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AN ANALYSIS OF METHODOLOGY USED IN COMMERCIAL GEOHISTORY AND GEOCHEMISTRY PROGRAMS: BURY 5.41, BASINMOD 2.55 AND MATOIL 1.4

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ANDRZEJ P. RADLINSKI

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CONTENTS

1. PREAMBLE.

I critically review the methodology used in three commercial programs (Matoil 1.4, BasinMod 2.55 and Bury 5.41) for geohistory analysis in sedimentary basins. Various elements of this methodology have been described in the original literature. However, in the view of increased utilisation of the computerised geohistry analysis in BMR there is a need to provide a geologically-minded user with a comprehensive information about the requirements, capabilities and limitations inherent in current technology, particularly in the context of recent research developments.

This document is not intended to replace the instruction manual. In fact, I do not discuss the practical aspects of data input, running the programs and extracting the required output at all. These subjects are well covered by the original program documentation (Matoil 1988, BasinMod 1990, Bury 1991). I also do not discuss many details covered by the original papers on methodology.

My intention is, on one hand, to provide an inexperienced user with a geological background with detailed information about the principles and inner workings of geohistory analysis, and, on the other hand, to create a quick reference text. This is reflected in the structure of this document. Sections 2, 3 and 4 concentrate on the methodology, whereas Section 5 contains a table that lists consecutive stages of the geohistory analysis process, indicates the particular implementation employed in a given software package and cross-references the user to the main body of text for more details. Section 6 lists major theoretical and procedural limitations of the commercial software packages.

2. INTRODUCTION.

Matoil, BasinMod and Bury are commercial software packages developed for PCs by different companies in the period 1988-1991 for the purpose of one-dimensional simulation of geohistory and hydrocarbon generation in single wells. In BMR, Matoil has been used by geochemistry groups and Bury by the Marine Program and Petroleum Resource Assessment Branch.

These packages are designed in a user-friendly manner, which means they can be used by people with little computing experience. However, the underlying geological models and numerics are not necessarily transparent to the user. This fact, combined with rather brief documentation refering to a variety of original papers (with the most recent references missing) encourages a 'black-box' approach to basin analysis. Therefore, a situation may arise where the results obtained using the best geological input available to the user will be uncritically looked upon as the best possible outcome of state-of-the-art basin modelling.

Such a perception may be wrong for two main reasons. Firstly, there are some realistic geological scenarios that by design cannot be handled by these programs. Anything that is not one-dimensional falls into this category - for instance, strongly dipping beds may cause the heat-flow field to have a significant horizontal component. There are other examples of this sort of difficulties, which are discussed below. They may be characterised by stating that the user is aware of the problem but cannot force the modelling program to accomodate their preferred geological picture.

Secondly, the geoscientific models used by the programs are themselves approximate and sometimes controversial. More advanced or alternative approaches can be found in recent literature. In particular, this comment applies to the concept of instantaneous (Airy) isostasy and the oil and gas generation models universally used by all of the programs analysed here. These problems are a natural consequence of the fact that commercial computer implementations tend to lag behind the pioneering research in geosciences and, once developed, are of limited flexibility. One can be only aware of these problems by critically following the current literature.

In this document we attempt to critically review the numerical procedures used for modelling of various geological phenomena in the commercial software packages Bury 5.41, Matoil 1.4 and BasinMod 2.55. This analysis is based on the accompanying commercial documentation and relevant literature. I did not have access to the proprietary computer code and it is assumed that there are no errors or discrepancies between the theory and numerics at the coding level. In other words, throughout this document we accept that programs are really doing what the manufacturers claim they should be doing. It should be stressed that the analysis presented here may not reflect all the features available in the latest releases of the programs; information on this subject should be sought directly from the software companies.

Another important, but more subjective aspects of these programs are the versatility, i.e. ability to accomodate new sets of model parameters, ease of use and the graphical appeal. These matters usually depend on the user profile and are not commented upon here except in general terms. I believe that one can only develop an informed opinion in this area by actively using the programs.

This document is organised in the following way. Firstly, I review the major steps involved in geothermal and geochemical modelling (Section 3). Secondly, for each step the results of appropriate quantitative approach are summarized and discussed both in the geoscientific and mathematical context (Section 4). At this stage, a critical review of some aspects of these models is given and possible improvements (based on existing literature) are suggested. Thirdly, methods employed in various programs are directly compared (Section 5). Results are presented in form of a table which refers the reader to particular sections of this document for more details. Throughout this document a particular effort is made to compile full list of references on which the existing methodology is based (Section 6).

3. MAJOR STEPS.

The three commercial programs reviewed here simulate the hydrocarbon generation in sedimentary basins along the lines of the same general model. According to the model, transformation of kerogen into oil and gas occurs as a series of chemical reactions whose rates depend exclusively on the temperature and the kerogen-type-related parameters. The hydrocarbon generation temperature window is from approximately 90 to 130 degrees Celsius. The main purpose of the modelling excercise is, therefore, to determine the temperature variation of the source rock formation versus geological time; some programs are also designed to reproduce basin subsidence history.

This has to be achieved in a way consistent with the overall geological knowledge of the region using the present day stratigraphic and biostratigraphic data. From the mathematical point of view the problem is underdetermined, i.e. it is possible to find many (technically - an infinite number) different paths leading to the same present day outcome. The role of the user is to identify the geologically reasonable ranges of parameters and select the most probable geohistory scenario by trial and error. Typically, this is done by adjusting two time-dependent quantities: palaeo-heat flow and unconformities. Programs themselves do not contain any 'intelligent' geological diagnostic device - they merely accept input data, facilitate speedy calculations according to fixed formulae and present the results in a variety of user-selected graphic forms. There is no provision that an illogical (not to mention incorrect) input will be automatically rejected by a program.

The major processes whose temporal evolution determines the present day geological record are sedimentation (including erosion), compaction, basin subsidence and heat flow. All of these processes are ultimately driven by the gravity field and, therefore, in the long run are dominated by their vertical components. This lends credibility to the notion of prevailing one-dimensionality (in the vertical direction) of the basin evolution process. However, it should be stressed that in the presence of a horizontal deposition processes or tectonic activity, a transient state may develop for which the one-dimensional approach is not appropriate. This issue is expanded on later.

All of the programs analysed here assume strictly one-dimensional basin evolution kinetics. Because of the assumed vertical temperature gradient in the core, the appropriate temperature regime (oil window or gas window) may be eventually reached by a particular formation as the result of (i) sediment compaction under its own weight (lithostatic load) combined with the water pressure in the marine locations, and (ii) the vertical movements due both to the isostasy and tectonics. Note that in order to properly model these processes one has to know the density distribution in sediment down to the basement level.

Palaeo-heat flow is believed to vary for various stages of basin development. For each point of time, the palaeo-temperature at given depth depends on the thermal conductivities of all deposited strata (these in turn being related to their lithology and the degree of compaction) as well as palaeo-surface temperature. Therefore, in order to model the hydrocarbon generation it is necessary to fully analyse the basin evolution down to the basement and, in particular, reconstruct the burial history of every formation, including the sea level variations.

4. THEORETICAL AND NUMERICAL PROCEDURES.

4.1 COMPACTION AND VERTICAL TECTONICS - GENERAL CONCEPT.

The task of unscrambling a plausible geohistory scenario from the present day record has two main components: mechanical and thermal. These two components remain uncoupled, except when thermal metamorphism is considered, which is not the case for the commercial software packages analysed here.

