行政院及所屬各機關出國報告

（出 國 類 別：研　究）

（報 告 題 名：石油系統盆地分析）

服務機關：中國石油服份有限公司
台灣油礦探勘總處
姓　　名：張　森　吉

出國地區：美　　國

出國期間：八十九年八月一日
至十一月十七日

報告日期：民國九十年三月二日

目　　次

『石油系統盆地分析』研習報告

摘　　要

熱力裂解為有機物生成油氣主要機制，此機制可視為由三個互相關係之盆地分析主題：①盆地地層之埋藏史；②熱力變化史及③油氣之生成、移棲、聚集等。這些主題之研究方法漸漸演變作電腦軟體模擬，因此數學公式逐漸成為主要工具之一。模型的過程中，熱及液體流、地層壓密作用。油氣之生成及驅逐及第二次移棲等為盆地模擬考慮之因素，利用數學公式計算其地質年代中之歷史，進而評估模擬之盆地地層中是否是有機物成熟之要件以及油氣儲存之目標。

『石油系統盆地分析』電腦應用軟體著重於考慮因素使其達到較高的準確度。其方法在於利用現今所得之地質剖面資料轉為過去地質年代中盆地由初始至現今的一切埋藏史、熱力流動史，以及油氣生成之模擬。"PROBAS"為此次研習中，所應用之『盆地分析』電腦軟體，它可應用於平原區及麓山區之油氣探勘，並以圖型或表格資料呈現其結果，進而可模擬油氣儲存量及可能儲存位置，進而有助油氣之探勘。

『石油系統盆地分析』研習報告

一、前言：

本出國研習主題為『石油系統盆地分析』，大致上有關此主題可分為原理理論與實際電腦軟體操作。本主題研習之主要目的在幫助瞭解一個油氣探勘區域生油岩、儲油岩與油氣蓋層三者在一個沈積盆地內，所經過時間之各種變化，並利用數學模式及電腦軟體，以廓繪出對該地區油氣之探勘潛能及風險評估。本公司因應未來油氣探勘愈形困難處境，針對上述三種岩體在空間與時間之分佈，在選擇鑽井井位時先行透徹瞭解，因而對此問題甚為重視。故於八十九年度之研究計劃指派筆者赴美國柏克萊大學研習本主題。在此除感謝上級主管之指派外，並提出此次出國研習報告，期望對本主題有較深入之瞭解外，並對油氣探勘有直接之幫助。

本研習係以修課以及單獨面對面討論等方式計對本主題之研習，研習地點為美國柏克萊大學地球及行星科學系(Dept. of Earth and Planetary Sciences)，此系前身為地質及地球物理科學系，本系內設有『石油系統』小組(petroleum system project)，其領導人為 Dr. Wang 及 Dr. Berry，筆者

研習之期間恰為秋季學期之開始，故在此期間修了兩門課程：工程數學及石油地質，完整地修完這兩門課程，工程數學課程由 Dr. Wang 指導，主要課程包括偏微分方程及向量分析等。此二主題係計對油氣石油系統數學模擬所必須之課程。具備工程數學之基礎，對於數學模擬較容易吸收。另一門課程"石油地質"由 Dr. Berry 指導，此課程主要教授內容包括油氣之化學成份，油氣之生成步驟，油氣之探勘方法，最後綜合主題為『油氣石油系統』等，作有系統之瞭解。單獨面對討論研習方式，則與 Dr. Wang 單獨討論石油系統盆地分析之理論內容及電腦模擬之操作與應用。筆者在此研習利用上述二種方法，甚感收獲不少，尤其對於數學方程式在模擬中之物理意義獲得較佳之瞭解。

本報告內容包括『石油系統盆地』分析基本原理與須考慮之內容外，並作有系統之描述，並對於未來一盆地之分析有所幫助。最後並附有研習過程中，電腦應用軟體所須輸入之基本資料。

二、『盆地分析』之主題沿革與進展大綱

盆地分析之主要學派(main school)：

1、德國學派(German school)

Welte and Yukler(1981)強調 3-D 模式之整合，針對液體流動壓密作用以及熱傳輸正確地預測沈積盆地之油氣生成。Welte(1983,1988)將水力傳導係數(hydraulic conductivity)加入流體方程式，但滲透力(permeability)並沒有列入其方程式。文章諸如 Yalcin et al(1987)、Wygrala(1988)及 Yalcin(1991)，數學方程式利用 Eulerian frame，對孔隙率與應力之變化加以描述。

2、法國學派(French school)

注重 2-D 數值油氣生成及移棲之模擬，主要代表為 Institut Francais du Petrole (IEP)—Durand et al.(1984)、Tissoted et al.(1987)、Ungerer et al.(1990)、Burrns and Audebett(1990)、此學派利用 Lagrangian coordinate system,且將滲率力、流體密度、黏度列入方程式，而求其流體之特性。著重於孔隙率之減少計值與實測值對有效應力之關係。

3、伊利若學派(Illinois school)

Bethke(1955)發表熱流與流體經過壓密沈積盆地之模式，其資料來自 Exxon Oil Co。其後之研究強調水流，超壓力之關係，且著重於次生礦物對油氣生成之影響。Sharp(1983)亦為此學派之一員。

4、南卡羅來納學派(The South Carolina school)

Lerche and Glezen(1984)，以 Gulf Oil Co 之資料模擬盆地。利用 Lagrangian coordinate system 為基礎，強調孔隙比例(void ratio)與有效應力之數學關係。孔隙率與深度之關係模式，並建立應用方程式。

5、柏克來學派(Univ. of cal, Berkeley)

此學派為筆者於本次研習所赴之小組，其主要研究重點為整合盆地之模擬，利用有限元素數學方程式，並建立軟體名為 PROBAS，對熱流(heat flow)、流體、脫水作用、碳氫化合物之成熟度，流體之傳輸等利用數學方程式描述其特性。這些控制因素於構造，如岩石破裂面、斷層，這些依據資料再作出與時間變化，模擬並回覆過去一幕一幕之變化歷史。筆者並於研習期間於 Dr. Wang 指導下，利用此軟體演練盆地分析模擬，所利用之軟體應用者手冊將列於後頁。

除了上述較重要之外，尚有其它之模擬方式，在此不另一一述之。

三、盆地分析要素

有機物在盆地內經過地質時間受熱裂解作用，產生碳

氫化合物，為油氣生成之主要機制，此機制包括三個主要因素：①埋藏史(burial history)；②受熱史(thermal history)及③油氣生成、移棲及儲存史。此三要素並非獨立無關，而是互相相關，其要點如下：

A、利用埋藏史之資料作為盆地之評估

埋藏史之計算資料可提供"石油地質師"下列資料，如盆地之地史對孔隙率之預料，以及地史對熱傳導率(thermal conductivity)，這些資料依深度及岩性而變。再加上由地殼下沈或不整合之處理，可預測有機物裂解成油氣之時間及溫度，此時間即所謂關鍵時間(critical time)。另外提供熱流量或成熟度之指數。所需資料包括地層頂面之深度，地層之岩性，地層孔隙與深度之關係，井孔底部之溫度或地層溫度；油母質含量，以及鏡煤素反射率等與深度變化之資料。資料來源可能來自井下電測，地質報告或震測剖面等。建立地史之因數(parameters)包括可能生油岩之成熟度時間與深度之關係、生油岩熱量分佈、沈積速率與盆地下沈速率對時間之關係、壓密導致下沈之量、沈積物負載之大地平衡(isostatic response to sediment load)及脫

