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Study of methane gas migration in coal sorption tests

Boni B.S.N. Siahaan

University of Wollongong.
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STUDY OF METHANE GAS MIGRATION IN COAL BY SORPTION TESTS

A thesis submitted in fulfilment of the requirements
for the award of the degree of
Doctor of Philosophy

from
THE UNIVERSITY OF WOLLONGONG
Wollongong, New South Wales, Australia

by

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DEPARTMENT OF CIVIL AND MINING ENGINEERING
1990
They that wait upon the Lord shall renew their strength; they shall mount up with wings as eagles; they shall run, and not be weary; and they shall walk, and not faint.

Isaiah 40:31 (KJV)
DECLARATION

I declare that this work has not been submitted for a degree to any University or similar Institution except where specifically indicated.

BONI B.S.N. SIAHAAN

July, 1990
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ABSTRACT

The research reported in this thesis is concerned with a study of the mechanism of methane gas flow in coal. An indirect method of adsorption-desorption tests was conducted on cylindrical coal samples to simulate coal seam gas migration. The gas content of the cores was determined and physical and parametric characteristics of isotherms were investigated using the Langmuir equation as the representation of an ideal single molecular layer system. An attempt to investigate a potential outburst condition was carried out by pressurising a coal cylinder trepanned normal to the bedding plane provided with a central hole which was filled with coal fines.

The innovative computer-based method developed for direct data collection of gas desorption employs gravimetric methods with progressive desorbed gas escape (in contrast to the method of collecting desorbed gas for progressive volume measurement).

Nguyen's theoretical treatment of the problem using both diffusive and laminar flow and interchange between adsorbed and free gas phases is explained and demonstrated in some detail. This unified theory is most appropriate for solution using the numerical model involving flow only for gas and moisture and couple codes for gas and stress-deformation problem.

Finally, detailed recommendations are proposed to the existing adsorption-desorption tests for any follow-up work.
Keywords

Adsorption, carbon dioxide, coal rank, Darcy's law, depth of cover, desorption, diffusion, Fick's law, Freundlich's equation, gas pressure, isotherms, laminar flow, Langmuir's equation, methane, mixed gas, moisture content, permeability, porosity, seam gas, sorption, stress, temperature, unified model, volatile matter.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Chapters</th>
<th>Pages</th>
</tr>
</thead>
<tbody>
<tr>
<td>TITLE PAGE</td>
<td>i</td>
</tr>
<tr>
<td>DECLARATION</td>
<td>iii</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>iv</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>v</td>
</tr>
<tr>
<td>KEYWORDS</td>
<td>vi</td>
</tr>
<tr>
<td>TABLE OF CONTENTS</td>
<td>vii</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td></td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td></td>
</tr>
<tr>
<td>NOTATION</td>
<td></td>
</tr>
</tbody>
</table>

## CHAPTER I INTRODUCTION

1.1 General ......................................................... 1 - 1
1.2 The source of seam gas ........................................ 1 - 2
1.3 Gassiness of coal seams ...................................... 1 - 3
1.4 Emission of gas into mine workings ....................... 1 - 5
1.5 Dilution and gas drainage .................................... 1 - 5
1.6 Purpose and scope ............................................ 1 - 6

## CHAPTER II LITERATURE REVIEW OF METHANE GAS FLOW IN COAL

2.1 Physical properties of methane in coal .................. 2 - 1
2.1.1 General .................................................. 2 - 1
2.1.2 Determination of porosity ................................ 2 - 4
2.1.3 Permeability ............................................. 2 - 7
CHAPTER III PREDICTION OF METHANE EMISSION INTO MINE WORKINGS

3.1 Introduction ................................................. 3 - 1
3.2 Methane emission as a limit to production ................. 3 - 2
3.3 Methane emission into mine working ...................... 3 - 3
3.4 Factors affecting gas emission into mine workings ...... 3 - 7
    3.4.1 Depth of coal seam ................................. 3 - 7
    3.4.2 Rank of coal ...................................... 3 - 8
    3.4.3 Thickness of coal seam ......................... 3 - 8
    3.4.4 Structural characteristics of coal and strata .... 3 - 8
    3.4.5 Nature of roof and floor ......................... 3 - 9
    3.4.6 Geological features .............................. 3 - 10
    3.4.7 Mining method .................................. 3 - 10
        (i) General ........................................... 3 - 10
        (ii) Development ................................... 3 - 11
        (iii) Advancing longwall ......................... 3 - 11
        (iv) Retreating longwall and pillar extraction ... 3 - 12
        (v) Abutment area ................................... 3 - 12
        (vi) Supporting openings ........................... 3 - 13
        (vii) Adjacent workings ............................. 3 - 13
        (viii) Mine ventilation .............................. 3 - 13
        (ix) Period of activity .............................. 3 - 14
3.5 Methane prediction methods .............................. 3 - 14
3.5.1 France ........................................ 3 - 18
3.5.2 Belgium ....................................... 3 - 19
3.5.3 West Germany ................................. 3 - 23
3.5.4 Poland ......................................... 3 - 31
3.5.5 U.S.S.R ......................................... 3 - 39
3.5.6 The United Kingdom ........................... 3 - 42
3.5.7 The United States of America .................. 3 - 52
3.5.8 Australia ....................................... 3 - 55

3.6 A comparison and summary of emission prediction methods ........................................ 3 - 58

CHAPTER IV  INFLUENCE OF DESORPTION PROCESS ON GAS FLOW

4.1 Introduction ..................................... 4 - 1

4.2 Adsorption-desorption test ....................... 4 - 2

4.3 Coal seam gas content determination ............ 4 - 4

4.3.1 Direct methods ................................ 4 - 4

4.3.2 Indirect methods ............................. 4 - 7

4.3.3 Gravimetric method .......................... 4 - 11

(i) Determination of bomb volume ............... 4 - 12

(ii) Pressurizing the coal sample and adsorption 4 - 12

(iii) Desorption tests ............................. 4 - 13

4.4 Data acquisition and processing for gas desorption 4 - 18

4.4.1 General ...................................... 4 - 18

4.4.2 High pressure gas sorption apparatus (and also for subsequent desorption testing) 4 - 19

4.4.3 Electronics and hardware ..................... 4 - 23
4.5 Experimental studies on adsorption and desorption of gases on coal

4.5.1 Adsorption tests

4.5.2 Adsorption of CH₄

4.5.3 Adsorption of CO₂

4.5.4 Adsorption of mixed gas

4.6 Physical and parametric characteristic of isotherms

4.6.1 Langmuir's and Freundlich's models

(i) Effect of the nature of gas

(ii) Effect of the temperature

(iii) Effect of the moisture content

(iv) Influence of rank

(v) Effect of the ash content

4.7 Desorption of gas from coal

4.7.1 Desorption of CH₄ gas from coal samples

4.7.2 Desorption of CO₂ gas from coal samples

4.7.3 Desorption of mixed gas from coal samples

4.7.4 Discussion

CHAPTER V SUMMARY OF THE UNIFIED THEORY OF METHANE GAS MIGRATION IN COAL

5.1 Introduction

5.2 The unified theory

5.3 Basic flow equation

5.3.1 Darcy's flow in a compressible system
5.3.2 Diffusive flow in the adsorbed phase

5.3.3 Stress deformation equation

5.4 Gas flow rate

5.4.1 Small equivalent permeability

5.4.2 Variation of gas flow rate with time

5.5 Computer application

5.5.1 The flow equation

5.5.2 The method of dipole reflection

5.6 Program desorb

5.6.1 Description of the program

5.6.2 Illustrative example

CHAPTER VI CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER WORK

6.1 Conclusions

6.2 Recommendations

REFERENCES

APPENDIX 1

APPENDIX 2

APPENDIX 3

APPENDIX 4
LIST OF TABLES

Table Description pages

Chapter 3
3 - 1  The Classification of coal Seam Used in Poland
(developed from Curl, 1978) ........................................ 3 - 34
3 - 2  Factor taken into consideration by various national
prediction methods .................................................... 3 - 60

Chapter 4
4 - 1  Investigation of seam gas pressure and temperature
gradient (developed from Hargraves, 1963) ...................... 4 - 10
4 - 2  Desorption of CO2 from coal sample Bomb B2, type 2,
Sept. 1989 ................................................................. 4 - 26
4 - 3  Desorption of CO2 from coal sample Bomb B2, type 2,
Sept. 1989 ................................................................. 4 - 27
4 - 4  Desorption of CH4 gas from bomb Pressure vs Time
curve for Bomb L, Sept. 1989 ........................................ 4 - 32
4 - 5  Ratio of CO2/CH4 adsorption at different pressures for
Australian and European coals ..................................... 4 - 44
4 - 6  Effect of nature of gas on sorptive capacity Australian*,
Australian (1985), European (1980), and French (1965)
Langmuir's equation ............................................... 4 - 48
4 - 7  Effect of rank on coal sorptive capacity
French, American, and European coal, Langmuir's equation .... 4 - 49
4 - 8  Effect of VM on coal sorptive capacity
Australian adb (1985), Australian afd (1985) and German coal (1980), Langmuir's equation ........................................ 4 - 50

4 - 9 Effect of moisture content on coal sorptive capacity
Australian*, Australian (1985) and American coal (1973)
Langmuir's equation ........................................... 4 - 51

4 - 10 Effect of ash on coal sorptive capacity
Australian coal (1985), Langmuir's equation ................. 4 - 52

4 - 11 Effect of moist CH4 and moist on coal sorptive capacity
Australian coal (1985), Langmuir's equation .................... 4 - 52

4 - 12 Effect of temperature on coal sorptive capacity
Australian (1985) and European coal (1980)
Langmuir's equation ........................................... 4 - 53

4 - 13 Effect of nature of gas on coal sorptive capacity
Freundlich's equation .......................................... 4 - 54

4 - 14 Effect of rank on coal sorptive capacity, French, American, and European coal, Freundlich's equation ......................... 4 - 55

4 - 15 Effect of VM on coal sorptive capacity, Australian adb (1985), Australian afd (1985), and German coal (1980)
Freundlich's equation .......................................... 4 - 56

4 - 16 Effect of moisture content on sorptive capacity
Australian*, Australian (1985), and American coal (1973)
Freundlich's equation .......................................... 4 - 57

4 - 17 Effect of ash on sorptive capacity Australian coal (1985)
Freundlich's equation .......................................... 4 - 58

4 - 18 Effect of moist CH4 and moist on coal sorptive capacity
Australian coal (1985), Freundlich's equation .......................... 4 - 58

4 - 19  Effect of temperature on coal sorptive capacity

Australian (1985) and European coals (1980)

Freundlich's equation .................................................................. 4 - 59

4 - 20  n and T constants for CH4 adsorption test ......................... 4 - 88
### LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Pages</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Chapter 1</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.1.</td>
<td>The interrelationship between sorptive capacity, coal rank and depth (Kim, 1977)</td>
<td>1 - 4</td>
</tr>
<tr>
<td><strong>Chapter 2</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.1.</td>
<td>Adsorption isotherms for Bulli Seam coal</td>
<td>2 - 5</td>
</tr>
<tr>
<td><strong>Chapter 3</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.1.</td>
<td>Total gas emission plotted against output and desorbable gas content. The straight lines denote weekly averages (Curl, 1978)</td>
<td>3 - 4</td>
</tr>
<tr>
<td>3.2.</td>
<td>Specific gas emission plotted against output and desorbable gas content. The trend curves denote weekly averages (Curl, 1978)</td>
<td>3 - 4</td>
</tr>
<tr>
<td>3.3.</td>
<td>Distinguished zones around a face</td>
<td>3 - 6</td>
</tr>
<tr>
<td>3.4.</td>
<td>Gunther's Method (Curl, 1978)</td>
<td>3 - 20</td>
</tr>
<tr>
<td>3.5.</td>
<td>Gunther's Prediction Compared with Measured Emission (Curl, 1978)</td>
<td>3 - 21</td>
</tr>
<tr>
<td>3.7.</td>
<td>Zones of Gas Emission Used in West Germany (Curl, 1978)</td>
<td>3 - 24</td>
</tr>
<tr>
<td>3.8.</td>
<td>Zones of Gas Emission Used in West Germany (Curl, 1978)</td>
<td>3 - 26</td>
</tr>
<tr>
<td>3.10.</td>
<td>Schultz's Method (Curl, 1978)</td>
<td>3 - 29</td>
</tr>
<tr>
<td>3.14.</td>
<td>Curves for residual methane pressure in adjacent coal seam as a function of strata dip ratio of distance from the worked seam to the extrac thickness is used in the roof strata (Curl, 1978)</td>
<td>3 - 37</td>
</tr>
<tr>
<td>3.15.</td>
<td>Example of the method of pressure difference prediction (Curl, 1978)</td>
<td>3 - 38</td>
</tr>
<tr>
<td>3.16.</td>
<td>Lidin's method (Curl, 1978)</td>
<td>3 - 41</td>
</tr>
<tr>
<td>3.17.</td>
<td>Curve for Degree of Emission Against Face Advance (Curl, 1978)</td>
<td>3 - 45</td>
</tr>
<tr>
<td>3.18.</td>
<td>Degree of gas emission at 900m (Curl, 1978)</td>
<td>3 - 46</td>
</tr>
</tbody>
</table>
3.19. Correction of height before using 900m curves (Curl, 1978) .......... 3 - 47
3.20. An example curve for the degasing during coal clearance (Curl, 1978) .. 3 - 49
3.21. Example presentation of prediction (Curl, 1978) ............................ 3 - 51
3.22. Actual emission against estimate using direct method for some USA mines ................................................................. 3 - 53
3.24. Factor taken into consideration by various national prediction methods ... 3 - 60

Chapter 4

4.1. Glass test tube for determination of desorbed gas Q2 ................................................................. 4 - 6
4.1a. Seam gas composition for the Bulli Seam Illawarra area
(based on Hargraves, 1986b) ................................................................. 4 - 9
4.2. Investigation of seam gas pressure and temperature gradient ahead of borehole (developed from Hargraves, 1963) ................................. 4 - 11
4.3. Calibration curves for CH4, CO2 gas and mixed gas in bombs .......... 4 - 14
4.4. Relationship between gas adsorbed Ca and quantity of gas directly adsorbed for CH4 Qdir in the coal sample .................... 4 - 15
4.5. Relationship between gas adsorbed (Ca) and quantity of gas directly adsorbed Qdir by coal sample in CO2 ......................... 4 - 16
4.6. Relationship between gas adsorbed (Ca) and quantity of gas directly adsorbed Qdir by coal sample in mixed gas .......... 4 - 17
4.7. High pressure adsorption - desorption apparatus .......................... 4 - 20
4.8. High pressure adsorption - desorption system ............................... 4 - 21
4.9. High pressure adsorption-desorption system ................................. 4 - 21
4.10. Gas container (bomb) - Schematic ................................................. 4 - 22
4.11. General arrangement for data acquisition on gas adsorption) .......... 4 - 25
4.12. Graph for 'gas desorbed' against 'direct gas desorbed'
for CO2 gas (Bulli Seam coal, West Cliff Coliery) ............................... 4 - 28
4.13. General arrangement for data acquisition and pressure reading .......... 4 - 29
4.14. The equipment to measure the pressure in the bomb ....................... 4 - 30
4.15. Typical time against pressure within the bomb in the first two hours ................................................................. 4 - 33
4.16. Sieve analysis of coal fires (Bulli Seam, West Cliff Colliery .......... 4 - 35
4.17. Bulk coal samples, Bulli Seam ............................................. 4 - 38
4.18. Cylindrical coal samples, Bulli Seam ..................................... 4 - 38
4.19. Cylindrical coal samples, type 3 Bulli Seam ............................... 4 - 39
4.20. Adsorption isotherms for Bulli Seam coal for CH4 (West Cliff Colliery) ........................................................................ 4 - 40
4.21. Adsorption isotherms for Bulli Seam coal (West Cliff Colliery), dry CO2 in dry coal ...................................................... 4 - 41
4.22. Adsorption isotherms for Bulli Seam coal, dry mixed gas in dry coal .............................................................................. 4 - 43
4.23. Adsorption isotherms for Australian coal, dry CH4 and dry coal (developed from Bartosiewicz and Hargraves, 1985) .......... 4 - 60
4.24. Adsorption isotherms for Australian coal in dry CO2 gas (developed from Bartosiewicz and Hargraves, 1985) ............. 4 - 61
4.25. Effect of temperature and rank on CH4 gas adsorption isotherms for European coal (developed from Boxho et al, 1980) .... 4 - 62
4.26. Effect of temperature on sorption isotherms for moist CH4 and moist at 20oC and 30oC (developed from Bartosiewicz and Hargraves, 1985) ................................................. 4 - 63
4.27. Influence of natural moisture content on the adsorption of CH4 by pure coal (developed from Boxho et al, 1980) .......... 4 - 65
4.28. Effect of moisture content on the adsorption of CH4 in high pressure adsorption test as expressed by
4.29. Increase of degree of coalification with depth (Stach et al, 1982) 4 - 67

4.30. Effect of moisture content on adsorption isotherms
   for American coal (developed from Kissel et al, 1973) 4 - 68

4.31. Effect of moisture content on Langmuir's A for
   American coal ...................................................... 4 - 69

4.32. Effect of moisture content on adsorption isotherms for
   Pittsburgh from Joubert et al, 1973) .................................. 4 - 70

4.33. Effect of moisture content on Langmuir's A on
   Pittsburgh I coal ...................................................... 4 - 71

4.34. Effect of moisture content on adsorption isotherms for
   Pittsburgh II coal (developed from Joubert et al, 1973) .............. 4 - 72

4.35. Effect of moisture content on Langmuir's A for
   Pittsburgh II coal ...................................................... 4 - 73

4.36. Effect of moisture content on adsorption isotherms for
   Pocahontas coal (developed from Joubert et al, 1973) .............. 4 - 74

4.37. Effect of moisture content on adsorption isotherms for
   Hartshorne coal (developed from Joubert et al, 1973) .............. 4 - 75

4.38. Effect of moisture content on sorptive capacity for
   Bulli Seam coal (CH4 gas) ............................................ 4 - 76

4.39. Effect of moisture content on Langmuir's constant for
   Bulli Seam coal ...................................................... 4 - 77

4.40. Effect of moisture content on sorptive capacity for
   Australian coals (developed from Bartosiewicz and Hargraves, 1985) 4 - 78

4.41. Sorption capacity for moist coal in moist CH4
   (developed from Bartosiewicz and Hargraves, 1985) .................. 4 - 79
4.42. Effect of rank on adsorption isotherms for American coal (developed from Kim, 1977) ......................... 4 - 81

4.43. Effect of volatile matter on CH4 adsorption isotherms for German coal (developed from Boxho et al, 1980) .................................................. 4 - 82

4.44. Effect of volatile matter on Langmuir's A for German coal (developed from Boxho et al, 1980) ............... 4 - 83

4.45. Effect of volatile matter (afd) on Langmuir's A for Australian coal (developed from Bartosiwicz and Hargraves, 1985) .................................................. 4 - 84

4.46. Effect of volatile matter (adb) on Langmuir's A for Australian coal (developed from Bartosiwecz and Hargraves, 1985) .................................................. 4 - 84

4.47. Effect of ash content on Langmuir's A for Australian coal (developed from Bartosiewicz and Hargraves, 1985) .......... 4 - 85

4.48. Desorption of CH4 gas from bomb for Bulli Seam coal .......... 4 - 87

4.49. Desorption of CO2 gas from coal sample (Bulli Seam coal) .......... 4 - 89

4.50. Desorption of mixed gas from coal sample (Bulli Seam coal) .......... 4 - 90

4.51. Composition of mixed gas against time during desorption by mass spectrograph analysis ........................................ 4 - 91

4.52. Airey's desorption test result ........................................ 4 - 93

4.53. Lama and Nguyen's desorption results ........................................ 4 - 93

Chapter 5

5.1. Variation of equivalent permeability with gas pressure (Nguyen, 1989) 5 - 15

5.2. Variation of composite compresibility with gas pressure (Nguyen, 1989) 5 - 15

5.3. Data against unified model for CH4 desorption from intact coal ........ 5 - 24
5.4. Desorption data against empirical model ........................................... 5 - 25
Notations

A : Langmuir's constant, cm$^3$/g
A : the cross-sectional area perpendicular to the macroscopic velocity vector, cm$^2$
A : Freundlich's constant, cm$^3$/g kPa$^{-1}$
$\alpha$ : internal angle of prism
$\alpha$ : the effective rock compressibility
AR : degree of gas emission in roof, %
AF : degree of gas emission in floor, %
B : Langmuir's constant, kPa$^{-1}$
B : Freundlich's constant
$\beta_S$ : the compressibility of the rock matrix
$C_a$ : the quantity of adsorbed gas at pressure $P$, cm$^3$/cm$^3$, or m$^3$/t
$C_V$ : the quantity of the free gas per unit volume of coal, cm$^3$/cm$^3$
$D_F$ : the diffusivity of CH$_4$ gas in coal
$\mu$ : the fluid viscosity, kPa-s
$\mu$ : the weakness number
n : number of moles
$\Phi$ : the porosity of coal
h : the height in the roof or depth in the floor, m
K : the intrinsic permeability of the porous medium, cm$^2$/s
l : the length of the face, m
P : pressure, kPa
Qt : the quantity of gas emitted up to time $t$, cm$^3$/g
Q : the initial gas content in the coal samples, cm³/g
Qd : the quantity of gas directly adsorbed by coal
R : the universal gas constant = 8.3044 kPa/kmol/oK
ρ : the density of fluid
ρₚ : the density of rock solid
t : time, second
T : absolute temperature, oK
V : the total volume of rock unit, including both pores and solids
Vᵥ : the volume of pore space of rock unit
Z : the gas deviation factor, defined as the ratio of volume actually occupied
   by a gas at pressure P and temperature T to the volume occupied
   if it behave ideally
CHAPTER I
INTRODUCTION

1.1. General

Methane gas from coal seams is an important substance both from the aspect of coal mine safety and as an unconventional natural gas resource. The liberation of methane into nearby mined roadways and the occurrence of outbursts are both dangerous (Kininmonth and Mould, 1982). On the other hand, the recognition that proven fuel reserves could be exhausted within the foreseeable future has focused increasing attention on methane gas as an economic source of natural gas production (Price and Ancell, 1978).

It is apparent that a sound comprehension of the mechanism underlying the flow process of CH4 gas in coal is essential for safe coal winning and for design of ventilation and for any gas drainage system. But the mechanism is still an imperfectly understood matter. In literature a variety of mathematical models may be observed for gas emission from coal. Some models are empirical (Owili-Eger, 1973), while others are based on Darcy's laminar flow (Price et al, 1973), or Fick's diffusive flow involving diffusion along a concentration gradient (Sevenster, 1959). Some involve a two-step process namely diffusion in micropores followed by laminar flow in a macropore system (Acell, 1980 and King et al, 1983).

Seam gas in a virgin seam, before any activity takes place, is in equilibrium with:

(i). the seam gas generation related to the particular rank of coal and its time rate of generation,
(ii). the back pressure against escape of seam gas to zones of lower pressure and ultimately atmospheric pressure, and

(iii). the channel of gases from other sources, normally other coals.

Coal mining exposes a seam below surface and induces a new gas pressure gradient into the strata, the pressure gradient is from virgin gas pressure at some distance into the strata to atmospheric pressure at the site exposed. The parameters which affected this gradient are the virgin gas pressure, the permeability of the coal, the sorptive capacity of the coal, the composition of the gas, the geometry of mining, and some other factors. Gas emissions from virgin coals are high immediately after their exposure, and gradually settle to a steady-state. For virgin pillars which had a finite quantity of gas content, the gas emission rate falls with time as the amount of gas remaining in the pillar reduces, until the gas content reaches equilibrium with atmospheric pressure.

Coal seams naturally are not homogenous or completely isotropic, so gas emission into workings is not uniform per unit area of coal exposed due to planes of weakness such as bedding planes, cleat, and faults, to changing properties and to other parameters.

1.2. The source of seam gas

Firedamp is a by product of the coalification process, and is mainly contained in coal. It is estimated that up to 13026m$^3$ of all types of gases are produced during the formation of one tonne of coal (Hargraves, 1962; Patching, 1970). The main products are methane (CH$_4$), carbon dioxide (CO$_2$), N$_2$, and H$_2$O as water vapour.

During the early stages of the transformation of plant substances to coal, there is usually only a thin and permeable covering over the deposits, and most of the gases generated can escape. As a result, little gas is found in most low-rank
coal seams. By contrast, the compact higher-rank coals usually have been more deeply buried and are covered by more compact rocks. Coal has a stronger affinity for CO₂ than CH₄, but the greater production of CH₄ in the later stages of maturation is able to progressively replace most of any CO₂ retained from the earlier stages. This results in the seam gas of higher rank coals, bituminous to anthracite coal being essentially retained CH₄ (Hargraves, 1982).

Over geological time, diffusion and other processes such as geological disturbances in the earth's crust result in the removal of all but up to 14.2m³ to 42.6m³ of gas per tonne of high rank coal of the total gas generated during coal metamorphism. This residual gas is the usual primary concern when coal measures are mined underground. Quantities of CH₄ and air in the proportions from 5% to 15% CH₄ constitute an explosive mixtures which when ignited, may cause disastrous explosions.

1.3. Gassiness of coal seams

The sorptive capacity of coal for gas depends on the porosity of the coal, which is related to rank, on the nature of the gas and on the pressure of the gas. Figure 1.1 shows the interrelationship between sorptive capacity for CH₄, coal rank and depth (gas pressure related to depth).

Gassiness is specified in terms of volume of gas per tonne of coal (m³/tonne, cm³/g). When seam thickness is ignored, an approximation of the quantity of gas per tonne of coal can be made on the basis of seam gas pressure (depth) and laboratory adsorption isotherms for the appropriate gas composition at this pressure. Alternatively a direct measurement of gas pressure may be made, replacing depth as the determining factor of gas pressure, or the quantity of gas may be measured directly from a virgin coal sample.
Fig. 1.1. The interrelationship between sorptive capacity, coal rank and depth (Kim, 1977)
1.4. Emission of gas into mine workings

The seepage of gas from virgin seam to the surface is a compromise between the permeability of escape channels to the surface and the gas pressure of the seam. In practice this results in the virgin gas pressure being at nearly hydrostatic pressure from the surface.

Gas emission into workings results essentially from the pressure gradient developed between seam gas at virgin pressure in the coal ahead of the workings and the atmospheric pressure at exposure. As a face advances, the gas pressure in the virgin coal falls and disturbs the adsorption equilibrium, resulting in the liberation of some previously adsorbed gas from coal micropores into the macro fracture system in the face area. When such gas reaches the workings, it disperses into the air, if the gas is largely CH$_4$ (specific gravity of 0.555 relative to air) it may accumulate at the roof, if largely CO$_2$ (specific gravity of 1.529) it may layer at the floor, while intermediate compositions depend on the proportions of CH$_4$ and CO$_2$, and may be lighter or heavier than air.

Factors affecting gas emission into mine workings and various CH$_4$ prediction methods are more detailed in Chapter 3.

1.5. Dilution and gas drainage

All seam gases in the mine ventilation dilute the mine air, reducing its oxygen content. CH$_4$ is flammable, CO$_2$ is extinctive and has physiological effects. Both CH$_4$ and CO$_2$ can cause coal to have instantaneous outbursts of coal and gas during face advance.

To minimise the problems of seam gases, by statutory regulation the CH$_4$ concentration in the working areas must be maintained at for instance 1%, and in the main returns at 1.5%. As above at 5% - 15% in pure air CH$_4$ creates an
explosive mixture. To meet the dilution requirements, great quantities of fresh air are demanded.

*Mosgrove and Budzak (1981)* say that poor ventilation leads to low productivity, that high productivity could not be achieved while trying to maintain air at 4.2 m³/s at the last open crosscut. They say a rule of thumb in laying out a coal mine is to provide enough entries in the main entry system to keep air velocities at 2.5 m/s or less; at this flow rate good ventilation may be expected.

A general rule of thumb for seam gas drainage is that drainage is successful if one half of the gas is drained separate from the ventilation (*Hargraves*, 1982). He states that for the U.S.S.R., to safeguard against instantaneous outburst, the gas pressure in the seam should be reduced to 9 kPa before faces can advance.

### 1.6. Purpose and scope

To simulate coal seam gas migration the indirect method of adsorption-desorption tests was conducted on cylindrical coal samples. The gas contents of the cores were determined and physical and parametric characteristics of isotherms were investigated using the Langmuir equation as the representation of an ideal mono-molecular layer system. A computer based method of direct data collection was also developed. Normally gas emission is measured by the conventional volumetric method for which rather complicated equations are required to obtain the quantity of gas desorbed (*Bertard et al*, 1970). The procedure developed used a gravimetric method, the gas desorbed being released to atmospheric air (*Siahaan et al*, 1989). A program written in *BASIC* is used to initiate, collect data, and terminate data acquisition. It is important to note that the volumetric method and
the gravimetric method developed are very much different in the duration of the process, the gravimetric method used being much shorter in time.

