (%)	-0.98	V9 (%)