離地殼下沉量(backstripped crustal subsidence)，此即為總下沉量減去壓密以大地平衡之反應量。這些因素最後利用電腦程式計算，並用圖表示其結果。時間間隔之古構造圖油氣隨時間之移棲路線圖，以及生油岩因時間變化之熱力成熟度均可利用圖示表示之。利用構造地層圖、地質圖或震測剖面圖，以表示油氣生成之時間與油氣移棲可能路徑，最後關鍵點即為儲存之位置。

地層埋藏史係由震測剖面，地質剖面或由井下地層資料所建立之地層埋藏深度與時間之變化。若不考慮壓密效應(compaction effects)，所有地層界限之上升速率最上層為相同，在目前最上層界限在地表，則由地層厚度可知其它地層界限之深度，利用反撥法(backstripping process)可建立"地層埋藏史"。但這只是模式，真正實際必須考慮地層之深度可能因孔隙率之變化而有不同。目前建立的只是壓密後的深度，沈積時壓密程度輕小，故地層厚度較壓密後為大，故必須考慮去壓密作用(decompaction effects)，所得之沈積地層厚度以推算埋藏深度才較合真實。Hinte(1978)說明

若 R：沈積物堆積速率；A：經過時間；T：目前地層厚度，且孔隙率為ϕ；ϕ_0：沈積時孔隙率，則 R=T(1－ϕ)/A-(1－ϕ_0)，此式表示地層之厚度為時間之函數，亦即為深度之函數。Sclater and Christie(1980)建立孔隙率之經驗公式$\phi=\phi_0 e^{-cz}$，ϕ：孔隙率在深度為 z，ϕ_0：孔隙率在地表 z＝0 時，C＝常數(依不同岩性而變)。

另一種模式由 Falrey and Middleton (1981)提出，他們的模式孔隙率遞減除了因深度外，另考慮載負效應(loading effects)，其基本公式為 $d\phi/\phi=-kedL$；而 $e=\phi/1-\phi$且 dL=(1-ϕ)/dz；dz 代表負載所影響深度之變化，k：岩性常數。則上式之解為 $1/\phi=1/\phi_0+kz$；ϕ_0：初始孔隙率，z：深度。此式依岩性之不同，有不同之經驗公式，如：

頁　岩：$1/\phi=1/0.7+2.43z$

砂　岩：$1/\phi=1/0.4+1.20z$

粉砂岩：$1/\phi=1/0.53+2.18z$

壓密效應修正利用$\phi=\phi_0 e^{-cz}$，$d\phi/\phi=-kedL$，則總厚度於沈積物為 hs，其深度為 z_1 為 z_2，則

$hs=[1-\phi(z)]dz$

$$hs=(z_2-z_1)-(\phi_0/c)(e^{-cz1}-e^{-cz2})$$

$$(z_2-z_1)-(1/k)$$

進一步推論：

$$z_4-z_3=hs+(1/k)\ln[(1/\phi(s)]/(1/\phi_0+kz_3)$$

如果已知下列壓密係數、鑽井深度、年代及古水深，則利用上列方程式，可繪出埋藏史。

另外與孔隙率有重要之因素為不整合之模擬，有下列三種方式可模擬不整合：

1、沈積間斷(depostional hiatus)

2、沈積或侵蝕在剖面之厚度及年代由地區性地質決定(如鏡煤素反射率之間斷或電測等)。

3、利用估計法計算侵蝕厚度

$$AGE_E=(R_1\times AGE_1+R_2\times AGE_2)/(R_1+R_2)$$

$$侵蝕厚度=R_1\times(AGE_E-AGE_1)$$

AGE_E：開始侵蝕之年代、AGE_1、AGE_2：不整合上下之年代，R_1及R_2為不整合面上下沈積物之沈積速率。

經過上述之修正後，各層之厚度及深度為時間之函數，再依岩性及密度，即可估算地殼因負載而

沈之量度，下列公式可作為下沈量之估算(Steckler and Watts,1978)：

$Y=S[(Pm-Ps)/(Pm-Pw)]+Wd-\Delta_{SL}[Pm/(Pm-Pw)]$，

Pm：平均地函密度、Pw：平均水密度、Ps：平均沈積物密度、Δ_{SL}：平均海水面之上下、Y：無沈積物或水負載岩盤之深度，Y：亦代表大地構造力影響之地殼下沈量，Wd 及Δ_{SL}由古沈積環境估算。

B、碳氣化合物之生成及熱量史

建立地層埋藏史主要目的之一在於預測生油岩之成熟度及潛能之程度，主要在於評估沈積盆地油氣產量是否是儲存至開關經濟價值。下列諸點必須知悉：(1)在盆地任何位置，其每立方公里可產油氣之量；(2)油氣形成時間、蓋層建構時間，以及構造形成時間而封閉；(3)多少量之油氣已遠移離生成岩，剩下多少殘有於生油岩；(4)評估油氣最後儲存之位置。

上述必須以定量方法才能作到，數學模式有有助於上述問題之達成。Tissot and Welte(1978)

應用現象模式預測碳氫化合物含量對時間與溫度之變化。第一級化學反應動能假設全部消耗於油母質之裂解如下公式：

$$dx_i/dt = k_i x_i \text{；} k_i = A_i e^{-Ei/kbT(t)}$$

x_i：第 i 種化合物之密度、k_i：反應速率、k_B：波滋曼常數、A_i：反應速率(在溫度上限)、E_i：活化能、T(t)：x_i 化合物時間為溫度之函數。一般認為油母質有三種類型(type Ⅰ、Ⅱ、Ⅲ)，每種可視為有 6 個不同之化學鍵，其活化能之範圍約 10～80Kcal/mole，所以有機物 X_i 第 i 個反應之總反應熱為 $E_1+E_2+\cdots\cdots+E_6$，利用有不同之油母質對 i 反應有不同之 E_i、A_i 及 X_i 值。這些數值為定量計算油氣生成量所需之變數，且必須決定時間對溫度之方程式。Tissot and Welte(1978)利用固定地溫梯度於此模式，且把熱流量(heat flux)視為隨時間變化，可改善此模式。散熱方程式：

$$\partial_T/\partial_t = (\rho c)^{-1}\nabla\bullet(k\nabla T)+(\rho c)^{-1}Q(t)\delta(z-z_{besement})$$

，其中 c：比熱、ρ：密度、k：熱傳導率 δ(z)：

Dirac function、Q(t)：熱流量為時間之函數。在 3-5km 深處，此散熱方程式之解為：

$T(t)=T_t(t)+Q(t)D(t)/k(t,z)$，其中 $T_t(t)$：每層頂部之溫度為時間之函數，D(t)：該層之厚度亦為時間之函數、k(t,z)：為平均熱傳導為時間及深度函數。欲預測盆度之成熟度，必須知道 Q(t)、D(t)及 k(t,z)，而 k(t,z)及 D(t)可由埋藏史及岩性得知，但 Q(t)較難估算。欲估算古地溫，須知熱傳導係數與時間之關係，但很難由外插法求得，只應用於砂岩，而砂岩只限於偏部空間與時間，頁岩與石灰岩則由實驗方法求得。熱傳導係數主要受制於孔隙率。在無資料可應用之處，吾人可假設 $k_s=k_r(k_w/k_r)^{\phi}$，k_r、k_w 及 k_s 分別為岩基(rock matrix)、水及沈積物之熱傳導係數，ϕ為孔隙率。