In an attempt to investigate a potential outburst condition, a hole is drilled in the centre of the coal core and the hole is filled with coal fines; then the whole sample is pressurised in gas. This experiment is based on Ruff's "nest theory" where nests or pockets of low strength coal (already crushed in-situ) and saturated with gas are suddenly intersected by an advancing face may triggering an outburst (Lama, 1981). The assessment of adsorption-desorption tests is presented in Chapter 4.

The scope of the work did not extend to design and provision of major high pressure equipment. Such was available from previous work of others and was made used of as an economic expedient. It would have been preferred to have used freshly designed equipment more specific to the task with the extra expense in part compensated by greater economics in gas usage, etc.

The model used to simulate gas desorption from coal samples termed unified theory combines diffusion flow and laminar flow and allows of phase interchange taking place at any time during the flow of gas in the coal samples (Lama and Nguyen, 1987; Nguyen, 1988; Nguyen, 1989). Langmuir's model (Langmuir, 1916) is adopted to described the process of methane adsorption onto coal. From desorption test results "history matching" is conducted to determine the Darcy permeability for laminar flow component of the composite effective permeability. The resulting differential equation is solved using Crank-Nicholson. After determining coal porosity, boundary conditions for the real problem requiring simulation is established and simulation is conducted using the finite difference method. It is strictly based on fundamental theories of fluid flow in porous media, and has a form analogous to the soil consolidation problem. Therefore it is most suitable for application of modern numerical techniques. Chapter 5 is devoted to detailed presentation of the unified theory.
CHAPTER II

LITERATURE REVIEW OF METHANE GAS FLOW IN COAL

2.1. Physical properties of methane in coal

2.1.1. General

The study of the physics of flow through porous media has become basic to many branches of science and engineering. Disciplines such as soil mechanics, ground water hydrology, and petroleum engineering all rely on it as fundamental to their individual practical applications. In recent years, an increasing interest has been shown in mining engineering, in relation to the prediction of gas emission into mine workings.

To study the flow of gas through coal, coal seam is treated as a porous medium. The physical nature of the gas-coal bond normally is given in the following simplified way. Coal is a porous medium with natural fracture networks which provide storage and conduits for transport of fluid. Gas may be contained in coal as free gas in the macropore system and as an adsorbed layer on the internal surface of coal (Patching, 1970). The greater part of gas in coal is held at the surface of the coal pores and microfissures in adsorbed form as a monomolecular layer.

The behaviour of free gas which is present in the fissures and macropores of the coal, can be described by Boyle's law and the kinetic theory of gases (Boxho et
al, 1980 and Ancell et al, 1980). In the adsorbed state, gas molecules adhere to the large internal surface area of coal which has been estimated to be \(20 \text{ m}^2/\text{g}\) to \(200 \text{ m}^2/\text{g}\). The large surface area available because of the very fine pore structure of the coal makes it possible to hold a large quantity of gas. At normal seam pressure (at depths of 500m to 1000m) adsorbed gas is roughly 90% to 95% of the total gas occupying coal, and there is a continual interchange of molecules between the free gas and the adsorbed gas. The content of the adsorbed gas is related to the free gas pressure in equilibrium with the coal. Curves depicting this relationship can be determined experimentally in the laboratory by pressurising coal with gas at various pressures, and at constant temperature and by determining either volumetrically, gravimetrically, or chemically the amount of gas adsorbed at each pressure (Hargraves, 1966).

There are many models which could be used to describe the process of CH4 adsorption or desorption from coal, but Langmuir's model seems to be favoured. The adsorption of pure gas on Australian coal can be described by the Langmuir equation fairly accurately (Lama and Bartosiewicz, 1982, and Saghafi et al, 1987). Treatment of the Langmuir's equation of the ideal localised single layer has been extended to binary mixtures (Young and Crowell, 1962).

The quantity of free gas present in the coal pore space of coal can be described by Boyle's law:

\[
P V = Z n R T \tag{2.1}
\]

where:

- \(P\) : pressure, kPa
- \(V\) : pore space volume, m\(^3\)
- \(n\) : number of moles
- \(R\) : the universal gas constant (8.3044 kPa/kmol/°K)
- \(T\) : absolute temperature, °K
Z: the gas deviation factor, defined as the ratio of volume actually occupied by a gas at pressure $P$ and temperature $T$ to the volume occupied if it behave ideally (when $Z = 1$).

At the temperatures existing in mines (which vary from 20°C to 30°C in Australia), departure of $Z$ from unity is negligible at pressures up to 4000 kPa.

The quantity of the free gas per unit volume of coal, $C_v$ (cm$^3$/cm$^3$) depends on the porosity of the coal and absolute pressure and temperature, and in terms of coal porosity can be calculated by:

$$C_v = \phi \frac{P}{P_0} \frac{273}{T}$$  \hfill (2.2)

where:

- $\phi$: the coal porosity, i.e. fraction of pore space to total coal volume
- $P_0$: standard atmospheric pressure (101.3 kPa)
- $P$: absolute pressure in kPa
- $T$: absolute temperature °K

The free gas in coal makes up a small fraction, usually 5% to 10% of the total gas content. The volumetric free gas content, $C_v$ is proportional to the coal porosity, which is affected by the pressure of the overburden and the moisture content of coal or rock. Porosity can vary between 0.01 to 0.11 cm$^3$/cm$^3$ for coal (Boxho et al, 1980).

At equilibrium, a unique relationship exists between the quantity of adsorbed gas $C_a$ and the free gas pressure $P$ which is commonly described by Langmuir's equation:

$$C_a = \frac{ABP}{1+BP}$$  \hfill (2.3)
where:

\( C_a \) : the quantity of adsorbed gas at pressure \( P \), cm\(^3\)/g, or m\(^3\)/t

\( P \) : absolute gas pressure, kPa

\( A \) and \( B \) : Langmuir's constants depending on the nature of gas and the rank, moisture content, and the temperature of coal, cm\(^3\)/g, and kPa\(^{-1}\) respectively.

When the unit of cm\(^3\)/g is used, the conversion to cm\(^3\)/cm\(^3\) is obtained by multiplication with the coal dry density (g/m\(^3\)). *Equation (2.3)* suggests that there is a limit of quantity of gas adsorbed, even if pressure \( P \) is increased to infinity. *Figure 2.1* shows the adsorption isotherms for Bulli seam coal.

### 2.1.2. Determination of porosity

The porosity of coal which governs the free gas storage capacity of coal, can be stated simply as the ratio of the pore volume to the total volume of coal. It is a function of lithological factors such as heterogeneity of original grain size, packing and cementation of the grains, and is generally expressed as a percentage or a fraction as:

\[
\phi = 100 \frac{V_v}{V}
\]  

*Equation (2.4)*

where:

\( V_v \) : the volume of pore space of rock unit

\( V \) : the total volume of rock unit, including both pores and solids

The pore structure of a coal or rock may or may not be interconnected. Some terms have been introduced to describe physical measures related to porosity. Absolute porosity and effective porosity are two of the terms commonly used to
describe the degree of interconnection of the pores. Absolute porosity is the total percentage of the pores in the medium whereas effective porosity is that fraction of the pore structure that is interconnected. In the laboratory conventionally, porosity is determined by displacement of liquids by coal as follows:

A coal sample is enclosed in a container of known volume, which is then filled with mercury. Mercury does not penetrate into pores with size of less than 7.5\(\mu\). The volume of mercury is determined gravimetrically. After the mercury has been removed, the container is filled with helium (He). This gas penetrates into the finest cavities of the coal; it is lightly adsorbed in the pores. The volume of He
which is determined gravimetrically would be equal to the sum of the volume of mercury and that of the coal pores if He were not adsorbed at all. The porosity determined by this method gives a somewhat high result. Porosity of rocks varies with depth, and at depths greater than 7,000m, the porosity of most rocks will cease to exist (Pirson, 1958).

To characterize coal porosity quantitatively, the pore volume, surface area, and pore size distribution need to be determined (Mahajan, 1982). In the conventional way, densities and pore volumes are measured using displacement of liquids, whereas physical adsorption of gas and the heat of immersion method are used to measure the surface area.

Adsorption isotherms of CO₂ at 25 °C are used to determine pore size distribution. The International Union of Pure and Applied Chemistry (1972) classifies pores of different sizes in the following manner:

- pores greater than 500 Å in diameter are macropores,
- pores with diameter in the range 20-500 Å are mesopores, and
- pores with diameter in the range 8-20 Å are micropores.

In the laboratory investigation of coal reservoir properties (Price et al, 1978) it was reported large differences in porosities between those measured with He and those with water as saturating fluids. Porosities by He determined on five samples varied from 2.5% to 8.6% while water determined porosities varied from 0.4% to 1.1%. The porosity of the fracture or cleat system probably is better represented by the water determined porosities due to consideration that this is a function of pore size that the respective molecules could penetrate. Porosity for American coal could be best taken as 0.01% to 4%. Kneuper (1972) as quoted by Price and Ancell (1978) predicts an effective porosity of 1.3% to 3.9% for European coals.

For Australian bituminous coals the general range of porosity is 1% - 3% for coals of 20% - 40% volatile matter (a.f.d.) (Hargraves, 1983).
2.1.3. Permeability

Permeability can be defined as the ability of gas to flow through coal or the ability of coal to transmit the gas when a pressure gradient is developed across it. Basically it is a function of the porosity and the tortuosity of any interconnected network of void spaces in the coal. It is independent of the density and viscosity of the gas flow through the medium. In-situ it is also dependent on environmental stresses. The overall permeability of the coal along the CH$_4$ flow channel should be considered. The permeability of a medium can be derived from the result of an empirical discovery of the French hydrologist D'arcy (1856) to the effect that it proportionately relates the velocity of flow of a flowing gas of viscosity $\mu$, to the pressure gradient and the path length. The permeability of the coal has been subdivided into micro and macropermeability by Hargraves (1973). He considered micropermeability to be the permeability of the pores within the coal lumps through which gas flows by diffusion, and macropermeability as the permeability of fissures and fractures through which gas flows according to Darcy's law. Unfractured solid coal has a very low permeability and in some instances is virtually impermeable (Kissell and Bielicki, 1972). Patching (1973) states that macropores can be penetrated by mercury, while micropores can only be penetrated by He. This is related to remarks above concerning porosities.

It is not a simple work to accurately measure permeabilities of fracture systems in laboratory samples. Trepanned cores which have been disturbed by the drilling process and relieved of confining stresses throw doubts on the accuracy of such a method. Macropermeability of coals determined in laboratory experiments however, may be of value for comparisons of permeability between samples. Based on results of laboratory measurements in the USA, Dabbous et al (1974) have shown that coal permeability exhibits an effect of stress hysteresis.
This led them to the conclusion that the flow of methane is dependent on the stress history of the coal.

The stress history or the cycles of stress change due to mining (Mordecai and Morris, 1974; Gawuga, 1979) may also affect the coal permeability. It is possible that internal structural modifications of coal due to stress change are irreversible (it is simple to imagine new asperities being broken off at each restressing). The stress concentration around a mine opening is usually relieved by incipient fracture including sometimes roof sagging, floor heaving, resulting in an increase in flow permeability through the cracks and joints opened up.

The process of degasification could result in shrinkage in coal volume which lead to further release of gas molecules or an increase in permeability. It was suggested by many including Hargraves (1963), Patching (1971), and McColl-Stewart (1971). For coal from Metropolitan Coal Mine (New South Wales, Australia) an average strain of 0.00182 may result from 1000 kPa change in equilibrium sorption pressure using CO₂ gas, as reported (Hargraves, 1984).

Adsorption of water may lead to coal expansion as reported by Reznik et al (1974) that the gas permeability increases rapidly as water is removed from the coal. It appears that drainage of water results in better availability of internal surface area for surface diffusion of adsorbed molecules.

Permeability of flow through fine cracks is also directly dependent on seam gas pressure, that is flow rate decreases with decreasing pressure; as shown by field observations of CH₄ gas emission from coal seams (McColl Stewart, 1974). This so-called ‘negative’ Klinkenberg effect has also been reported by King et al (1983) and by Lam and Nguyen (1987) from desorption experiments on a cylindrical coal sample. The existence of an abutment area ahead of a working face may also affect the coal permeability. This region, which is under higher confinement than the virgin coal, may exhibit higher permeability due to fracturing.
Universally coal seams exhibit a natural system of fractures. The fracture system is generally perpendicular to the bedding planes of the coal, except in areas of high tectonic activity. This system of joints and fracture is commonly referred to as cleat (Ancell et al, 1980). Traditionally coal mines used to be planned to take advantage of the cleat by mining in the direction in which coal breaks most easily. To take bedding and cleats into consideration, cores drilled normal and parallel to the bedding plane are used. Where face (primary, major) and butt (secondary, minor) cleats are prominent, the coal seam is more permeable in the direction of the face cleat (Price et al, 1973). Modern mechanised mines have less advantage from orienting workings relate to cleat.

The permeability of a coal seam to CH4 is also influenced by the concentrations of other fluid phases including water. At high strata pressure the permeability of coal to water is less than or equal to the gas permeability (Curl, 1978). However at low strata pressure the water permeability may be greater than the gas permeability because under the shear stress of the flowing water the coal tends to fracture internally.

Constraint dramatically reduces gas permeability of coals, for instance from 0.01 md to 0.0004 md as a result of increasing hydrostatic constraint from 1 to 10 MPa has been observed (Bartosiewicz and Hargraves, 1985). Lama and Nguyen, (1987) using radial techniques at varying pressure also observed drop in permeability by a factor of 2 - 3 with increase of stress from 0 to 10 MPa.

The permeability of rock at any point is therefore a function of the rock type, its location with respect to mine workings and time.

2.2. Transport modes
Since coal exhibits two types of pore structure, flow of gas through it will be of a mixed type and it will be difficult to separate the different types of flow. Flow of gas through coal can be by molecular diffusion through the micropore system, permeation through the macropores or by a combination of both. These two distinct transport modes are interdependent.

Flow through microporosity is a diffusion mechanism. Diffusion was defined as the process which leads to an equalisation of concentration within a single-phase (Jost, 1952). It was further stated that the value of the diffusion current can be approximately called permeability, under standard conditions. The driving force for this mode of transport is the concentration gradient, i.e. in isotropic substances the rate of transfer of diffusing substance through unit area of section is proportional to the concentration gradient measured normal to the section (Fick, 1855).

A second mode of transport of gas flow through coal is permeation. Permeation is the passage of gas through the fracture system of a porous medium. The driving force for this transport mode is the gas pressure gradient, which is caused by the gradient between in-situ gas pressure and the near atmospheric pressure of coal face. Flow within the fracture system is considered to be laminar in accordance with Darcy's flow equation. Darcy's law requires fluid flow to be viscous, with the fluid adhering to the walls of fractures through which it flows. With a gas flow this does not happen and slip occurs along the walls of fractures.

2.2.1. Previous models

A variety of mathematical approaches have been presented for describing the emission of CH₄ from coal seams into mine workings. Basically the equations used are equations describing fluid flow in porous media (Darcy's law or Fick's
law) and the principle of continuity. A brief overview of some models are presented.

Airey (1968, 1971) suggested a model based on observation of gas emission from broken coal:

(i). the initial rate of release of CH₄ is very large regardless of the size of coal,
(ii). the total volume of emitted CH₄ approaches a constant after a very long time,
(iii). the quantity of gas released is greater for smaller sized coal pieces, and
(iv). the total volume of CH₄ released increases with time and the rate of emission decreases with time.

These observations led to an algebraic equation in which the volume of gas desorbed was an exponential function of a time variable as follows:

\[ Q_t = Q(1 - \exp(- \frac{t}{T})^n) \]  

(2.6)

where:

\[ Q_t \] : the quantity of gas emitted up to time \( t \), cm³/g
\[ Q \] : the initial gas content in the coal samples, cm³/g
\[ t \] : time, second
\[ n, T \] : constants

Two approaches to modelling emissions based on Darcy's equation for single-phase gas flow have been reported in the Russian literature. In the simpler case (Gorbachev et al, 1973, Vylegzhanin, 1973, and Karagodin et al, 1974), desorption was modelled in terms of the Langmuir adsorption relation. The quantity of adsorbed gas is assumed to be always in equilibrium with the free gas pressure. The assumption of equilibrium between adsorbed and free gas means that the adsorption phenomenon can be treated as an extra or enhanced gas
compressibility term in the usual single-phase equation and, in terms of the models corresponds to very fast desorption times.

Owili - Eger (1973) developed a two dimensional steady-state (time independent) model for gas emission based on solution of the diffusion equation. The source term corresponding to a constant desorption rate and gas influx from adjacent strata was formulated empirically. O'Shaugnessy (1980) extended this model for the case of nonsteady flow from a longwall face using a finite element technique. Both approaches produced single-phase models.

Price and Abdalla (1972) developed a two dimensional two-phase model for simulating the emission of gas and water into workings. The primary limitation of this model, which employed state-of-the-art petroleum reservoir numerical simulation techniques, was that the source term due to adsorbed gas was assumed to be simply proportional to free gas pressure.

Price and Ancell (1973, 1978, 1980) and Chase (1980) have developed two-phase, transient models for the flow of gas and water in coal seams with a diffusion model for the desorption process in a dual porosity medium. These models were formulated to predict production of coal seam fluids by an array of vertical wells and by an isolated vertical well respectively.

2.2.2. The unified model

Nguyen (1988) developed the unified model of CH$_4$ gas flow in coal. CH$_4$ gas flow in coal is characterized by strong sorptive behaviour of gas molecules to the internal surface of coal. The 'permeability' is thus largely influenced not only by the mechanisms of laminar flow (Darcy's law) and diffusive flow (Fick's law) but also by rate of interchange between the adsorbed and the free gas phases. The model is most appropriate for solution using the finite element technique involving
parallel and coupled codes, one for gas and moisture flow and the other stress-desorption analysis.
CHAPTER III

PREDICTION OF METHANE EMISSION INTO MINE WORKINGS

3.1. Introduction

Gas emission into mine workings originates from the worked seams and adjacent seams and strata. Gas from the worked seam migrates through the seam to the face, and gas can migrate from adjacent strata to relaxed zones about mine workings. Any gas which has not been released before the coal is cut may be released on cutting and during transportation, although the release may not be complete by the time the coal reaches the surface. It is obvious that quantifying the emission of methane into mine workings is a complex combination of processes and circumstances.

The in-situ gas pressure in equilibrium with the pressure of its environment (such as strata stress due to over burden, ground stresses because of formation and hydrostatic pressure because of pressure of water and other gases). Coal winning disturbs the strata and upsets the equilibrium of the gas contained in the coal seam. Relaxing and the resultant fracturing of the strata opens extra flow paths for the gas to migrate into the workings. Gas pressure in "virgin coal seam" may be over 4000 kPa, while workings contain air at virtually atmospheric pressure (according to the depth below surface). Therefore there is a gas pressure gradient developed from in-situ virgin pressure to roadway air pressure. The gas release process starts once a fall in pressure at the adsorbing coal surface takes place on the exposure of
coal face and continues till such time when a new equilibrium is established. As a face advances the rate of release of adsorbed gas into surrounding workings increases. The rate of emission and the quantity of gas emitted depend on the extent of pressure relief which itself depends on the quantity of coal or rock won in relation to factors such as the coal and strata disturbed, the rate of mining, the in-situ gas pressure, gas content and permeability of strata.

Determination of gas emission from coal seams is of basic importance in the planning of ventilation systems and any gas drainage requirements in coal mines. Its importance has increased very rapidly in recent years mainly due to the increase in use of highly productive equipment. The increased use of highly powered equipment for winning, loading, and transporting coal has had an important effect on the gas production of an operation. CH4 emission into workings and its control in the context of such environmental conditions as would ensure safe and efficient operation of power equipments in coal mines are two of most important factors. The highly productive equipment is mostly electrically driven. As has been stated methane-air mixtures containing 5% to 15% methane are explosive. Ignition of methane-air mixtures from electrical sparking due to short circuits etc may initiate hazardous explosions in coal mines. Thus the concentration of CH4 needs to be maintained below the statutory limit.

3.2. Methane emission as a limit to production

CH4 emission into workings appears to have a close link with the coal face production related to the rate of face advance. The following equation correlating output, the rates of gas emission and other variables (Chugh, 1977) has been evolved:
\[ P_{\text{max}} = \frac{10080 \cdot m \cdot Q}{U \cdot (100 - c) \cdot q} \]  

\( P_{\text{max}} \): the maximum daily output, tonnes  
\( m \): the permissible percentage of methane in the air  
\( Q \): the quantity of air, m\(^3\)/min  
\( q \): the total rate of gas emission, m\(^3\)/tonne  
\( c \): the percentage of gas captured by degasification  
\( U \): the irregularity factor for gas emission

From measurements which were taken on 364 faces in the Ruhr coalfield, \( P_{\text{max}} \) was plotted against the rates of gas emission which to produce hyperbolic curves.

*Noack (1976)* describes CH\(_4\) emission at a face as having inert and energised components (*Curl, 1978*). The inert component is the release at zero coal output, while the energised component is the increase in CH\(_4\) emission per unit of production.

Plotting daily output (t/d) against CH\(_4\) emission (m\(^3\)/min), and applying regression analysis, a straight line would be obtained giving a shape of the energised component and on intercept of the inert component, which is shown in *Figure 3.1* (*Curl, 1978*). The straight lines denote weekly averages at specific desorbable gas contents.

*Figure 3.2* (*Curl, 1978*) shows the graphs of specific methane are hyperbolic because the inert gas component is distributed amongst increasingly large tonnages of coal as the output and energised component increase. From examination of *Figure 3.1* it is obvious that in the planning of any operation in gassy mines, possible maximum specific gas emissions must be known in advance so that suitable ventilation and any gas drainage requirements can be arranged.

### 3.3. Emission of methane into mine workings
Fig. 3.1. Total gas emission plotted against output and desorbable gas content (Curl, 1978)

Fig. 3.2. Specific gas emission plotted against output and desorbable gas content (Curl, 1978)
The permeability of intervening strata is generally low and and may be considered to be practically unaffected by stress, in the cases where fractures are not produced. For coal, permeability reduces under the effect of compression and increases under that of tension because the macropore and micropore systems naturally tend to close in the first case and to open in the latter. If the permeability of the compressed coal before excavation is close to that of the strata, the permeability of the relaxed coal will be greater.

Coal mining induces a modification of the stress pattern in the surrounding ground. This changed stress pattern produces fissures in a zone enveloping the excavation, but this fissured zone is not as extensive as the whole zone in which the stress has changed. These changes are generally characterized by a zone of relaxation enveloped by a zone of compression. Fractures can occur in the compression zone or in the relaxed zone but they open only in the relaxed zone.

The characteristics and the rate of fissuring are functions of distance and position relative to the excavation, the shape and size of the excavation, the initial stress levels (which depend on the depth), and the thickness and nature of the strata.

CH₄ gas contained in the seams emits particularly if it is able to flow through open fissures developed in the strata where seams are relaxed. Around a face three zones may be distinguished, the first zone nearest the opening, the second zone completely enveloping the first, and the third zone where the ground is relaxed but where the rocks are hardly influenced by fissuration (Figure 3.3).

The zone nearest the excavation where the seams and strata fracture into blocks, which are displaced relative to each other, constitutes a very permeable region around the working. The roof zone being assisted by gravity is more important, since the floor zone being resisted by gravity is very small. The height of this roof zone is 3 to 10 times the face height for a typical caved face, the particular figure depending on the nature of the strata; the height is less for stowed
Fig. 3.3. Distinguished zones around a face
faces. The voids forming in this zone constitute a reservoir of CH₄ gas which, at a time of falling barometric pressure can release CH₄.

In the second zone the strata fracture and separate from each other. When the ground recompresses, the natural micropores partially close bringing together the sides of the fissures and the broken pieces so that even if the permeability does not return to its initial low value, it is decreased. In the roof it may extend to about 100m and in the floor it may extend to over 50m below the face.

The height of the first and the second zones is affected by factors such as the working thickness of the seam, whether the waste is caved or stowed, the length of face, and the presence of adjacent panels.

The third zone is the relaxed zone which allows for coal seams to become more permeable and the gas to escape providing there are channels such as bore holes or roads.

3.4. Factors affecting gas emission into mine workings

Factors such as depth of coal seam, rank of coal seam, structural characteristic of coal and strata, nature of roof and floor, geological features, and mining method affecting gas emission into mine workings.

3.4.1. Depth of coal seam

As has been discussed above, the quantity of the free gas present in the macropore system of the coal can be described by Boyle's law PV=nRT. The quantity of the free gas per unit volume of coal Cᵥ (cm³/cm³) is a function of the porosity of coal and pressure and temperature; which is expressed as
\[ C_v = \phi \frac{P}{P_0} \frac{273}{T} \]

\( C_v \) is directly related to pressure of overburden which means the greater the depth (=pressure), the higher will be the gas content. In the formula developed by the *Bureau of Mines (USA)* to estimate the methane content of coal, which incorporates corrections for moisture, ash, and temperature, pressure and temperature were expressed as a function of depth (*Kim, 1977*).

### 3.4.2. Rank of coal

Properties of coal such as total carbon, volatile matter and moisture contents are commonly used as a measure of rank. In general rank of coal increase with increase in fixed carbon contents and decrease in moisture and volatile matter contents. It should also be noted that in general, rank increases with depth (*Hilts’ Law*) (*Cook, 1982*).

Among others the *U.S.B.M.* has found that in general the adsorptive capacity and hence CH4 content for American coal increases with rank (*Kim, 1977*)

### 3.4.3. Thickness of coal seam

A thick seam will be proportionately more gassy than a thin seam, for seam of the same rank and the same depth and the same temperature. If the surrounding strata are thick and tight in structure, gas will remain in the strata. Conversely, if fissures are well developed in the strata, gas will release easily.

### 3.4.4. Structural characteristics of coal and strata
The gas sorptive capacity of coal and strata at a given strata stress, depends on gas pressure, temperature and the porosity. In the case of coal porosity is related to rank. The flow of gas through coal and strata is the ability of the rocks to transmit the gas when a concentration and pressure gradient of the gas develops across them. Gas migration and emission, depends on the number, size and orientation of the flow channels available for gas determining the flow capacity of coal and strata. McCulloch et al (1974) in U.S.A. have shown that holes drilled perpendicular to the face cleat yield from 2.5 to 10 times the amount of gas released as compared with holes drilled perpendicular to the butt cleat. Also Lidin (Chugh, 1977) has shown that Russian coal permeability along or parallel to the bedding planes was about 10 times the permeability at right angles to them. Coal develops higher induced permeability than strata and coal and strata in the roof develop higher induced permeabilities than they do when in the floor of the workings.

3.4.5. Nature of roof and floor

The magnitude of pressure relief and the extent of the zone of relaxation depends on the strength of rocks in roof and floor in relation to the magnitude and direction of the ground stresses. Strong roof, for instance massive sandstone, experiences lowering of the roof beginning far behind the area of extraction which results in delayed and also slight bed separation and induced fissuration. For a soft weak roof like shale in the immediate roof, bed separation starts only a short distance behind the working face and fissuration of the roof is quite intensive and uniform. As expected this results in a uniform rate of gas emission narrow limits.
3.4.6. Geological features

The gassiness is generally high in geological and tectonically disturbed formations such as those folded, faulted or where sill and dyke intrusions are found. The intrusive rocks sometimes act as a barrier and prevent gas migration until penetrated when abnormally high rates of gas emission may be experienced. Tensile fractures are conducive to gas escapes whereas compressive fractures tend to tighten the structures where gas accumulates. Large differences in gas content have been measured on opposite sides of geological faults. This has been reported in Belgium and Poland (Curl, 1978), more usually for faults with large throws but sometimes with throws as small as 1.5 m. When CH4 gas has to flow up dip in water bearing strata it must first displace the water, which has been found by McCulloch et al (Curl, 1978) to reduce considerably CH4 flow rates in the U.S.A.

In dipping seams, the larger the seam inclination, the more gas escapes since flow along the bedding planes is much greater than flow normal to them. Consequently gas content will be lower. Conversely, the lower the inclination, the more gas remains in the coal seam.

3.4.7. Mining method

(i). General

In relatively thick flat working seams all the development is in the seam itself, except shaft sinking; while in inclined seams and thinner seams a larger proportion of the development is in rock whereas significant methane flow is related to total coal exposure.

Coal mining in the form of headings and faces introduces artificial "channels" for gas escaping. Steep gas pressure gradients will be developed
around the openings, where virgin coal seam pressures are high. Advancing faces will set up steeper gradients, and the steepness increases with the rate of advance.

(ii). Development

Headings into virgin coal are normally horizontal, so gas sorption in the coal could be expected to be uniform, for that horizon. The gas will enter headings from the solid at rates increasing with advance rates. In general faces and ribs emit gas at maximum on first exposure, and gradually flow diminishes to some finite value. For room and pillar development or possibly for development of longwall panels, the choice of number of headings is to some extent influenced by the gas problem. The magnitude of pressure relief and the extent of zone of relaxation around a narrow heading are small, and the gas release in such headings may be small. But in a wide heading (or a number of small headings in close proximity) the span of the arch of deformation encompasses a large volume of relaxed coal and strata surrounding the opening and the rate of gas release may be great. In gassy seams, the gas flow into the workings may dictate a maximum advance rate without increasing the quantity of ventilating air. Very rarely are single headings driven in gassy situations. Twin entries provide a separate intake and return. In very gassy conditions multiple headings may be more practical to reduce gas concentrations in the ventilating air.