The mechanical component is the sum of two conceptually different processes: compaction and vertical tectonics. Compaction can be mathematically quantified using specific models, whereas the tectonic basement movement is unpredictable. However, since the position of the palaeosurface relative to the sea level can be inferred from the biostratigraphic record and assuming that the global sea level variations are known, the net result of these two processes at any point of time can be determined. Subsequently, the effect of tectonic movement can be calculated by simple subtraction. It is clear that the results of such an analysis depend on the underlying models of compaction and isostasy. In the context of commercial package these models are usually taken for granted without further thought thus introducing 'hidden' assumptions.

By far the least constrained assumptions are, however, introduced in a case of missing record (unconformity), in particular when it is a long-lasting one. The unavoidable user intervention in the form of the temporal pattern of elevation rise and erosion belongs to the realm of science-fiction. Every effort should be made to relate the quantitative description of an unconformity to a broader picture of basin evolution, palaeoclimate, etc. In the view of mathematically underdetermined character of the geohistory problem it is simply wrong to justify the selected elevation pattern just by using the 'it gets the right answer' type argument.

4.2. COMPACTION AND DECOMPACTION.

4.2.1. Compaction Models.

Compaction is a process in which under the load of overlying layers, the solid particles of sediment collapse on each other squeezing the formation liquids out of the pore space. It is assumed that the density of solid sediment material (skeleton, matrix) is not affected by the overburden pressure. The increase of overall density of the compacted material is thus achieved by replacing formation liquids with more dense sediment. Note that chemical reactions and/or mass transport in the rock undergoing compaction that in general may take place are ignored.

If the formation liquids are free to move around (normally pressured rocks) then it is postulated on the basis of extensive wireline log analysis that for given basin and lithology the rock density (and, thus, porosity) depends only on the maximum depth of burial. It is obviously only an approximate, empirical fact. We note in passing that one would expect the sediment density to depend on the lithostatic pressure rather than depth, but these are approximately proportional due to only small differences in densities of various lithologies.

For numerical analysis a mathematical formula for porosity versus depth is required. According to the philosophy presented above, it would have a general form:

$$\text{porosity} = \text{function}(\text{basin, lithology, depth}) \quad (1)$$

where the specific form of the function is selected to fit best the experimental data collected for given basin. The usual procedure is to calculate the porosity using the sonic log data, as described in detail in Appendix A of Sclater and Christie (1980). It is important to note that at least for shales and sandstones the dependence of function in equation 1 on the basin can be very strong. In other words, this function is not universal for a given lithology and, consequently, as a rule the sonic log analysis should be performed for every specific basin in order to determine the values of compaction parameters .

A variety of functions have been used over the years and their particular form does not really matter as long as it closely approximates the field data. The commercial programs discussed here use as a default either an exponential form, as documented for the North Sea area by Sclater and Christie (1980) (and previously postulated by Athy 1930, Hedberg 1936, Ruby and Hubbert 1960), or a hyperbolic form adopted by Falvey and Middleton (1981) (and previously applied by Horowitz 1976 to shales). Maximum differences between these two functions may reach about 15% and are particularly pronounced for shallower strata.

The Sclater and Christie (SC) function is:

$$f = f_0 \exp(-cz) \quad (2)$$

where f_0 is the porosity at the surface, $-c$ is the (negative) slope of the porosity-depth line on a logarithmic scale and z is the depth. Sclater and Christie (1980) demonstrate that for the North Sea locations the slope $-c$ is different for different lithologies. Its typical values are several tenths per thousand metres and get larger for more compressible lithologies (for detailed values see Table A1a, page 3732 of Sclater and Christie 1980). For an incompressible medium, $c=0$.

The Falvey and Middleton (FM) function is:

$$f = f_0/(1+f_0kz) \qquad (3)$$

where k is the lithology-dependent parameter whose typical value varies from 0.4 to 10.0 per thousand metres (for detailed values see section 'D.1.5. Lithologic Parameters Files' of version 5.41 Bury manual, May 1991). The value of k is larger for more compressible rocks and equals zero for an incompressible medium.

4.2.2. Decompaction by Method of Slices.

The purpose of decompaction procedure is to calculate the variation of thickness of lithological units versus depth and determine the evolution of the lithostratigraphic column as a function of time. The appropriate numerical procedure (method of slices) was first derived by Perrier and Quiblier (1974) and was later used by other authors. It can be briefly outlined as follows.

Consider a total volume of porous sediment, v_t, contained in an infinitesimally small, fictious cylinder located somewhere inside the sedimentary column, whose axis is vertical and base area is S. As new sediment is added on top of the stratigraphic column, S remains unchanged but v_t decreases by the volume of the expelled formation liquids, v_l. However, the volume of solid sediment contained inside the shrinking cylinder, v_s, remains constant:

$$v_s = (1-f)\ v_t \qquad (4)$$

where the volume of expelled formation liquids is $v_l=fv_t$. It is implicit in equation 4 that both the porosity f and total volume v_t depend on depth z at which the cylinder is buried. Now, lets expand the cylinder vertically so it would extend from depth z_1 to z_2 that delineate a deposition zone we wish to decompact. The amount of liquid, V_l, in the pore spaces inside the expanded cylinder now is:

$$V_l = S \int_{z_1}^{z_2} f(z)dz \qquad (5)$$

and the depth-invariant volume of the solid sediment, V_s, is:

$$V_s = V_t - fV_t = S\{(z_1-z_2) - \int_{z_1}^{z_2} f(z)dz\} \qquad (6)$$

Both sides of equation 6 can be divided by the base surface area, S, yielding the expression for the <u>depth-invariant</u> thickness of the solid component of sediment, H_s:

$$H_s = z_1 - z_2 - \int_{z_1}^{z_2} f(z)dz \qquad (7)$$

This form of decompaction equation is quite general and can be applied to any functional dependence of porosity on the depth, f(z). Since the left-hand-side of (7) is depth-invariant, equation 7 holds for the pair of depths (z_1,z_2) being replaced by any other pair (z_3,z_4), providing the new pair corresponds to the upper and lower limits of the originally selected deposition zone at some geological time. In other words, if we had a way to mark all the solid sediment particles in this zone, the choice of z_3 and z_4 would have to be such that all of the marked particles and no others, should be contained between z_3 and z_4 at some fixed point of time in the past.

If, for instance, z_1 and z_2 are selected from the present day record as the top and bottom of the zone to be decompacted, and z_3 is the arbitrarily selected top of this zone at some point in the past, then z_4 can be calculated from equation 7 using a numerical (non-analytical) procedure. It is simply a matter of numerically solving one nonlinear equation with one unknown quantity. In order to do that the integral in equation 7 has first to be evaluated using an integrand given by equation 2, equation 3, or any other expression consistent with the field data. The values of integrals of functions given by equations 2 and 3 can be calculated analytically and are given by the original authors (Sclater and Christie 1980, Falvey and Middleton 1981).

What remains to be done after z_3 and z_4 have been determined is identifying the point of time that corresponds to the depth z_3. In order to do this in a systematic way for the whole stratigraphic column one may use the method of slices, as originally described by Perrier and Quiblier (1974).

The idea is to first divide the column in a well (or a number of wells) into layers (called stages) delineated by dated, synchronous boundaries. Stages may consist of layers of various lithologic type. In order to enable further numerical analysis it is necessary to assume a specific deposition rate and Perrier and Quiblier use constant deposition rate for a given lithology within a stage. However, the rate may be different for different lithologies within a stage and may differ for the same lithology between stages.