依 Friedimger(1988)，熱傳導係數可寫為：

$$k_n=k_f^{\phi}k_s^{(1-\phi)}$$

熱傳導係數一般隨溫度增加而下降，在油氣溫度窗中，其溫度之效應更為明顯。而任何古熱

流量之模式必須符合現令之熱流量，此由井底地層溫度、地表溫度及熱傳導係數可估算總熱流量。

C、盆地回撥下沈(back stripped subsidence)及熱流史(heat flow history)

回撥下沈(Y)可利用地質模式預測之，對特一地質模式比較回撥下沈及預測下沈(predicted subsidence)；其目的為經由兩者下沈之差異：(1)可評估該地質模式之可靠性；(2)利用此地質模式預測熱流史；(3)可用來修正地質模式對鏡煤素反射率之差異及(4)預測潛能生成岩之成熟度與時間之關係，其離井位之下沈量，可用震測剖面解釋之。

地質模式可提供熱流變化與時間之重要來源，熱源之估算對一模式可能增加，而對另一模式可能減少。大致上有四種模式應用於地殼之下沈：(1)Mckenzie 岩石圈延展模式；(2)火成岩脈入侵模式；(3)熱力膨脹模式及(4)深部地殼變質模式。各種模式所估算地殼高度隨時間、溫度變化

之估算公式，各有差異不在此詳述。

D、依鏡煤素反射率估算熱流

各種地質模式所算出之熱流均有差異，由鏡煤素反射率估算熱流為一較佳之方法，熱流利用此方法估算之誤差可能來自埋藏史之評估以及輸入之資料。其它方法尚有黏土礦物之轉變、孔隙率對深度與溫度之變化、油氣中碳元素之對稱性、油氣中分子之重量分佈。同位素之變化、礦物之退火性質地磁歷史、液體包、花粉之透明度、生物指標等，可作為估算熱流之方法。此熱流之估算進而可預測盆地各深度地層之成熟度。

一般"盆地分析"之模擬輸出之資料可分為三種：埋藏史、熱力成熟度以及相關資料。埋藏史資料包括各地層對時間之深度變化圖、地殼下降與時間圖、壓縮下沈圖、地平衡及負載下沈圖、沈積物沈積速率圖、基般下沈與時間之關係圖、海平面對時間之關係圖。熱力成熟度計算圖包括目前時間溫度相積(TTI)對深度圖，目前鏡煤素反射率對時間圖、鏡煤素反射率對 TTI 圖，每一層每一種油母質

產生油氣之百分比與時間之變化圖。至少有七種情況，其熱流對時間變化可被模擬，如：具有固定之溫度梯度，目前之熱流假設固定且可由井底或地層之溫度及岩性決定，利用 Makenzie 模式，其它模式決定其熱流。

結合熱力成熟度資料及埋藏史計算，可作出熱力成熟度之影響結果，如計算油母質裂解成油氣量與地質年代之變化，此為"盆地分析"主要目的之一。

E、油氣生成及驅逐模擬

"盆地模擬" 目前為油氣探勘普遍工具之一，未來亦將如此，而盆地模擬亦盆地分析首要之事，至於它是否有用呢？至於是否有必要去作呢？回答此問題，須先知油氣形成之活化能及其驅逐之方式。本次研習對此問題之大綱整理出較重要之幾點。

1、為何要作動力學模擬？

數學模式指出溫度與地質年代影響因素？

一般而言，動力控制之化學反應具有時間與溫

度互相補償之特性，但因古溫度無法確定，故時間溫度只能定性。動力模式包括活化能、反應速率，初始及次生反應等問題。

Lopatin－Waples method 係假設化學反應速率每溫度增 10℃，其加速為兩倍，此粗略估計尚可，若要精確計算，則誤差很大。而且時間亦有時會高估，例如當地層有受侵蝕時，地溫下降 20℃，此時成熟度可能停止增加。除時間與溫度外，尚有其它因素可影響碳氫化合物之生成？很明顯對某一有機物之種類，壓力亦會影響其裂解速率。一般而言，壓力低於 200bar，其影響較大，200-200bar 影響不大，且高壓可使之缺乏不飽和碳氫化合物。然而壓力一般在"盆地分析"不列入考慮之因素。

同樣地，含水量亦不確定之因素。硫分量可能加速成熟度，其效應在熱裂過程中，伴演降低黏度。氧元素之存在亦可加速有機物之裂解。黏土礦物可能不如預測之重要。

2、何種動力模式較重要？

一般模式均利用第一級為其反應速率，此反應只考慮動力之裂解，通當並不考慮第二級反應，此反應可能因成熟度之增加而使油氣進一步分解。一般而言，活化能並非完全消耗於化學鍵之破壞，在熱裂分析若利用封閉系統，可得較佳之結果。並且利用區段溫度分佈熱裂比連續溫度較佳。

其它問題如：如何得到動力模擬參數，以降低其不準確度？鏡煤素模擬之特性？何種模式可用來描述油氣驅逐？

其次問題如盆地模擬、地化資料拌演之角色，如由地化資料決定其成熟度或地化資料決定其氣驅逐模式等。最後如可否預測化學成份或盆地中之液氣相狀態，均為"盆地分析"之主題

F、熱力模擬

決定熱力分佈之歷史之因素為目前之測量溫度(地面及井下溫度)，目前之測量成熟度地質資料(構造史、熱流史、氣候變化、沈積環境、侵蝕史等)，其它如物理性質(有機物組成熱傳係數、孔隙率、孔

隙填充物等)。模擬之方法一般利用電腦軟體，孔隙率可用公式模擬。熱傳導係數可根據孔隙率及氣候摸擬，熱流根據構造運動及目前之地溫修正之。成熟度可用 TTI 觀念依鏡煤素反射率計算，碳氫化合物計算依據第一級反應方程式，地溫資料取自電測或 DST 溫度，並作井底溫度之修正。

不正常熱流可能來自特有之地質現象(如冰川效應、盆地近代下沈、高壓帶及孔隙液體及流動之變化)，近年之不確定等因素。高壓帶併演重要之角色，其產生原因為不滲透層、快速沈積、厚層積物等。

四、結論：

『石油系統分地分析』係一門相當繁複之工作，且為目前石油探勘重要的工具之一，尤其在對一處女地之探勘，由少量現有之資料，對一盆地作歷史性之描述，由每一時間間隔所作的描繪，即為此分析之主要工作。主要工作為：①盆地埋藏史之模擬；②熱力之摸擬；③碳氫化合物之生成與驅逐之摸擬；④孔隙率、液相流以及油氣移棲之模擬等，這些問題均涉及艱深之數學公式運算，故均以電腦軟體運算。

在探勘應用上，有許多種電腦軟體針對盆地分析之模擬作特定性之用途。如：筆者本次研習中，所用之軟體PROBAS，可應用於平原區及麓山區，且可依需要精確度，作較細之時間分割，得到較正確及詳細之模擬。本次研習之主要目的除了理論與原理之探討外，並利用 PROBAS(如附件)電腦軟體應用於地質或震測剖面，作上述各種主要之模擬。研習之報告除以書陳述外，並附上 PROBAS 應用程式之資料手冊，以利未來應用此程式之先前準備，並將應用於未來油氣探勘上

此次研習筆者感覺數學是現代科技電腦軟體之重要工具，過去均認為數學之艱難，但此次之研習中，將數學作生活化之講解，因此感覺並非想像中之艱難，此為研習中意外之收穫。

五、研習心得與建議

『石油系統盆地分析』為探勘界累積百年來之知識，對石油之探勘在一盆地之地層作整合性之研究，亦為目前對一探勘區域之整合性評估。我們知道，一個盆地經過地質年代之時間，經歷了自然界之作用包括物理、化學以及