Standing pillars in unextracted zones, will emit gas at rates varying inversely with their age. The older the age the less gas will remain and, the slower will be the rates.

(iii). Advancing longwall

Longwall advancing can be considered as a huge heading in regard to the gas in the working seam; with a wider face and a correspondingly slower rate of advance, the slower advance results in a flatter gas gradient ahead of the face.
pressure drop from the intake across the face to the return causes air leakages across the goaf and also from the face to the return ribside. This leakage is an advantage as it holds CH4 back in the waste and avoids the problems of accumulated gas in the waste moving out onto the face at times of falling barometric pressure. The ventilation current is progressively enriched in CH4 as it passes along the face and along the return.

If longwall mining with the full-caving method is used, the gas originally stored in the roof and adjacent seams will be released and will flow into the ventilation networks. This is more accentuated during the periodic roof weighting when the main roof disintegrates and caves over large areas, becoming more permeable.

(iv). Retreating longwall and pillar extraction

The gate roadways are developed before the face starts into production, so to some extent the mined panel of coal is predrained of CH4. The longwall face and the pillar emit gas at rates which are inversely related to age of the blocks and are directly related to the size of the individual pillar. There is also a possibility of gas migrating onto the face line particularly if the goaf of a retreating longwall is not ventilated by bleeders (leakage to a separate return at the starting end of the block).

(v). Abutment area

As has been discussed above the existence of the abutment area may change the coal permeability. The solid coal ahead of a working face can be divided into two sections, one section on the face side of the (front) abutment, and the other beyond the abutment into the virgin solid coal. McColl-Stewart (1971) and Kissell (1972) showed the face side of the front abutment (crushed zone), including its increased permeability compared to zone beyond the abutment due to fracturing.
As the face advances the previous crushed zone is mined and a new crushed zone is formed ahead of the face.

(vi). Supporting openings

The characteristics (sizes, depths, and rates) of fissuration on which the orientation of migration and flow channels in the relaxed zone depend, also depend on the efficiency of the support system (speed of setting, adequacy and strength of support) in the face area and in the goaf behind. Delay in setting support or inadequate support results in more intense fissuration and permanent bed separation than if the roof control is good. The breaks and cracks are much wider and extensive in a poorly supported face area.

(vii). Adjacent workings

If multiple seam mining is involved, the mining operation in one seam disturbs the surrounding strata. The stratigraphic section above and below the working is of great importance, because the zone of strata relaxation extends into the strata both above and below the working. As a considerable proportion of the methane entering the working originates from surrounding seams and strata, the number and position of adjacent coal seams is important to be considered. The rates of gas emission are generally much higher in such areas where remnant pillars are found above and below them, because of these pillars being stressed and deformed not only forming gas channels but, on getting crushed, causing extension of the relaxed zone above and below thus increasing the rates of emission considerably.

(viii). Mine ventilation

Mine ventilation variations include air quantity, direction of air flow, absolute pressure and humidity and these affect rates of gas emission. In Germany,
Winter (Chugh, 1977) has shown that gas emission in mines consists of two parts, the basic emission which is from the working seam and the supplementary emission originates from the surrounding strata. The basic emission is almost constant irrespective of the quantity of air flowing, whereas the supplementary emission is affected by environmental factors. Thus in a mine where the basic emission is significant, an increase in air quantity will cause a permanent increase in the gas flow rate because of greater 'scouring action' and 'ejector effects' of the ventilating air than before the increase.

In a mine where the basic gas emission is insignificant a sudden decrease in ventilation air quantity will usually be accompanied by an immediate decrease in gas emission rate (m³/min), but it will rise again until an equilibrium equal to the earlier rate is reached.

When air pressure is taken into consideration, if mine ventilation is the exhausting type, the quantity of gas release will increase with increasing (negative) air pressure. Conversely, if the ventilation is the forcing type, it decreases with increasing (positive) air pressure.

(ix). Period of activity

Gas release continues even during the period when no mining activities are in progress, although the rate of gas emission is very much reduced compared to that during active mining. Irani et al (1972) showed that rates of gas emission in some U.S. mines were 20,000m³/day during the eight week strike compared to 28,750m³/day during active mining. Dunmore (1979) also obtained a typical recording of U.K. CH₄ concentration which showed the general rise in level throughout the working week, together with peaks taking place during production shifts and the gradual reduction of release over the weekend.

3.5. Methane prediction methods
Various CH₄ emission prediction techniques are under development or in use in many coal mining countries throughout the world. The gassiness of coal is stated conventionally as the total of gas released into the working related to the coal output (mined saleable coal). Mine gassiness depends on the coal won, and also on the extent of virgin rib exposed, the extent of goafs and the release of gas from any adjoining seams in the roof and floor mainly through the goafs and any prior mining in adjoining seams.

The quantity of gas emission in an underground coal mine can be expressed either by the absolute quantity or the relative quantity of emission. The absolute quantity of emission is the absolute quantity of emission per unit time in the whole mine. In volumetric unit it will be m³/day or m³/min. The relative quantity of emission is the average quantity of emission per ton coal produced within a certain period of time (week, month, etc).

In absolute units indices of gassiness available include (Hargraves, 1980):
1. mean gas emission, the rate m³/d and litre/s averaged over long periods, such as one week,
2. the real gassiness of a coal, the volume of gas m³/tonne contained in the coal in its virgin state,
3. as a comparative index to the gassiness of face coal, expressed as the emission of gas taken from the coal, over a standard length of time after detachment of the coal, expressed as the emission value, cm³/g.

Some well known predictive techniques have been proposed by authors including Jeger (1977), Koppe (1975), Airey (1971, 1978), Lidin (1965) and others are outlined.

Release of CH₄ into workings takes place from both the worked seam and adjacent coal seams and strata. The basic parameters considered are
(i).the stratigraphy of the worked seam, above and below the worked seam, and
the zone of gas emission.
(ii). the gas content of the source expressed in m$^3$/t of source material
(iii). the degree of gas emission from the worked seam, adjacent seams and strata
(iv). the desorbable gas content of all involved seams and strata

A knowledge of the location and thickness of strata components of the worked seam and its surrounding is essential for any overall prediction method. The extent of the stratigraphic column under consideration depends on the zone of gas emission. This is the three-dimensional area surrounding the workings from which gas is released as a result of mining operations. The major sources of gas emission in the strata are taken to be the coal seams disturbed by the working which is estimated starting from the coal seam up to 200m above the worked seam in the roof and down to 100m below the worked seam in the floor.

The gas content of the source is measured using either 'direct method' or 'indirect method'. In the direct method coal samples are sealed as soon as possible after retrieval from a borehole and gas desorbed from the samples is measured in the laboratory; in the French version (CERCHAR) 10g of cuttings of above 2mm size are sufficient, whereas in the UK version (MRDE) a portion of core sample of 30g mass is taken. In the indirect method gas pressure and temperature are measured in-situ and these are interpreted in terms of the gas content of the seam by means of a laboratory measured adsorption isotherm curve. Investigations of seam gas pressure involve setting of seals deep in boreholes and allowing the inbye enclosed volume to build up to full seam pressure for measurement. The measurement requires a near-perfect seal in a borehole and is subject to problems of gas leakage and strata water pressure.

There are two different interpretations of the quantity of gas content of a coal sample or coal seam. The first theory which is used in Belgium, France, and Federal Republic of Germany, methane desorbs from coal until it is in equilibrium with free methane in its crack system at atmospheric pressure. The other interpretation, which is used in the UK in the application of the theory of Airey,
based on the observation that large blocks of coal can desorb completely. In consequence the gas content value used in the UK is of the order of $1 \text{m}^3/\text{t}$ greater than other prediction methods (Boxho et al, 1980).

Prediction methods vary in their definition of the zone of gas emission and in the way they determine the degree of gas emission from various portions of a zone. Most methods vary the degree of gas emission as a function of height within a zone of gas emission represented by a physical model. They differ because of the differences in the shape on which they are based. All methods require knowledge of at least the gas content of the worked seam, and preferably the gas contents of all adjacent seams and strata. However, it is not possible to obtain all gas contents due to physical and economic restrictions. Assumptions commonly made where complete data are not available such as adjacent seams having the same gas content as the worked seam and that intervening strata such as shale and sandstone have a percentage of the worked seam gas content.

CH$_4$ emission from coal measure strata can be subdivided into emission from each bed of strata. Each is considered separately. Total gas emissions can be determined from the input of emissions from the worked seam, adjacent seams and strata, and any gas that may be emitted while clearing coal from the mine. CH$_4$ emission from the worked seam is determined by applying a degree of gas emission to the content of the seam. The degree of gas emission is then multiplied by the relative thickness of the particular seam to be considered. The relative thickness is the ratio of the thickness of the seam under consideration to the thickness of the worked seam. This product is then multiplied by the gas content of that particular seam to give the methane emission in cubic metres per tonne of coal produced at the face from that seam. Use of the relative thickness leads to the dependence of methane emission on coal face production. The effect of gas emission from each layer is so calculated and the sum of each of the adopted
partial emission values then gives the total predicted methane from surrounding strata.

The degree of gas emission from adjacent seams and strata is usually related to their distances from the worked seam. Relationships for the degree of gas emission using the various prediction methods can be defined mathematically or graphically. Most methods assume a fixed degree of gas emission which is often 100%. However, there is now an attempt to vary the degree of emission according to mining parameters. For example, the Mining Research and Development Establishment (M. R.D.E.) method in the U.K. uses a degree of emission varying with face advance rate (Figure 3.2) (the complement reaching the surface in the coal).

Gas emission from coal during clearance affecting a particular mining site should be considered because this emission flows inbye with the intake air. The degree of gas emission from coal being cleared should relate to the time elapsed between when the coal is cut and when it has been loaded away to where any emissions from the coal will not enter the intake roadways of the working district. The remnant CH₄ content of the coal being cleared is the original in-situ content minus the methane emitted before cutting.

Overall total gas emission is obtained by summing the gas emission from the worked seam, adjacent seams and strata, and the gas emitted during coal clearance. Predicted CH₄ emissions are usually presented as specific gas emission in cubic meters per tonne of coal production (m³/t). This can be converted to a mean CH₄ emission rate (m³/d or l/s) by multiplying by face production (t/d or kg/s) averaged over a period of time.

Prediction techniques developed and/ or used by different countries are presented as follows:

3.5.1. France
French prediction methods were initially developed at CERCHAR by Gunther (1967). He considered that there was 100% degree of gas emission from the roof strata to 100m above the workings. In the floor the degree of emission decreased linearly from 100% to 0% at a depth of 100m below the worked seam (Figure 3.4). The zone of emission in the roof and floor strata was considered to be a parallelogram depending on the gradient of the coal face. This appears to be a simplified representation of the emission zone and CERCHAR acknowledge this by stating that it is not the actual zone but merely a simulation. Fifty percent of the desorbable gas content of the worked seam is assumed to enter the ventilation current. Correlations have been made between this prediction method and actual emissions. Some of these correlations are plotted in Figure 3.5. Figure 3.5 shows that in some cases the predicted emissions were more than 20% in error. Within the zone of emission Gunther considers emission on the basis of 100m of stone being equivalent to 1m of coal (Boxho et al, 1978).

Gunther's method was greatly improved by Jeger (1977). Work by Jeger revised the geometrical configuration for the variation of the degree of gas emission with distance from the worked seam. The revised configuration is based on practical measurement and is shown in Figure 3.6. He considers the thickness of 100m of shale or fine sandstone with shaly partings, and 10m of coarse sandstone is equivalent to 1 m of coal. French experience has shown that a minimum of 1m³/t to 3m³/t remains in coal seams affected by mining operations. Accordingly the degree of gas emission from adjacent seams are now calculated from the initial gas content less 2m³/t; e.g for distance from 30m to 120m the degree of gas emission is equal to (initial gas content - 2)/(initial gas content) x 100%. The revised method has been shown to have an accuracy of better than 20% on correlation with actual emissions.

3.5.2. Belgium
Fig. 3.4. Gunther's method (Curl, 1978)
Fig. 3.5. Gunther's method compared with measured emission (Curl, 1978)
Fig. 3.6. Jeger's method (Curl, 1978)
The Institute National des Industries Extractives (INIEX) have adopted a prediction method which is basically a modification of the French method. Initially they employed Gunther's convention of 100% emission to a height of 100m in the roof. But their investigations have led them to believe that emission does not then immediately drop off to 0%. One hundred percent emission to a height $x$ above the worked seam with emission then reducing linearly to 0% at a further height $d$ is the configuration now used for roof emissions (Figure 3.7) Boxho (1978) (Curl, 1978) has adjusted the values of $x$ and $d$ so that the predicted emission agrees exactly with the measured gas make recorded in a number of longwall workings. In the floor the degree of gas emission is considered to be 100% for the first 20m and then reducing linearly to 0% another 30m below (Figure 3.7). In considering the gas content of strata about the worked seam, standard assumptions are used. Sandstone 10m thick is taken to have a gas content equivalent to 1m of coal, as is a 100m thick shale layer. For non-coal strata in the roof, the CH$_4$ content of the coal seam below it is used for the above calculations. For strata in the floor, the content of the seam above the stratum to be considered is used for the calculations. If the CH$_4$ content of the worked seam is the only content known then it is used for all calculations (Curl, 1978). In Belgian mines it has been found that the CH$_4$ make from non-coal strata can be up to half of the total emission. It appears that INIEX has modified the CHERCHAR method to suit Belgian mining conditions.

3.5.3. West Germany

CH$_4$ prediction methods in present use in West Germany are those developed by Flugge, Schultz and Winter (Curl, 1978). All three methods use the perpendicular distance from the worked seam to adjacent strata in their calculations. They appear to be most accurate for strata with gradients of less than
c) INIEX method, Belgium
Experimental variation in roof

Fig.3.7. INIEX method
18°. Originally the non-coal strata was disregarded in terms of CH4 emission. However, the rock strata is now assumed to have a gas content of 1%-10% of the content of adjacent coal seams. Koppe (1976) has found that 4% generally gives the best correlation between predicted and actual emissions.

Flugge's method considers the flow of CH4 into longwall workings from a triangular prism imposed on the workings (Figure 3.8). Another triangular prism is considered beneath the workings. The prisms represent the zone of gas emission. The internal angle of the floor prism is a constant 22.5°. Internal angles of the roof prism vary depending on the intensity of any CH4 drainage program in use. More intensive drainage is considered to result in a larger zone of gas emission, and hence a greater internal angle is applied. Flugge's method assumes a 100% of gas contained in strata within the prismatic zone is assumed to enter the working. However, this can be thought of as partial emission from rectangular blocks above and below the seam for which the degree of gas emission is given by

\[
\text{Degree of emission } \% = 100 - \left( \frac{200 h \cot \alpha}{l} \right) \tag{3.2}
\]

where:

- \( h \) : the height in the roof or depth in the floor, m
- \( l \) : the face length, m
- \( \alpha \) : internal angle of prism

The variation of degree of gas emission with distance from the worked seam according to Flugge's method is shown in Figure 3.9.

Schultz method models 100% emission from a semi-cylindrical zone for emission from roof strata. The diameter and hence volume of this zone are governed by the longwall face length. The diameter is half the face length (Figure 3.8). If this zone is considered rectangular in section the degree of gas from the roof is given by:
a) FLÜGGE, Triangular prisms

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_R$</td>
<td>50 gon</td>
<td>60 gon</td>
<td>65 gon</td>
</tr>
<tr>
<td>$\alpha_F$</td>
<td>25 gon</td>
<td>25 gon</td>
<td>25 gon</td>
</tr>
</tbody>
</table>

A No drainage  
B Medium drainage  
C Intensive drainage

b) SCHULTZ, Semicylinder

c) WINTER, Rectangular prism

\[ AR = 100 \exp (-\mu (h-20)) \]
\[ AF = 100 \exp (\mu (h+8)) \]

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_R$</td>
<td>0.016</td>
<td>0.014</td>
<td>0.012</td>
</tr>
<tr>
<td>$\mu_F$</td>
<td>0.070</td>
<td>0.050</td>
<td>0.030</td>
</tr>
</tbody>
</table>

A Strong strata  
B Medium strength strata  
C Weak strata

**Fig.3. 8. Zones of gas emission used in West Germany (Curl, 1978)**
3.9. Flugge's method (Curl, 1978)

d) Flugge's method, FRG
Face length = 200m
A No drainage
B Medium drainage
C Intensive drainage
Degree of emission \( \% = \frac{100}{l} \sqrt{\left( l^2 - 4h^2 \right)} \) \hspace{1cm} (3.3)

where:

- \( h \) : the height or depth from worked seam, m
- \( l \) : the face length, m

Schultz method considers that there is 100% emission to 5m depth in the floor and then emission decreases linearly to 0% at 20m depth. The profile of Schultz’s method is shown in Figure 3.10.

Winter’s model is different from the previous ones. It gives the degree of emission more directly. Winter assumes a rectangular zone of emission (Figure 3.8) for both the roof and floor strata. He calculates the degree of emission via the following relationships:

Degree of gas emission (roof) \( \% : 100 \left( \mu (h - 20) \right) \) \hspace{1cm} (3.4)

Degree of gas emission (floor) \( \% : 100 \left( \mu (h + 8) \right) \) \hspace{1cm} (3.5)

where \( \mu \) is termed the weakness number. The value of \( \mu \) depends on how easily strata surrounding the worked seam fracture to form CH4 flow paths. The upper and lower limits of the emission zone are defined by a minimum degree of emission of 10%. Practical measurements have ascertained that this zone has extended between 164m and 212m in the roof and between 41m and 85m in the floor. Winter’s curves are shown in Figure 3.11.

In West Germany as in other countries it is common for the zone of gas emission of new workings to intercept old workings. For this situation a prediction is first made for the gas that has been emitted from the old workings, allowing for a degree of gas emission from these workings when intercepted.
Chapter 3 - 29

e) Schultz's method, FRG
Face length = 200m

Fig. 3.10. Schultz's method (Curl, 1978)
f) Winter’s method, FRG

A. Strong strata
B. Medium strength strata
C. Weak strata

Fig. 3.11. Winter's method (Curl, 1978)
To calculate emission from the worked seam into mine workings, it is considered that between 30% and 70% of the CH₄ content is remnant in the coal when it leaves the ventilation district. The actual percentage depends on the desorption rates for different coals and on mining parameters. A slower desorption rate obviously means more remnant gas. If a specific desorption rate is not known for a particular seam to be investigated, 50% emission is assumed.

The floor emission prediction methods of Flugge, Schultz and Winter have now been checked by Koppe (1975); Koppe used borehole measurements to define the extent of the emission zone in the floor. His plots of the degree of gas emission against depth incorporate a variable to account for the variation of gas emission which he has found to exist along a longwall face (Figure 3.12). The plotted curves are simplified representations of statistically derived mathematical expressions for the variation of the degree of gas emission with depth and location along the face length. Roof emissions are still calculated by the methods of Flugge, Schultz and Winter. An earlier attempt to define the extent of the gas emission zone was made by Noack (1969, 1970) (Curl, 1978). His work failed to provide a direct model of the emission zone but it did give the general indications that the upper limit was 130m above the workings, the lower limit was 50m below them and that the lateral limit was 30m either side and ahead of a longwall face.

Kaffanke (1971) (Curl, 1978) has compared actual emissions with predictions from the Schultz and Winter methods for coal mines in the Ruhr basin. The results were not satisfactorily successful. From one hundred predictions of CH₄ emission, only 49 were within 25% of the actual emission measurements. Attempts are now being made to develop computer programs for CH₄ prediction application in West Germany. Reuther (1975) (Curl, 1978) has done work to develop such a program using a method comparable to that of Flugge.

3.5.4. Poland
Fig. 3.12 Koppe's curves for degree of gas emission in floor strata (Curl, 1978)
In Poland coal seams are classified according to CH₄ content of the seam or the gas emission into workings depending on which gives the more severe classification (Table 3-1). As with prediction methods in other countries the Polish consider CH₄ emission in component parts, namely emission from the coal face, from coal being cleared out of the mine, from the coal sides of gate roads and from underlying and overlying strata. The development of Polish prediction methods is based on work carried out at the Barbara Experimental Mine.

Emission of gas from the worked seam is related to the surface area of coal exposed at the face. A fixed value of gas emission per unit area (m³/m²/min) is used according to the category of the coal seam on the basis of the in-situ gas content. It is assumed that, during clearance, 80% of the remnant CH₄ in the cut coal desorbs into mine airways, with 20% remaining in the coal on its arrival at the surface. Emission from coal in the roadway sides is taken to depend on the age of the development. With roadways developed well in advance of longwall operations this source of emission is frequently considered negligible. CH₄ emission prediction from adjacent seams is similar to that in Western Europe where the degree of the emission is related to distance from the worked seam (Figure 3.13). The % emission curve for upper seams is defined by:

\[ AR\% = 64.7(-0.03957h/t) \] (3.6)

where:

\( A_R \) : degree of gas emission in the roof, %

\( h \) : height or depth from worked seam, m

\( t \) : extracted seam thickness, m

For seams in the floor the % emission curve is given by:
TABLE 3 - 1

The classification of coal seams used in Poland
(reproduce from Curl, 1978)

<table>
<thead>
<tr>
<th>Category of CH₄ hazard</th>
<th>CH₄ content of worked seam, m³/t</th>
<th>Specific measured CH₄ emission in a development heading, m³/t</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non gassy seam</td>
<td>&lt;0.002</td>
<td>-</td>
</tr>
<tr>
<td>I</td>
<td>0.02 - 2.50</td>
<td>&gt;5</td>
</tr>
<tr>
<td>II</td>
<td>2.50 - 4.50</td>
<td>5 - 10</td>
</tr>
<tr>
<td>III</td>
<td>4.50 - 8.00</td>
<td>10 - 15</td>
</tr>
<tr>
<td>IV</td>
<td>&gt;8.00</td>
<td>&gt;15</td>
</tr>
</tbody>
</table>
Fig. 3.13. The Barbara Mine method (Curl, 1978)
\[ AF\% = 54.1(-0.0372/ h/t) \quad (3.7) \]

where:

\( AF \): degree of gas emission in the floor, \%

These relationships were established on the basis of results of gas content measurements in adjacent seams both before and after they were affected by mining operations. The maximum degrees of emission are 54.1\% in the floor and 64.7\% in the roof. These values are very low in comparison with Western European methods, many of which have 100\% emission to a considerable distance from the worked seam. The Polish do not take into consideration the gas content, if any, of adjacent strata other than coal. They have standardized the Barbara mine method to yield the best correlations with actual emissions from their mines. A coefficient of irregularity has been included in their methods to account for peaks of methane emission. A factor of 1.65 is used for development roadways and the factor is 4.6 for longwall gate roadways and faces.

A method based on seam seam gas pressure is used in some mines in Poland. This method is much different from the methods discussed thus far which have all been based on the degree of gas emission from an emission zone. The residual pressure in adjacent seams after they have been influenced by mining operations is predicted using curves such as that shown in Figure 3.14. This prediction was enabled by work by Ajruni (1970). It can be seen that the dip of the strata has a great effect on the residual pressure at a particular distance from the worked seam. To make a prediction of the CH4 emission from adjacent seams, the relevant residual CH4 pressure curve is selected from Figure 3.14. This curve is then superimposed on the virgin CH4 pressure curve for the worked seam and surrounding strata (Figure 3.15). The virgin pressure is a function of depth below the surface. The positions of worked and adjacent seams are also plotted on Figure 3.15. For each seam the difference between the virgin and residual CH4 pressure is
Fig. 3.14. Curves for residual methane pressure in adjacent coal seams as a function of strata deep ratio of distance from the worked seam to the extracte thickness is used in the roof strata

(Curl, 1978)
Fig. 3.15. Example of the method of pressure difference prediction
A: original in-situ methane pressure curve
B: residual methane pressure curve after mining
(Curl, 1978)
noted. The drop in gas pressure due to mining results in decreased gas sorption in the coal and hence CH₄ desorbed and emitted into mine workings. The quantity which can be retained by the coal at the residual gas pressure can be derived from the adsorption isotherm for that coal. This residual content is subtracted from the initial content to give the quantity of CH₄ emitted. Emissions from all adjacent seams are summed to give the total predicted CH₄ flow into workings. However, this method does not enable differentiation between CH₄ emission from the coal face and that from coal being transported from the mine.

No data have been obtainable on the accuracy of the Polish methods. However, it appears that the Barbara mine method has an advantage over Western European methods in that it considers gas volume emitted per unit area per unit time as compared to volumes emitted per tonne of coal mined. This seems to be more useful when determining air flow quantity requirements. Also the Polish have attempted to use a pressure based prediction which is more useful in developing a laminar Darcian flow model.

3.5.5. U.S.S.R.

Russian mines are often extremely gassy and hence CH₄ prediction is of primary importance in the design of mine ventilation systems. A standard method of ventilation design has been developed and it includes CH₄ prediction techniques. The prediction techniques consider separately the emission into extraction workings, development roadways and old workings. Much of the prediction development work has been conducted by Lidin et al (1965).

Prediction methods used in Russia appear to use the in-situ CH₄ content of the worked seam and the remnant CH₄ content of the coal during clearance to the
surface. The Russians used the mathematical expressions include terms for the in-situ CH₄, and also employ a coefficient which depends on the system of working.

There are two methods which are commonly used to determine CH₄ emission from surrounding coal seams. One is comparable to Western European methods using the degree and zone of emission concepts. The emission zone is rectangular with the extent of the rectangle depending on the thickness of the coal to be extracted, the dip of the strata and whether caving or stowing techniques are practiced. The degree of emission for each adjacent coal seam is directly related to its distance from the worked seam as shown in Figure 3.16. As with Western European methods the gas emission is calculated from the degree of emission by considering the thickness of each seam and its desorbable CH₄ content. Russian experience has shown that surrounding strata excluding coal seams contribute between 10% and 15% of the total emission. Emission from surrounding strata is therefore calculated on this basis. Degree of gas emission is expressed as:

\[
\text{Degree of gas emission} \% = 100 \left(1 - \frac{h}{h_{\text{max}}} \right) \tag{3.8}
\]

where:

h : vertical distance from worked seam, m

A residual pressure method is also used in Russia. It involves determination of the residual pressure in under and overlying seams. This uses the distance from the seam under consideration to the worked seam, the dip of the strata and the extraction thickness. The measured or predicted virgin CH₄ pressure and the predicted residual pressure are applied to the adsorption isotherm for the coal to give the predicted emission (= content at measured/predicted virgin pressure - content at predicted residual pressure) from each seam being considered. These emissions are summed for all others seams and gas from the worked seam to yield
1.5m, level seam with full caving.

Fig. 3.16. Lidin's method (Curl, 1978)
the total emission.

In development roadways CH4 emission from broken coal and exposed coal surfaces contribute to total methane make. The gas flow from exposed coal surfaces is given by an empirical equation which includes terms for roadway dimensions, seam thickness, the rate of advance and the rate of initial CH4 emission from a freshly exposed coal surface (m3/m2/min). The initial rate of CH4 emission is considered as a function of percentage of volatile matter in the coal. Emission from broken coal in development headings is calculated from a remnant gas content and the tonnage which has been cut.

Gas emission from old workings has been found to contribute between 5% and 20% of the total emission from other sources in Russian mines. The percentage depends on the number of levels being mined. Prediction of emission from old workings is made on the basis of such a percentage. This predicted emission is added to the CH4 make from the face and development workings to give the total CH4 emission for the mine.

3.5.6. The United Kingdom

*M.R.D.E.* is working on a CH4 prediction model based on theory of *Airey* (1968, 1971, 1978) of gas emission from coal. Airey developed a gas emission model which regards the coal seam as an assembly of lumps of broken coal.

Theory of Airey may be summarized as follows:

In his earlier study (1968), he had derived an equation to fit the observed emission of gas from pieces of coal of different size as:

\[ Q_t = Q(1 - \exp(-t/T)^n) \]  \hspace{1cm} (3.9)

where:
Qt : the quantity of gas emitted in time t, cm³/g
Q : the initial gas content, cm³/g
t : time, second
n, T : constants

Then in his subsequent work (1971), the coal seam ahead of the face was visualised as fragmenting into 'lumps' which decreased in size with the increasing stress associated with approaching coal face. The fracture structure developing around the lumps was considered to provide the channel for gas to escape to the airways of the working. The fractures were considered to give negligible resistance to gas flow (even in the region of maximum stress) and the rate of emission to be determined entirely by the emission characteristics of the lumps.

Then Airey used his work in the field of rock mechanics to extend the theory to include all the seams in adjacent seams disturbed by the working.