The next step is to divide each stage into a number (typically several tens) of slices in such a way that (i) each slice contains only one lithology and (2) each slice was deposited in the same period of time, Δt. This can be done using equation 7 and the previously selected deposition rates for various lithologies. Thus, within one stage the thickness of slices will vary between the lithologies and, for given lithology, will decrease as depth increases. Note that this procedure will keep the slices synchronous between various wells.

Finally, all the slices are removed and fully decompacted and the evolution of stratigraphic column in time is reconstructed slice by slice, starting from the oldest slice deposited on top of the basement. Both these steps are performed using equation 7. The palaeo-water depth is not required at this stage if the surface porosity f_0 of equation 2 or eqquation 3 is taken as the porosity of the top sediment layer. Since the slices constitute the obvious time calibration marks, the outcome of this procedure is the evolution of stratigraphic column with time.

Note that the above reconstruction of evolution of the stratigraphic column provides sufficient structural information for the kerogen maturation modelling. However, adding corrections for the water depth (paleobathymetric) and relative sea level changes enables one to get an extra bonus in the form of the tectonic component of basement position. This requires a specific model of isostasy, which is discussed next.

4.3 ISOSTASY.

All of the commercial programs analysed here use the concept of instantaneous (Airy) isostasy. This means that the lithosphere is assumed to have no flexural strength and, consequently, it is viewed as an assemblage of independent columns, each composed of solid rock, surface water (where appropriate) and the atmospheric air (which is usually neglected owing to its very small overall contribution equivalent to 10 metres of water column). Every column is buoyantly supported by an isobaric (constant pressure) datum inside the aesthenosphere and in response to a changed load it adjusts its vertical position instantaneously. The most general expression for the Airy equilibrium states that for every column its elevation is such that:

$$\int_{\text{datum}}^{\text{surface}} g(z)\rho(z)dz.=.\text{constant} \qquad (8a)$$

where $\rho(z)$ is the vertical distribution of rock density for a given column and $g(z)$ is the acceleration of gravity. Since typical distances between datum and surface (about 30 km) are small compared to radius of the Earth, $g(z)$ can be assumed constant and incorporated into the constant on the right hand side of equation 8a. Thus, the Airy equilibrium condition becomes:

$$\int_{\text{datum}}^{\text{surface}} \rho(z)dz = \text{constant} \qquad (8b)$$

Equation (8b) is both precise and impractical. For want of more specific data, it is usually approximated as a sum of contributions from five strata: sea water (indicated by subscript w), sediment (s), igneous and metamorphic crust (c), mantle lithosphere (m) and mantle aesthenosphere (a):

$$\rho_w h_w + \rho_s h_s + \rho_c h_c + \rho_m h_m + \rho_a h_a = \text{constant} \qquad (9)$$

where the datum from which h_a is measured is an isobaric surface in the aesthenosphere. The meaning of equation 9 is that in order for this surface to remain isobaric under arbitrary load conditions (mathematically expressed by altering the thickness of water or sediment layer) the remaining three layer's thicknesses will vary in some way to satisfy equation 9. This 'some way' is usually constrained by geological circumstances that form the framework of the geological model quantified by the isostatic equations. Two examples of specific geological models will be discussed in detail later.

Equation 9 can be also expressed in a fully equivalent, differential form:

$$\rho_w \Delta h_w + \rho_s \Delta h_s + \rho_c \Delta h_c + \rho_m \Delta h_m + \rho_a \Delta h_a = 0 \qquad (10)$$

where the corresponding change of surface elevation (or relative sea level), ΔE, is:

$$\Delta E = \Delta h_w + \Delta h_s + \Delta h_c + \Delta h_m + \Delta h_a \qquad (11)$$

Equations 10 and 11 are the fundamental equations of differential isostasy (Suppe 1985). Mathematically, they are a system of two linear equations with six unknowns (all the layer thicknesses differentials, Δh_i, i=w,s,c,m,a, and the elevation differential, ΔE). The densities ρ_i are usually assumed to be known (ρ_w=1030, ρ_s=2100-2700 (depending on lithology and depth, as discussed in the section on compaction), ρ_c=2700-3000, ρ_m=3400 and ρ_a=3300, all expressed in kg/m^3).

In order to enable exact solution of a practical isostatic problem four of the six unknowns have to be somehow determined. Firstly, it seems to be a common practice to blur the difference between the mantle lithosphere and mantle aesthenosphere by the device of using just one common density, ρ_m=3350 kg/m^3. This formally eliminates the aesthenosphere layer thickness, h_a, from equation 9, and, consequently, the corresponding differentials from equations 10 and 11. Physically, it corresponds to shifting the isobaric datum from its original position in the aesthenosphere up to the deepest position occupied by the mantle\crust interface in the course of the geological events under consideration.

Secondly, biostratigraphy and sedimentology is used to determine the palaeo-water depth, h_w. Additionally, biostratigraphically derived information can be used in conjunction with decompaction algorithms based on equation 7 in order to yield the palaeo-sediment thickness, h_s.

Thirdly, the relative sea level changes are studied by independent means, thus providing information on the values of ΔE in submarine situations. In terrestrial environments the uplift and erosion parameters have to be estimated using whatever knowledge is available (which, as mentioned before, is one of the weaknesses of the procedure).

Application of the concept of Airy isostasy can be well illustrated by reworking a textbook example using our notation. We use the Airy isostasy principle to demonstrate that the sediment thickness accumulated in marine environment is proportional to the water depth, thus limiting the maximum possible total sediment thickness caused by sediment loading alone.

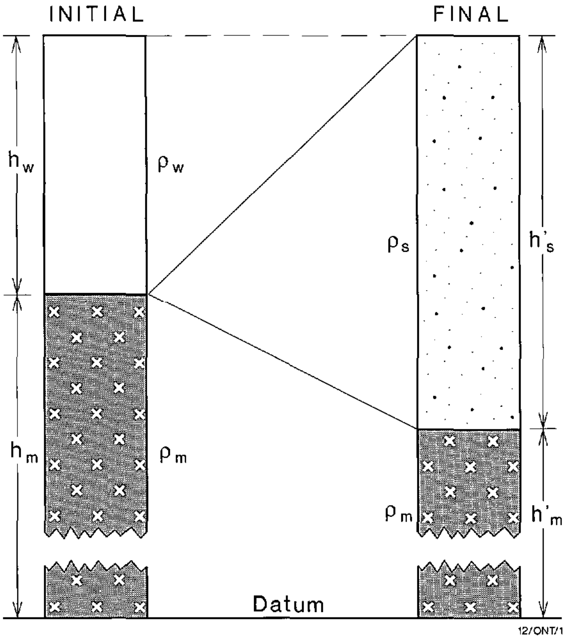

Figure 1. Stratigraphic column before (initial) and after (final) sediment accumulation in a submarine basin. Notation is explained in the text. Note that crust is not shown; its presence is also ignored in equations 12 and 13 since $\Delta h_c = 0$.

The initial and final situation is depicted in Figure 1. Sediment is being deposited on an initially sediment-free basement in the water depth h_w until it fills the basin to the brim. Our aim is to determine the final sediment thickness, h_s.