生物等，盆地內地層經過這些變動，再加上熱力與流動之過程，最後之結局為現今我所看到的事實。這些事實是過去長久時間累積的結果，而『石油系統盆地分析』主要之工作在於對過去某一斷地質年代利用模擬，回後過去之歷史，這些歷史該我們能掌握未知之地下地層對油氣儲存數量及位置。這些工作是繁複且艱辛的，但對油氣探勘而言，它們是先前的工作，其主要目的在於預知油氣的移棲路徑，以及最後的儲存位置。

『石油系統盆地分析』在應用方面，已知甚多種類之軟體，應用於模擬應用軟體程式之設計工程數學大為重要。培養程式設計人員，將有助於模擬應用程式之改進，建議本公司應加強電腦軟體程式設計工作。

PROBAS 軟體應用程式操作要點：

此次赴柏克萊大學研習『石油系統盆地分析』課程，除理論之探討外，其部份時間研習電腦應用程式之操作。

此節主要描述電腦程式所輸入之資料列出其要點，程式名稱為『PROBAS』。係由此大學所設計之電腦程式，除用於平原區之盆地外，亦可用於盆地構造山運動之麓山區。故此軟體適合用於台灣麓山區之盆地模擬，此點與大多數模擬軟體不同之處。

"PROBAS" 主要有兩大部份需要瞭解：(1)輸入檔案；(2)圖形輸出，輸入檔案又可分為五個資料：(1)沈積層及斷層之幾何資料(sediment layer and fault geometry data material property data)；(2)物質之特性資料；(3)幾何分割資料(mesh geometry data)；(4)地質時間資料(geologic time data)及(5)液體來源資料。(其詳細操作方法如附件)，各資料性質簡述如下：

(1)沈積及斷層幾何資料：將地質剖面或震測剖面(時間已換為深度)、圖上之地質資料(包括地層界限及斷層或其它構造)，先界定出座標，再將各地質界限利用數位化讀存至電腦檔案，為首先之工作。即各地層之

界限座標數位化，讀存資料包括地層之上下界限座標，以及地層各地塊界限之性質等。

(2)物質之特性資料：總共有17種物質資料需要輸入，此為針對地塊中各地層之物性質料，包括孔隙率poro(地表條件)、可壓縮係數(b1：負載狀下、b2：非負載狀下)、地表面積(Sxo：在x軸方向、Syo：在y軸方向)、熱產生率(heat：W/kg)、黏土比例(earth：%)、顆粒密度(ds：kg/m^3)、沈積物之比熱(cs：J/kg ° k)、熱傳導係數(w/m° k)、岩石指數(equation number)、①：頁岩、②：砂岩(斷層厚度(米))、有機碳百分比(TOC%)、油母質(ker1、ker2、ker3、ker4)碳酸鈣含量($CaCO_3$：%)

(3)幾何分割資料：總計沉積地層之總數，斷層之總數等

(4)地質年代資料：各地層界限之絕對年代。

(5)液體來源資料：水之產生量、地溫、碳氫化合物之產出量、二氧化碳之產出量，所用單位均為gm/kg of rock。

上述利用電腦運算及繪圖，為所需之基本資料，其所運用之公式如操作手冊。

"PROBAS"盆地模擬資料輸入手冊：

Ⅰ、輸入資料：

1、沈積層及斷層幾何資料

2、沈積物特性資料

3、幾何分割資料

4、地質年代資料

5、流體來源資料

Ⅱ、輸出資料：

1、數值資料

2、繪圖資料

Ⅲ、基本方程式

PROBAS
- a Basin Modeling Program

User's Manual

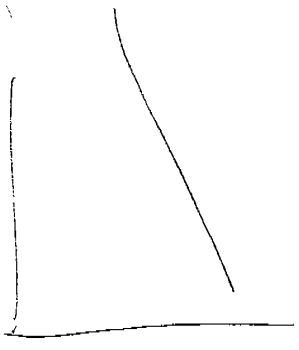
by
Chi-yuen Wang and Pengtao Sun

Spring, 2000

CONTENTS

$$\beta \equiv \frac{1}{V}\frac{dV}{dP} \approx \frac{1}{V_0}\frac{\Delta V}{\Delta P}$$

$$\Delta V = V_0 \beta \Delta P$$



I. Introduction

Sedimentary basin is a dynamic system in which complex processes, such as heat flow, the creation of fluid through compaction, dehydration and hydrocarbon maturation, fluid transport, etc., interact with each other. Fracturing, faulting, and the formation of fluid compartments further complicate the situation. Furthermore, these processes are time-dependent nonlinear and may significantly impact the expulsion and migration of hydrocarbons in basins. Through the effort over the past decade, we have developed a modeling tool, ***PROBAS***, for integrated analysis of the thermal evolution, hydrocarbon maturation and fluid migration in sedimentary basins. The software tool is a two-dimensional finite-element code for accurate and site-specific simulation of a rift basin with listric growth fault. This code allows the users to simulate time-dependent sedimentation and faulting at prescribed geologic rates, and to reconstruct the thermal evolution and fluid (water, oil and gas) migration in the basin.

Most basin models neglect the processes of faulting and fault diagenesis. It is well known, however, that faults sometimes provide major pathways for fluid transport and, on other occasions, become major barriers for fluid movements. Significant oil and gas fields are associated with fault zones, but the question why some faults are sealing while others are leaking remains to be one of the most challenging problems in hydrocarbon exploration. Thus it would be vital to integrate the processes of faulting, fault diagenesis, and their time-dependent changes, together with sediment and hydrocarbon maturation, and migration, in basin models.

The ***PROBAS*** system consists of four major components: 1. User specified input, 2. automatic generation of finite element meshes, 3. finite element calculation, and 4. graphic output of the calculated results. Only the first and the last components of the system will be of concern to the users. The first component (user specified input) allow users to define the necessary input files. The last component (graphic output of the calculated results) allows the user to make various graphic outputs of the computed results. Generation of the finite element mesh (the second component) and subsequent finite element computation (the third component) are fully automatic and require no effort from users.

II. User Input Files

The required input files by the ***PROBAS*** system consist of two categories: geometrical data and material data. These files contain user-specified information for sedimentary layering and time of sedimentation, fault geometry, mesh density, and sediment properties. All these files are stored in the "data" subdirectory. The nature and the required format for these files are described in the following:

1. Geometric data

The geometric data for the ***PROBAS*** basin modeling come from the 2D seismic profiles. It consists of a vertical cross-section of a sedimentary basin, with the vertical dimension converted from the seismic travel time to depth (in km). The major boundaries between the sedimentary layers and faults on the cross-sections are digitized at selected key-points and the coordinates (in distance and depth) of these boundaries and faults are tabulated and stored as the basic input information for modeling. Back-stripping of this digitized cross-section, performed by a separate program, is carried out one layer after another, until the basement is exposed. The results of the back-stripping, each marks a specific time frame, of a basin with *n* layers of sediments, are stored in the files ***mesh.0, mesh.1, ..., mesh.n***, where ***mesh.0*** is the cross-section for the present time, **mesh.1** is the cross-section with the topmost layer stripped, etc., and ***mesh.n*** is the cross-section with the basement exposed, i.e., at the very beginning of basin formation. All these files have the same format described as follows:

1) Geometric data for sedimentary layers

File names: mesh.#

Sedimentary layers are arranged from top to bottom in the order of 0, 1, 2, ... n. The 1st number on the line immediately preceeding the x- and y-coordinates gives the layer number. Each layer are defined by the positions of their upper and lower boundaries and separated in the lateral direction by faults (or the vertical continuation of faults for those that do not reach the surface or the basement). The uppermost surface of the sedimentary column (at depth 0) is not specified. The faults in turn are arranged from the left to the right in the order of 0, 1, 2, ... Their positions are specified by the x-

coordinate (the horizontal distance from a chosen origin) and the y-coordinate (the vertical depth from the surface of the sedimentary column) of selected key-points on the fault. Thus there are two side-boundaries for each layer; they can either be a model boundary or a fault (or a vertical line). The nature of the side-boundaries of a layer is indicated by the 2nd and the 3rd number on the line. A number of -1 means the left boundary if it lies in the 2nd, and the right boundary if it lies in the 3rd. The number 0 means the first fault (or vertical line), and 1 means the second fault (or vertical line). When both the 2nd and 3rd numbers are 0, the x- and y-coordinates marks the position of a fault, and the 1st number gives the fault number (or vertical line).

All the layers, including those back-stripped, must be included in each of the ***mesh.#*** files. For the back-stripped layers, the vertical coordinates are specified as '0'. The following format is used in prescribing the positions of the sedimentary boundaries in each ***mesh.#*** file:

(1st boundary beneath the surface)

layer number *(nolay)* | fault on the left *(nolfau)* | fault on the right *(norfau)* | no. of key-points *(numdlay)*

horizontal coordinate (x) vertical coordinate (y)

.

.

(a total of *numslay* rows)

.

.

horizontal coordinate (x) vertical coordinate (y)

.

.

.

layer number *(nolay)* | fault on the left *(nolfau)* | fault on the right *(norfau)* | no. of key-points *(numdlay)*

horizontal coordinate (x) vertical coordinate (y)

.

.

(a total of *numslay* rows)

.

.

horizontal coordinate (x) vertical coordinate (y)

(2^{nd} boundary beneath the surface)

(etc.)

where *nolay, nolfau, norfau, numdlay* are integers, x and y are real numbers, and distance and depth are in km.

2) Geometric data for faults

Additional files are needed to describe the position of faults in the sedimentary basin. The fault geometry is also stored in the ***mesh.#*** files, when both the 2nd and 3rd numbers are zero. The format of these files is as follows:

(1st fault from left)
fault number, 0, 0, no. of key-points
(nofau) (numdfau)
horizontal coordinate (x) vertical coordinate (y)
.
.
(a total of numdfau rows)
.
.
horizontal coordinate (x) vertical coordinate (y)

(2nd fault from left)
fault number, 0, 0, no. of key-points
(nofau) (numdfau)
horizontal coordinate (x) vertical coordinate (y)
.
.
(a total of numdfau rows)
.
.
horizontal coordinate (x) vertical coordinate (y)

where *nofau, numdfau* are integers, x and y are real numbers, and distance and depth are in km.

2. Material property information

Two categories of data are used in defining the material properties of a specific layer: 1) geometrical coordinates for the material property data in the present cross-section, and 2) a library of the material property of rocks. The use of geometrical coordinates for the material property data enables the use of multiple kinds of material within the same layer, for example, river channel deposits within a layer of fine sands. The x- and y-coordinates for the layers must be accurate enough so that the entire cross-secction is covered with assigned material properties. No x- and y-coordinates for the basement are needed.

1) geometrical coordinates for the material

File name: mate.dat

material index (norock) no. of key-points (numdrock)
horizontal coordinate (x) vertical coordinate (y)
.
.
(a total of numdrock rows)
.
.
horizontal coordinate (x) vertical coordinate (y)
.
.
.

material index (norock) no. of key-points (numdrock)
horizontal coordinate (x) vertical coordinate (y)
.
.
(a total of numdrock rows)
.
.
horizontal coordinate (x) vertical coordinate (y)

(etc.)

where *norock and nundrock* are integers, x and y are real numbers in km.

2) Material Parameter File

File name: rift.mat

This file supplies a table of material properties parameters for sediments and fault.

The first row specifies (1) the number of different kinds of material in the table *(mmate)* and (2) the number of different properties for each material *(nmate).*

The second row specifies the first kind of sediment properties, the third line gives the second kind of sediment properties, etc.

The last two lines (*nmate-1* and *nmate*) specify the properties of faults and of the basement, respectively.

A total of 17 material properties are listed as separate columns in the table; these are:

poro: porosity at surficial condition,

b1: compressibility parameter in the Athy's relation during loading (in Pa^{-1}),

b2: compressibility parameter in the Athy's relation during unloading (in Pa^{-1}),

sx0: specific surface area in the X-direction (in m^2/m^3),

sy0: specific surface area in the Y-deirection (in m^2/m^3),

heat: rate of heat production (in W/kg),

earth: clay content (in percentage),

ds: density of the solid grains (in kg/m^3),

cs: specific heat of the bulk sediments (in unit of $J/kg\ ^oK$),

sk: thermal conductivity (in $W/m\ ^oK$),

"equation number" for porosity calculation: 1 for shale (Athy's law), 2 for sands; or fault thickness (in *m*),

toc: total organic content (in percentage),

ker1: kerogen type I (in relative ratio),

ker2: kerogen type IIa (in relative ratio),

ker3: kerogen type IIb (in relative ratio),

ker4: kerogen type III (in relative ratio),

CaC03: carbonate content (in percentage).

3. Mesh generation data

File name: mesh.dat

The total number of sedimentary layers is *numlay*, and the total number of faults (or vertical lines) is *numfau*. The faults (or vertical lines) cut each sedimentary layer into *numfau+1* lateral subdomains. For the finite element calculation, each of the subdomains is further divided into a number of meshes. The first line in this file specifies the number of lateral divisions in each subdomain. The second line in this files specifies the number of verical divisions in each sedimentary subdomain. The number of vertical meshes for all the subdomains in a particular sedimentary layer is the same. Thus the format for this file is:

nx(1), nx(2), ..., nx(numfau+1)
ny(1), ny(2), ..., ny(numlay)

where nx(i) indicates the number of meshes in the lateral direction in the ith subdomain; ny(j) indicates the number of meshes in the vertical direction in the jth sedimentary layer.

4. Geologic age data

File name: re_time0

Each boundary between sedimentary layers corresponds to a particular geologic age. For a basin with *numlay* sedimentary layers, there are *numlay+1* boundaries, corresponding to *numlay+1* distinct geologic ages. In this file, the beginning of basin formation is taken to be 0.0 and is listed at the top line. The *lapsed* time between this beginning and the other sedimentary boundaries are listed in sequence in the subsequent lines. The format for this file is then:

0.0
time(1)
time(2)
.
.
time(numlay)

where *time(i)* indicates the accumulated time since the beginning of basin formation to the complete deposition of the *ith* sedimentary layer.

5. Fluid source data

There are five files for fluid sources: The first of the these specifies the rate of water production from clay dehydration in the sediments. The other four files specify the rate of production of natural gases from the four types of kerogen.