Emission from lumps of coal of a particular size is characterized by the time constant denoted by t₀, or t₁ where it varies with lump size, and summation from a seam depends on knowledge of the distribution of lump size and hence of t₁ in the seam. For the worked seam an exponential distribution was applied:

for x>0 , t₁ = T exp (x/x₀)
for x<0 , t₁ = T

where x is the distance ahead of the position of maximum stress (front abutment), x₀ is constant and t₀ is the minimum time constant which takes place at and behind the front abutment position.

Extending this for application to adjacent seams, he assumed that t₁ depends on function of stresses in the seam, and by taking the ratio of principal stresses (σ₁/σ₃) as a criterion for rock failure, he deduced that surfaces of equal t₁ in the strata are coincident with surfaces of equal value of the principal stress ratio. By using analytic solutions for the stresses around a coal face, he was able to compute
the distribution of time constants around the face in a coal seam, and hence the degree of gas emission from seams in adjacent strata as a function of distance from the face line.

He has found a good agreement when comparing model curves with curves based on experimental results for emission from coal samples taken from three British coal mines. For calculation of the degree of degasing of surrounding strata, age of the worked district and face advance rate are required.

There are two parts of to the _M.R.D.E._ method. Firstly the prediction calculations are tabulated and the degree of gas emission is presented graphically. In the second part a computer program enables emission to be determined as a function of time. This program considers the shift by shift face advances, gives the required airflow to dilute methane to acceptable concentration levels and allows for peaks of CH4 emission during production. The program also enables the gas make at various locations in gate roadways to be predicted.

Total CH4 emission is divided into three categories in the _M.R.D.E._ method:

1. emission from the worked seam
2. emission from adjacent coal seam
3. emission from broken coal during clearance

The degree of gas emission from the worked seam before the coal is cut is a decreasing function of the rate of face advance (Figure 3.17) Initially the _M.R.D.E._ method considered the relationship between the degree of emission and distance from the worked seam to be the same for both underlying and overlying seams. As a result of work by Airey on the effect of the distribution of stress around longwall workings on gas emission, a non-symmetrical distribution of degree of emission is used. Figure 3.18 shows the degree of gas emission plotted against distance from a worked seam at a depth of 900m. At other depths a correction factor from Figure 3.19 must be applied. As can be seen from Figure 3.18 the degree of gas emission increases with the age of the district. It may be
Fig. 3.17. Curve for degree of emission against face advance (Curl, 1978)
Fig. 3.18. Degree of gas emission at 900m
(Curl, 1978)
3.19. Correction of height before using 900m curves
(Curl, 1978)
noted that only coal seams are considered as potential sources of CH4 in the 
*M.R.D.E.* method. However, gas release from other strata could be included 
without undue difficulty. But it is believed that such strata does not usually 
contain significant quantities of CH4. In their predictions the M.R.D.E. prefers to 
know the gas content of each individual seam. If such data are not available the 
gas content of the worked seam is used.

The degree of emission from coal being transported away from the face 
along the intake depends on the time that elapses while the coal remains exposed 
to the ventilating air of the district. *Figure 3.20* shows an *M.R.D.E.* curve for the 
degree of emission from a bituminous coal against exposure time to the ventilation 
current. This curve is based on coal cut by a longwall shearer. Different curves 
would be applicable for other mining machines such as continues miners in 
development, or ploughs on longwall (commonly used in West Germany), since 
they produce a different coal size distribution of won coal. Such differing curves 
are a consequence of the dependence of degree of emission on the degree of coal 
breakage. *Kissell and Deul (1974)* has concluded that the CH4 emission resulting 
from coal breakup contribute only a small proportion to the total gas emission from 
the working district.

When CH4 drainage is practised, an arbitrary criterion is used to estimate 
the quantity of CH4 being drained. All of the gas emitted from the coal strata 
which is above and below the worked seam and behind a vertical plane passing 
through the face line is assumed to enter the drainage system. Gas from ahead of 
the face in the worked and adjacent strata and seams is assumed to enter the 
ventilating air. CH4 from cut coal also enters the air flow. In *Figure 3.18* the 
curve for zero age is used to predict the CH4 emission entering the ventilating air 
from from adjacent seams. Predicted flow into the drainage system is the 
difference between the zero and district age curves. Knowing the degree of gas 
emission the *M.R.D.E.* method enables the remaining CH4 content in adjacent
Fig. 3.20. An example curve for the degassing during coal clearance (Curl, 1978)
seams to be calculated at any time during the mining of the worked seam. Therefore, if a second seam is to be worked, the expected CH$_4$ make from the surrounding and partially degased seams can be determined.

There is provision for taking into account any increase in CH$_4$ make which may occur towards the end of a working week in in the M.R.D.E. prediction model. It is confirmed that such an increase does occur in many countries including Australia (Hargraves et al, 1964). To take this variation of emission into account, the degree of degasing is varied as a function of face advance from the beginning of the week. This function thus allows variable advances and even holiday periods to be brought into predictions.

A French concept of a coefficient of irregularity or peak factor to account for sudden peaks in emission above the mean level has been adopted by M.R.D.E. This coefficient is used to calculate the air flow required to dilute peak CH$_4$ levels to below statutory limits. At the return end of the face predicted emission is multiplied by a factor of 2.0 and the outbye end of the return airway of the panel by a factor of 1.5 to give expected peak emissions. These peak factors are somewhat arbitrary and may be modified with further experience.

Considerable importance has been placed on the presentation of its predictions by the M.R.D.E. They present predictions in a form that they feel best indicates to a ventilation engineer what he has to do to reduce CH$_4$ concentrations. Examples of emission to an acceptable level and predicted collection by CH$_4$ drainage in Figure 3.21 are given as a function of weekly face advance. The equivalent ventilation is the additional air quantity required if drainage is not practised and a steady emission is assumed.

Development of the M.R.D.E. method appears to have much promise. Predicted CH$_4$ concentrations have been compared with actual concentrations in several U.K. coal mines with results correlating reasonably well. However, in certain cases the predicted CH$_4$ concentrations have been below actual
Fig. 3.21. Example presentation of predictions (Curl, 1978)
concentrations. If this difference is significant, a ventilation engineer may underestimate the air quantity required for dilution of methane to acceptable levels resulting in an inadequate ventilation. One way to overcome this is to increase the peak factor. As stated before, this will occur with further experience.

3.5.7. United States

In European longwall operations a large part of the CH4 emission originates from adjacent seams and strata. This is due to the great strata relaxation associated with longwall mining. In the U.S.A. bord and pillar mining is used more widely than longwall mining (although the use of longwall is increasing rapidly (Peng, 1986), consequently much reduced gas emission can be expected from adjacent seams and strata. Hence, it is generally associated with emission from the worked seam. CH4 prediction research in the U.S.A. has concentrated on forecasting the flow of CH4 from the worked seam. There has also been considerable interest in seam gas predrainage (Davis and Krickovic, 1973 and Deul and Elder, 1973) and seam gas production (Price and Ancell, 1978).

Kissell et al (1973) have found that a good estimate of CH4 emission into mine roadways can be made from a direct determination of the in-situ CH4 content of the worked seam. This appears to be applicable in large deep mines where coal production is constantly in excess of 2000 tonnes/day. Figure 3.22 shows a plot of direct CH4 content against actual emission for six United States coal mines. An almost linear relationship is evident despite the fact that the mines are producing from widely different coal seams surrounded by different adjacent strata. Although such a relationship can only be considered as a tentative correlation, it should provide a good approximate CH4 prediction technique for coal mining conditions commonly encountered in the United States.
Fig. 3.22. Actual emissions against estimate using direct method for some U.S.A. mines (Curl, 1978)
Owili-Eger (1973) and Owili-Eger and Ramani (1974) have developed a computer model to simulate CH4 flow from coal seams and intervening strata into mine workings. Their initial model was a steady-state model. Owili-Eger develops the model by combining laminar flow, a mass balance equation and the general equation of strata for a gas obeying Boyle's law. He gives a final flow equation which is a second order non-linear partial differential equation. He solves this equation for CH4 emissions using a finite difference scheme and a computer to obtain the solutions. His computer program requires input parameters to define model size, initial conditions and boundary conditions. These conditions include initial gas pressure and face pressure, properties of the coal seam and strata such as directional permeabilities, porosity and temperature of coal seam, and properties of the flowing gas. The output yields the predicted gas pressure distribution and the CH4 flow rates on a time basis (m3/day, m3/min). In a correlation exercise this method predicted a flow of 500m3/day into a face area which compared to a subsequently measured mean flow of 450m3/day. Ramani and Owili-Eger have extended their work to cover unsteady-state flow. They have found that unsteady-state predictions were in better agreement with field measurements than steady-state predictions, but that the difference was small and in practice either condition could be used. The Owili-Eger and Ramani model will be used as an integral part of mine ventilation planning in the U.S.A.

In underground mining operations considerable volumes of water can flow from both the worked seam and adjacent strata. Dewatering leads to increased permeability to CH4 flow. Therefore it would be a great advantage to have a model of the two-phase flow of water and CH4 as compared to the single-phase flow of CH4 alone. Such a model has been developed for the United States Bureau of Mines (U.S.B.M.) in the form of two computer programs. These programs were developed by specially adapting reservoir models used regularly in the petroleum industry to give very accurate predictions. The area of the coal seam under
consideration is divided into grid blocks typically about 3m square. Parameters affecting flow such as porosity, permeability, seam thickness and depth may be defined for each block in the model. The coal seam is assumed to have a finite boundary within which the mine workings are described by internal moving boundaries. A source is incorporated in the model which simulates the desorption of CH\textsubscript{4} from coal and its diffusion through the coal mass into the fracture system. The model then considers the flow of CH\textsubscript{4} through the fracture system in the coal to the mine workings. Flow is assumed to be laminar and Darcy's law is used. Darcian based flow relationships are solved by numerical solution techniques (e.g. finite difference schemes). Output from these programs yield prediction of CH\textsubscript{4} concentration gradients and pressure distributions within the seam. More importantly, the flow of CH\textsubscript{4}, or CH\textsubscript{4} and water into mine workings is given as a function of time.

American methods are much different from European methods, mainly due to the difference in the dominant mining method. In the U.S.A. there appears to be little attention paid to the determination of degrees or zones of emission, because emission from adjacent strata is considered much less significant. However, American prediction methods offer much promise when attempting to forecast emissions in bord and pillar mining operations. Bord and pillar mining is widely practised in Australia, although longwalls are coming to the fore quite rapidly. Therefore, the development of both European and American techniques for methane prediction is required so that they can be applied to Australian coal mining conditions.

3.5.8. Australia

For Australian coal mining, no standard method has been developed to predict gassiness associated with the various geological and mining conditions,
and the relationship between coal output and total CH4 make has not been established.

Up to this stage, only a proposal by Hargraves (1986) and the investigation by Lunarzewski and Larkings (1985, 1986) could be accounted for prediction method.

The following factors are considered by Hargraves (1986) for Australia to develop its own method:

(i). although in retreating method the retreat is faster than in advancing longwall faces, as the longwall block is mined with only some of the original contained gas, the gassiness of the coal mined is less than in advancing

(ii). differences in sorptive capacity and permeability between the likely Carboniferous European and Permian Australian coals

(iii). differences in the caving characters of the overburden shown by differences in European and Australian subsidence experience suggests differences in strata permeability

(iv). the degree of emission of gas from seams presented by Curl (1978), irrespective of coal rank; whereas the higher sorptive capacity and lower permeability of higher rank leads to proportionately more gas liberated more slowly

(v). European methods do not consider that the minimum span of goaf has great bearing on the distance to which caving extends in the roof and changes in the floor occur.

In spite of the fact that there is a great difference between European coal and Australian coal, he proposed the following curves:

1. a minimum gas emission curve, which is a combination of Schultz, Barbara Mine, INIEX, and Lidin methods
2. a maximum gas emission curve, which is a combination of Flugge, Lidin, Jeger, INIEX, and Gunther methods

3. an average gas emission curve of all authorities

These European predictions for longwall advancing operations consider the gas content of the working seam reduced by, any gas retained in the coal on reaching the surface. For longwall retreating, the discounting also includes gas emitted from the longwall block of the working seam prior to commencement of mining. For pillar extraction, considerations are the same as for longwall retreating, but usually pillars for extraction have emitted all their gas within six months of formation (40m dimension in high rank bituminous coal) and desorbable gas content could be taken as zero (Hargraves, 1986).

Lunarzewski and Larkings (1986) have investigated the relationship between coal output and total CH4 make by systematic gas balance measurement during longwall extraction. Then a computer method was used to approximate the mathematical equation from the initial graphs of coal production against quantity of CH4 in the ventilation system for various conditions.

The predictions made at the early stage were based on empirical and theoretical formula and graphs which considered factors such as coal volatile matter, seam thickness, distances to other seams, coefficient of degasing, CH4 content of working and adjoining seams, and specific rates of gas emission for different production levels. Their analysis included stratigraphic columns, measurements of gas content and gas macropermeability, gas balance surveys, and the assessment of gas drainage applications.

In investigations monitoring the absolute gassiness for the overall workings in the mine as well as for the individual panels, occasional gas balance measurements around the working and development panels and gas flow rate measurements from cross-measure and in-seam drainage holes were conducted
(Lunarzewski and Larkings, 1985). The results obtained from investigations indicated the need for some modifications to the emission levels predicted initially.

3.6. A comparison and summary of emission prediction methods

The prediction techniques reviewed are irrespective of coal rank, whilst rank is generally accepted as an important factor in coal sorptive capacity.

The factor of the minimum span of goafs which has bearing on the distance to which caving in the roof and relaxation in the roof and floor extend is not taken into consideration. The presumed height of roof caving depends only on height of extraction.

Most Western European methods have evolved purely from practical experience and correlation with actual emissions. The West German methods of Flugge, Schultz and Winter and the Russian method (Lidin) give very similar predictions. Gunther’s method (France) gave far higher prediction than these methods but it has now been superseded by Jeger’s method which gives lower predictions comparable to the West German and Russian predictions. The M.R.D.E.-method has always given higher predictions than European methods. When comparing any method against actual measured emission in a mine it is likely there will be an error in the measured. This error is due to to the inherent inaccuracies in measuring ventilating air velocities and seams gas contents. The M.R.D.E. suggest that measured emission could itself have an error as great as 32%. Jeger believes his prediction method to have an accuracy of 20%. Noack (West Germany) considers the accuracy of present prediction methods to be far from satisfactory. He estimates that errors of 100% are possible. The assessment of anomalous conditions in coal measure strata appears as one of the greatest difficulties in making an accurate forecast of methane emissions. Personal
assessments of these conditions may always remain an important part of prediction methods.

Each of the degree of gas emission type prediction methods is different in its detail. The Gunther and Jeger methods have fixed degree of emission curves. Flugge and Schultz consider the longwall face length. Flugge includes the intensity of CH4 drainage. Winter considers the strength of the surrounding strata. Polish and Russian methods have terms for the thickness of the extracted seam incorporated in them. The M.R.D.E. methods consider seam depth and the age of the district. The Barbara Mine method of Poland has unusually low maximum degrees of gas emission. However, it can be concluded that as all these methods are largely empirical, such diversity is not surprising.

A major difference between prediction methods is their means of determination of emission from adjacent non-coal strata. In some methods hypothetical or assumed contributions to total gas make are included. All degree of emission type methods can predict CH4 emission into new workings, the zone of emission of which intercepts old workings providing all necessary data are available.

There are differences of opinion with regard to how much of the desorbable gas content of the worked seam is emitted into mine workings. Gunther and Jeger believe that 50% enters mine workings while the West German believe that between 30% and 70% enters them, depending on desorption rate of the coal. If the desorption rate is not known by the West Germans a value of 50% is assumed, which is the value that the French always use in any case. The M.R.D.E. method has an expression for emission from the worked seam as a function of weekly face advance. Polish methods use measured values of face emission and apply them to the exposed coal surface area to determine worked seam emissions on a time basis in m3/m2/min. All of these different approaches are depicted in Table 3.2
## TABLE 3 - 2

Factor taken into considerations by various national prediction methods

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<td>Emission from conveyor</td>
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<td>Gas content of adjacent seams</td>
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<td>Gas content of other strata</td>
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Opposing opinions on how much of the CH$_4$ content of coal can be desorbed are quite evident. The gas content of a coal seam or a coal sample is possibly interpreted in two ways, namely the quantity of gas (m$^3$/tonne, cm$^3$/g) which will desorb down to atmospheric pressure, and the other is the quantity of gas which can desorb down to zero absolute pressure. According to the former theory, methane desorbs from coal until it is in equilibrium with free CH$_4$ in its fracture system at atmospheric pressure. This method is used in Belgium and West Germany, while the French consider the maximum desorbable gas content for mining conditions to be the content desorbable to atmospheric pressure less 2m$^3$/t. The latter interpretation is based on the observation that large blocks of coal can degas completely. This method is used in the United Kingdom (*M.R.D.E.* ) in the application of Airey's method.

A very great distance exists between European and American approaches to the CH$_4$ emission problem. In the United States the emphasis has been on emission from the worked seam. This is due to American mining methods not resulting in as great an emission from adjacent strata as occurs in the predominant longwall mining methods of Europe, where emission from adjacent strata is significant.
CHAPTER IV

INFLUENCE OF DESORPTION PROCESS ON GAS FLOW

4.1. Introduction

The measurement and prediction of the gas that can be adsorbed in coal is important, but it does not explain the gas flow in coal. Gas which was also formed during the coalification process is partly retained by coal because of its affinity to adsorb on coal surface. If the process makes gas available to the coal surfaces, then the coal-CH₄ system will exist in equilibrium at the prevailing temperature, pressure and moisture content.

If the coal in equilibrium with a particular gas pressure is suddenly exposed to a lower pressure, the coal will desorb some of its adsorbed gases. The quantity which would be desorbed may be calculated by the difference between equilibrium volume at initial conditions and that at the reduced pressure.

Patching (1970), Cervik (1970) and Kissell (1972) postulate that gas flow in coal can take place in two ways. In unfractured coal, the flow is thought to be a diffusion process with a concentration gradient as the driving force. In fractured coal, the gas flow is thought to be through fractures with pressure gradient as the driving force.

In laboratory work gas flow may be modelled by adsorption - desorption. A good understanding of the desorption process will help to elucidate the mechanics of gas flow in coal. This chapter presents the results of laboratory work on the adsorption - desorption process in coal.
4.2 Adsorption-desorption tests

When a gas is in equilibrium with solid, the concentration of gas molecules is always greater in the layer close to the surface of the solid than in the free gas phase, regardless of the nature of the gas and the solid. The process of the increase in the concentration of the gas molecules and their physical hold onto the solid surface is called adsorption. Adsorption is a reversible and a reproducible process.

Although the adsorption is instantaneous, the penetration of the gaseous phase to the less accessible internal surface of a porous medium is dependent on the process of fluid flow through absorption. Absorption describes a more or less uniform penetration of gas into solid, therefore a process which involves diffusion to a certain extent. Absorption is not considered to play a significant role in the flow of methane from coal (Patching, 1970). Therefore in this context, the use of the term adsorption is chosen for the gas content of coal.

The pressures and the equivalent adsorptive capacities are normally defined graphically by adsorption isotherms. The graphs plot the volume of gas adsorbed against pressure at constant temperature.

For low absolute gas pressure (< 100 kPa) the quantity of adsorbed gas at pressure P C_\text{a} is almost directly proportional to pressure. Above 5000 kPa, C_\text{a} shows no further increase with pressure. Measurement in European 'virgin seams' shows in 80% of the cases in-situ pressures varying from 400 kPa to 4000 kPa (Boxho et al, 1980), while in Australia they vary from 1500 kPa to 4200 kPa (Lama and Bartosiewicz, 1982). For some coal mines which mine Bulli seam coal, at varying depths from 480m to 610m, gas pressure may vary from 3000 kPa to 4200 kPa. Assuming the magnitude of in-situ pressure is available, one practical use of the adsorption isotherms is an indirect method of estimating the total gas content of the coal seam as discussed below.
The moisture content of coal has an important effect on the quantity of gas adsorbed. The general effect of moisture content is a reduction in sorptive capacity. At a given partial pressure and temperature CO$_2$ is much more readily adsorbed than CH$_4$. At the same equilibrium pressure the quantity of gas adsorbed decreases as the temperature rises, hence it is important that all adsorption determinations be conducted at constant temperature. The adsorptive capacity of coal increases with coal rank.

As desorption is a reverse process of adsorption, factors affecting adsorption also affect desorption. If coal in equilibrium with one gas pressure is suddenly exposed to a lower pressure, the quantity of gas adsorbed in it will drop. The gas emission process starts once a fall in pressure occurs at the adsorbed coal surface. A number of studies have been carried out to model gas desorption. Certain empirical formulations, based on simplified relationships, such as (Lama and Bartosiewicz, 1982) are:

\[ Q_t = A^3(t)^{0.5} \]  
\[ Q_t = A^2(t)^{0.5} \]  
\[ \frac{Q_t}{Q} = \sqrt{1 - \exp \left( \frac{-4 \pi D t}{d^2} \right)} \]  
\[ \frac{Q_t}{Q} = \left[ 1 - \exp \left( \frac{t}{T} \right)^n \right] \]  
\[ Q_t = Q \left( \frac{t}{T} \right)^n \]

where:

\( Q_t \): gas desorbed cm$^3$/g in time \( t \)

\( Q \): initial gas quantity, cm$^3$/g
4.3. Coal seam gas content determination

Methods for determining the gas content of coal seams can be grouped into two categories, direct and indirect methods. Direct methods are based on sampling a coal lump, placing in a sealed chamber and then measuring the gas desorbed. Indirect methods are based on laboratory gas sorption characteristics of coal, related to particular pressure and temperature conditions measured in the mine.

4.3.1. Direct methods

The direct method was first developed by CERCHAR in France and has been widely accepted ever since. The original method consists of extracting coal samples and enclosing the cuttings in a container as soon as possible, then the gas content desorbed on enclosure Q2 is determined volumetrically (Bertard et al., 1970). The gas content of a particular sample is composed of lost, desorbed, and residual gas.

In taking a sample, a certain time will elapse between cutting of the sample from the coal seam and when it is enclosed in a container for transport.
During this time it will lose a quantity of gas, normally denoted as $Q_1$. During transport from the field to the laboratory the coal sample releases a quantity $Q_2$ of methane into its container. The gas released with time $Q_2$ is measured by displacement of water (Figure 4.1). Desorbed gas is released into the upper chamber of the inverted graduated cylinder. It is expected that the gas desorbed by the sample will be in the chamber at a slight difference of pressure from atmospheric and will displace an equivalent amount of water. The volume measurement is continued until the gas emitted from the sample is less than 0.05 cm$^3$/g per day for five consecutive days. Testing can be carried out on a part sample or the complete sample. After completing desorption to atmospheric pressure, the sample is removed from the container and the sample is prepared for determination of its content of residual gas.

In the laboratory the sample is crushed in a sealed bomb using steel rods or steel balls and a further quantity of gas $Q_3$ is released. Crushing is done at atmospheric pressure in the U.S. A (Kissell et al, 1973).

The volume of gas lost $Q_1$ is calculated using the relationship $Q_1 = k(t)^n$. The desorbed quantity is at first proportional to the square root of the time (that is when $n=0.5$). The coefficient $k$ is determined experimentally or assumed. A desorption meter which consists of a polyethylene flask of one litre capacity, in order for the counter pressure (=pressure rise) $\Delta P$ not to impede the gas desorption a copper fitting and a U-tube manometer is used in such determination. In estimating $Q_1$, lost time $t$ has to be established very carefully. The amount of the lost gas depends on the drilling flushing medium and the time required to retrieve, measure and describe the sample, and seal the sample in the container. The shorter the lost time $t$, the greater will be the confidence in the calculation of lost gas. If $t_1$ is the time elapsed between the moment when the sample was extracted from the seam and when it was enclosed in the desorption meter, then the sample is left in the desorption meter for an equal length of time $t_1$ and the
Fig. 4.1. Glass test tube for determination of desorbed gas Q2 (Bertard et al, 1968)
quantity of gas desorbed during this time is measured, using \( q = k (t_1)^n \), the quantity of gas \( q \) desorbed between the instants \( t_1 \) and \( 2t_1 \) is \( q = k \sqrt{2t_1} - k \sqrt{t_1} \) if \( n = 0.5 \).

The value of \( n \) was taken as equal to 0.5 by Bertard et al (1970) and Kissell et al (1973), and as between 0.25 - 0.3 by Airey (1968). The total gas content is then given by \( Q = Q_1 + Q_2 + Q_3 \). The size and shape of the sample is an important consideration in this method. It was taken as cuttings of 2mm size and above and a total mass of 10g by CERCHAR and a sample of 30g by Airey and up to 800g by Diamond (1981).

Smaller particle size increases the proportion of 'lost gas' \( (Q_1) \) in \( Q \). A geometric shape should be a better model for analysis than a random chip. Apart from considerations of duration of experiment a drill core would appear to offer the best opportunity for analysis of adsorption and desorption.

4.3.2. Indirect methods

These methods involve basically measurement of seam gas pressure and laboratory determination of the quantity of gas content of the particular coal at this pressure. The indirect method was originally developed by Ettinger (1958) in the U.S.S.R (Curl, 1978) in an attempt to overcome the problems associated with the direct methods. A hole is bored into the seam to be investigated from either underground or the surface. The drillhole is sealed off near its inby end and by either a hydraulically, mechanically or pneumatically expanded rubber collar (Hargraves, 1963, 1986) and the maximum gas pressure measured is taken as the in-seam gas pressure. Also in-seam temperature must be determined. Then gas content of the coal seam \( (cm^3/g, m^3/t) \) can be determined from the relevant
adsorption isotherm curve at the constant temperature of the seam under consideration.

The adsorption isotherms can be either determined in the laboratory by pressurising a coal sample with gas at various pressures, and by determining volumetrically, gravimetrically, or chemically the amount of gas at each pressure. The determinations are conducted with coal samples, either of cuttings of small size or of geometric shape. The determinations are performed at the expected temperature of the seam as mined. The range of normal virgin coal temperatures in Australian mines is 20° to 30°C. For Australian coal, every gas composition between pure CH4 and pure CO2 exists so the influence of composition must be recognised (Hargraves, 1986b). Figure 1a shows seam gas composition for the Bulli Seam, Illawarra area, New South Wales.

The seals set deep in boreholes take some time to build up to full seam pressure. The validating of the results obtained depends on the efficiency of sealing and the presumption that the drilling of the hole has not had the effect of affecting the maximum pressure to be investigated behind the seal.

It is accepted that the gas content of coal depends upon the stress on the coal. But it has become conventional to utilise adsorption isotherms of gas in coal as an absolute basis, with the only stress applying to the coal being the load applied by the confining and surrounding gas.

To prepare an adsorption isotherm on this basis and to use the isotherm along with the measured gas pressure in the seam assumed to be the virgin gas pressure, suggests a particular figure of gassiness to be applied to the coal.

It can be seen that the determination of seam gas content by the indirect method may incorporate assumptions as input data. This suggests that gas content of the seam (m³/t) resulting from such determination may need to be qualified by such assumptions, i.e. that the borehole has reached the position of 'virgin pressure', that the condition of stress existing in the seam does not affect sorptive
Fig. 1a. Seam gas composition for the Bulli Seam Illawarra area (based on Hargraves, 1986b)
capacity measured without stress, providing there are no problems of gas leakage and strata water pressure, and that the temperature is correct. Hargraves (1963) showed that a temperature gradient exists ahead of working faces, as depicted in Table 4-1 and Figure 4.2.

### TABLE 4 - 1

Investigation of seam gas pressure and temperature gradient  
(Developed from Hargraves, 1963)

<table>
<thead>
<tr>
<th>Date</th>
<th>Mine</th>
<th>Site</th>
<th>Depth of hole, m</th>
<th>Gas pressure, kPa</th>
<th>Temperature, °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>26-5-60</td>
<td>Collins.1</td>
<td>No.1 Tunel No.2 Hdg</td>
<td>2.44</td>
<td>6.90</td>
<td>25.78</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5.94</td>
<td>482.75</td>
<td>27.33</td>
</tr>
<tr>
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<td></td>
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<td>9.45</td>
<td>627.58</td>
<td>28.5</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>12.04</td>
<td>675.857</td>
<td>28.89</td>
</tr>
<tr>
<td>31-8-60</td>
<td>Collins.2</td>
<td>No.1 Tunnel No.2 Hdg</td>
<td>3.05</td>
<td>24.14</td>
<td>27.22</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>6.10</td>
<td>186.89</td>
<td>27.94</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>12.50</td>
<td>393.10</td>
<td>27.78</td>
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<td></td>
<td></td>
<td>17.98</td>
<td>358.62</td>
<td>27.78</td>
</tr>
<tr>
<td>17-6-60</td>
<td>Metrop.</td>
<td>3/N.No.4 Hdg</td>
<td>1.83</td>
<td>0</td>
<td>25.72</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>6.40</td>
<td>18.62</td>
<td>27.72</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>9.30</td>
<td>21.38</td>
<td>27.72</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>12.19</td>
<td>26.90</td>
<td>27.39</td>
</tr>
</tbody>
</table>

Collins. : Collinsville  
Metrop. : Metropolitan  
Hdg : Heading
4.3.3. Gravimetric method

In this method the gas adsorbed at each pressure is determined gravimetrically. The equipment consists of a gas supply cylinder with pressure regulator which is connected to a manifold through pressure regulating valves. The manifold has independently controlled outlets to which sample containers ('bombs') are attached using high pressure plastic hoses and fittings. The manifold has connection to a vacuum pump and to the sample bombs. Pressure release
valves are incorporated to release pressure in the manifold line on any of the sample bombs independently.