For this situation, the isostasy equations have the form:

$$\rho_w \Delta h_w + \rho_s \Delta h_s + \rho_m \Delta h_m = 0 \tag{12}$$

$$\Delta E = \Delta h_w + \Delta h_s + \Delta h_m = 0 \tag{13}$$

where $\Delta E = 0$ because (1) the basin fills to the brim and (2) there is no change of sea level during sedimentation. One can calculate Δh_m from equation 13: $\Delta h_m = -(\Delta h_w + \Delta h_s)$, and substitute into equation 12. After simple rearrangements of terms one gets the known result:

$$\Delta h_s = \Delta h_w \ ((\rho_w - \rho_m)/(\rho_m - \rho_s)) \tag{14}$$

There is a subtle point of convention here. By definition, any thickness differential Δh is a difference between the final and initial thickness, the final value being indicated with a prime. Therefore, Δh is positive if the thickness increased with time and negative if the thickness decreased with time. It is much safer to consequently adhere to this (or some equivalent) convention in one's calculations and interpret the results after the final formula has been obtained rather than introduce an *ad hoc* notation every time a new problem is to be solved. In the case of equation 14, the numerator ($=\rho_w - \rho_m$) is negative and Δh_w ($=0-h_w$) is negative, so the resulting sediment thickness h_s' ($=\Delta h_s$, since there was no sediment initially) is positive, as expected.

Substituting the values of densities to equation 14 one gets the following well-known relation between the maximum possible final sediment thickness and water depth:

$$h_s' = A\ h_w \tag{15}$$

where A varies from about 0.86 (for $\rho_s = 2.1\ kg/m^3$) to about 2.6 (for $\rho_s = 2.7\ kg/m^3$).

4.4 TECTONIC DRIVING FORCE (SUBSIDENCE).

4.4.1. Airy Isostasy.

In this section we define the concept of, and derive the formula for, the tectonic driving force of basement using the Airy isostasy principle as presented in equation 8. The results are also presented in a notation cosistent with the original formulation of this problem by Steckler and Watts (1978).

The fact that many basins contain much thicker shallow-water sediments than predicted by formula 15 can be only explained by invoking the tectonic driving force. The tectonic driving force is defined by Steckler and Watts (1978) as the hypothetical position of the palaeo-basement (relative to the present day sea level) had there been no sediments deposited. Thus, the driving force (sometimes called the basement subsidence curve) is a function of geological time.

The principles of calculation as well as the possible origins of the tectonic driving force are discussed by Steckler and Watts (1978). Here we derive their results (using the general notation of equations 10 and 11) in a more detailed way than was presented in the original paper.

The concept of calculation of the tectonic driving force is presented in Figure 2. The three sedimentary columns schematically shown there correspond to (a) the present day column, (b) a reconstructed palaeo-column representing some point of time in the past and (c) a hypothetical column obtained from column (b) by removing the sediment ("backstripping") and matching the sea level with its present day position. Sea floor position in column (c) relative to the present day sea level is by definition the tectonic driving force.

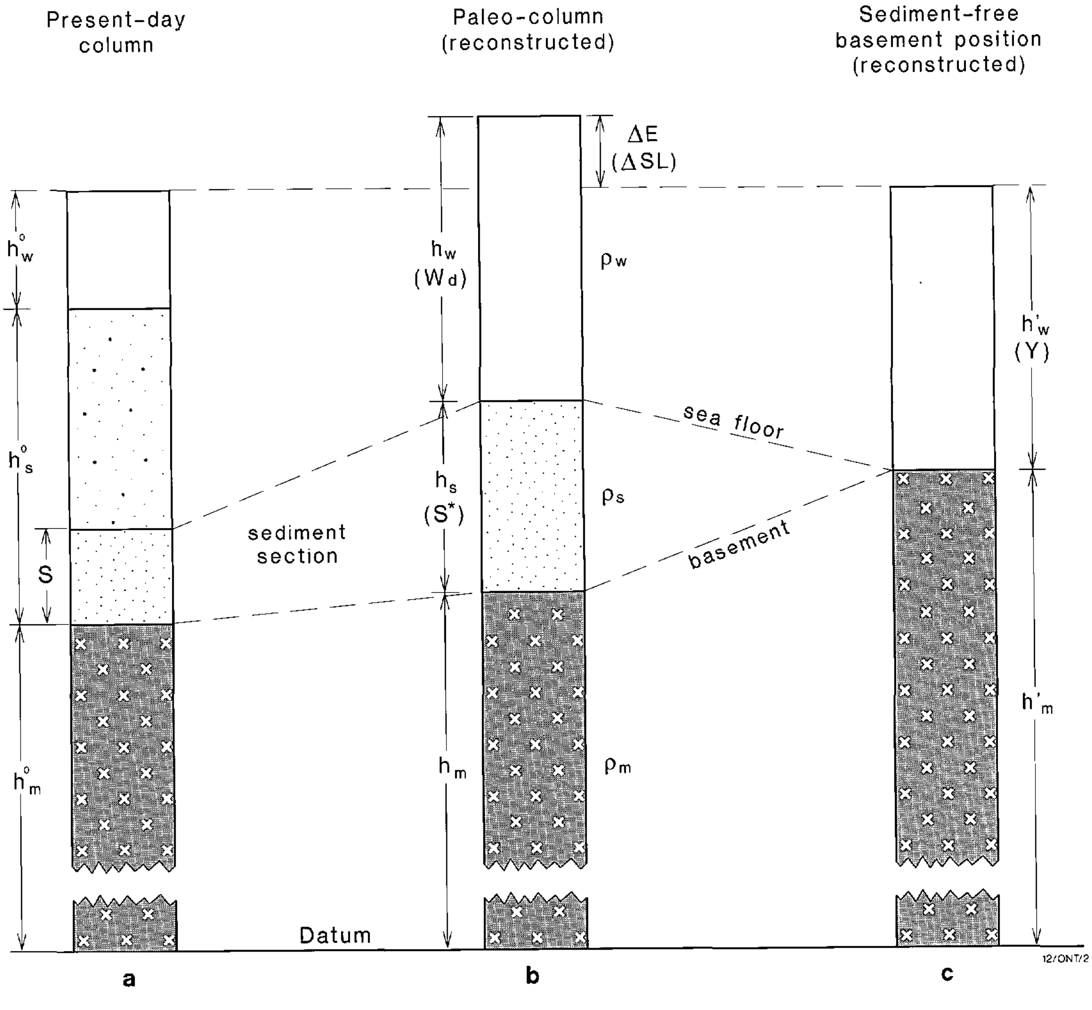

Figure 2. Three stratigraphic columns used to calculate the tectonic driving force. Notation is explained in the text. Note that crust is not shown; its presence is also ignored in equations 16a and 16b since $\Delta h_C = 0$.

Columns (b) and (c) are derived from column (a) using the following procedure. Firstly, biostratigraphy is used in order to determine age versus depth in the sediment column $h_s{}^0$. A section deposited prior to some point of time is then selected (of height S in column (a)). The younger sediment is then removed and water depth adjusted to the appropriate palaeo-value. Next, the sediment section is decompacted along the lines of equation 7, finally yielding the reconstructed palaeo-column (b).