1) The production of water

File names: h2os.mat

The production of water from clay dehydration is a function of temperature. The format of this file is:

Number of rows (num1) number of columns (numc=2)
Temp(1) water-production (gm/kg of rock)
Temp(2) water-production (gm/kg of rock)
.
.
Temp(num1) water-production (gm/kg of rock)

2) The production of hydrocarbons

File name: ch4s.mat

The production of hydrocarbons (currently limited to methane gas) is calculated from kerogen maturation (which itself is a function of temperature). Since each type of kerogen contributes to the hydrocarbon production, the format of this file is:

Number of rows (num1) number of columns (numc=5)
Ro(1) HC (gm/kg of rock) HC (gm/kg of rock) HC (gm/kg of rock) HC (gm/kg of rock)
Ro(2) HC (gm/kg of rock) HC (gm/kg of rock) HC (gm/kg of rock) HC (gm/kg of rock)
.
.
Ro(num1)HC (gm/kg of rock) HC (gm/kg of rock) HC (gm/kg of rock) HC (gm/kg of rock)

3) The production of carbon dioxide

File name: co2s.mat

The production of carbon dioxide is calculated from kerogen maturation (which itself is a function of temperature). The format of each of these files is:

Number of rows (num1) number of columns (numc=2)
Ro(1) CO_2-production (gm/kg of rock)

Ro(2)	CO_2-production (gm/kg of rock)
.	
.	
Ro(num1)	CO_2-production (gm/kg of rock)

III. GRAPHICS OUTPUT

The calculated temperature, HC-maturation, excess pore pressures, fluid flow, hydrocarbon migration, and porosity at each time step are output as two-dimensional diagrams. The calculated results are first converted into a format for graphics output by editing the file *demofile* by typing **write *demofile***. Changing the number on the first line, where "1" = "excess pore pressure", "2" = "temperature", etc., will allow the user to convert different types of results for graphics output. To execute the graphics, type: ***movie.bat***.

IV. APPENDIX

1. Basic Equations

The basic equations used consist of two major types: (1) differential equations which govern heat transport, fluid transport and solute transport, and (2) empirical (or theoretical) relations which connect material properties with pressure, temperature and porosity.

• Differential Equations:

There are three types of differential equations in the **IBM** system: one for heat transport, one for fluid transport, and (to be implemented later) one for each of the solute components in the pore fluids. In order to closely simulate the *in situ* processes, these transport equations are fully coupled and solved together.

1. Heat transport equation:

$$c\rho\frac{DT}{Dt} = \nabla\cdot(K\nabla T) - c_w\rho_w\mathbf{q}\cdot\nabla T + H$$

where DT / Dt is the rate of change of T in the Lagrange coordinate system, c and ρ are, respectively, the specific heat and density of the bulk sediments, the subscript w indicate the corresponding properties of the pore fluids, K is thermal conductivity of the bulk sediments, $\mathbf{q}$ is Darcy velocity of fluids with respect to sediments, and H is heat source per unit volume of sediments per unit time.

The boundary conditions used in **IBM** for solving the heat transport equation are:

(1) 0 ^{o}C at the surface of the sedimentary sequence,

(2) 1300 ^{o}C at the base of the lithosphere (100 km below sealevel),

(3) no lateral loss or gain of heat at large distances from the two sides of the basin.

2. Fluid transport equation:

$$S\frac{DP}{Dt} = \nabla \cdot (\frac{k}{\eta} \nabla P) + \beta \frac{DP_t}{Dt} + \phi \alpha_w \frac{DT}{Dt} + Q$$

where S is the specific storage of the sediments, P is the excess pore pressure, P_t is the effective overburden pressure, k is permeability, η is fluid viscosity, β is the bulk compressibility of sediments, ϕ is porosity, α_w is the thermal expansivity of pore fluid, and Q is fluid source per unit volume of sediments per unit time.

The boundary conditions used by **IBM** for solving the fluid transport equation are:

(1) zero excess pore pressure at the surface of the sedimentary sequence,

(2) no flow across the boundary between the basement and the sedimentary sequence,

(3) no lateral loss or gain of fluids at large distances from the two sides of the basin.

3. Solute transport equation (not yet implemented in the available 2D model):

$$\phi\rho_w \frac{DC_i}{Dt} = \nabla \cdot (\boldsymbol{D}\rho_w \nabla C_i) - \rho_w \mathbf{q} \cdot \nabla C_i + E_i$$

where C_i is the i th component of the solute, where i =1,2,...,n, $\boldsymbol{D}$ is the coefficient of dispersion, and E_i is the source of the i th component of the solute per unit volume of sediments per unit time.

• Major Material Property Relations:

Porosity:

$\phi = \phi_0 \exp(-bP_e)$ (Athy's relation)
for shales (and limestones)

$P_e = 59.4 - 1.37\phi + 100/\phi$ (Ungerer et al., 1987)
for sandstones

Permeability:

$$k = \frac{\phi^3}{5S_o{}^2(1-\phi)^2}$$ (Koseny-Carmen's relation)

Thermal conductivity:

$$K = K_s(\frac{K_w}{K_s})^{\phi}$$ (Lewis and Rose, 1970)

where K_w and K_s are, respectively, the thermal conductivity of pore fluid and solid sediment grains.

Specific Storage:

$$S = \beta + \phi\beta_w$$

where β and β_w are the compressibility of the bulk sediments and pore fluid, respectively.

Bulk Sediment Density:

$$\rho = \phi\rho_w + (1-\phi)\rho_s$$

where ρ_w and ρ_s are, respectively, density of pore fluid and the solid sediment grains.

Bulk Sediment Specific Heat:

$$c = \phi c_w + (1-\phi)c_s$$

where c_w and c_s are, respectively, density of pore fluid and the solid sediment grains.

The viscosity of pore fluid is calculated from temperature according to the following empirical equation:

$$\eta^{-1} = 5380 + 3800A - 260A^3$$

where $A = (T-150)/100$, T is in ^{o}C, and η in kg m^{-1} s^{-1}.

輸入資料之表列格式：

1、地層界限及斷層 X 軸、Y 軸之座標：

—X 軸代表剖面水平與原點之距離

—Y 軸代表特點深度

—數字分別界限之種類

2、沈積層之化學物理特性資料

0	-1	0	18
	-3.000000284984715		2.010000190241267
	-2.235294329988611		2.010000190241267
	-1.470588374992508		2.010000190241267
	-7.058824199964040E-001		2.010000190241267
	5.882353499969954E-002		2.010000190241267
	8.235294899958031E-001		2.010000190241267
	1.588235444991907		2.010000190241267
	2.352941399988011		2.010000190241266
	3.117647354984114		2.010000190241267
	3.882353309980217		2.010000190241267
	4.647059264976321		2.010000190241267
	5.411765219972425		2.010000190241267
	6.176471174968527		2.010000190241267
	6.941177129964632		2.010000190241267
	7.705883084960735		2.010000190241267
	8.470589039956838		2.010000190241267
	9.235294994952943		2.010000190241267
	10.000000949949050		2.010000190241267
1	-1	0	18
	-3.000000284984715		4.020000380482533
	-1.647058979991607		4.020000380482532
	-2.941176749985018E-001		4.020000380482534
	1.058823629994606		4.020000380482533
	2.411764934987712		4.020000380482531
	3.764706239980820		4.020000380482535
	5.117647544973923		4.020000380482534
	6.470588849967035		4.020000380482536
	7.823530154960137		4.020000380482534
	9.176471459953250		4.020000380482533
	10.529412764946360		4.020000380482535
	11.882354069939470		4.020000380482534
	13.235295374932570		4.020000380482534
	14.588236679925680		4.020000380482534
	15.941177984918780		4.020000380482536
	17.294119289911880		4.020000380482535
	18.647060594905000		4.020000380482537
	20.000001899898100		4.020000380482536
2	-1	0	18
	-3.000000284984715		6.030000570723798
	-1.058823629994604		6.030000570723803
	8.823530249955044E-001		6.030000570723799
	2.823529679985614		6.030000570723800
	4.764706334975726		6.030000570723803
	6.705882989965829		6.030000570723805
	8.647059644955943		6.030000570723805
	10.588236299946050		6.030000570723807
	12.529412954936170		6.030000570723815
	14.470589609926270		6.030000570723830
	16.411766264916380		6.030000570723845
	18.352942919906490		6.030000570723876