Sample bombs have both isolation valves and quick release valves (to atmosphere) mounted on them and are placed in a temperature controlled water bath surrounded by a copper sleeve to keep the bombs dry. The main steps of the gravimetric method can be summarized as follows.

(i). Determination of bomb volume

Before starting tests, the sample bombs are calibrated to determine the gas holding capacity of the bombs individually. First the bombs are weighed. Then bomb volumes at atmospheric pressure are determined using distilled water of known density. Then, when the bombs have been cleaned and dried, the capacities of bombs are determined by pressurizing them with gas to equilibrium at various pressures and at a defined temperature. Then calibration curves for bombs can be produced using the volume and capacity of the bombs. Figure 4.3 shows a typical calibration curve, volume related to internal pressure.

(ii). Pressurizing the coal sample and adsorption test

A coal sample is placed inside a sample bomb and the bomb is then closed and weighed to determine the weight of the coal. When all connections to the bombs have been made, gas is introduced and constant pressure is maintained at the predetermined level. Once daily isolation valves are closed, the bomb detached and weighed and then returned to the manifold and repressurised. Each bomb is continually pressurized until equilibrium weight has been reached. After equilibrium has been reached, the amount of gas adsorbed \( (\text{cm}^3/\text{g}) \) is calculated as exemplified in Appendix 1. Gas adsorbed in 1g of coal
is a while 'direct gas volume adsorbed in 1g of coal' is a measured quantity of gas adsorbed, obtained merely by divided weight of gas adsorbed (weight difference between two pressure level = the total gas compressed to the bomb between two pressure level) with gas density divided by sample mass. This 'direct gas adsorbed' is a function of volume of free space in the bomb, i.e. the higher this volume, the higher will be the 'direct gas adsorbed' and this is an undesirable condition. The ideal condition is direct gas adsorbed = gas adsorbed, which can be obtained by completely eliminating free gas space. Figure 4.4 to Figure 4.6 shows the relationship between gas adsorbed and the direct gas adsorbed, both calculated from this current work.

The process is repeated at sufficient different pressures to enable the sorption isotherm to be produced at the chosen temperature.

(iii). Desorption tests

When the equilibrium at the highest pressure in the range has been reached, the pressurised bomb is placed on the balance and the quick release valve is opened for desorption. Adsorption is a reversible process, so the experimental procedure for the desorption test is the reverse of the previous experiment in three stages, thus:

(i). The final weight of the bomb at a given pressure is recorded
(ii). The pressure release valve is opened gently and gas is desorbed to the atmospheric air.
(iii). Weight readings are taken after 15, 30 and 45 seconds, and thereafter every minute over a period of 30 minutes, and every five minutes over a period of 30 minutes and every 15 minutes over the next four hours adopting the method of Lama (1983).

The weight is monitored continuously every day until no significant further weight change occurs indicating that desorption has ceased.
Fig. 4.3. Calibration curves for CH4, CO2 and mixed gas in bombs.
Fig. 4.4. Relationship between gas adsorbed $C_a$ and quantity of gas directly adsorbed for $CH_4$ $Q_{dir}$ by the coal sample.
Fig. 4.5. Relationship between gas adsorbed (Ca) and quantity of gas directly adsorbed Qdir by coal sample in CO2
Fig. 4.6. Relationship between gas adsorbed ($C_a$, cm$^3$/g) and quantity of gas directly adsorbed $Q_{dir}$ by coal sample in mixed gas.
4.4. Data acquisition and processing for gas desorption

4.4.1. General

Conducting tests using the conventional direct method, as developed by Bertard (1970) and modified by the U.S.B.M. (Kissell, 1973), led to errors in their gas content estimations because of high loss of gas in the initial stages (Q1). However, the automation of the measuring system is difficult and costly (Lama and Bartosiewicz, 1982).

The method adopted in conducting the laboratory work is a direct gravimetric technique which was chosen as the most practical method.

Manual recording and processing of data especially in conventional gas desorption tests (volumetric method) are often inaccurate because

(i). gas is released into and stored in upper the chamber of an inverted graduated cylinder filled with water, not to the atmospheric air at atmospheric pressure,

(ii). as the consequence of the above, there may be a build-up of pressure in the upper chamber which results in the volume read is not normally exactly at atmospheric pressure, and also may lead to developing 'counter pressure' (Hargraves, 1963) which eventually takes more desorption time, and

(iii). after determining Q1 and Q2 the sample is crushed in the laboratory and the further quantity Q3 must be determined, leading to another error due to lost gas during preparation and crushing.

Because of these factors, an innovative computer based gravimetric method of direct collection for presentation of the desorption isotherm was developed.
4.4.2. High pressure gas sorption apparatus (and also for subsequent desorption testing)

The basis for the experiment is the high pressure gas sorption apparatus shown in Figure 4.7 to Figure 4.9. The details and principles of the apparatus and the method for determining the amount of gas adsorbed in the coal sample is described by Lama and Bartosiewicz (1982). As stated above basically the apparatus consists of a means to connect the sample containers to a variable pressurized gas source and also to a vacuum pump.

Briefly, the sorption apparatus consists of six aluminium bombs which are designed to withstand pressures up to 5000 kPa at temperature ranges to 50°C. A vacuum of less than 0.01 kPa can be reached. The gas supply is connected to a manifold through a storage reservoir and a pressure regulating valve. The manifold supplies the bombs via six independently controlled outlets. Each gas line is fitted with an isolation valve to release the pressure in the line when a bomb is to be removed. The bombs are attached to the manifold with flexible nylon hoses and quick release snap fittings. The vacuum pump is also connected to the manifold to evacuate the bombs. This provides for either pressure or vacuum in the manifold. The bombs are cylindrically shaped containers of 58.82 mm bore with internal volumes from 352 cm$^3$ to 423 cm$^3$. Lids are secured to the bombs with eight bolts each and sealed with neoprene O-rings. Each bomb lid is fitted with two valves, one being an isolation valve and the other (quick acting) is used to permit the continuous circulation of gas through the bomb. Figure 4.10 shows a bomb in detail.

Shortage of finance precluded the usage of bombs with standardized size and unstandardized size bombs (which were available) were used instead. Standardized
Fig. 4.7. High pressure adsorption - desorption system
1 - 6 Primary supply system
7 - 12 Pressure release system
13 - 18 Isolation valves
A - F Sample

Gas supply
Pressure transducer

Vacuum shut off valve

Vacuum gauge
Vacuum pump

Temperature regulator

Coal sample

water
Fig. 4.8. High pressure adsorption-desorption system

Fig. 4.9. High pressure adsorption-desorption system
Figure 4.10. Gas container (bomb) - Schematic
bomb sizes would have been better to avoid comparative errors from bomb to bomb.

4.4.3. Electronics and hardware

(i). Equipment

A high resolution, precision balance is used to determine the bomb weight at different pressures on a daily basis (while adsorbing) and the bomb weight at any time during desorption. The balance (Mettler PK 2000S electronic balance with measuring range between 0.001g to 2500g with readability of 0.01g) is connected via an interface to a computer system. This arrangement enables the direct acquisition of the amount of gas desorbed for a bomb. Figure 4.11. shows a general arrangement for data acquisition.

(ii). Hardware

Data transfer from the balance to the computer system is accomplished using a serial bus at maximum transfer rate of 9600 baud. An a-synchronous communication adapter made it possible to connect the balance provided with a current loop data interface and the microcomputer. Required hardware parts are:
- CL-RS232 Adapter: CL249 manufactured by Mettler,
- Connection cable: computer-adapter (Data communication equipment DCE), and
- Galvanically separated connection cable-interfaces. The data are transferred without processing and without storage, i.e. the instrument does not have a data storage.
Transmitting and receiving character strings are made through the operating system of the microcomputer (IBM Personal Computer) which supports communication with external instruments so that the interface card can be addressed directly from the BASIC program.

A short program 'BGDES' is written in BASIC (Appendix 2) to start the test, record the change in the weight of the bomb and calculate the gas desorbed, and stop the test as follows.

(i). The final weight of the bomb at a given pressure is recorded.
(ii). The pressure release valve is opened and simultaneously the program run is started, thus readings are commenced.

Desorption of gas (cm³/g) against time elapsed from the opening of the valve can be plotted, and diffusivity can be determined. The BGDES program performs the following:

(i). It records the time elapse since the opening of the pressure release valve.
(ii). Simultaneously it records the weight of the bomb at any time according to time elapse (= current weight).
(iii). It calculates the weight difference, i.e. initial weight minus current weight.
(iv). It calculates the 'direct quantity of gas desorbed', i.e. weight difference divided by gas density divided by sample weight.
(v). It converts 'direct gas desorbed' to 'gas desorbed' using 'converting factors' obtained from the adsorption isotherm. The converting factors have been calculated beforehand, by using 'XYUTI' program available for this purpose.

This program is written in BASIC; it has the ability to convert the polynomials up to order of 5 in the forms of normal, normal-log, and log.

The output of BGDES program is presented in Table 4.2. It consists of four columns, which are:

<table>
<thead>
<tr>
<th>t, sec</th>
<th>time elapsed since the opening of the bomb's valve, seconds</th>
</tr>
</thead>
<tbody>
<tr>
<td>cw, g</td>
<td>current weight, g</td>
</tr>
</tbody>
</table>
Fig. 4.11. General arrangement for data acquisition on gas desorption
TABLE 4 - 2
Desorption of CO2 from coal sample
Bomb B2, type 2, September 1989

<table>
<thead>
<tr>
<th>t, sec</th>
<th>cw, g</th>
<th>wd, g</th>
<th>Q, cm³/g</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>1604.671</td>
<td>0.636983</td>
<td>2.762332</td>
</tr>
<tr>
<td>30</td>
<td>1604.061</td>
<td>1.246983</td>
<td>4.479556</td>
</tr>
<tr>
<td>45</td>
<td>1603.486</td>
<td>1.821984</td>
<td>5.961882</td>
</tr>
<tr>
<td>105</td>
<td>1601.366</td>
<td>3.941984</td>
<td>10.44484</td>
</tr>
<tr>
<td>165</td>
<td>1599.492</td>
<td>5.815984</td>
<td>13.37685</td>
</tr>
<tr>
<td>225</td>
<td>1597.82</td>
<td>7.487983</td>
<td>15.38858</td>
</tr>
<tr>
<td>285</td>
<td>1596.333</td>
<td>8.974983</td>
<td>16.81931</td>
</tr>
<tr>
<td>345</td>
<td>1594.993</td>
<td>10.31498</td>
<td>17.8895</td>
</tr>
<tr>
<td>405</td>
<td>1593.789</td>
<td>11.51898</td>
<td>18.71477</td>
</tr>
<tr>
<td>465</td>
<td>1592.703</td>
<td>12.60498</td>
<td>19.37259</td>
</tr>
</tbody>
</table>

wd, g : weight difference, i.e. initial weight minus current weight, g
Q, cm³/g : quantity of gas desorbed, cm³/g

With the additional lines in the program, the command to print quantity of direct gas desorbed Qd, cm³/g, such output presented in Table 4-3 can be obtained. When output data is plotted, i.e. time t against 'gas desorbed' Q and 'direct gas desorbed' Qd, curve such as Figure 4.12 is obtained.

Most likely Lama and Bartosiewicz (1982, 1983) misinterpreted this quantity of 'direct gas desorbed' as quantity of 'gas desorbed'.

An attempt is made to improve the existing system to provide pressure-time curve as well during desorption. The pressure reading during desorption may be obtained by installing a pressure transducer connected to an ADDA (Analog-
TABLE 4 - 3

Desorption of CO₂ from coal sample Bomb B2, type 2, September 1989

<table>
<thead>
<tr>
<th>t, sec</th>
<th>cw, g</th>
<th>wd, g</th>
<th>Qd, cm³/g</th>
<th>Q, cm³/g</th>
</tr>
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<td>0.636983</td>
<td>2.312074</td>
<td>2.762332</td>
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<tr>
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<tr>
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<tr>
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<td>1601.366</td>
<td>3.941984</td>
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<tr>
<td>465</td>
<td>1592.703</td>
<td>12.60498</td>
<td>45.75262</td>
<td>19.37259</td>
</tr>
</tbody>
</table>
Digital Digital-Analog) converter in the system. ADDA card (IBM PC version) is a high precision data conversion system. It contains 16 channels 12 bits analog to digital conversion. Figure 4.13 shows the general arrangement for this data acquisition and Figure 4.14 shows the equipment to measure the pressure in the bomb. Presently, a serious problem while conducting this experiment is the effect of the drag of the wire on the sensitivity in weighing during desorption. Hence at this stage time-pressure curve is obtained only by sacrifice of the curve of time.
Fig. 4.13. General arrangement for data acquisition and pressure reading
Fig. 4.14. The equipment to measure the pressure in the bomb
against quantity of gas desorbed. The program used for this special condition 'BGDESPRE' is shown in the Appendix 3.

The output of the BGDESPRE program, Table 4.4 consists of five columns, which are:

- \( t, \text{sec} \): time elapsed since the opening of the quick release valve, seconds
- \( cw, g \): current weight, g
- \( wd, g \): weight difference, i.e. initial weight minus current weight, g
- \( Q, \text{cm}^3/g \): quantity of gas desorbed, cm\(^3/g\)
- \( P, \text{kPa} \): current gas pressure in the bomb, kPa

As has been stated above, due to problems with handling the pressure transducer and its cable, current weight \( cw \), weight difference \( dw \), and gas desorbed \( Q \) must be sacrificed to obtain current gas pressure in the bomb \( P \). Figure 4.15 shows a typical time-pressure curve for first two hours for CH\(_4\) gas. Again, this is not the desirable condition, because in the condition of atmospheric pressure during gas desorption, time needed to reach atmospheric pressure within the bomb should be minimised approaching 0.0 second which means as soon as the quick release valve is open, the pressure within the bomb is equal to atmospheric pressure. This condition may be approached by virtually eliminating free gas space in the bomb, i.e. by using a coal sample of volume nearly equal to the volume of the bomb (Of course this would involve standard samples, and redesign of the bomb to suit).

4.5. Experimental studies on adsorption and desorption of gases on coal

4.5.1. Adsorption tests
### TABLE 4 - 4

Desorption of CH₄ gas from bomb
Pressure vs Time curve for Bomb L, Sept - 1989

<table>
<thead>
<tr>
<th>t, sec</th>
<th>cw, g</th>
<th>dw, g</th>
<th>Q,cm³/g</th>
<th>P,kPa (G)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>1950.238</td>
<td>3.662025</td>
<td>6</td>
<td>3873</td>
</tr>
<tr>
<td>30</td>
<td>1950.149</td>
<td>3.751025</td>
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<td>3783</td>
</tr>
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<td>45</td>
<td>1950.068</td>
<td>3.832024</td>
<td>6</td>
<td>3680</td>
</tr>
<tr>
<td>105</td>
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<td>4.137025</td>
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<tr>
<td>165</td>
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</tr>
<tr>
<td>345</td>
<td>1948.852</td>
<td>5.048024</td>
<td>6</td>
<td>2423</td>
</tr>
<tr>
<td>405</td>
<td>1948.686</td>
<td>5.214025</td>
<td>6</td>
<td>2291</td>
</tr>
<tr>
<td>465</td>
<td>1948.534</td>
<td>5.366025</td>
<td>6</td>
<td>2130</td>
</tr>
</tbody>
</table>
All samples come from West Cliff Colliery, New South Wales (Australia). The cylindrical coal samples are of Bulli Seam coal of approximately 50 mm diameter and height of 50 mm which were trepanned both perpendicular and parallel to the bedding plane. The ends of the samples were lapped and then sealed using epoxy and aluminium foil to prevent axial flow. There are three kind of samples used, namely type 1 for intact coal sample trepanned normal to bedding plane, type 2 for intact coal sample trepanned perpendicular to the bedding plane, and type 3 for coal sample trepanned normal to bedding plane with a central hole.
filled with coal fines. Type 3 samples were used in an attempt to obtain some information on gas outbursts. This type 3 experiment is based on Ruff's theory (1930) where nests or pockets of low strength coal (already crushed in-situ) and saturated with gas are suddenly exposed by an advancing face triggering an outburst (Lama, 1981). There are two basic theories which have been proposed to explain the phenomenon of outburst. The most commonly accepted is the dynamic theory (Lama, 1981). According to this theory both rock pressure and gas play the important role. Rock pressure causes fracturing and release of a large volume of gas which causes the displacement of coal. The second theory was proposed by Ruff and is known as the 'nest theory'.

As has been discussed above, the gassiness is generally high in geological and tectonically disturbed formations such as those folded and faulted. It may be supposed that all areas where coal is weak and fractured caused by geological and tectonical disturbs are 'nests'. When these nests are penetrated, abnormally high rates of gas emission or gas outburst may be experienced.

The moisture content of samples was determined by thermal drying tests. The average density of samples was 1.386 g/cm³ determined using 'Test for porous material method T606' (Department of Main Roads, NSW, 1980). In calculation of adsorption, specific gravity of coal is taken nominally as 1.4 g/cm³ (Aziz, pers. comm.). The diameter of the central hole was chosen 8 mm and the size of coal fines is between 53μ and 75μ. Apparent specific gravity of coal fines was 1.371 g/cm³ determined using British Standard BS 1377, 1975. Grading of aggregate as results of sieve analysis is shown in Figure 4.16

The weight of samples varied from 128.612g to 154.257g which means the average volume of bomb occupied by the sample was about 27%. The rest (about 73% of the volume of bomb) to be occupied by gas could cause the following problems:

(i). wasted gas during the adsorption process, which
Fig. 4.16. Sieve analysis of coal fines
(ii). leads to obtaining two kind of gas adsorbed, i.e. 'direct gas adsorbed' and 'gas adsorbed' during adsorption process and consequently will produce two kind of gas desorbed, i.e. 'direct gas desorbed' and 'gas desorbed' while desorbing as discussed above, and (iii). the inability to monitor pressure within the bomb during desorption concurrent with weighing the bomb during desorption and knowing that ideally, desorption should be to atmospheric pressure through out desorption. The condition of atmospheric pressure within the bomb while desorbing could not be obtained even though gas is emitted to atmospheric air as supported by output of 'BDESPRE' program discussed above.

To simulate gas flow in a coal seam the samples were pressurized with gas at various pressures to saturation, as identified by repeat weighings. Samples were pressurized to various (gauge) pressures of 100 kPa - 4000 kPa at room temperature (17°C - 25°C) and constant bath temperature at 25°C. A temperature of 25°C was chosen on advice as representing in situ virgin temperature of West Cliff coal. The maximum pressure of 4000 kPa was adopted on advice (Aziz, pers.comm.) as representing in situ virgin pressure of West Cliff coal.

During adsorption gas pressure dropped rapidly in the first few hours and became more stable after a few days (pressure was only admitted to the bombs intermittently, because inevitable line losses occurred and were minimized for economy and safety reasons).

Carbonaceous substances such as charcoal, coal, and coke can adsorb gases readily, and these characteristics give these substances their filtration properties. The capability to store CH₄ and other gases in coal may be explained by the same mechanism. As stated above, in the adsorbed state the gas molecules are "tightly packed and closely held" to the walls of the very fine sized pores in the coal structure (Patching, 1970).
This ‘packing’ is thought to be single molecular and its density increases with pressure. At low pressures with rise of pressure, the quantity of gas adsorbed increases rapidly and almost linearly. At higher pressures when the adsorbed layer becomes more dense with rise of pressure, the rate of adsorption slows and finally, at extremely high pressures, it nearly stops. Figure 4.17 to Figure 4.19 show the coal samples used in the laboratory work.

4.5.2. Adsorption of CH₄

Diameter of samples varied from 46.95 mm to 47.67 mm, and height varied from 46.81 to 52.94 mm. The moisture content of the samples ranged from 1.06% - 2.32%. The gas used was dry methane with density of 0.00072 g/cm³ at 0°C and 1.013 kPa.

Cylindrical intact coal samples and cylindrical coal samples with central hole filled with coal fines were pressurized in the bombs. A typical adsorption isotherm is shown in Figure 4.20. The gas quantity adsorbed at 4101.3 kPa by sample type 1 is 10.209 cm³/g (at moisture content of 2.3%), and 12.116 cm³/g for coal sample type 2 (at moisture content of 1.21%) and 15.946 cm³/g for coal sample type 3 (at moisture content of 1.18%).

Type 3 sample has a higher sorptive capacity. In a simple way this can be explained as follows: when two samples with different weight (type 3 less than type 1 due to its smaller specific gravity of 'central core') are saturated with approximately the same quantity of gas, then the sample with smaller weight will adsorb more.
Fig. 4.17. Bulk coal samples, Bulli Seam

Fig. 4.18. Cylindrical coal samples, Bulli Seam
Fig. 4.19. Cylindrical coal samples, type 3

*Bulli Seam*
4.5.3. Adsorption of CO₂

The diameters of samples varied from 51.31 to 52.11 mm, and height varied from 52.11 to 53.20 mm. Gas used was dry CO₂ with density of 0.001848 g/cm³ at 15°C and 1.013 kPa.

A typical adsorption isotherm is shown in Figure 4.21. The gas quantity adsorbed by sample type 1 was 25.738 cm³/g at 4101.3 kPa, and as much as 25.374 cm³/g and 28.738 cm³/g for coal sample type 2 and type 3 respectively. As
expected from the CH$_4$ experiments coal sample type 3 adsorbed more gas than intact coal samples. The average moisture content was 1.17%.

4.5.4. Adsorption of mixed gas

The diameter of the sample varied from 49.2 to 49.80 mm; the height varied from 51.35 to 56.08 mm. There were three samples of type 1 and 2 and three samples of type 3. The average moisture content of coal sample was 1.22%. Gas
used was dry mixed gas (50% CO₂ and 50% CH₄) with density of 0.001347 g/cm³ at 0°C and 101.3 kPa.

A typical adsorption isotherm is shown in Figure 4.22. The gas quantity adsorbed by sample type 1 was 19.376 cm³/g at 4101.3 kPa and as much as 20.197 cm³/g and 20.518 cm³/g for coal sample type 2 and type 3 respectively. The coal sample provided with central hole filled with coal fines adsorbed more than the intact samples at peak pressure.

The adsorption capacity of coal for CO₂ is higher than CH₄. The ratio is due to a number of factors, such as polarity of the molecule and liquifaction temperature of the gas. Ettinger et al (1967) studied two coals of different rank, which showed the ratio at low pressure to lie between 3 and 4. With increase in pressure, the adsorption of CO₂ reaches its peak at 4012 kPa and the ratio at this pressure decreases to 1.5 - 1.7. Table 4-5 gives the ratio of sorptions of CO₂ and CH₄ various pressure for Australian (developed from Bartosiewicz and Hargraves, 1985, and this current work) and European (developed from Boxho et al, 1980) coals as determined in laboratory high pressure adsorption tests.

4.6. Physical and parametric characteristics of isotherms

4.6.1. Langmuir's and Freundlich's models

Langmuir's and Freundlich's models could be used to describe the process of gas adsorption onto coal. The models relate the quantity of a gas adsorbed per unit mass of solid to the partial vapour pressure of the gas. Langmuir's theory gives the fraction of the adsorbent surface which is covered by molecules of adsorbed gas (Ruppel et al, 1974).
fig. 4.22. Adsorption isotherms for Bulli seam coal, dry mixed gas in dry coal.
### TABLE 4 - 5

Ratio of CO2/CH4 adsorption at different pressures for Australian and European coals

<table>
<thead>
<tr>
<th>MINE</th>
<th>SEAM</th>
<th>Adsorption pressure, kPa</th>
<th>Absolute Ratio of CO2/CH4 adsorbed</th>
</tr>
</thead>
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<tr>
<td></td>
<td></td>
<td>100</td>
<td>200</td>
</tr>
<tr>
<td>Moura 1</td>
<td>'C'</td>
<td>2.886</td>
<td>2.60</td>
</tr>
<tr>
<td>Metrop. 1</td>
<td>Buli</td>
<td>3.007</td>
<td>2.553</td>
</tr>
<tr>
<td>Appin 1</td>
<td>Buli</td>
<td>3.120</td>
<td>2.823</td>
</tr>
<tr>
<td>Collins. 1</td>
<td>Bowen</td>
<td>3.378</td>
<td>3.07</td>
</tr>
<tr>
<td>Ellalong 1</td>
<td>Greta</td>
<td>3.725</td>
<td>3.411</td>
</tr>
<tr>
<td>Laleham 1</td>
<td>'B'</td>
<td>3.133</td>
<td>3.019</td>
</tr>
<tr>
<td>Tahmoor 1</td>
<td>Buli</td>
<td>3.62</td>
<td>3.186</td>
</tr>
<tr>
<td>West Cliff 2</td>
<td>Buli</td>
<td>4.209</td>
<td>4.03</td>
</tr>
<tr>
<td>French 3 (Cev.)</td>
<td>2.828</td>
<td>2.386</td>
<td>1.9</td>
</tr>
<tr>
<td>Europe, A 3</td>
<td>?</td>
<td>1.85</td>
<td>1.816</td>
</tr>
<tr>
<td>Europe, B 3</td>
<td>?</td>
<td>2.977</td>
<td>2.493</td>
</tr>
</tbody>
</table>

A = Anthracite 5% VM (afd)
B = Bituminous 27% VM (afd)
(Cev.) = Cevennes Basin
1. develop from Bartosiewicz and Hargraves, 1985.
2. this current work
3. develop from Boxho et al, 1980.
The shape of the isotherms of methane adsorption on coal can be classified as being of type I which is associated with a system where adsorption does not proceed beyond a single molecular layer (Brunauer et al, 1940). The critical temperature of methane is 190.5°K and its critical pressure is .00463 kPa (463.03 N/cm²). Keen (1977) states that a second layer does not become apparent in coal at pressures less than 50 atmospheres. At normal temperatures in coal mining, and at gas pressures at depths of 500m - 1000m, it is almost impossible that adsorption with more than single molecular layer may take place (Keen, 1977 and Patching, 1970).

The best representation of an ideal single molecular layer system is given by Langmuir's isotherm. The necessary and sufficient assumptions of Langmuir's isotherm are that the molecules of the gas are adsorbed as complete entities on to definite points of attachment on the surface of the adsorber. Each point of attachment can accommodate one and only one adsorbed atom independent of the presence or absence of other adsorbed atoms on neighbouring points of attachment.

In the kinetic derivation, the adsorbed layer is regarded as in dynamic equilibrium with the gas phase. The number of molecules hitting unit surface in unit time is given by kinetic theory as:

\[ \mu = \frac{P}{(2\pi mkT)^{1/2}} \]  \hspace{1cm} (4.6)

where:

- \( P \): pressure
- \( m \): mass, g
- \( k \): universal constant
- \( T \): absolute temperature, °K
Those molecules striking sites which are already occupied will immediately be 'reflected'. Of the molecules coming down on uncovered sites, a certain fraction \( \alpha \) will condense and be held by the surface forces for a finite time (regarded as adsorbed), the remainder will be reflected. If the fraction of the site which is already filled is \( \theta \), then the rate at which molecules pass into the adsorbed state is \( \alpha \mu (1 - \theta) \). The rate at which they leave the adsorbed state is \( v\theta \).

At equilibrium the number of molecules in the adsorbed state at any instant is constant, therefore:

\[
\alpha \mu (1 - \theta) = v \theta \tag{4.7}
\]

where:

\( v \): the rate of evaporation from a fully covered surface.

By combining equation (4.6) and (4.7) and putting

\[
\frac{\alpha}{v (2\pi \mu kT)^{1/2}} = b \tag{4.8}
\]

\[
bP = \frac{\theta}{1 - \theta} \quad \text{or} \quad \theta = \frac{bP}{1 + bP} \tag{4.9}
\]

which is known as Langmuir's adsorption isotherm.

Equation (4.9) could be written in the form:

\[
C_a = \frac{ABP}{1 + BP} \tag{4.10}
\]

Equation (4.10) can be rearranged as:
Plotting $1/C_a$ against $1/P$, a straight line should be obtained giving a shape of $1/AB$ and on intercept of $1/A$. A and B constants could be deduced, and also coefficient of correlation ($r$) and error ($e$) could then be determined.

Freundlich equation could be written as:

$$C_a = AP^B$$

$$\log (C_a) = B \log AP$$

Plotting log $C_a$ against log $P$ leads to obtaining of A and B constants, and coefficient of correlation ($r$) and error ($e$) could be determined as well.