Secondly, the sediment is totally removed and water level adjusted back to the present day value (this is done in order to provide a convenient datum for the change of basement position versus time). The columns (b) and (c) are now mathematically coupled by the Airy isostasy principle. In our notation this principle states:

$$\Delta E = \Delta h_w + \Delta h_s + \Delta h_m \qquad (16a)$$

$$0 = \rho_w \Delta h_w + \rho_s \Delta h_s + \rho_m \Delta h_m \qquad (16b)$$

Note that we have used notation as shown in Figure 2. Symbols in parentheses in this figure correspond to the original notation of Steckler and Watts (1978). By calculating Δh_m from (16a) and substituting it into (16b) one gets:

$$0 = (h_w{}' - h_w)\rho_w - h_s\rho_s + (\Delta E + h_w - h_w{}' + h_s)\rho_m \qquad (17)$$

Our aim is to calculate the "backstripped" basement position, hw'. It is a matter of simple algebra to arrive at the formula:

$$h_w{}' = h_w + h_s((\rho_m - \rho_s)/\rho_m - \rho_w)) + \Delta E(\rho_m/(\rho_m - \rho_w)) \qquad (18)$$

where, according to our convention $\Delta E<0$ for situation as in Figure 2. This is the master equation for the tectonic driving force. Note that we have consistently used $\Delta h = h' - h$ for all the indices (w, s, m).

It can be easily seen by consulting Figure 2 that using the Steckler and Watts notation their original result is exactly reproduced:

$$Y = W_d + S^*((\rho_m-\rho_s)/(\rho_m-\rho_w)) - \Delta_{SL}(\rho_m/(\rho_m-\rho_w)) \qquad (19a)$$

where the change of sign of the last term is caused by the fact that Steckler and Watts's sea level change , Δ_{SL}, is calculated relative to the present day sea level. Equation (19a) is frequently presented in an equivalent form:

$$h_w' = \{h_s((\rho_m-\rho_s)/(\rho_m-\rho_w)) + \Delta E(\rho_w/(\rho_m-\rho_w))\} + \{h_w+\Delta E\} \qquad (19b)$$

or, in the original notation (Steckler and Watts 1982):

$$Y = \{S^*((\rho_m-\rho_s)/(\rho_m-\rho_w)) - \Delta_{SL}(\rho_w/(\rho_m-\rho_w))\} + \{W_d-\Delta_{SL}\} \qquad (19c)$$

Expressions (19b) and (19c) are useful because in this particular form response of the basement to the sediment weight and changes in sea level (first term in curly brackets) is separated from the water depth relative to the present day sea level (second term in curly brackets).

4.4.2. Flexural and Visco-elastic Models.

The concept of Airy isostasy has two intrinsic assumptions which substantially simplify the task of computer programming: one-dimensionality (caused by lack of lateral interaction between adjacent stratigraphic columns) and instanteneous response to load. Both of these assumptions are not very realistic owing to the elastic and/or viscous behaviour of lithosphere under load. There has been a considerable effort to incorporate these features into the basin modelling, particularly during the last decade. None of these results have been reflected in the commercial programs reviewed here. Therefore, for the benefit of general interest, I give only a brief overview of these studies and quote only the most recent papers in which references to previous work can be found.

There have been two schools of thought regarding the response of lithosphere to load: the elastic (flexural) approach (Walcott 1970) and viscoelastic model (Beaumont 1978). Various aspects of these models were developed over the years to describe the subtle features of basin formation (for instance, see Sinclair et al. 1991, Beaumont et al.1988, and references cited therein).

Both the elastic and viscoelastic models are capable of taking into account the spatial and temporal distribution of load in a basin. Thus, the calculated response of the basement is two-dimensional and time-dependent.

For the simplest flexural models (e.g. Steckler and Watts (1978), Bond and Kominz (1984)) the steady-state response of lithosphere to a fixed sediment distribution is calculated and compared with the Airy isostasy results. There seems to be little difference between the results obtained using the flexural and Airy models, at least for the particular basin structures analysed in these papers. Steckler and Watts (1982) estimate that those differences do not exceed 10 percent near the basin center, the tectonic subsidence being greater in the flexural models. Towards the basin edges, however, all the subsidence may be of exclusively flexural origin.

The time dependence of the lithosphere response is an inherent part of the viscoelastic models (so far limited to load being applied at discrete time intervals, (Beaumont 1978)) and of most recent sophisticated flexular models (that take into account continuous deposition and erosion, Sinclair et al. 1991). It is apparent that at least in the case of viscoelastic models the time constant of the load response may be of the order of 10 m.y., which would have dramatic effect on the geohistory modelling for young basins (of the lifetime of the order of 10 m.y.) as compared to the Airy isostasy based models. It has to be noted, however, that the Airy model may be sufficient for very young basins because the early stages of rifting are usually accompanied by active faulting that results in strong fragmentation of the basement into mechanically decoupled horsts and grabens, thus possibly destroying the flexular strength of lithosphere depending on the rheological conditions.

4.5. HEAT FLOW.

Heatflow is a fundamental property of the lithosphere that drives and characterizes consecutive stages of basin development. It also directly affects the thermal history of various strata, which makes it one of the most critical factors in the modelling process.

The commercial programs analysed here use the palaeo-heatflow values supplied by the user to calculate the temperature at the boundaries of each lithological unit versus time, thus providing data for maturation calculations. Matoil additionally offers an in-built option of a rift heat-flow pattern based on the work of McKenzie (1978). In any case, the mathematical model is strictly one-dimensional, i.e. vertical heat flow is assumed. The heat flow algorithms used in BasinMod and Bury use a purely conductive model (discussed below), whereas in Matoil the convective component due to water expulsion is also taken into account (Ungerer et al. 1984). Additionally, any heat generated in the sediment (for instance originating from radioactive decay) is ignored. The above assumptions are restrictive and they should be geologically verified in order to substantiate the results of one-dimensional modelling. A comprehensive review of these issues is given by Allen and Allen (1991).

In one (vertical) dimension, z, the relationship between the heatflow, Q, and temperature, T, is given by:

$$Q = \kappa(z)\ dT/dz \tag{20}$$

where κ is thermal conductivity of infinitesimally thin layer, dz, at depth z. Equation 20 demonstrates the <u>local</u> proportionality between the heatflow and temperature gradient. Generically, the temperature gradient develops as a consequence of heat flow and, therefore, heat flow is considered to be a more fundamental quantity. In particular, various stages of basin development are best characterized in terms of heat flow values. Although the commercial programs analysed here enable one to use either heat flow or temperature gradient input values (which is computationally equivalent in view of equation 20), it is a better practice to use heat flow as primary data and perhaps employ fixed temperature points (for instance, at the bottom of the hole and/or on the surface) for control purposes.

Thermal conductivity is a weighted average of the solid matrix (which makes it dependent on the rock lithology) and formation liquid (usually brine). The relative amount of these two components is 1-f and f, respectively, where f is the porosity determined using the porosity-depth relations described in Section 3.2 above. The weighted average thermal conductivity, κ_{total}, is calculated according to:

$$\kappa_{total} = (\kappa_{solid})^{f}\ (\kappa_{liquid})^{1-f} \tag{21}$$

where the solid component of thermal conductivity for rocks of mixed lithology is expressed as the following weighted average:

$$\kappa_{solid} = (\kappa_{solid1})^{p}\ (\kappa_{solid2})^{1-p} \tag{22}$$

where p is the proportion of solid1 (of given lithology) in the mixture and 1-p is the proportion of remaining rock, which may be of mixed lithology (solid2).

Equation 22 presents but one possible scheme of calculating the composite thermal conductivities (this particular scheme is used in Bury). Other possible ways of averaging are discussed in Allen and Allen (1991). In general, it is not important what algorithm is used to obtain the average as long as the results are consistent with experimental data. However, I have not examined this area in detail and, therefore, cannot recommend any particular averaging procedure. Besides, the commercial programs do not allow the user to alter the in-built averaging procedures.