20.294119574896600	6.030000570723908
22.235296229886700	6.030000570723957
24.176472884876820	6.030000570724011
26.117649539866920	6.030000570724093
28.058826194857030	6.030000570724185
30.000002849847150	6.030000570724310
3 -1	0 18
-3.000000284984715	8.040000760965063
-4.705882799976018E-001	8.040000760965071
2.058823724989510	8.040000760965064
4.588235729976621	8.040000760965073
7.117647734963733	8.040000760965071
9.647059739950846	8.040000760965077
12.176471744937960	8.040000760965087
14.705883749925080	8.040000760965112
17.235295754912190	8.040000760965144
19.764707759899290	8.040000760965199
22.294119764886410	8.040000760965269
24.823531769873520	8.040000760965361
27.352943774860630	8.040000760965482
29.882355779847740	8.040000760965622
32.411767784834860	8.040000760965791
34.941179789821960	8.040000760965986
37.470591794809070	8.040000760966201
40.000003799796200	8.040000760966432
4 -1	0 18
-3.000000284984715	10.0
-1.764706049991023E-001	10.0
2.647059074986511	10.0
5.470588754972124	10.0
8.294118434957737	10.0
11.117648114943360	10.0
13.941177794928960	10.0
16.764707474914580	10.0
19.588237154900200	10.0
22.411766834885820	10.0
25.235296514871430	10.0
28.058826194857040	10.0
30.882355874842650	10.0
33.705885554828260	10.0
36.529415234813860	10.0
39.352944914799490	10.0
42.176474594785090	10.0
45.000004274770720	10.0
0 0	0 6
10.000000949949050	0.000000000000000E+000
10.000000949949050	2.010000190241267
20.000001899898100	4.020000380482536
30.000002849847150	6.030000570724310
40.000003799796200	8.040000760966432
45.000004274770720	10.0

12 17 0

No sand shale lime coal

```
0.7  8.0e-8  6.9E-8  6.E8  6.E9  5.e-13  0.0   2450.  1000.  2.0  1  0
.0   1.0  0.0  0.0  0.0  0.0  phase   7   10   85   0     0
0.5  4.9E-8  6.9E-8  3.E6  3.E7  5.e-13  0.0   2650.  1000.  3.0  1  0
.0   1.0  0.0  0.0  0.0  0.0  phase   1  100    0   0     0
0.5  4.9E-8  6.9E-8  3.E6  3.E7  5.e-13  0.0   2650.  1000.  3.0  1  0
.0   1.0  0.0  0.0  0.0  0.0  phase   1  100    0   0     0
0.7  8.0e-8  6.9E-8  6.E8  6.E9  5.e-13  0.02  2450.  1000.  2.0  1  0
.0   1.0  0.0  0.0  0.0  0.0  phase   7   10   85   0     0
0.5  4.9E-8  6.9E-8  3.E6  3.E7  5.e-13  0.0   2650.  1000.  3.0  1  0
.01  1.0  0.0  0.0  0.0  0.01 phase   1  100    0   0     0
0.7  8.0e-8  6.9E-8  6.E8  6.E9  5.e-13  0.0   2450.  1000.  2.0  1  0
.0   1.0  0.0  0.0  0.0  0.0  phase   7   10   85   0     0
0.5  4.9E-8  6.9E-8  3.E6  3.E7  5.e-13  0.0   2650.  1000.  3.0  1  0
.0   1.0  0.0  0.0  0.0  0.0  phase   1  100    0   0     0
0.5  4.9E-8  6.9E-8  3.E6  3.E7  5.e-13  0.0   2650.  1000.  3.0  1  0
.0   1.0  0.0  0.0  0.0  0.0  phase   1  100    0   0     0
0.7  8.0e-8  6.9E-8  6.E8  6.E9  5.e-13  0.02  2450.  1000.  2.0  1  0
.0   1.0  0.0  0.0  0.0  0.0  phase   7   10   85   0     0
0.5  4.9E-8  6.9E-8  3.E6  3.E7  5.e-13  0.0   2650.  1000.  3.0  1  0
.01  1.0  0.0  0.0  0.0  0.01 phase   1  100    0   0     0
0.6  6.5e-8  6.9E-8  3.E8  3.E9  0.e-9   0.0   2550.  1000.  2.5  1  0
.0   1.0  0.0  0.0  0.0  0.0  fault  11   75   25   0     0
0.0  5.0e-8  6.9E-8  3.E8  3.E9  5.e-11  0.0   2650.  1000.  3.0  1  0
.0   1.0  0.0  0.0  0.0  0.0  base   13    0    0   0     0
```

```
Poro,   b1,     b2,    sx0,  sy0,   heat, earth,  ds,     cs,    sk, No.,
cot, ker1,ker2,ker3,ker4,CaCo3
      1/pa 1/pa  m^2   m^2   W/kg/t        kg/m^3 J/(kg*K) W/(m*K)
```

```
 4    6
 0.        0.
10.        0.
10.        2.
 0.        2.
 4    7
 0.        2.
10.        2.
20.        4.
 0.        4.
 4    8
 0.        4.
20.        4.
30.        6.
 0.        6.
 4    9
 0.        6.
30.        6.
40.        8.
 0.        8.
 4    10
 0.        8.
40.        8.
45.        10.
 0.        10.
 4    1
10.        0.
90.        0.
90.        2.
10.        2.
 4    2
10.        2.
90.        2.
80.        4.
20.        4.
 4    3
20.        4.
80.        4.
70.        6.
30.        6.
 4    4
30.        6.
70.        6.
60.        8.
40.        8.
 4    5
40.        8.
60.        8.
55.        10.
45.        10.
 4    6
```

1. The specific volume (inverse of density) of water:
Let V be the specific volume of water in cubic meter per kg, P the total pressure in pascal, (excess + hydrostatic), and T temperature in centigrade.

V = 0.001 + T(2) x (a + b x P(2)) + P(c + d x T(3))

where T(2) is the square of T, P(2) is the squate of P, T(3) is the cube of T,
a = 3.85x10(-9),
b = 3.45x10(-26),
c = -4.32x10(-13),
d = -5.42x10(-20).

For interpolation purpose, you could use this eqaution to generate V in a P-T space that includes the maximum values of P and T in the models. Naturally, the more points you use in the interpolation, the more accurate your results will be.

2. The specific volume of methane gas is obtained from solving the following equation:

[P + a/V(2)] x (V - b) = RT

where a = 0.225, b = 4.28 x 10(-5), R is the gas constant (8.314 J/mole/K), and T is in degree Kelvin.

3. The density of oil may be obtained from the following formula:

rho = 850 x exp [-7.20x10(-4)x(T-To) + 5x10(-10)xP]

where rho (oil density) is in kg/m(3), T is in oC, To is surface temperature in oC, P is total pressure in Pa.