These calculations were applied to some published adsorption isotherm curves both for CH$_4$ and CO$_2$ and also from this current work. The sources of coal sorption data of others used was Australian (Bartosiewicz and Hargraves, 1985), German (1980), European (Boxho et al, 1980), French (Gunther, 1965) and American (Kissel et al, 1973). Results of the calculations are shown in Table 4 - 6 to Table 4 - 12 (Langmuir's equation) and Table 4 - 13 to Table 4 - 19 (Freundlich's equation).

(i). Effect of the nature of gas

At a given partial pressure and temperature, carbon dioxide is much more readily adsorbed than methane. The quantity of CO$_2$ adsorbed is 2 to 4 times that of CH$_4$, due to higher affinity of the CO$_2$ gas to coal.

Figure 4.20 and Figure 4.21 derived from this current work, Figures 4.23 and Fig.4.24 developed from Bartosiewicz and Hargraves (1985) show the effect of nature of gas on sorptive capacity for Australian coals. Table 4-6 embraces these data expressed in effect of the nature of gas on Langmuir's constant.
TABLE 4-6

Effect of nature of gas on coal sorptive capacity
Langmuir's equation

<table>
<thead>
<tr>
<th>Gas</th>
<th>A, cm³/g</th>
<th>B, kPa⁻¹</th>
<th>Coef.of correlation</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Type 1</td>
<td>18.32264</td>
<td>0.0004015</td>
<td>.9976</td>
<td>.1409</td>
</tr>
<tr>
<td>Type 2</td>
<td>19.4339</td>
<td>0.0004855</td>
<td>.9992</td>
<td>.1158</td>
</tr>
<tr>
<td>Type 3</td>
<td>29.9326</td>
<td>0.0003454</td>
<td>.9985</td>
<td>.4172</td>
</tr>
<tr>
<td></td>
<td>20.69402</td>
<td>0.001467</td>
<td>.9921</td>
<td>.6774</td>
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<tr>
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<td>19.0544</td>
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<td>0.00109</td>
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<td>.5201</td>
</tr>
<tr>
<td>Ant.</td>
<td>5% VM</td>
<td>30.1419</td>
<td>0.004681</td>
<td>.9854</td>
</tr>
<tr>
<td></td>
<td>Ant.Cev.</td>
<td>24.71638</td>
<td>0.002242</td>
<td>.9936</td>
</tr>
<tr>
<td>CO₂</td>
<td></td>
<td></td>
<td></td>
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</tr>
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<td>Type 1</td>
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<td>.9917</td>
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</tr>
<tr>
<td>Type 2</td>
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<td>.9973</td>
<td>.2327</td>
</tr>
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<td>29.23119</td>
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<td>.9825</td>
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<td>32.30425</td>
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</tr>
<tr>
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<td>Ant.Cev.</td>
<td>35.6372</td>
<td>0.005492</td>
<td>.9791</td>
</tr>
</tbody>
</table>

*Australian  this current work
Type 1 = intact coal sample drilled normal to bedding plane
Type 2 = intact coal sample drilled parallel bedding plane
Type 3 = coal sample with central hole which filled with coal fines
Cev. = Cevennes
TABLE 4-7

Effect of rank on coal sorptive capacity
French, American, and European coal
Langmuir's equation

<table>
<thead>
<tr>
<th>Rank</th>
<th>A, g/cm³</th>
<th>B, kPa⁻¹</th>
<th>Coefficient of correlation</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ant</td>
<td>24.71638</td>
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<td>0.9936</td>
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<td>Bit</td>
<td>21.93147</td>
<td>0.001259</td>
<td>0.999</td>
<td>0.0754</td>
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<td>Lvb</td>
<td>35.7532</td>
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</tr>
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<tr>
<td>Ant. 27%M</td>
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<td>0.002045</td>
<td>0.9939</td>
<td>0.5679</td>
</tr>
</tbody>
</table>

Ant = Athracite
Bit = Bituminous
Lvb = Low volatile bituminous
Mvb = Medium volatile bituminous
Hvb = High volatile bituminous
VM = Volatile Matter
TABLE 4-8

Effect of VM on coal sorptive capacity
Australian adb(1985), Australian afd (1985), and
German coal (1980)
Langmuir's equation

<table>
<thead>
<tr>
<th>%VM</th>
<th>A, cm³/g</th>
<th>B, kPa⁻¹</th>
<th>Coefficient of correlation</th>
<th>Error</th>
</tr>
</thead>
<tbody>
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</tr>
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<td>.9929</td>
<td>.8132</td>
</tr>
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<td>.6774</td>
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TABLE 4-9
Effect of moisture content on coal sorptive capacity
Australian*, Australian (1985), and American coal (1973)
Langmuir'equation

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*Australian, this current work
### TABLE 4 - 10

Effect of ash on coal sorptive capacity  
Australian coal (1985)  
Langmuir's equation

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### TABLE 4 - 11

Effect moist CH₄ and moist on coal sorptive capacity  
Australian coal (1985)  
Langmuir's equation

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**TABLE 4 - 13**

Effect of nature of gas on coal sorptive capacity
Freundlich's equation

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*Australian - this current work
## Table 4-14

**Effect of rank on coal sorptive capacity**  
**French, American, and European Coal**  
**Freundlich’s equation**

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### TABLE 4 - 15

Effect of VM on coal sorptive capacity
Australian adb (1985), Australian afd (1985), and
German coal (1980)
Freundlich's equation

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TABLE 4 - 16

Effect of moisture content on sorptive capacity
Australian*, Australian (1985), and American coal (1973)
Freundlich's equation

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<td>.532</td>
<td>.9901</td>
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<td>.9807</td>
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<td>.7544</td>
<td>.9841</td>
<td>.2743</td>
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</table>

*Australian, this current work
### TABLE 4 - 17

**Effect of ash on coal sorptive capacity**  
*Australian coal (1985)*  
*Freundlich's equation*

<table>
<thead>
<tr>
<th>%ash</th>
<th>A, cm³/g kPa</th>
<th>B</th>
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<th>Error</th>
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<td>5.4</td>
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<td>10.9</td>
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<td>.6105</td>
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<td>.5121</td>
<td>.9927</td>
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<td>.5710</td>
<td>.9745</td>
<td>2.0196</td>
</tr>
</tbody>
</table>

### TABLE 4 - 18

**Effect of moist CH4 and moist on coal sorptive capacity**  
*Australian coal (1985)*  
*Freundlich's equation*

<table>
<thead>
<tr>
<th>Location</th>
<th>A, cm³/g kPa</th>
<th>B</th>
<th>Coefficient of correlation</th>
<th>Error</th>
</tr>
</thead>
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<td>Moura</td>
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<td>.9927</td>
<td>.7824</td>
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<td>Collinsville</td>
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<td>.5722</td>
<td>.989</td>
<td>1.1296</td>
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<td>Metropolitan</td>
<td>.2841</td>
<td>.5211</td>
<td>.9905</td>
<td>.905</td>
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<td>Lalleham</td>
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</table>
### TABLE 4 - 19

Effect of temperature on coal sorptive capacity
Australian (1985) and European coals (1980)
Freundlich's equation

<table>
<thead>
<tr>
<th>Gas</th>
<th>$A$, cm$^3$/g kPa$^{-1}$</th>
<th>B</th>
<th>Coefficient of correlation</th>
<th>Error</th>
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<tr>
<td>CH$_4$</td>
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<td></td>
<td></td>
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</tr>
<tr>
<td>20°C</td>
<td>.3877</td>
<td>.4764</td>
<td>.9953</td>
<td>.3539</td>
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</tr>
<tr>
<td>20°C</td>
<td>.2802</td>
<td>.4932</td>
<td>1.0292</td>
<td>.3677</td>
</tr>
<tr>
<td>30°C</td>
<td>.2522</td>
<td>.4932</td>
<td>.9932</td>
<td>.2979</td>
</tr>
<tr>
<td>Ant.5% 26°C</td>
<td>2.9199</td>
<td>.2894</td>
<td>.9755</td>
<td>2.6885</td>
</tr>
<tr>
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<td>2.6057</td>
<td>.2894</td>
<td>.9755</td>
<td>2.3548</td>
</tr>
<tr>
<td>Bit.27% 26°C</td>
<td>.5467</td>
<td>.4388</td>
<td>.9764</td>
<td>1.8508</td>
</tr>
<tr>
<td>44°C</td>
<td>.4681</td>
<td>.4388</td>
<td>.9764</td>
<td>1.3557</td>
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<tr>
<td>CO$_2$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ant.5% 26°C</td>
<td>7.4922</td>
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<td>.9622</td>
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</tr>
<tr>
<td>44°C</td>
<td>6.683</td>
<td>.2223</td>
<td>.9622</td>
<td>4.9321</td>
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<tr>
<td>Bit.27% 26°C</td>
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<tr>
<td>44°C</td>
<td>1.307</td>
<td>.3761</td>
<td>.9769</td>
<td>3.0288</td>
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</table>

Ant.5% : Anthracite 5% VM (Volatile Matter)
Bit.27% : Bituminous 27% VM
Fig. 4.23. Adsorption isotherms for Australian coal, dry CH4 and dry coal (developed from Bartosiewicz and Hargraves, 1985)
(ii). Effect of temperature

The quantity of gas adsorbed decreases as the temperature increases, at the same equilibrium pressure (Figure 4.25). Starting from 299 K it falls 0.8% per degree for bituminous coal, and 0.6% per degree for anthracite (Boxho et al, 1980). For Australian coal the decrease is 1% of sorptive capacity per 1°C rise in temperature (Bartosiewicz and Hargraves, 1985) which is shown in Figure 4.26.
Fig. 4.25. Effect of temperature and rank on CH4 gas adsorption isotherms for European coal (developed from Boxho et al, 1980)
The effect of temperature on sorptive capacity expressed as the effect of temperature on Langmuir's constant is presented in Table 4-12 developed from Boxho et al (1980) and from Bartosiewiecz and Hargraves (1985).

(iii). Effect of moisture content

Increasing rank in the brown-coal stage is primarily characterized by decrease of total inherent moisture content. The porosity, inherent surface and moisture vary together with rank. Moisture and porosity decrease with increase of
rank from the brown coal stage to that of medium volatile bituminous A coals and with further increase of rank these properties decrease to the anthracite stage (Stach et al, 1982).

The general effect of increasing moisture content is a reduction in adsorptive capacity. At the same in-situ methane pressure, a naturally moist coal is less gassy than if it were naturally dry. Ettinger's formula gives an approximate value for the effect of moisture:

\[
\frac{C_{amo}}{C_{adr}} = \frac{1}{1 + 0.31w}
\]  

(4.14)

where:

- \(w\) : moisture content in %
- \(C_{amo}\) : gas content of moist coal in m3/t
- \(C_{adr}\) : gas content of dry coal in m3/t

This formula represented in Figure 4.27 (reproduced from Boxho et al, 1980) and is valid up to 5% moisture. Above that moisture level, saturation occurs and the ratio then becomes almost constant. Lama developed a curve up to 16% moisture which depicts the relationship between the moisture content and the adsorption of CH4 in a high pressure adsorption test (Lama, 1986), which is shown in Figure 4.28. Such a high inherent moisture content would only appear to be feasible for very low rank coal, as shown by Figure 4.29.

Investigation on the effect of moisture content on quantity of gas adsorbed by Joubert et al, (1973) gives a decreasing Langmuir's constant as moisture content decreases. Figure 4.30 to Figure 4.37 show the effect of moisture content on sorptive capacity for American coals and Table 4-9 shows this effect expressed as effect of moisture content on Langmuir's constants. Figure 4.38 to Figure 4.40 show the effect of moisture content for Australian coal. Figure 4.38 and Figure
Fig. 4.27. Influence of natural moisture content on the adsorption of CH4 by pure coal (developed from Boxho et al, 1980)
Fig. 4.28. Effect of moisture content on the adsorption of CH4 in high pressure adsorption test as expressed by Langmuir's A (reproduced from Lama, 1986)
Fig. 4.29. Increase of degree of coalification with depth
(Stach et al, 1982)
Fig. 4.30. Effect of moisture content on adsorption isotherms for American coal (developed from Kissel et al, 1973)
Fig. 4.31. Effect of moisture content on Langmuir's A for American coal
Fig. 4.32. Effect of moisture content on adsorption isotherm for Pittsburgh I coal (developed from Joubert et al, 1973)
Fig. 4.33. Effect of moisture content on Langmuir's A on Pittsburgh I coal
Fig. 4.34. Effect of moisture content on adsorption isotherms for Pittsburgh II coal (developed from Joubert et al., 1973)
Fig. 4.35. Effect of moisture content on Langmuir's A for Pittsburgh II coal.
Fig. 4.36. Effect of moisture content on adsorption isotherms for Pocahontas coal (developed from Joubert et al, 1973)
Fig. 4.37. Effect of moisture content on adsorption isotherms for Hartshorne coal (developed from Joubert et al, 1973)
4.39 shows the results from this current work, while Figure 4.40 was reproduced from Bartosiewicz and Hargraves (1985).

Moist CH$_4$ gas with moist coal samples also results in reduced sorptive capacity from 15% to 27% for different coals, which is shown in Figure 4.41 (reproduced from Bartosiewicz and Hargraves, 1985) and Table 4-11 shows this effect expressed in Langmuir's constants.
Fig. 4.39. Effect of moisture content on Langmuir's constant for Bulli Seam coal.
Fig. 4.40. Effect of moisture content on sorptive capacity for Australian coals (developed from Bartosiewicz and Hargraves, 1985)
(iv). Influence of rank

Properties of coal which commonly are used as a measure of rank are mean maximum reflectance of vitrinite, total carbon content, volatile matter yield, moisture content, and specific energy (Cook, 1982). Volatile matter and total carbon are expressed on an ash-free, dry basis - the coaly component only.

At given pressure and temperature, the quantity of gas adsorbed by dried coal is at maximum between 20% and 40% volatile matter content. At first Langmuir's
constant "A" decreases with increasing volatile matter, and then rises again with further volatile matter increases (Boxho et al, 1980).

The \textit{U.S.B.M.} has found that in general the adsorptive capacity and hence methane content of coal increases with rank. It is obvious that more gas can be adsorbed at higher seam gas pressures. Langmuir's constant shows decrease from anthracite coal to high volatile bituminous coal, as illustrated in \textit{Table 4-7} and \textit{Figure 4.42} for American coal (developed from Kim, 1977), and in \textit{Figure 4.43} and \textit{Figure 4.44} for German coal (developed from Boxho et al, 1980), and \textit{Figure 4.45} - \textit{Figure 4.46} and \textit{Table 4-8} for Australian coal (developed from Bartosiewicz and Hargraves, 1985) and in the results from this current laboratory work.

(v). Effect of ash content

The gas is only adsorbed by the carbonaceous matter of coal substance.

\[
\frac{C_{a\Pi}}{C_{a\alpha}} = \frac{1}{1 - 0.01a}
\]  

(4.15)

where:

\(C_{a\Pi}\): gas content of pure coal, \(m^3/t\)

\(C_{a\alpha}\): gas content of ashy coal, \(m^3/t\)

\(a\): actual ash content \%

Effect of ash content for Australian coal is shown in \textit{Figure 4.47} and \textit{Table 4.10} expressed this effect on Langmuir's constants.

4.7. Desorption of gas from coal
Fig. 4.42. Effect of rank on adsorption isotherms for American coal (developed from Kim, 1977)
Fig. 4.43. Effect of volatile matter on CH4 on CH4 adsorption isotherms for German coal (developed from Boxho et al, 1980)
Fig. 4.44. Effect of volatile matter on Langmuir's A for German coal (developed from Boxho et al, 1980)
Fig. 4.45. Effect of volatile matter (afd) on Langmuir's A for Australian coal (developed from Bartosiewicz and Hargraves, 1985)

Fig. 4.46. Effect of volatile matter (adb) on Langmuir's A for Australian coal (developed from Bartosiewicz and Hargraves, 1985)
Desorption of gas from coal is the reverse process of gas adsorption, in other words, the higher the amount of gas adsorbed, the higher gas quantity will be emitted. The initial rate of gas desorption is very high and it drops progressively with increasing time.

4.7.1. Desorption of CH4 gas from coal samples
The quantities adsorbed by intact coal samples are 10.209 cm\(^3\)/g for sample drilled perpendicular to bedding plane, and 12.116 cm\(^3\)/g for sample drilled parallel to bedding plane, and 15.946 cm\(^3\)/g for coal sample provided with central hole filled with coal fines consecutively.

*Figure 4.48* shows that by the time that desorption time \(t\) reached 1000 seconds about 60% - 70% of the adsorbed gas had been released from intact coal samples and by the same time about 50% of the adsorbed gas from coal sample provided with central hole filled with coal fines. By the time \(t\) reached 22545 seconds about 90% of the adsorbed gas had been emitted, and after five days (430,000 seconds) no more gas desorption was detected.

As has been stated above, a specific empirical relationship between time and the quantity of gas desorbed has been formulated, as follows:

\[
Q_t = Q (\frac{t}{T})^n \tag{4.16}
\]

\[
Q_t = A \sqrt{t} \tag{4.17}
\]

where:
- \(Q_t\) : gas desorbed cm\(^3\)/g in time \(t\)
- \(Q\) : initial gas present, cm\(^3\)/g
- \(t\) : time, seconds
- \(n,T\) : constants

Proceeding from *equation (4.12)*:

\[
Q_t = Q (\frac{t}{T})^n
\]

\[
\log Q_t = \log Q + n \log t - n \log T
\]
Fig. 4.48. Desorption of CH4 gas from bomb for Bulli seam coal

\[
\log Q_t = n \log t + \log \left( \frac{Q}{T^n} \right)
\]  

(4.18)

Plotting \( \log Q_t \) against \( \log t \), a straight line would be obtained giving a shape of \( n \) and on the intercept gives \( \log \left( \frac{Q}{T^n} \right) \). In laboratory desorption tests, the value of \( Q \) is known, so the value of \( T \) may be calculated.

For the early stages of desorption the conditions shown in Table 4-20 apply:
TABLE 4 - 20
n and T constants for CH4 gas desorption test

<table>
<thead>
<tr>
<th>Range of elapsed time, sec</th>
<th>n</th>
<th>Qt, cm³/g</th>
<th>T</th>
</tr>
</thead>
<tbody>
<tr>
<td>45</td>
<td>.287</td>
<td>2.980</td>
<td>.000303</td>
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<td>165</td>
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<tr>
<td>645</td>
<td>.337</td>
<td>8.831</td>
<td>.001007</td>
</tr>
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</table>

Table 4-20 shows that diffusivity is not constant.

4.7.2. Desorption of CO₂ gas from coal samples

Desorption of CO₂ gas is given in Figure 4.49. The figure shows the significant difference in quantity of desorbed gas from intact coal samples and from coal sample provided with central hole which is filled with coal fines.

The quantities adsorbed by tested coal samples are 25.738 cm³/g, and 25.374 cm³/g and 28.738 cm³/g for coal samples type 1, type 2 and type 3 respectively.

Figure 4.49 shows that by the time t reached 1000 seconds about 60% of the adsorbed gas had been released. And by the time t reached 22545 seconds about 90% of the adsorbed gas had been released. After five days (430,000 seconds) practically no more gas desorption was identified.
4.7.3. Desorption of mixed gas from coal samples

Desorption of mixed gas is given in Figure 4.50. Although sample type 3 adsorbed gas more than type 2 at 4000 kPa, the difference is not very significant. Consequently the quantity of desorbed gas from type 3 sample does not show the significant difference from the quantity of desorbed gas from intact coal samples. At this stage the explanation given for this 'abnormality' is that whilst the desorptions expressed in cm³/g the weights of samples were 149.941g, 132.663g, and 141.967g for type 1, type 2, and type 3 samples.
respectively. Accordingly one would expect that type 2 sample would adsorb and desorb (in total) more gas than the others at the same pressure level. Figure 4.50 shows that by the time $t$ reached 6345 seconds about 60% of the adsorbed gas has been released for sample type 1, which took 1545 seconds and 3045 seconds for type 2 and type 3 respectively. From the results obtained, again it suggests the need for standardization of the opening of the outlet valve while desorbing gas from bombs. For gas desorbed reached 80% gas release of the adsorbed gas took 4545 seconds and 9045 seconds for type 2 and type 3 samples respectively.

Analysis of gas quantity at desorption was conducted on mixed gas using mass spectrograph. Figure 4.51 shows time against composition of mixed gas
Fig. 4.51. Composition of mixed gas against time during desorption by mass spectrograph analysis

\[ \frac{\text{CH}_4}{\text{CH}_4 + \text{CO}_2} \] since the opening of the outlet valve. The results confirmed that pressure on the free space of the bomb has the significant role on gas desorption.

4.7.4. Discussions
Adsorption

Both Langmuir's and Freundlich's equation were used to model gas adsorption isotherms. At this stage, it may be stated that Langmuir's model shows the better agreement with the results obtained from adsorption laboratory work. In some cases, it produced the better description of coal properties, as shown in the effect of volatile matter on sorptive capacity for German coal (*Figure 4.44*).

The adsorption isotherms shows that normally type 2 adsorbed slightly higher gas than type 1, which confirmed that orientation of flow channels for gas influences the gas flow capacity of coal.

Desorption

*Figure 4.52* shows the desorption curve of CH4 obtained by Airey (1968) for various size of coal (from 200 - 52 mesh up to .625cm - 1.25 cm). *Figure 4.53* shows another desorption curve for core sample (diameter of 50 to 55 mm and length of 50 mm to 120 mm) in CH4 gas (*Lama and Nguyen, 1987*). These two curves were obtained by conducting the conventional volumetric desorption method.

For work by Airey, the general observations are:

(i). the initial rate of release of CH4 is very large for all sizes, and it subsequently falls off progressively with increasing time.

(ii). for the smallest coal size, the total of the CH4 desorbed reaches its ultimate value after about 20 hours, while the larger coal still giving out methane after 600 hours.

Hargraves (1962), working in very fine closely sized coal from drill cuttings and plotting desorption-time at the coal face showed a strong direct relation between granulometry and time to completion of desorption. Hargraves (pers.comm) reports desorption testing on numerous Australian coals of -100mm size lasting at least 4 months.
Chapter 4 - 93

Coal size: B.S. sieve sizes as marked
Coal prepared at 50% moisture and saturated with methane at 300 lb/in²

Fig. 4.52. Airey's desorption test result (1968)

Test 11 W 1
D₀ = 0.000165 cm²/s

Fig. 4.53. Lama and Nguyen's desorption results (1987)
For work by *Lama and Nguyen*, the period of desorption tests varied between 850 hours and 1000 hours, and excluded time elapsed between the opening of the bomb and the transfer of the core samples to the temperature controlled bath which inexplicably was a period varied from 90 hours to 120 hours.

It appears that the desorption period achieved in this work by the gravimetric method with releasing gas to the atmospheric air is much shorter compared to the conventional volumetric method described by others.

Desorption for CO₂ gas showed curves of type 1 and type 2 cross. At this stage, this phenomenon could be explained as the role of reversibility of adsorption process (compare Figure 4.21 and Figure 4.49). Although no adsorption-time curve has been presented.

As has been discussed previously, the volume of the bomb which is not occupied by sample has raised the problems of obtaining two kinds of quantities of gas desorbed and also the condition of atmospheric pressure within the bomb during desorption can not be obtained even though gas has been released to atmospheric air. At this stage there is no correction needed for quantity of gas desorbed obtained, because 'direct gas desorbed' has been converted to gas desorbed.

These problems may be overcome by minimising or virtually eliminating the volume of bomb not occupied by coal sample (free space); which could be better achieved by standardizing the size and the shape of the sample used first and following this by standardizing the volume (size) of the bomb accordingly.
5.1 Introduction.

A complete understanding of the mechanisms underlying the flow process of CH$_4$ gas in coal is essential for safe coal mining and design of ventilation and gas drainage systems. But the understanding still appears to be incomplete. As has been discussed the literature is not in total consensus on the mechanisms of CH$_4$ flow in coal. This can be observed from the variety of models postulated for CH$_4$ gas emission from coal, some models being purely empirical, some being based on Darcy's laminar flow with a pressure gradient as driving force, some on Fick's diffusive flow with the concentration gradient as the drive, and some involving a two-step process with diffusion in the micropores followed by laminar flow in the macropores (Airey, 1968; Kissel and Bielicki, 1972; Bielicki et al, 1972; Hemala et al, 1982; Jones et al, 1982; and King et al, 1983).

Many models which employ Fick's law compare gas concentration in the coal pore-space derived from the gas pressure by some modified form of the ideal gas law, and the diffusion mechanism presented is equivalent to Darcy's laminar law with a gas pressure gradient as the driving force. Furthermore, the gas drainage model describes the gas desorption process from coal specimens by assuming an empirical form with the amount of gas desorbed being an exponential function of time (Bertard et al, 1970; Lama and Bartosiewicz, 1982).

In the following unified theory of CH$_4$ gas in coal, the flow will be described with special emphasis on application of the theory in predicting changes in the gas
flow rate with time. The unified theory has been formulated and developed by 
Nguyen (1988) relying on his earlier work on moisture movement in porous media 
under gradient of temperature (Nguyen, 1975). The main premises of the theory are 
that the flow of CH₄ gas through coal is an interactive flow of the free gas phase 
and the adsorbed gas phase and the interchange of molecules between the two 
phases is influenced by presence of any moisture in the pores, and occurs in the 
manner as depicted by sorption isotherms.

5.2. The unified theory

Methane gas

Under normal conditions, the rate of CH₄ emission into mine workings is 
essentially dependent on seam gas content (which is related to pressure) and 
permeability of coal (which is dependent on porosity).

Normally CH₄ present in coal is described in the following way: it exists in 
two states, namely as the free gas state and as the adsorbed state. Free gas is 
present mainly in the macropores, and its behaviour can be described by Boyle's 
law and the kinetic theory of gases. At normal coal seam pressures, adsorbed gas 
occupies roughly 90% to 95% of the total gas content in coal (Boxho et al., 1980), 
and there is a continual interchange of molecules between the free gas and the 
adsorbed (Patching, 1970).

The quantity of free gas present in the pore space of coal can be described 
by:

\[ PV = ZnRT \]  \hspace{1cm} (5.1) (same as 2.1)

Consequently the quantity of free gas per unit volume of coal, \( C_v \) is 
calculated by:
The volumetric free gas content, $C_v$, is proportional to the coal porosity, $\phi$ which is affected by changes in in-situ stresses and the moisture content of coal or rock.

Likewise the content of the adsorbed gas $C_a$ is related to the free gas pressure in equilibrium by laboratory determined isotherms. It is commonly described by the Langmuir equation:

$$C_a = \frac{ABP}{1 + BP} \quad (5.3) \text{ (same as 2.3)}$$

In general, gas pressure tends to comply with a hydrostatic profile (Patching, 1970; Kim and Douglas, 1973), which means that the deeper the strata the higher the quantity of gases, CH$_4$ gas in particular. Hargraves (pers.comm) feels that the profile commences at about the water table.

### 5.3. Basic flow equations

For practical purposes, the complex mechanism of CH$_4$ transmission in coal is considered to take place under two simultaneous and parallel process: Darcy's laminar flow in the pore space and Fick's diffusive flow of adsorbed gas along the internal surface. The mechanisms of the two gas flow are interactive through the process of phase interchange, or adsorption-desorption as depicted in relevant isotherms, between free gas and adsorbed gas. Influence of rock and gas
compressibilities on the flow rate is also taken into consideration. A complete solution to the mechanism of the gas migration requires the coupling of the equation with a stress-deformation equation.