Note that in order to calculate the composite thermal conductivity for mixture of several lithologies, equation 22 should be applied several times, starting from a mixture of two lithologies. In the consecutive steps solid1 will then represent the newly added component and solid2 the mixture whose thermal conductivity was determined in the preceding step. In practical application for the commercial programs analysed here the temperature dependence of thermal conductivity is ignored (for detailed discussion of this issue see Palciauskas 1986).

As the result of the above procedure κ_{total} (formally identical with κ in equation 20) is determined. This enables one to calculate the temperature differential, $\Delta T = T_1 - T_2$, across the layer of a constant (possibly mixed) lithology extending from depth z_1 to z_2, simply by integrating equation 20:

$$T_1 - T_2 = \kappa^{-1} Q \ (z_1 - z_2) \qquad (23)$$

where Q is, of course, heatflow.

Note that equation 23 enables one to calculate the vertical temperature profile using appropriate values of κ for different lithologies, starting either from the top (sea bottom or surface temperature) or bottom hole (TD temperature). If both of these temperatures are known (which may be the case for present day sedimentary column), equation 23 is overdetermined and can be used as a test for a particular choice of heat flow and/or lithologies. This option is taken advantage of in Bury and BasinMod.

This brings us to the question of heatflow time profiles (palaeo-heatflow). The fact that commercial programs do not offer any default options (except for Matoil which has a rift option, (McKenzie 1978)) is not accidental - it reflects the ongoing contention in the literature regarding the thermal origins of basin formation and evolution. There are detailed palaeo-heatflow models developed for particular basin formation scenarios (for details see McKenzie 1978, Falvey 1982 and literature cited therein), but the applicability of these scenarios is difficult to verify. As a guide to the art of palaeo-heatflow reconstruction one could use the values compiled by Allen and Allen (1991, Fig. 9.18) for various geological settings (extensional, compressional and strike-slip basins as well as basement). These values vary from 0.5 heat flow units (for old oceanic crust) to 5 heat flow units for active ocean ridges and volcanoes. Also radiogenic component of heatflow will not remain constant during the basin forming process, since the thinning of both upper and lower crust can be extended in time. In any case, responsibility for creating a plausible heat flow pattern which would be consistent with the geological perception of basin evolution is squarely with the user.

4.6. KINETICS OF CHEMICAL REACTIONS.

4.6.1. Kerogen Transformation.

The kinetics of chemical processes that transform kerogen into hydrocarbons can only be inferred from laboratory experiments. The experimental data thus obtained are then scaled up to the geological conditions assuming that (1) the transformation rate, dx/dt, where x is the amount of organic matter transformed and t is time, is expressed by the same mathematical formula over the 12 orders of magnitude of time variation (from 10 minutes typical for a laboratory experiment to 10 million years typical for a geological hydrocarbon generation period), and (2) the chemical reactions occuring in a sample extracted from a core are exactly the same as in the natural conditions.

Although none of these assumptions can be directly verified, the latter one has been proven wrong at least in some cases. In particular, it has been demonstrated that, in contrast to the laboratory evidence, light hydrocarbons in field conditions cannot be produced by cracking oil. Instead, a steady-state catalytic process has been postulated for generation of gas and some components of oil (Mango 1990a, 1990b and 1991). As the process of catalysis is extremely sensitive to the minute amounts of chemically active constituents, it is susceptible to major changes caused by the core extraction and/or preparation procedures and, therefore, may not be evident in laboratory experiments.

Transformation of kerogen into hydrocarbons occurs by a series of complex chemical reactions of which little is known (typical pyrolysis experiments provide information about the total amount of organic matter transformed and are not reaction-selective). Consequently, the aim of present-day mathematical modelling has been to provide a way of quantifying the kinetics using simplified hypotheses that can be tested against the pyrolysis experimental data obtained in laboratory. However, the commercial programs analysed here use these numerical models developed for laboratory data to describe the kerogen transformation in the field conditions, thus relying on assumptions (1) and (2) above. Although this is the best which can be done given the current state of research, the results should be treated with caution.

On the other hand, it is essential to have a predictive model of hydrocarbon generation. Very recently there have been attempts to identify, characterize and model the specific thermal transformations in kerogen for which the single reactant/product path is not affected by catalysis (Alexander et al. 1991). Such transformations have a potential to be used for testing various geohistory scenarios as well as the precise indicators of kerogen maturity.

Whatever is the detailed nature of kerogen thermal transformation, it must occur by breaking chemical bonds (characterised by bonding energy E_i) using the molecule's vibrational energy (of the order of kT, k being the Boltzmann constant and T the absolute temperature in Kelvin). The rate at which a typical molecular bond vibrates upon thermal excitation, A_i, is of the order of 10^{12} - 10^{14} sec^{-1}. If bonds of a given type (lets say, i) do not interact either with each other or with any other types of bonds , it follows that statistically the number of bonds, dn, that break in a given interval of time, dt, is simply proportional to the number of bonds of type i, n_i:

$$-dn_i = k_i\, n_i\, dt \qquad (24)$$

where the minus sign on the left hand side is used to indicate that the total number of unbroken bonds is decreasing with time. Note that equation (24) is fully equivalent to the radioactive decay law (for exactly the same reason: the decaying nuclei do not interact with each other and perish in absolute solitude).

We intend to use equation (24) to determine the number of broken bonds (which is proportional to the amount of matter transformed) versus time. At a constant temperature it could by done by simple integration since the rate constant k_i depends only on the interplay between the molecular bonding energy, E_i, and the thermal energy, kT (which, by omission, means that k_i does not depend neither on time, t, nor on the number of remaining unbroken bonds, n_i). However, in any realistic geological situation the temperature does change in step with subsidence and, consequently, k_i varies as well. Under these circumstances the kinetic problem based on equation (24) can be only solved by numerical means.

It follows from the form of equation (24) that k_i equals the probability that a single bond will break in the time interval between t and t+dt. Such a process is properly described only at the quantum-mechanical level. Without going into details, it can be shown that k_i is:

$$k_i = A_i \exp(- E_i/(kT)) \tag{25}$$

where A_i is the vibrational frequency of the bond i in the molecule and E_i is the binding energy (called activation energy in the context of the thermal transformation process). Equation (25) is called the Arrhenius formula. Sometimes, instead of the Boltzmann constant, k, the gas constant, R, is substituted. These two forms of Arrhenius formula are equivalent, the difference being caused by using different units of energy.

It is worthwhile to discuss equation (25) in considerable detail because from reading the literature one may get an impression that both E_i (activation energy) and, in particular, A_i (pre-exponential factor) are merely fitting parameters with little a'priori constraints imposed on their values. This is a wrong impression. A_i is related to the molecular vibrational energy (which can be determined for instance by the infrared spectroscopy, Raman spectroscopy or neutron scattering), and for organic carbon compounds typically remains within the range 10^{12} - 10^{14}

sec^{-1}. Consequently, for breaking a single bond in an isolated molecule value of A_i greater than 10^{14} sec^{-1} makes little physical sense, although values smaller than 10^{12} sec^{-1} can be expected for the so-called forbidden transitions. (Units are important since in the hydrocarbon generation context A_i may be occassionally expressed in $(m.y.)^{-1}$!).

As mentioned above, the activation energy, E_i, is related to the dissociation energy of chemical bond under consideration. These dissociation energies for organic carbon compounds are of the order of several electronvolts per bond or, in other units, several tens of kilocalories per mole. In order to be prepared for shock of other units it is useful to keep handy the following relations: 100kcal/mole=4.338eV/bond, 100kJ/mole=1.037eV/bond, 1kcal/mole= 4.184J/mole.