4. The viscosity of water (with 5% brine):

u = 10(-3) x [5.38 + 3.80xA - 0.26xA(3)]

where A = (T - 150 oC)/100 oC

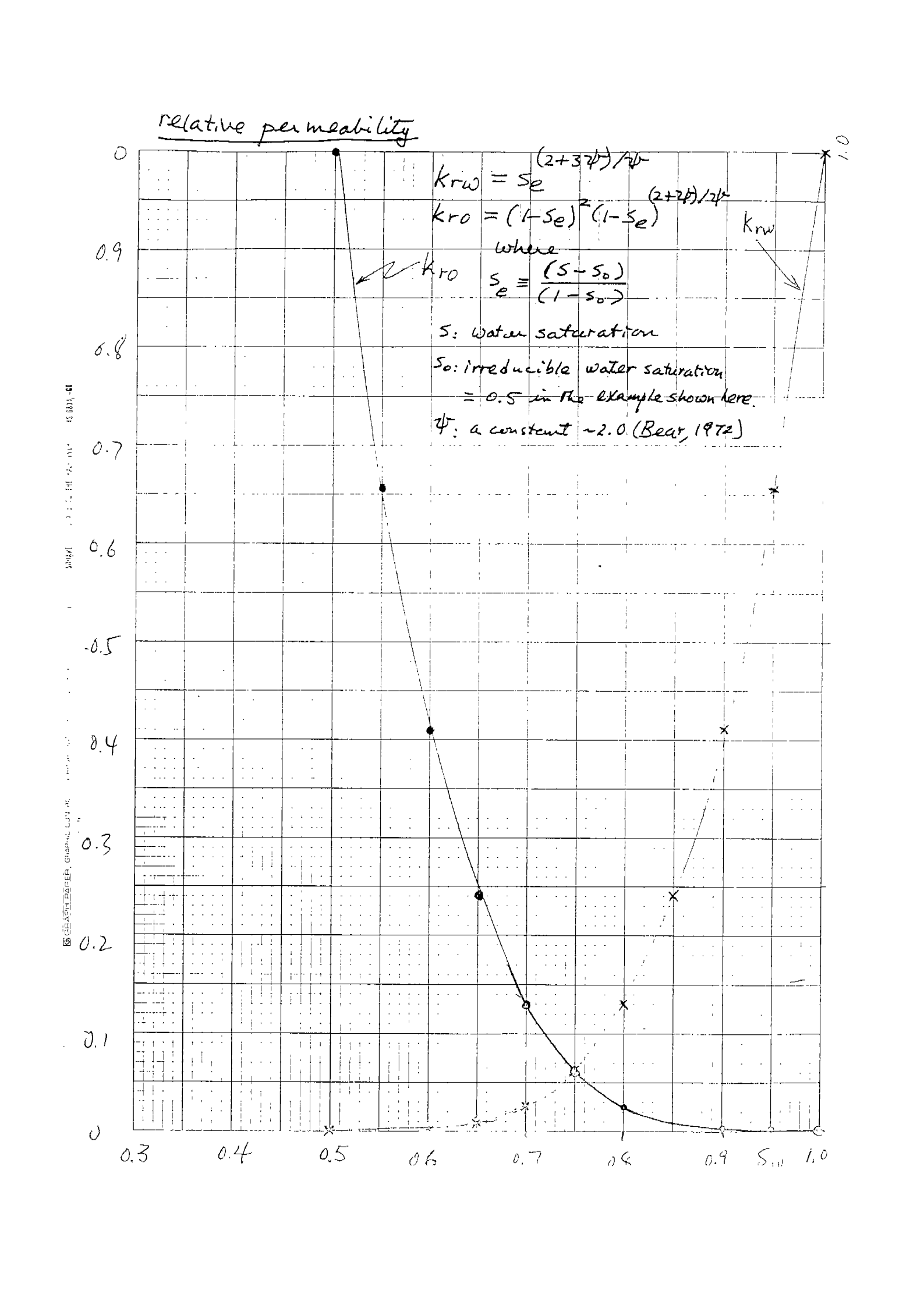
u is in Pa-s and T is in oC.

5. The viscosity of hydrocarbon fluid:

u = wg x ug + wo x uo

where
wg is the mass fraction of gas,
wo is the mass fraction of oil,
ug in Pa-s is the vicosity of gas, given by the following formula:
ug = 1x10(-5) + 1.5x10(-8)xP/rhs - 2.2x10(-7)x(T - To)
rhs is the bulk density of sediments,
To is the surface temperature,
uo is the viscosity of oil, given by the formula below,
uo = 1.4186x10(-6)xexp(6597/T)
T is in oK,
P is total pressure in Pa.

		DELTA G (cal/mol)	DELTA H (cal/mol)	S (cal/mol/K)	V (cc/mol)		Cp (cal/mol/K)	
25.000	400.000	1.014	-3.108	4240.	-3004.	-24.28	36.38	63.54
25.000	600.000	1.022	-3.235	4413.	-2930.	-24.62	35.96	66.11
25.000	800.000	1.030	-3.360	4584.	-2851.	-24.92	35.59	68.49
25.000	1000.000	1.038	-3.484	4753.	-2767.	-25.21	35.26	70.70
25.000	1200.000	1.045	-3.607	4921.	-2678.	-25.48	34.96	72.76
25.000	1400.000	1.052	-3.729	5087.	-2586.	-25.72	34.69	74.68
25.000	1600.000	1.059	-3.850	5253.	-2490.	-25.96	34.45	76.49
25.000	1800.000	1.065	-3.971	5417.	-2391.	-26.17	34.23	78.18
25.000	2000.000	1.072	-4.090	5580.	-2289.	-26.38	34.03	79.77
25.000	2200.000	1.078	-4.209	5742.	-2184.	-26.57	33.84	81.27
25.000	2400.000	1.084	-4.327	5903.	-2077.	-26.75	33.67	82.68
25.000	2600.000	1.089	-4.445	6064.	-1967.	-26.93	33.51	84.00
25.000	2800.000	1.095	-4.562	6224.	-1856.	-27.09	33.36	85.26
25.000	3000.000	1.100	-4.679	6383.	-1742.	-27.24	33.23	86.44
50.000	200.000	.997	-3.115	4606.	-1720.	-19.56	38.36	49.18
50.000	400.000	1.005	-3.238	4788.	-1608.	-19.78	37.76	50.31
50.000	600.000	1.013	-3.359	4967.	-1492.	-19.98	37.24	51.35
50.000	800.000	1.020	-3.479	5144.	-1375.	-20.16	36.77	52.32
50.000	1000.000	1.027	-3.597	5319.	-1255.	-20.33	36.36	53.22
50.000	1200.000	1.034	-3.714	5492.	-1133.	-20.49	35.99	54.06
50.000	1400.000	1.041	-3.830	5663.	-1009.	-20.64	35.65	54.84
50.000	1600.000	1.048	-3.944	5832.	-884.	-20.77	35.35	55.58
50.000	1800.000	1.054	-4.058	6001.	-757.	-20.90	35.07	56.27


relative permeability
$k_{rw} = S_e^{(2+3\psi)/\psi}$
$k_{ro} = (1-S_e)^2 (1-S_e)^{(2+2\psi)/\psi}$
where
$S_e \equiv \frac{(S-S_o)}{(1-S_o)}$
k_{ro}
k_{rw}
S: water saturation
S_o: irreducible water saturation
= 0.5 in the example shown here.
ψ: a constant ~2.0 (Bear, 1972)
0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.3
0.4
0.5
0.6
0.7
0.8
0.9
S_w
1.0