5.3.1. Darcy's flow for a compressible system

Darcy's law holds that flow rate of a fluid through a porous medium is proportional to the potential or pressure gradient \( \frac{\partial P}{\partial x_i} \):

\[
q_{Di} = - \frac{KA}{\mu} \frac{\partial P}{\partial x_i} \tag{5.4}
\]

where:

- \( K \) : the intrinsic permeability of the porous medium \((\text{cm}^2/\text{s})\)
- \( A \) : the cross-sectional area perpendicular to the macroscopic velocity vector, \(\text{cm}^2\)
- \( \mu \) : the fluid viscosity, \(\text{kPa-s}\)

The relative bulk velocity of methane gas in rock is defined as:

\[
V_i = \phi \left( \frac{\partial \mu_{lf}}{\partial t} - \frac{\partial \mu_{ls}}{\partial t} \right) \tag{5.5}
\]

where:

- \( \phi \) : the rock porosity
- \( \mu_{lf} \) and \( \mu_{ls} \) : displacement of the fluid and rock respectively, and
- \( t \) : time
If $V_{\text{if}}$ and $V_{\text{is}}$ are used to denote velocities of fluid and solid, equation (5.5) can be rearranged as:

$$
\phi V_{\text{if}} = V_i + \phi V_{\text{is}}
$$  \hspace{1cm} (5.6)

where $V_i$ can be described by Darcy's law as:

$$
V_i = -\frac{K}{\mu} \left( \frac{\partial P}{\partial x_i} + \rho g_i \right)
$$  \hspace{1cm} (5.7)

where:

- $K$: the intrinsic permeability of the porous medium (assumed to be isotropic), $\text{cm}^2/\text{s}$
- $\mu$: the fluid viscosity, kPa-s
- $P$: the fluid pressure, kPa
- $\rho$: the fluid density, g/cm$^3$
- $g_i$: the acceleration of gravitational in the $i$th direction

The principle of mass conservation (continuity) for the free gas phase can be written as:

$$
- \frac{\partial}{\partial x_i} \left( \rho \phi V_{\text{if}} \right) = \frac{\partial (\phi \rho)}{\partial t} + \Gamma
$$  \hspace{1cm} (5.8)

where:

- $\rho$: the density of fluid (gas)
\[ \Gamma : \text{the rate of gas transfer from the adsorbed state to the free phase} \]

*Equation (5.7)* gives:

\[
\frac{\partial}{\partial x_i} \left( \rho \phi \nu_{ij} \right) = \frac{\partial (\rho \nu_i)}{\partial x_i} + \phi \frac{\partial \nu_{is}}{\partial x_i} + \nu_{is} \frac{\partial (\phi \rho)}{\partial x_i} \tag{5.9}
\]

Assuming the effects of gravitation are negligible, and noting that the total derivative of time \( \frac{d}{dt} \) can be written as:

\[
\frac{d}{dt} \frac{\partial (\phi \rho)}{\partial t} = \nu_{is} \frac{\partial (\phi \rho)}{\partial x} + \frac{\partial (\phi \rho)}{\partial t} \tag{5.10}
\]

and also:

\[
\frac{d}{dt} \frac{\partial (\phi \rho)}{\partial t} = \phi \frac{d\rho}{dt} + \rho \frac{d\phi}{dt} \tag{5.11}
\]

*Equation (5.3)* can be combined with *equations (5.7), (5.9) and (5.10)* to yield:

\[
\frac{\partial}{\partial x_i} \left( \frac{\rho K}{\mu} \frac{\partial \rho}{\partial x_i} \right) - \phi \rho \frac{\partial \nu_{is}}{\partial x_i} - \nu_{is} \frac{\partial (\phi \rho)}{\partial x_i} = \frac{\partial (\phi \rho)}{\partial t} + \Gamma \tag{5.12}
\]

which, from (5.10) and (5.11), becomes:
The equation of continuity for rock solid can be written as:

\[
\frac{\partial}{\partial x_i} \left( \rho \frac{k}{\mu} \frac{\partial P}{\partial x_i} \right) - \phi \rho \frac{\partial V_{is}}{\partial x_i} = \phi \frac{\partial p}{\partial t} + \rho \frac{\partial \phi}{\partial t} \Gamma 
\]  

(5.13)

where:

- \( \rho_s \): the density of rock solid
- \( V_{is} \): the tensor notation denoting the rate of volumetric strain

It can be shown that equation (5.14) can be rearranged:

\[
- \frac{\partial}{\partial x_i} \left( (1 - \phi) \rho_s V_{is} \right) = \frac{\partial}{\partial t} \left( (1 - \phi) \rho_s \right) 
\]  

(5.14)

where:

- \( V_{is} \): the tensor notation denoting the rate of volumetric strain

Substituting (5.15) for the time derivative of porosity in (5.13), continuity equation of the free gas becomes:

\[
\frac{\partial}{\partial x_i} \left( \rho \frac{K}{\mu} \frac{\partial P}{\partial x_i} \right) = \phi \frac{\partial p}{\partial t} + \rho \frac{1 - \phi}{\rho_s} \frac{\partial p_s}{\partial t} + \rho \frac{\partial V_{is}}{\partial x_i} + \Gamma 
\]  

(5.16)
Defining the compressibility of the rock matrix:

\[ \beta_s = \frac{1}{\rho_s} \frac{d\rho_s}{dP} \]

the effective rock compressibility:

\[ \alpha = (1 - \phi) \beta_s \]

and the fluid compressibility:

\[ \beta_f = \frac{1}{\rho} \frac{d\rho}{dP} \]

*Equation (5.16)* becomes:

\[ \frac{\partial}{\partial \chi_i} \left( \rho \mu \frac{\partial P}{\partial \chi_i} \right) = \rho (\alpha + \phi \beta_f) \frac{dP}{dt} + \rho \frac{\partial V_{is}}{\partial \chi_i} + \Gamma \quad (5.17) \]

5.3.2. Diffusive flow in the absorbed phase

Concurrent with gas movement in the free phase, is the diffusion process taking place by adsorbed gas molecules in the micropore system, under a concentration gradient:
\[ q_{F_i} = -D_F \frac{\partial C_a}{\partial x_i} \] 

(5.18)

where:

- \( D_F \): the diffusivity of CH\(_4\) gas in coal, cm\(^2\)/s
- \( C_a \): the volumetric concentration of adsorbed gas (corresponding to free pressure \( P \))
- \( q_{F_i} \): the rate of surface diffusion per cross-sectional area, g/cm\(^3\)

The continuity equation for the adsorbed phase:

\[ -\frac{\partial}{\partial x_i} (\rho_o q_{F_i}) = \frac{\partial}{\partial t} (\rho_o C_a) - \Gamma \] 

(5.19)

where:

- \( \rho_o \): the density of gas at normal temperature and pressure (NTP)
- \( C_a \): the quantity of gas adsorbed, cm\(^3\)/g

Noting that approximately:

\[ \frac{\partial}{\partial t} (\rho C_a) = \rho_o \frac{\partial C_a}{\partial t} \] 

(5.20)

and:

\[ \frac{\partial C_a}{\partial t} = \lambda \frac{\partial P}{\partial t} \]

where, using Langmuir's equation (5.3):
\[ \lambda_a = \frac{\partial C_a}{\partial P} = \frac{AB}{(1 + BP)^2} \]  

(5.21)

\[- \frac{\partial}{\partial x_i} \left( \rho_o \ D_F \ \lambda_a \ \frac{\partial P}{\partial x_i} \right) = \rho_o \ \lambda_a \ \frac{\partial P}{\partial t} - \Gamma \]  

(5.22)

The combined gas flow equation can now be obtained by adding equation (5.17) and equation (5.22):

\[ \frac{\partial}{\partial x_i} \left( (\rho_o \ D_F \ \lambda_a + \rho \ \frac{K}{\mu}) \ \frac{\partial P}{\partial x_i} \right) = (\rho \ (\alpha + \beta_f \phi) + \rho_o \ \lambda_a) \ \frac{\partial P}{\partial t} + \rho \ \frac{\partial v_{is}}{\partial x_i} \]  

(5.23)

The composite permeability of CH4 gas in coal can be further defined:

\[ K_g = D_F \ \lambda_a \ \mu + \rho \ \frac{K}{\rho_o} \]  

(5.24)

and total compressibility comprising gas, rock matrix compressibility and a phase interchange component:

\[ c_T = \frac{\rho}{\rho_o} \ (\alpha + \beta_f \phi) + \lambda_a \]  

(5.25)

The differential equation describing flow of CH4 gas in coal becomes:
\[
\frac{\partial}{\partial x_i} \left( \frac{K_g}{\mu} \frac{\partial P}{\partial x_i} \right) = c_T \frac{\partial P}{\partial t} + \frac{\rho}{\rho_o} \frac{d\varepsilon_v}{dt} \tag{5.26}
\]

where:
\[
\varepsilon_v : \text{the bulk volumetric strain of coal}
\]

(i). **Stress-deformation equation**

The last term of the unified flow equation (5.26) requires output from the coupling of a stress-deformation equation which can be derived \(\text{(Biot, 1941)}\) as:

\[
G \frac{\partial^2 \mu_i}{\partial x_j \partial x} + (\lambda + G) \frac{\partial^2 \mu_j}{\partial x_i \partial x_j} + \chi \frac{\partial P}{\partial x_i} - f_i = 0 \tag{5.27}
\]

where:
- \(\mu_i\) : displacement in the \(i\)th direction
- \(f_i\) : body force in the \(i\)th direction
- \(\chi\) : rock parameter
- \(G\) : the shear modulus \(\left( G = \frac{E}{2(1 + \nu)} \right) \)
- \(\lambda\) : Lame's constant \(\left( \lambda = \frac{E\nu}{(1 - 2\nu)(1 + \nu)} \right) \)
- \(E\) : the elastic modulus
- \(\nu\) : Poisson's ratio

\[
\chi = 1 + \frac{\beta_s}{\beta} \tag{5.28}
\]

where:
- \(\beta_s\) : the rock matrix compressibility
- \(\beta\) : the bulk compressibility
\( \chi \) can be practically taken as unity (= 1)

The coupling of equations (5.26) and (5.27) yields the system of equations depicted by the theory of CH4 gas flow in coal from which complete solution to the problem of CH4 gas flow in (deformable) rock media can be obtained. Its formulation is appropriate for simulation by finite difference or finite element methods.

5.4. Gas flow rate

In the following, some basic characteristics of CH4 gas drainage from coal will be analysed using the unified theory.

5.4.1. Small equivalent permeability

Consider the simplified form of equation (5.26) in the case where interaction of stress-deformation of rock is negligible or non-existent:

\[
\frac{\partial}{\partial x_i} \left( \frac{K \partial P}{\mu \partial x_i} \right) = c_T \frac{dP}{dT} \quad (5.29)
\]

which can be used to determine flow parameters required for gas flow modelling for laboratory or field tests.

A large discrepancy between the equivalent permeability given computed from (5.29) and the gas permeability measured from a conventional permeability test was revealed from results of desorption tests on coal core samples (Lama and Nguyen, 1987). The permeability predicted by the unified theory is smaller than
the conventional flow permeability by two to three orders of magnitude. This discrepancy (Nguyen, 1989) explains in terms of constriction of coal pore channels by adsorbed gas molecules reducing the effective porosity of coal.

5.4.2. Variation of gas flow rate with time

Variations of the gas flow rates from seams with time have been frequently observed by gas drainage engineers (Truong, 1987). The flow rate itself, although it generally decreases with time, may also have a range of increasing flow. A number of factors such as permeability change, stress history, volume shrinkage due to the degasification process, volume expansion due to water adsorption, and slippage along the walls of the pores, may affect gas flow rate.

As has been discussed above, permeability may decrease by one order of magnitude for a stress change from 1 to 10 MPa, and permeability measurements under triaxial stress condition conducted by Mordecai and Morris (1974) showed a 30% decrease in permeability from initial to fractured conditions followed by a sharp increase of permeability to failure. Changes in gas flow rate also may be affected by the stress history or the cycles of stress change due to mining and the existence of an abutment region at some distance ahead of the coal face which is under higher confinement than the virgin coal. In the unified theory, influence of stress change on flow rate is incorporated by the coupling of the stress-deformation equation (5.27) to the flow equation (5.26).

Another factor which may affect the permeability is shrinkage of coal volume due to the degasification process as has been discussed above. In the unified theory increase in molecular gas release due to 'the shrinkage effect' can be incorporated by a more proper modelling of Darcy's permeability K within
equation (5.24) as a function of effective porosity to account for occupation of the pore space of adsorbed gas molecules.

The feature of 'negative' Klinkerberg effect which affect the flow permeability is explained by the theory as follows:

Typical variation of $K_g$ and $c_T$ with gas pressure, obtained by using realistic parameters from field and laboratory observations (Truong, 1981) and the literature and the equations (5.24) and (5.25) above, is shown in Figure 5.1 and 5.2, respectively. Neglecting stress-deformation and assuming constant effective porosity and pressure gradient, it can be seen from Figure 5.1 and 5.2 that as pressure decreases (from seam gas pressure of 4500 kPa) permeability $K_g$ will decrease (somewhat linearly) as surface diffusion $D_F$ is assumed to be negligibly small and composite $c_T$ will increase. Without influence of or interaction with mining-induced stresses and fracturing and with the assumptions stated above, therefore, the gas flow rate from a coal seam during drainage will tend to decrease with time.

5.5. Computer application

One of the basic aims of the unified theory formulation is to develop a more reliable model which is capable of predicting CH₄ gas flow rate over the entire range of flow regimes. At this stage computer application is restricted to single-phase flow of CH₄ gas in coal and the practical steps required for computer simulation are:

Step 1 : Conduct desorption test on cylindrical coal samples

Step 2 : Conduct adsorption test to determine Langmuir’s constants A and B.

Alternatively, A and B can be estimated from a desorption curve obtained in Step 1:
Fig. 5.1. Variation of equivalent permeability with gas pressure (Nguyen, 1989)

Fig. 5.2. Variation of composite compressibility with gas pressure (Nguyen, 1989)
A = maximum gas content of seam, cm$^3$/g

B = $P_{A/2}^{-1}$

where $P_{A/2}$ is the gas pressure corresponding to a seam content equal to half of the maximum gas content.

Step 3: From results of the desorption test perform history-matching to determine the Darcy permeability $K$ depicting the free gas (laminar) flow component of the composite effective permeability $K_g$. History-matching is performed by computer simulation of the desorption test using the finite-difference method.

Step 4: Assume $D_F$ is negligibly small, and determine coal porosity $\phi$, rock matrix compressibility $\beta_S$. The latter is required only in a coupled analysis.

Step 5: Establish boundary conditions for the real problem requiring simulation.

Step 6: Conduct simulation by a selected method, e.g. finite difference, finite element and boundary element, using the data and conditions established in Steps 2-5.

5.5.1. The Flow Equation

By approximation, equation (5.26) can be rewritten as:

$$
\frac{\partial}{\partial x_i} \left( D \frac{\partial P}{\partial x_i} \right) = \frac{\partial P}{\partial t}
$$

which is an uncoupled flow equation having a diffusion form, and
\[ D = \frac{K_g}{\mu c_T} \quad (5.31) \]

Equation (5.31) is the fundamental form of this formulation and it can be used to validate the model in conjunction with a desorption test (Vutukuri and Lama, 1986).

In cylindrical coordinate system, equation (5.31) is written in the form:

\[ \frac{\partial P}{\partial t} = \frac{1}{R} \frac{\partial}{\partial R} \left( D \cdot R \frac{\partial P}{\partial R} \right) \quad (5.32) \]

where \( D \) : equivalent diffusivity \( D(P) \), i.e. \( D \) is a function of gas pressure.

Equation (5.32) was applied to the desorption data on coal samples. Crank's solution of heat conduction in solids (Crank, 1956) was initially to solve the equation (Lama and Nguyen, 1987).

The Crank - Nicholson form equation (5.32) can be written as:

\[
P^n_j - P^{n-1}_j = \frac{\Delta t}{4_j(\Delta R)^2} \left\{ (2j + 1) D_{j+1/2} (P^n_{j+1} + P^{n-1}_{j+1}) \right\} \\
- \frac{\Delta t}{4_j(\Delta R)^2} \left\{ 2 \left( D_{j+1/2} + D_{j-1/2} \right) (P^n_j + P^{n-1}_j) \right\} \\
+ \frac{\Delta t}{4_j(\Delta R)^2} \left\{ (2j - 1) D_{j-1/2} (P^n_{j-1} + P^{n-1}_{j-1}) \right\} 
\]

(5.33)

which yields a system of linear equations in \( P^n_{j+1}, P^n_j, \) and \( P^n_{j-1} \). Subscript \( j \) denotes annular node and subscript \( n \) denotes the time \( t = n \Delta t \).
At the centre of the cylindrical sample, \( j = 0 \) and \( R = \frac{\Delta R}{2} \), the finite difference scheme can be approximated as:

\[
P^n_0 - P^{n-1}_0 = \frac{2\Delta t}{(\Delta R)^2} \left[ D_{1/2} (P^n_1 + P^{n-1}_1) - D_0 (P^n_0 + P^{n-1}_0) \right]
\]  

(5.34)

*Figure 5.3. (Lama and Nguyen, 1978)*, indicates that the analytical solution to equation (5.32) using constant values of equivalent diffusivity \( D \) (Crank, 1956), gives poor history to experimental data. A sharp kink is observed at around 85% - 90% of the total gas content desorbed, in contrast with a more gentle pattern of gas desorption (Airey, 1968). The slope of desorption curve is a measure of the gas diffusivity or equivalent permeability \( K_g \), and a gently changing slope with increasing time or decreasing gas pressure can be modelled by the permeability being a direct function of gas pressure, that is:

\[
D = D_0 \left( \frac{P}{P_0} \right)^e
\]  

(5.35)

or:

\[
k = k_0 \left( \frac{P}{P_0} \right)^e
\]  

(5.36)

where:

\[
k : \frac{K_g}{\mu}
\]
P: the original seam gas pressure or sorption pressure
laboratory coal specimen
e: an exponent

For the unified model of gas to be validated, the main focus should be on identification of parameter of equation (5.32) (or its permeability form (5.26)), that is determination of $D_0$ (or $K_0$) and exponent $e$.

5.5.2. The method of Dipole Reflection

Identification of parameter, which is also called back analysis was used as an optimisation search scheme. It is not a well-posed problem in the mathematical sense due to yielding not a unique solution but a multitude of solutions. Two type of parameter identification approach, the direct and the indirect may be differentiated.

The direct approach involves reformation of the matrix of equations, such as the potential flow equation or elastic stress-deformation equation, and the required parameters form the variable vector, for examples vector of transmissivities in hydrology, and vector of elasticity moduli in stress analysis, whilst the state parameters such as hydraulic heads and deformation or strain measurements are inverted and built into the matrix of coefficient.

The indirect approach involves unknown parameters not explicitly used in the forward solution system; for example back-figuring the shear strength parameters or as in the present modelling determining flow parameters. Solution to these problems normally requires the use of optimisation techniques, especially those by-passing evaluation of partial derivatives such as Powell's method, Rosenbrock's method, and the simplex reflection method (Nguyen, 1985). One can
consider that the indirect approach may be further sub-divided into two categories. One category involves the minimisation of a standard error function:

\[
f = \sum_{i=1}^{n} (t_i - m_i)^2
\]  

(5.37)

where:

- \( n \): the number of data points
- \( t_i \): the \( i^{th} \) computational
- \( m_i \): the experimentally value

The optimum of the error function \( f \) is not zero normally.

The other category is the back analysis of a failure which is equivalent to locating the minimum of function \( f \) (normally a limit state functional), which is equal to zero. Optimizing such limit state function can be effectively conducted by the Newton - Raphson method in conjunction with a Taylor's series expansion as exemplified by Nguyen (1985).

Identification of parameter which is normally found in electrical engineering literature, is to deal with the first data or the curve involving recursive relations. This is most appropriate with state variable or parameter being represented as a time series. Smoothing of the curve or filtering is also used to consider the uncertainty nature of the variables and parameters. In that capacity, its formulation tends to suppress the mechanistic nature of parameter relations. Due to the poor history matching of the analytical solution to the desorption data shown in Figure 5.3 and considering the principle of 'filtering', it is decided that identification of the parameter is best performed in two stages. The first stage is to determine the shape of the desorption curve as represented by exponent \( e \), and the second stage to determine \( k_o \) or \( D_o \). This approach has been found to give more meaningful results to the parameter values required in the formulation above.
A new optimisation search scheme has been devised to determine $D_0$ (or $k_0$) from desorption data. The scheme, called the Dipole Reflection technique, is a simplified and single parameter version of the simplex reflection technique, commonly used in geomechanics application in recent years (Nguyen, 1985). Its algorithm begins with evaluation of the objective function at two trial values of the unknown parameter. The values of the two 'poles' are then compared with each other, and the pole having a higher value is reflected to the other side of the other pole by the same separation distance. The function is again evaluated at the reflected pole and the process of comparing and reflecting is repeated until convergence is reached. To avoid 'swinging', a second reflection on the same pole uses only half the separation distance in reflection.

5.6. PROGRAM DESORB

5.6.1. Description of the program

The program DESORB has been written for the operation of microcomputers with MS - DOS (Trademark of Microsoft Inc.). The code contains a main program for data input and iterative computations for the Dipole Reflection Method, and six subroutines. Test data are supplied under free format from a file (FILINP), and consist of:

- Langmuir's A and B constants
- the universal gas constant $R$
- gas molecular mass
- absolute temperature
- gas viscosity
- coal porosity
coal density, and

- a number of desorption data, which used $10^{-5}$ seconds and $\text{cm}^3/\text{g}$ as the unit for the time and desorption respectively. The six subroutines are:

FULCOM: the main subroutine incrementing the time for computing distribution of pressure, quantity of desorption, and the error function in the history matching of desorption data. The error function is the objective which is employed in the search for the optimal value of equivalent permeability.

GASCON: the function routine calculating the total gas content of coal. The total gas content is the sum of adsorbed gas and free gas.

CTAD: the function routine which evaluates the total compressibility (equation 5.25).

ASSEMB: assembles the matrix equation to solve for new gas pressures at nodal points.

GAUSOL: makes CALL to subroutine SOLVER.

SOLVER: solves the system of simultaneous linear equations.

Program DESORB is given in Appendix 4.

5.6.2. Illustrative example

A computer run using desorption data obtained from this current work was performed.

The coal sample was a cylindrical core of 49.6mm diameter and of 55.4mm height, and assumed porosity of 0.025 on the basis of Bulli Seam coal. The circular cross section was divided into annular rings for the Crank - Nicholson finite difference computation. Using the Dipole Reflection method, after fifteen
iterations the optimum value of $K_0$ was determined to be 0.001817 mD. The results of the run are shown in Figure 5.3.

Figure 5.4 shows the data being matched with the exponent model given in Equation 4.16. At this stage it appears that both models did not produce the match expected; Figure 5.3 more simulates 'direct gas desorbed' (compare to Figure 4.12). Most certainly the empirical model simulate 'direct gas desorbed', because in fact (at this stage), actual gas desorbed is a curve converted from direct gas desorbed. Also, the result obtained from the desorption test is not 'the real desorption' due to free space in the bomb.
Fig. 5.3. Data against unified model for CH4 desorption from intact coal
Fig. 5.4. Desorption data against empirical model
CHAPTER VI
CONCLUSIONS AND RECOMMENDATIONS

6.1. Conclusions

General

This research is mainly concerned with assessments of the methane gas migration in coal based on sorption isotherms. It is also concerned with improvements in the existing adsorption-desorption measurement procedures by reducing the contribution of systematic errors.

Direct method

The direct method is a quick method to determine the gas content of coal seams. With the existing procedure, doubt is cast on its accuracy due to large values of 'lost time' while determining Q1, time preparing sample for determining Q2, and crushing time for the last stage to determine Q3. The 'lost time' in early stages is more accentuated due to the large quantity of gas desorbed.

Manual recording and processing of data especially in conventional gas desorption tests (volumetric method) are often inaccurate due to:

gas being released into the upper chamber of an inverted graduated cylinder filled with water, not to atmospheric air at atmospheric pressure, consequently there is a built-up of pressure in the upper chamber which results in the volume read not normally being exactly at atmospheric pressure.
**Indirect method**

The indirect method involves measurement of seam gas pressure and laboratory determination of the quantity of gas content of the particular coal at this pressure and in-seam temperature.

To measure seam gas pressure: the seal set deeply in the bore-hole takes some time to build up to full seam pressure. The validity of the results obtained depends on the efficiency of sealing and the presumptions that the drilling of the hole has not had the effect of affecting the maximum pressure to be investigated behind the seal and that the hole and seal are deep enough to reach the virgin gas condition.

To prepare an adsorption isotherm based on the indirect method and to use the isotherm along with the measured gas pressure in the seam as to be the virgin seam gas pressure, provides a particular figure of gassiness to be applied to the coal. Such a determination of seam gas content by the indirect method may incorporate assumptions as input data.

In the existing procedure of laboratory determination of the adsorption isotherm, free space in the bomb could cause the following problems:

(i). wasted gas during adsorption process, which

(ii). leads to obtaining two kinds of gas adsorbed, i.e. 'direct gas adsorbed' and '(actual) gas adsorbed' during adsorption process and consequently will produce two kinds of gas desorbed, i.e. 'direct gas desorbed' and '(actual) gas desorbed' while desorbing, and

(iii). the condition of atmospheric pressure within the bomb while gas was desorbing could not be achieved although gas is released to atmospheric
air as supported by output of 'BGDESPRE' program and mass spectrograph analysis on mixed gas.

The results of gas desorption suggest that a control for standardised opening of the pressure release (outlet) valve is needed to ensure laminar flow takes place.

**6.2. Recommendations**

To minimise the possibility of obtaining two kinds of gas adsorbed during the adsorption process, and to minimise the time needed to reach atmospheric pressure within the bomb during desorption (approaching 0.0 second), free gas space in the bomb should be minimised and virtually eliminated.

This condition may be achieved by using a coal sample of volume approximately equal to the volume of the bomb, allowing for the slight coal expansion during adsorption.

Standardised bomb and sample sizes should be used to minimise comparative errors from bomb to bomb.

A geometric shaped sample should be a better model for analysis than a random chip, and apart from considerations of duration of experiment a drill core would appear to offer the best opportunity for analysis of adsorption and desorption.

At this stage, the maximum standardised opening for the outlet valve during desorption in order to obtain laminar flow is recommended to provide an initial rate of weight decrease of 0.001g/second - 0.003g/second.
The direct and indirect methods combined to obtain measurement of greater accuracy of determination of seam gas content is recommended as follows:

A fresh sample from the seam under consideration is investigated by enclosing the sample in the standardised bomb (with the minimum free space) as soon as possible, take it to the laboratory and measure the gas release from the coal sample using the gravimetric method. The lost time during the transportation is recorded. The measurement in the laboratory is taken continuously by data acquisition system, for instance for the first twelve hours, and then reading manually once per day until the rate of emission becomes insignificant.