Although the dissociation energies for isolated bonds can be in principle determined very precisely from their optical spectra, in practice it is very difficult to separate from the multitude of bonds present in kerogen the particular type that breaks at a given temperature. Therefore, the description of thermal maturation process has been by necessity semi-empirical. In this approach, the laboratory kerogen decomposition curves (that account for the total amount of kerogen decomposed up to certain temperature under the constant heating conditions) are fitted by a distribution of a number of simultaneous processes described by equation (24), A_i and E_i being the fitting parameters.

There are several approaches to the fitting procedure described in the literature. The two most advanced and important are the Tissot model (Tissot and Welte 1983; see also Ungerer 1990) and the LLNL model (Braun and Burnham 1987, Braun et al. 1991). Among other approaches there are the early Tissot and Espitalie (1975) model and TTI graphical method (Hunt et al. 1991 and references cited therein). Some oil companies use alternative methods of geochemical prospect appraisal that do not involve computer models (for description of procedures adopted by BP see Mackenzie and Quigley 1988).

The commercial programs reviewed here rely on different approaches to geochemical analysis. Matoil 2.0 uses the Tissot and Espitalie (1975) model, Bury 5.42 employs the later Tissot model (Tissot and Welte 1983) and BasinMod 2.55 uses the algorithm developed by LLNL (Lawrence Livermore National Laboratories), (Braun and Burnham 1987).

These models are discussed in detail in the literature cited. The Tissot-derived models are based on the recognition of three main kerogen types (I, II, and III of lacustrine, marine and terrestial origin, respectively). On these models, it is proposed that the oil and gas generation from kerogen and then oil cracking to gas is performed by a series of parallel first-order chemical reactions (equation 24) that can be fully described by a set of material (percent of organic matter transformed) and kinetic (E_i, A_i) parameters that depend on the kerogen type only. These parameters, determined by fit to laboratory pyrolysis data, are in-built in the programs. Consecutive models differ in the degree of sophistication, the later versions offering greater number of parallel reaction channels and more complex description of gas generation.

The LLNL algorithm is also essentially based on the Tissot model, but it gives the user more flexibility by offering him a choice of one of the three kerogen types, a mixture of types or an independent input of source rock parameters.

The improvements to Tissot model (Matoil and Bury) are being introduced in step with new research at the Institut

Francais du Petrole (for recent developments see Behar et al. 1991), whereas the algorithm used by BasinMod has been originally developed at LLNL for their kinetic studies (Braun et al. 1991).

We conclude this section by repeating that the kinetic models have been developed to describe the results of laboratory pyrolysis experiments and their application for estimation of hydrocarbons generated in field conditions may be misleading.

4.6.2. Maturity.

Measurements of maturity constitute an independent way of getting (indirect) information about the temperature history of sampled formation. A number of organic maturation indices (Time Temperature Index - TTI, Thermal Alteration Index - TAI, Spore Colouration Index - SCI, Vitrinite Reflectance - R_0, pyrolysis maximum temperature - Tmax) have been used, but each of them can be only determined with some degree of subjective judgment.

A comprehensive review of this subject has been published by Tissot et al. (1987). The reader interested in details should refer to this work. In this section only the most important aspects related to the primary maturation indices used by Matoil, BasinMod and Bury are discussed.

Vitrinite reflectance is the most widely used maturation index. However, there are various types of vitrinites and, therefore, caution should be excercised while using R_0 data. In coals, there are two vitrinite types (Buiskool Toxopeus 1983): highly reflective, hydrogen-poor, non-fluorescing vitrinite 1 and less reflective, richer in hydrogen and weakly fluorescing vitrinite 2. These two types originate from different plants and/or gelification processes. The widely used coal rank scale is based on vitrinite 1.

The dominant macerals encountered in lacustrine (kerogen type I) and marine (kerogen type II) series are called alginite and bituminite, respectively. However, unlike normal coal vitrinite 1, they are not derived from higher plants. Although their physical appearance is similar to vitrinite 1, their chemical composition resembles vitrinite 2. To make things even more confused, for type I and II kerogen these macerals commonly contain particles of the same maturation but markedly different reflectances. Furthermore, the 'proper' vitrinite 1 is normally present in low concentrations in rocks dominated by lacustrine and marine macerals, making reliable reflectivity measurements difficult.

These complications make the measurement of R_0 on common maceral types rather difficult and subjective matter. This is illustrated in a study by Dembicki (1984), where vitrinate reflectance of a number of samples determined by 17 different laboratories exhibits a scatter all over the hydrocarbon generation window (e.g. for one of the samples the range is from 0.4 to 1.8%). In order to produce good results, the vitrinite reflectance measurements should be taken in a standardized manner by an experienced microscopist. Tissot et al. (1987) emphasize that if vitrinite reflectance data are collected with good control over the kerogen type and maceral type, the results are reliable.

In the context of practical application for computerized geohistory analysis, vitrinite reflectance (and other maturation indices) play central role. This is caused by the fact that there are methods to theoretically calculate R_0 for a given depositional sequence once the palaeo-temperature has been determined. In other words, the experimental values of vitrinite reflectance can be compared with corresponding theoretical values determined for a selected palaeo-temperature and depositional sequence (including non-deposition and erosion) scenario; the scenario can be subsequently changed to improve the overall agreement. This method of iterative search for the best set of parameters (called forward modelling) is used by all of the commercial packages analysed here.

Philosophically, the theoretical calculation of vitrinite reflectance (or other maturity index) is related to the problem of kerogen maturity itself. Therefore, all general comments regarding the kinetics of thermal transformation made in Section 4.6.1 apply. Consequently, there are two possible routes to determine vitrinite reflectance: (i) by direct calculation using a specific kinetic model or (ii) by correlation with other maturity indices (e.g. transformation ratio, T_{max}, etc.) that in turn can be determined by an independent laboratory measurement. The three commercial packages analysed here differ in their approach to this particular problem.

In Matoil, the maturity of kerogen of given type is determined in the following way. First, the transformation ratio (TR, i.e. the ratio of transformed kerogen to the total transformable kerogen expressed in %) is calculated using the kinetic model of Tissot and Espitalie (1975). Next, this ratio is used to determine a required maturation index using experimentally determined correlation tables (Espitalie et al. 1985 and Matoil 1988, Appendix C). Thus determined value of maturation index depends on the kerogen type.

In Bury, a quantification of Lopatin's time-temperature index of maturity, TTI, (Lopatin 1971, Waples 1980) is employed. The formula is (Falvey and Middleton 1981):

$$(R_0)^m = A \int_0^{tfd} \exp(\alpha T(t))dt + R_{init} \qquad (26)$$

where R_0 is vitrinite reflectance in %, T is temperature in Celsius, tfd is time from deposition in Ma, R_{init} is vitrinite reflectance in organic material at the surface (equivalent to $R_0 = 0.2\%$) and the values of constants are A $= 2.7 \times 10^{-6}$ Ma^{-1}, $\alpha = 6.8 \times 10^{-2}$ $(degC)^{-1}$, and $m = 5.635$.

Formula 26 was obtained by Falvey and Middleton by fitting the data of Hood et al. (1975) and Shibaoka and Bennett (1977). In the latter paper pre-1977 vitrinite reflectance data from Cooper Basin, North West Shelf, Gippsland Basin and some other geologically analogous Australian basins are compared with the predictions of the TTI model assuming constant geothermal palaeo-gradient and good agreement between the theory and field data is found. Therefore, the authors claim that their method should give "reasonably accurate estimate for Tertiary and possibly late Cretaceous rocks, because, in general, the geothermal gradient in recent geological times would be similar to the present-day gradient".