Simultaneously, an indirect method investigation should be conducted on the cutting of the same sample to confirm the result of the direct method and to obtain the lost gas Q1 during the lost time.
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**Appendix 1**
Calculation of gas quantity adsorbed

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<td>TYPE OF GAS</td>
<td>CH₄</td>
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<thead>
<tr>
<th>Weight of bomb, W₀ g</th>
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</thead>
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<td>Weight of bomb and coal, W₁ g</td>
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</tr>
<tr>
<td>Weight of coal in bomb, W₁ - W₀ g</td>
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</tr>
<tr>
<td>Density of coal, dc g/cm³</td>
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<tr>
<td>Density of gas (NTP), dg g/cm³</td>
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<td>Internal volume of bomb, V₀ cm³</td>
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<td>Volume of coal in bomb, cm³</td>
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<td>Free volume of bomb unoccupied by coal, cm³</td>
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<th>Pressure, kPa (gauge)</th>
<th>100</th>
<th>200</th>
<th>500</th>
<th>1000</th>
<th>2000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wt Bb+coal +Gas, W₂ g</td>
<td>1724.134</td>
<td>1724.334</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Gas wt in Bb, W₂-W₁</td>
<td>0.254</td>
<td>0.454</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Gas vol Bb Fr+ads, (W₂-W₁)/dg</td>
<td>385.082</td>
<td>688.296</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Gas vol as Cal Cur, V₁</td>
<td>275.076</td>
<td>554.454</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>V₁/V₀</td>
<td>0.790</td>
<td>1.593</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Free gas vol in Bb (V₁/V₀)* V₀- (W₁ W₀)/dc</td>
<td>191.802</td>
<td>386.605</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Vol of gas ads in coal at NTP [(W₂-W₁)/dg-V₁/V₀*{V₀-(W₁-W₀)/dg}]</td>
<td>193.280</td>
<td>301.690</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Gas vol ads in 1 g coal, cm³</td>
<td>1.310</td>
<td>2.045</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Gas vol dir ads in 1 g coal, cm³</td>
<td>2.611</td>
<td>4.666</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
A-2

APPENDIX 2

10 CLS
15 REM PROGRAM BGDES
20 REM ********************************************************************
30 REM This program is used to monitor gas desorption from bomb
40 REM It records the time vs weight at certain interval
50 REM It also records time vs gas desorb quantity
60 REM Coded by Boni Siahaan, 1988
70 REM Department of Civil and Mining Engineering
80 REM The University of Wollongong, NSW, Australia
90 REM ********************************************************************
100 A1 =.................. A2=................. A3=..................
110 A4 =.................. A5=............... A6=............... 
120 DEF FND(X) = A1 + A2*X + A3*X^2 + A4*X^3 + A5*X^4 + A6*X^5
130 INPUT "bomb number (bb)= ", BB
130 INPUT "initial weight (g)= ", WO
140 INPUT "sample weight (g)= ", WS
150 INPUT "gas density (g/cc)= ", DG
160 PRINT "bb,wo,ws", BB,WO,WS
170 REM set the current time
180 T$="000000"
190 ON ERROR GOTO 270
200 TIMES$=T$
210 OPEN "COM1: 2400,e,7,1,1f,pe" AS #1
220 OPEN "O",#2,"DESB6.DAT"
230 PRINT #1,"SNR"
240 T=TIMER
240 INPUT #1,S$
250 ON ERROR GOTO 900
260 REM ********************************************************************
270 record the weight after 15 sec elapsed, 3 times
280 REM ********************************************************************
290 T1=0
300 FOR Y=1 TO 3
310 T=TIMER
320 INPUT#1,S$
330 TM=ABS(T-15)
340 IF TM>.2 GOTO 250
350 IF VAL(S$)=0 THEN INPUT #1,S$
360 T1=T1+15
370 GOSUB 1020
380 WRITE #2,T1,VAL(S$),DW,Q,FND(Q)
390 PRINT "t,wc,dw,q,fnd(q)",T1,VAL(S$),DW,Q,FND(Q)
400 T$="000000":TIME$=T$
410 NEXT Y
420 REM *******************************************************
430 REM record weight 30 times for each 60 sec elapsed
440 REM *******************************************************
450 T$="000000":TIME$=T$
460 T1=45
470 FOR Y=1 TO 30
480 T=TIMER
490 INPUT #1,S$
500 ON ERROR GOTO 930
510 TM=ABS(T-60)
520 IF TM>.5 GOTO 420
530 IF VAL(S$)=0 THEN INPUT #1,S$
540 T1=T1+60
550 GOSUB 1020
560 DESOR=FND(Q)
570 PRINT "t,wc,dw,q",T1,VAL(S$),DW,Q,QA
580 WRITE #2,T1,VAL(S$),DW,Q
590 T$="000000":TIME$=T$
600 NEXT Y
610 REM *******************************************************
620 REM record weight 6 times for each 300 sec elapsed
630 REM *******************************************************
640 T$="000000":TIME$=T$:T1=1845
650 FOR Y=1 TO 6
660 T=TIMER
670 INPUT #1,$S$
680 ON ERROR GOTO 960
690 TM=ABS(T-300)
700 IF TM>.5 GOTO 590
710 IF VAL($S$)=0 THEN INPUT #1,$S$
720 T1=T1+300
730 GOSUB 1020
740 PRINT "t,wc,dw,q",T1,VAL($S$),DW,Q
750 WRITE #2,T1,VAL($S$),DW,Q
760 T$="000000":TIME$=T$
770 NEXT Y
780 REM ********************************************************
790 REM record weight 24 times for each 900 sec elapsed
800 REM ********************************************************
810 T$="000000":TIME$=T$:T1=3645
820 FOR Y=1 TO 24
830 T=TIMER
840 INPUT #1,$S$
850 ON ERROR GOTO 990
860 TM=ABS(T-900)
870 IF TM>.5 GOTO 760
880 IF VAL($S$)=0 THEN INPUT #1,$S$
890 T1=T1+900
900 GOSUB 1020
910 PRINT "t,wc,dw,q",T1,VAL($S$),DW,Q
920 WRITE #2,T1,VAL($S$),DW,Q
930 T$="000000":TIME$=T$
940 NEXT Y
950 CLOSE #1:CLOSE #2
960 END
970 COM(2) ON
980 INPUT#1,$S$
990 GOTO 200
1000 COM(2) ON
1010 INPUT#1,$S$
1020 GOTO 450
1030 COM(2) ON
1040 INPUT#1,S$
1050 GOTO 620
1060 COM(2) ON
1070 INPUT#1,S$
1080 GOTO 790
1090 DW=(WO-VAL(S$))
1100 Q=(DW/DG/WS)
1110 RETURN
1120 END
APPENDIX 3

10 DIM AD (5)
20 CLS
30 REM PROGRAM BGDESPRE
REM**************************************************
40 REM This program is used to monitor gas desorption from bomb
50 REM it records the time vs weight and press at certain interval
60 REM Also gas desorb volume vs time interval
70 REM Coded by Boni Siahaan, 1989
80 REM All right reserved
90 REM Department of Civil and Mining Engineering
100 REM The University of Wollongong, NSW,Australia
110 REM**************************************************
112 A1= A2= A3=
114 A4= A5= A6=
115 DEF FND(X)=A1+A2*X+A3*X^2+A4*X^3+A5*X^4+A6*X^5
120 INPUT "bomb number (bb) = ", BB
130 INPUT "original weight (g) = ", W0
140 INPUT "sample weight (g) = ", WS
150 INPUT "gas density (g/cc) = ", DG
160 PRINT "bb,wo,ws",BB,W0,WS
170 REM set the current time
180 T$="000000"
185 ON ERROR GOTO 270
190 TIME$=T$
200 OPEN "COM1:2400,e,7,1,if,pe" AS #1
210 OPEN "0",#2,"L6WEIGHT.DAT"
220 PRINT #1, "SNR"
230 T=TIMER
240 INPUT #1,$
250 IF VAL ($$) =0 THEN GOTO 240
260 GOTO 280
270 COM(1) ON:GOTO 240
280 REM ************************************************
290 REM record time vs weight and press after 15 sec elapsed, 3 times
300 REM ************************************************
310 T1=0
320 FOR Y=1 TO 3
330 T=TIMER
340 INPUT #1,S$
350 TM=ABS(T-15)
360 IF TM>.2 GOTO 330
370 IF VAL (S$)=0 THEN INPUT #1,S$
380 T1=T1+15
390 GOSUB 990
400 GOSUB 1020
410 PRINT "t,cw,dw,q,p",T1,VAL(S$),DW,Q,AC
420 WRITE #2,T1,VAL(S$),DW,Q,AC
430 T$="00000":TIME$=T$
440 NEXT Y

460 REM record time vs weight and press 30 times for each sec elapsed
470 REM *************************************************
480 T$="000000":TIME$=T$
490 T1=45
500 FOR Y=1 TO 30
510 T=TIMER
520 INPUT #1,S$
530 TM=ABS(T-60)
540 IF TM>.5 GOTO 510
550 IF VAL (S$)=0 THEN INPUT #1,S$
560 T1=T1+60
570 GOSUB 990
580 GOSUB 1020
590 DESOR = FND(Q)
600 PRINT "t,wc,dw,q,p", T1,VAL(S$),DW,Q,AC
610 WRITE #2,T1,VAL(S$),DW,Q,AC
620 T$="000000":TIME $=T$
620 NEXT Y
630 REM ****************************************************
640 REM record weight and press 6 times for each 300 sec elapsed
650 REM ****************************************************
660 T$="000000":TIME$=T$:T1=1845
670 FOR Y=1 TO 6
680 T=TIMER
690 INPUT #1,S$
700 TM=ABS(T-300)
710 IF TM>.5 GOTO 680
720 IF VAL (S$)=0 THEN INPUT #1,S$
730 T1=T1+300
740 GOSYB 990
750 GOSUB 1020
760 PRINT "t,wc,dw,q,p", T2,VAL(S$),DW,Q,AC
770 WRITE #2,T1,VAL (S$),DW,Q,AC
780 T$="000000":TIME$=T$
790 NEXT Y
800 REM ****************************************************
810 REM record weight and press 24 times for each 900 sec elapsed
820 REM ****************************************************
830 T$="000000":TIME$=T$:T1=3645
840 FOR Y=1 TO 24
850 T=TIMER
860 INPUT #1,S$
870 TM=ABS(T-900)
880 IF TM>.5 GOTO 850
890 IF VAL (S$)=0 THEN INPUT #1,S$
900 T1=T1+900
910 GOSUB 990
920 GOSUB 1020
930 PRINT "t,wc,dw,q,p" T1,VAL (S$),DW,Q,AC
940 WRITE #2,T1,VAL (S$),DW,Q,AC
950 T$="000000":TIME$=T$
960 NEXT Y
970 CLOSE #1:CLOSE #2
980 END
1000 Q=(DW/DG/WS)
1010 RETURN
1020 BA=&H278
1030 FOR Q=1 TO 4
1040 OUT BA,7
1050 A=INP(BA+3)
1060 FOR I=1 TO 7:A=INP(BA+4):NEXT I
1070 FOR I=1 TO 7:INP(BA+5):NEXT I
1080 C=INP(BA+2)
1090 HB=(C/16-INT(C/16)) *16
1100 LB=INP(BA+1)
1110 AD(Q)=HB*256+LB
1120 NEXT Q
1130 AC=0
1140 FOR Q=1 TO 5
1150 AC=(AD(Q)+AC)
1160 NEXT Q
1170 AC=(AC/50)*2
1180 RETURN
C
--------------
C PROGRAM DESORB
C
--------------
C
A FORTRAN to model gas desorption from
C cylindrical rock cores
C
C Coded by V. U. Nguyen
C Department of Civil and Mining Engineering
C University of Wollongong - NSW 2500
C
DIMENSION RJI (30), DIFF (30), DESORP (930), PMOD (930)
DIMENSION PRES (15), DFICO (3), GOP (3)
CHARACTER FILJNP*10, FILPRN*6, APR*1, FILOUT*10
COMMON/PHILIP/TIMAX, CTT, TSTEP, PREA, DR, NRIN, NUMD
COMMON/LARRE/RJI, DIFF
COMMON/NZ/IU, RTIO, PRECO, RGAS, AAV, BBV, DENS1, PHIM, RMAS,
$ TEMP, RMUOU
C
C -----------------------------------------------
C PREA: atmospheric pressure, kPa
C FILPRN: output print file
C FILINP: input data file
C AAV, BBV: Langmuir's constants
C RGAS: Universal gas constant
C RMAS: Molecular mass of gas
C TEMP: ambient temperature
C NUMD: No. of desorption data (time & desorption quantity)
C PHIM: Rock porosity (fraction)
C NRIN: number of annular rings used in F. D. model
C DENS1: rock density (g/cm3)
C RJI (K): time (10^5 seconds); DIFF (K); desorption (cm3/g)
C FILOUT; output disk file
C PRECO: initial sorption pressure, kPa
C
PREA= 101.3
FILPRN='PRINTF
WRITE(*,*) 'ENTER INPUT DATA FILENAME (10 CHARAC.
$ MAX.)'
READ(*,1023) FILINP
1023 FORMAT (A10)
OPEN (UNIT=4,FILE=FILINP,STATUS='OLD' ,
$ ACCESS='SEQUENTIAL' ,FORM='FORMATTED')
READ (4,*) AAV,BBV,RGAS,RMAS,TEMP,RMUOU
READ (4,*) NUMD,PHIM,NRIN,DENSI
C
C Converting AAV from cm³/g to cm³/cm³
C
AAV= AAV*DENSI
C
C Reading diffusion data
C
Do 215 I=1,NUMD
215 READ (4,*) RJI (I) ,DIFF (I)
C
NDIM=NUMD
PI=4.0*ATAN (1.0)
C
C Interactive data input
C
WRITE(*,*) 'Do you have a PRINTER connected ? (Y/N) '
READ(*,135) APR
135 FORMAT(A1)
WRITE(*,*) 'Give name to OUTPUT file (10 characters
$ maximum)'
READ9*136) FILOUT
136 FORMAT(A10)
IF(APR.EQ.'Y' .OR.APR.EQ.'Y') FILPRN='LPT1.'
WRITE(*,*) 'Enter Diameter & height of sample (mm)'
READ (*,*) DIAM,HEIGHT
DIAM=DIAM/10.0
RADIUS=DIAM/2.0
WRITE(*,*) 'ANALYSIS Type: 1 = Darcy; 2 = Diffusion; 3 & = Mixed'
WRITE(*,*) 'Enter Analysis Code (1,2 or 3):'
READ(*,*) IU
C
IF(IU.NE.2) GOTO 666
WRITE(*,*) 'Enter diffusivity (cm2/s)'
GOTO 667
666 WRITE(*,*) 'Enter initial trial value of K (of gas),
$ Darcy'
WRITE(*,*) '(If Viscosity in 1E-08 kPa-s)'
667 READ(*,*) DOR
RTIO=0.0
IF(IU.NE.3) GOTO 668
C
WRITE(*,*) 'Ratio of diffusion coefficient DF (in
$ cm2/s)'
WRITE (*,*) ' TO permeability K (in Darcy) - (Hint:
$ 0.05) '
READ(*,*) RTIO
C
668 WRITE (*,*) ' Enter seam gas (or sorption) pressure (KPa)'
WRITE(*,*) ' (if not available, enter 0 then press RETURN)'
READ(*,*) PRECO
C
C Time conversion to seconds
C
DO 121 I=1,NUMD
121 RJI(I)=RJI (I)*100000.0
IF (PRECO.EQ.0.0)THEN
WRITE(*,*) ' Enter gas content in cm3/g or m3/ton'
READ(*,*) CONTT
END IF

C Calculate initial gas content CTT (in cm³/cm³)
C
C IF (CONTT.LE.0.0) GOTO 2660
CTT = CONTT*Densi
write(*,*) contt, ctt

C CTT = ABP/(1+BP) + PHI*(P/Patm) (to be exact)
C
CALL SEAMP (PRECO, CTT, AAV, BBV, PHIM, TEMP)

C WRITE(*,*) 'Sorption pressure=', PRECO, 'kPa'
GOTO 2670

2660 CTT = GASCON (AAV, BBV, PRECO, PHIM, TEMP)
CONT = CTT/Densi
2670 CONTINUE

C WRITE(*,*) 'GAS CONTENT ', CONT, ' cm³/g'

C Input for F>D Calculation
C
DR = RADIUS/FLOAT(NRIN)
NRINS = NRIN + 1
DO 1 J = 1, NRIN
1 PRES(J) = PRECO
PRES(NRINS) = PREA

C TUY = PRECO
DORI = PERMG(TUY, DOR)
CBOT = CTAD (AAV, BBV, PRECO, PHIM)
THIG = 0.75*(DR**2.)/DORI
IF (THIG.GE.10000) THIG = 10000
WRITE(*,*) 'Compressibility: ',CBOT
WRITE(*,*) 'input time step (around ',THIG,'sec) '
READ(*,*) TSTEP

C
C VOL= PI*(RADIUS**2) *HEIGHT
C
C
DFICO(1)= DOR
DFICO(2)= 1.50*DOR

C
C DFICO(1) & (2) are two trial values of flow coefficient k0
IFLG=0
APR=''
WRITE(*,*) 'Do you want a quick run or $
$ optimizing run (q/o) ? '
READ(*,135) APR

C
C Output File
C
C
OPEN(UNIT=9,FILE=FILOUT,STATUS='UNKNOWN',ACCESS=
$ 'SEQUENTIAL')
OPEN(UNIT=7,FILE=FILPRN,STATUS='UNKNOWN',ACCESS
& ='SEQUENTIAL')

C
2840 IF(APR.EQ.'q'.OR.APR.AQ.'Q) THEN
ZOPT=DOR
GOTO 3110
END IF

C
C OPTIMIZING Run:
C Dipole Reflection Method to determine k0
C
C
WRITE (*,*) 'Enter number of interactions & accuracy
$ (eg. 0.002) '
READ(*,*) NSTOT,ERROE

C
DO 2870 I=1,2
GERR=0
GOP(I)=0.0
CALL FULCOM(DFICO(I),GERR,DESORP,PMOD,NDIM)
IF(I.EQ.2) GOTO 2870
WRITE(9,*) AAV,BBV,RGAS,RMAS,TEMP,RMUOU
WRITE(9,*) NUMD,PHIM,NRIN,DENSI
WRITE(9,*) DIAM,HEIGHT,PRECO,CONT,DOM,RTIO
WRITE(9,*) DFICO(I),',',GERR
WRITE(7,*) DFICO(I),',',GERR
2870 GOP(I)= GERR
JOLD=0
IF(GOP(I) .EQ.GOP(2) .AND.DFICO(I) .NE.DFICO(2) THEN
   ZOPT= .5*(DFICO(I)+DFICO(2))
   GOTO 3110
END IF
2930 IF(GOP(I).GT.GOP(2)) GOTO 3000
   JBIG=2
   JSMA=1
   GOTO 3010
3000 JBIG=1
   JSMA=2
3010 JNEW=JBIG
   RFAC=1
   IF (JNEW.EQ.JOLD) RFAC=.5
   DFICO(JNEW)=DFICO(JSMA)+RFA*(DFICO(JSMA)-DFICO(JBIG))
C
3040 JOLD=JBIG
   NREF=NREF+1
   CALL FULCOM(DFICO(JNEW),GERR,DESORP,PMOD,NDIM)
   WRITE(9,*) DFICO(JNEW),',',GERR
   WRITE(7,*) DFICO(JNEW),',',GERR,',',NREF
   GOP(JNEW)=GERR
   FUER=ABS(GOP(JNEW)-GOP(JSMA))
C
IF(FUER.LE.ERROE.OR.NREF.GE.NSTOT) THEN
ZOPT=DFICO(JSMA)
GOTO 3110
END IF
GOTO 2930

3110 IFLG=1
CALL FULCOM(ZOPT,EROP,DESORP,PMOD,NDIM)
WRITE(7,*) ZOPT,',',EROP
WRITE(9,*) 'OPTIMUM AT ',ZOPT,' ERROR: ',EROP

C
C Final output using optimum value of k0
C----------------------------------------------------------
DO 3210 I=1,NDIM
IF(RJI(I) .EQ.0.0.OR.DESORP(I) .EQ.0.0) GOTO 3210
WRITE(9,*) RJI(I),',',DESORP(I),',',DIFF(I),',',PMOD(I)
WRITE(7,*) RJI(I),',',DESORP(I),',',DIFF(I),',',PMOD(I)
3210 CONTINUE
CLOSE(UNIT=9)
CLOSE(UNIT=7)
STOP
END

C
C Quadratic equation to obtain Seam Pressure from CTT (cc/cc)
C----------------------------------------------------------
C
C SUBROUTINE SEAMP (PSEAM,CTOO,A01,B01,POROS,TND)
C----------------------------------------------------------
PATM=101.3
T00=298
ALI= B01*POROS*T00/TND*PATM
BLI= A01*B01-CTOO*B01+POROST00/(PATM*TND)
CLI= -CTOO
DETA= BLI**2  - 4.*ALI*CLI
PSEAM= )-BLI + SQRT(DETA))/(2.*ALI)
RETURN
C function GASCON calculates gas content

FUNCTION GASCON(A01,B01,PRX,POROS,TND)

GASCON = (A01*B01*PRX/(1.0+(B01*PRX)) +
POROS*PRX*298./(101.3*TND))
RETURN
END

C function CTAD(A01,B01,PRX,POROS)

FUNCTION CTAD(A01,B01,PRX,POROS)

BEF=1/PRX
RLAND = (A01*B01)/((1.0+B01*PRX)**2.)

ALLFA=0
CTAD=(PRX/101.4) * (ALLFA+BEF*POROS)+RLAND
RETURN
END

C function PERMG(PRX,PERK)

FUNCTION PERMG(PRX,PERK)

COMMON/NZ/IU,RTIO,PRECO,RGAS,AAV,BBV,DENSI,PHIM,RMAS,
$ TEMP,RMUOU

Kozeny-Carmen adjustment to permeability

EFFI= PHIM/(1.+BBV*PRX)
EFFK= PERK*(EFFI**3.)/(1.-EFFI)
SURDIF is Fick's coefficient of surface diffusion
SURDIF = RTIO*EFFK
TUY = 1.0
IF(IU.EQ.2) THEN
  TUY = 0.0
  SURDIF = PERK
END IF

RLAND = (AAV*BBV)/((1.0 + BBV*PRX)**2.)
DENG = PRX*RMAS/(RGAS*TEMP)
DENO = 101.3*RMAS/(RGAS*TEMP)
PERMG = (SURDIF*RLAND*RMUOU + TUY*(DENG/DENO)*EFFK)
$ /RMUOU
RETURN
END

SUBROUTINE FULCOM(DIFUS, EFRUN, THEO, PMOD, DIM)

DIFUS: amount of desorption cm^3/g, ERFUN: error function

DIMENSION AMA(15,15)
DIMENSION DIAN(750), RMETHA(750), APSUAT(750)
DIMENSION PRES(15), PNEW(15), RJ(30), DIFF(30),
$ THEO(30), PMOD(30)

COMMON /PHILIP/TIMAX, CTT, TSTEP, PREA, DR, NRIN, NUMD
COMMON/LARRE/RJ, DIFF
COMMON/NZ/IU, RTIO, PRECO, GAS, AAV, BBV, DENS1, PHIM, RMAS,
$ TEMP, RMUOU

DO 366 I = 1, NDIM
THEO(I)=0.0

INK=25
IWEN=NDIM - 1
NCOS=NRIN+1
DO 3340 J=1,NRIN

PRES(J)=PRECO
JR=0
PTT=PRECO
NU=0
TIM=0.0
TINC=TSTEP
NRINS=NRIN+1
DO 3370 K=1,750

GUIR=PTT/PRECO
IF(GUIR.GE.0.3.AND.GUIR.LT.0.6) TINC=TSTEP*2.0
IF(GUIR.GE.0.15.AND.GUIR.LT.0.3) TINC=TSTEP*5.0
IF(GUIR.GE.0.05.AND.GUIR.LT.0.15) TINC=STEP*15.0
IF(GUIR.GE.0.02.AND.GUIR.LT.0.05) TINC=STEP*25.0
IF(GUIR.LE.0.02) TINC=TSTEP*30.0
TIM=TIM+TINC
ROO=TINC/(DR**2)
TIMEX= RJI(NDIM)+10.0*TINC
IF(TIM.GE.RJI(NDIM)) INCK=4
IF (TIM.GE.TIMAX) GOTO 3630
DIFO= PERMG(PRES(1),DIFUS)
PRE12= .5*(PRES(1)+PRES(2))
DIF12= PERMG(PRE12,DIFUS)
PRES(NRINS)=PREA
PNEW(NRINS)=PREA

CALL ASSEMB(DIFUS,AMA,PRES,NCOS,ROO,DIFO,DIF12)
CALL GAUSOL(NRIN,PNEW,PRES,AMA)

C Calculate new pressure at nodes
DO 3480 J=1,NRIN
  IF(PRES(J).LT.PREA) PRES(J)=PREA+(1.0/(J+1.0))
  PTOT=PRES(J)*(2*J-1)+PTOT

CONATJ=GASCON(AAV,BBV,PRES(J),PHIM,TEMP)

CTOT=CONATJ*(2*J-1)+CTOT
CT=CTOT/(NRIN**2.0)
PTT=(CTT-CT)/DENSI

Modified isotherms: Max. Adsorbed Gas<Seam Gas Content

IF(EMIS.GE.DIFF(NDIM)) AAV=CTT

NU=NU+1
IBCHK=((NU/INCK)-INT(NU/INCK))
IF(IBCHK.NE.0) GOTO 3600
JR=JR+1
DIAN(JR)=TIM
RMETHA(JR)=EMIS
APSUAT(JR)=PTT
  WRITE(*,*) 't,P,D,C,TIM,PTT,EMIS,CT
  RMETHA(JR) is in "cc/g"
3600 CONTINUE
C
3370 CONTINUE
3630 CONTINUE
C
MAXJ=JR - 1
DO 3670 L= 1,NDIM
DO 3680 K=1,MAXJ
LA=0
IF(THEO(L).GT.0.0) GOTO 3670
IF(RJ(L).EQ.DIA.(K)) THEN
THEO(L)=RMETHA(K)
PMOD(L)=APSUAT(K)
GOTO 3670
END IF
IF(RJI(L).GT.DIAN(K).AND.RJI(L).LE.DIAN(K+1)) LA=K
IF(LA.NE.0) GOTO 3777
3680 CONTINUE
3777 CONTINUE
C
GRDM=(RJI(L)-DIAN(LA))/(DIAN(LA+1)-DIAN(LA))
DMET=RMETHA(LA+1)-RMETHA(LA)
DAPS=APSUAT(LA+1)-APSUAT(LA)
THEO(L)=RMETHA(LA)+DMET*GRADM
PMOD(L)=APSUAT(LA)+DAPS*GRADM
C
3670 CONTINUE
IF(THEO(NDIM).GT.25.0.OR.THEO(NDIM).LE.THEO(IWEN))$ THEO(NDIM)= RMETHA(MAXJ)+0.1
C
C Calculate error (optimal function to determine k0)
C
ERFUN=0.0
DO 3890 J=1,NDIM
3890 ERFUN= ERFU + (THEO (J) -DIFF(J))**2
ERFUN= SQRT(ERFUN/(NDIM-1))
WRITE(8,*0 'Error of prediction ',erfun
RETURN
END
C
SUBROUTINE GAUSOL(NRIN, PNEW, PRES, AAA)

DIMENSION PNEW(15), VECT(15), PRES(15), AAA(15,15)
NROW=NRIN
NCOL=NROW+1
CALL SOLVER(VECT, AAA, NROW, NCOL)

DO 4800 J=1, NROW
   PNEW(J)= VECT(J)
4800 PRES(J)= PNEW(J)
RETURN
END

SUBROUTINE ASSEMBLE(DIFUS, AAA, PRES, NCOL, ROO, DIFO, DIF12)

Assemble matrix system of equations with nodal pressures as variables

DIMENSION BUR(15,15), AAA(15,15), PRES(15), B(15)
COMMON /PHILIP/TIMAX, CTT, TSTEP, PREA, DR, NRIN, NUMD
COMMON/NZ/IU, RTIO, PRECO, RGAS, AAV, BBV, DENS1, PHIM, RMAS,$ TEMP, RMUOU

ICIR=1
C ICIR=1 is for case of SPHERE coal lump
NCOL=NRIN+1
NRINS=NCOL
CT11= CTAD(AAV, BBV, PRES(1), PHIM)

DO 11 J=1, NRIN
   BUR(1,J)= 0.0
   IF(ICIR.EQ.1) GOTO 5270
   BUR(1,1)= 1.0*CT11+3*ROO*DIFO
11
BUR(1,2) = -3*ROO*DIF12
B(1)  = 3*ROO*DIF12*PRES(2)+(1.*CT11-3*ROO*DIFO)*PRES(1)
GOTO 6290
5270 BUR(1,1) = 1.*CT11+2*ROO*DIFO
BUR(1,2) = -2*ROO*DIFO
B(1)  = 2*ROO*DIF12*PRES*(2)+(1.*CT11-2*ROO*DIFO)*PRES(1)
5290 CONTINUE
DO 5460 J=2,NRIN
   JL=J-1
   DO 5230 K=2,NCOL
5310 BUR(J,K)=0
   PREP=(PRES(J+1)+PRES(J))*0.5
   PREM=(PRES(J-1)+PRES(J))*0.5
   DMP=PERMG(PREP,DIFUS)
   DMM=PERMG(PREM,DIFUS)
IF(ICIR.EQ.1) GOTO 5400
   DJP1=(ROO/(2*JL))*(JL+1)*DMP
   DJ=-(ROO/(2*JL)*JL*(DMM+DMP)
   DJM1=(ROO/(2*JL)*(JL-1)*DMM
GOTO 5430
5400 DJP1=(ROO/(4*JL))*(2*JL-1)*DMP
   DJM1=(ROO/(4*JL)*(2*JL-1)*DMM
5430 CTJJ=CTAD(AAV,BBV,PRES(J),PHIM)
   BUR(J,J)=1.*CTJJ-DJ
   BUR(J,J-1)=DJM1
   BUR(J,J+1)=DJP1
   UJ=1.*CTJJ+DJ
   UJP1=DJP1
   UJM1=DJM1
   B(J)=UJ*PRES(J)+UJP1*PRES(J+1)+UJM1*PRES(J-1)
5460 CONTINUE
C
B(NRIN)=B(NRIN)-BUR(NRIN,NCOL)*PRES(NRINS)
DO 5550 I=1,NRIN
DO 5540 J=1,NRIN
5540   AAA(I,J)= BUR(I,J)
5550   AAA(I,NCOL)=B(I)
      RETURN
      END

C
SUBROUTINE SOLVER(C,A,NRO,NCO)
C
C Matrix solver
C
DIMENSION C(15),A(15,15)
C
DO 32 K=1,NRO
   PIVOT=A(K,K)
   IL=K
   K01=K+1
   DO 34 L=K01,NRO
   IF(ABS(A(L,K)).LT.ABS(PIVOT)) GOTO 38
   PIVOT=A(L,K)
   IL=L
34   CONTINUE
   IF (IL.EQ.K) GOTO 32
38   CONTINUE
   DO 39 LL=1,NCO
   TEMPOR=A(K,LL)
   A(K,LL)=A(IL,LL)
   A(IL,LL)=TEMPOR
39   CONTINUE
32   CONTINUE
C
C Calculate first row
C
DO 46 J=2,NCO
   A(1,J)=A(1,J)/A(1,1)
46   CONTINUE
C

DO 50 L=2,NRO
  L1=L-1
  DO 51 I=L,NRO
    SUM=0.0
    DO 53 K=1,1,L1
      SUM=SUM+A(I,K)*A(K,L)
    53 CONTINUE
    A(I,L)=A(I,L)-SUM
  51 CONTINUE
C

LP1=L+1
  DO 59 J=LP1,NCO
    SUM=0.0
    DO 61 K=1,L1
      SUM=SUM+A(L,K)*A(K,J)
    61 CONTINUE
    A(L,J)=(A(L,J)-SUM)/A(L,L)
  59 CONTINUE
C

C(NRO)=A(NRO,NCO)
NROM1=NRO-1
  DO 69 M=1,NROM1
    I=NRO-M
    SUM=0.0
    DO 72 J=I+1,NRO
      SUM=SUM+A(I,J)*C(J)
    72 CONTINUE
    C(I)=A(I,NCO)-SUM
  69 CONTINUE
RETURN
END