In Bury 5.41, formula 26 is used without constraints regarding geological time and/or geothermal palaeo-gradient. This may be a potential source of serious errors and, therefore, the applicability of equation 26 to a particular geological region should be scrutinized. (It should be noted that more recent models of thermal evolution of vitrinite reflectance are based on the activation energy distribution rather than a single value as in formula 26 (Larter 1989; Burnham and Sweeney 1989)). The package contains a look-up table that correlates R_0 with TAI, T_{max}, SCI and, optionally, two other user-defined maturation indices.

BasinMod offers a choice of the Lopatin's TTI method or a sophisticated kinetic model based on the recent work of Burnham and Sweeney (1989). The kinetic model of vitrinite maturation employs a semi-empirical approach, based on the same theoretical principles as discussed in Section 4.6.1 and calibrated using extensive experimental data to determine the distribution of activation energy. This is the most advanced model of vitrinite reflectance currently available. BasinMod has an option that enables use of SCI, TAI, and T_{max} as user-provided, measured maturation indices.

It should be pointed out that correlations between the kerogen transformation and various maturity indices (R_0, SCI, T_{max}, etc.) depend on the temperature/time path of the maturation process. This means that these correlations are not global. Therefore, indiscriminate use of the default look-up correlation tables should be discouraged.

5. DIRECT COMPARISON OF COMMERCIAL GEOHISTORY PROGRAMS.

This section pertains to the versions of Matoil, BasinMod and Bury indicated in Table 1. As the programs are being developed and updated, additional options and improvements become available. For example, Matoil has been superceded by a new package, Genex; a two-dimensional version of BasinMod (for workstations) is being introduced and a new version of Bury offers an improved maturity model (Burnham and Sweeney 1989) as well as comprehensive tutorial. This list is by no means exhaustive and it is best to seek information on the latest developments directly from the companies.

The main features of modelling algorithms used in Matoil, BasinMod and Bury are compared in Table 1. In most cases the particular model used is referred to the original work where it was first described; reference to an appropriate section of this document is also given.

General impression one gets from Table 1 is that the three programs do not differ much. This is true in particular in respect to Bury and BasinMod. Matoil is the oldest program and neglects the presence of oceanic water layer, which renders it inadequate for calculations of the tectonic driving force. The importance of differences between various kerogen maturation models are rather difficult to assess and may be immaterial anyway, because all of these models may be only roughly indicative of the true hydrocarbon potential.

Graphic presentation part is most advanced for Bury. It offers single and multi-well options, animation and does not require external plotting routines. BasinMod does not have the animation option and only prepares files for mapping using external packages. Matoil only offers single-well plots.

Table 1. Comparison of main features of Matoil, BasinMod and Bury.

FEATURE	MATOIL 1.4	BASINMOD 2.55	BURY 5.41
Compaction model	Falvey & Middleton (1981); section 4.2.1.	Falvey & Middleton (1981) or Sclater & Christie (1980); section 4.2.1.	Falvey & Middleton (1981); section 4.2.1.
Basin subsidence	Airy isostasy, Steckler & Watts (1978), section 4.4.1.	Airy isostasy, Steckler & Watts (1978); section 4.4.1.	Airy isostasy, Steckler & Watts (1978); section 4.4.1.
Decompaction model	Method of slices, Perrier & Quiblier (1974); section 4.2.2.	Method of slices, Perrier & Quiblier (1974), section 4.2.2.	Method of slices, Perrier & Quiblier (1974), section 4.2.2.
Heat flow model	One surface value. Choice of constant, user-defined or rifting HF (McKenzie 1978);section 4.5.	One surface value. Choice of user-defined HF, geothermal gradient or hole bottom temperature; section 4.5	One surface value. Choice of user-defined HF, geothermal gradient or hole bottom temperature; section 4.5.
Thermal conductivity	Automatic from lithology. Seven lithologies, combinations possible; section 4.5.	Automatic from lithology. Seven lithologies, combinations possible; section 4.5.	Automatic from lithology. Nine lithologies, combinations possible; section 4.5.
Palaeo-sea level	Not used.	User defined.	User defined or default.
Kerogen maturation model	Tissot & Espitalie (1975): three kerogen types, model calculates transformation ratio (TR); section 4.6.	LLNL model (Braun & Burnham 1987): three kerogen types, mixture or own pyrolysis data; simultaneous conversion of kerogen to oil and gas (4 components); oil cracking to gas and residue; default or user defined kinetic parameters; section 4.6.	Tissot & Welte (1983): three kerogen types or mixture; up to 10 bonds for transforming kerogen to oil, 5 for kerogen to gas, 3 for oil to gas cracking; default kinetic parameters. Maturity model after Falvey & Middleton (1981): modified TTI model giving R_0 vs temperature; section 4.6.

Table 1 (continued). Comparison of main features of Matoil, BasinMod and Bury.

Maturity model	Tissot & Espitalie (1975): maturation indices correlated with calculated TR; depends on kerogen type; section 4.6.2.	Burnham & Sweeney (1989); Waples (1980): choice of sophisticated kinetic model of R_0 or classical TTI method; section 4.6.2.	Falvey and Middleton (1981): modification of classical TTI method.; section 4.6.2.
Graphic display	Single well only. Limit of 10 plots, including: input data vs depth and time, thermal, burial, maturation and generation vs time.	Single well & multiwell, including: input data vs depth and time, thermal, burial, maturation and generation vs time.	Single well, multiwell and animation, including: input data vs depth and time, thermal, burial, maturation and generation vs time. Multiwell options: (1) basin and (2) cross-section; (1) plots same type of value (depth, temperature, etc) for same lithologic unit for up to 50 wells; (2) plots lithology & maturity at fixed time for up to 6 wells. Animation: cartoon of basin or cross-section option vs time within specified time interval.

6. QUICK GUIDE TO GEOHISTORY MODELLING.

The major features of methodology of the geohistory analysis and its implementation in the commercial software packages are listed below:

1. The kinetics of basin evolution (isostasy, tectonics, heat-flow, etc.) are strictly one-dimensional (in vertical direction).

2. Palaeo-heatflow and evolution of unconformities are the two most controversial and crucial pieces of input data.

3. Compaction of sediments is assumed to be purely mechanical (there is no chemical or mechanical mass transport). The curve of porosity versus depth is dependent on both lithology and basin. This porosity curve as a rule should be calibrated using sonic log data. In-built porosity defaults for various lithologies may be grossly misleading.

4. Airy isostasy (instantaneous, one-dimensional) is used. This may give grossly incorrect results at basin edges and for unfaulted, young basins (younger than approximately 10 Ma).

5. Tectonic subsidence results are only as good as the underlying isostasy model.

6. Unconformities and hiatuses should be modelled on the basin-wide scale, using regional geological and palaeo-climatic information.

7. Palaeo-heatflow should be reconstructed in the geological context of basin inception and evolution. Ocean floor (or surface) palaeo-temperature is very important.

8. Chemical kinetic models are based on the laboratory, not field data. Calculated hydrocarbon yields may be grossly incorrect.

9. Maturity models vary substantially between different packages. The source and input values of R_0 (and/or other maturation indices) should be carefully examined before use. This should include the type of macerals, number and the reproducibility of data points. Be particularly careful with type I and type II (lacustrine and marine origin) kerogen.

10. If possible, a number of wells in a basin should be analysed and the results checked for consistency with overall geological picture.

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