Vertical migration of hydrocarbons modelled with fractional flow theory

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Summary
We present a simple 1-D and one-lithology model of integrated hydrocarbon generation and vertical migration. Although the model is very simple, it captures some of the most basic features of the vertical migration process, like expulsion from source rocks, and vertical migration in carrier beds above and below the source rock. The dynamics in the model are caused by sedimentation, which is done at a constant rate. Owing to sedimentation, the source rock is brought down to the depths where kerogen breakdown starts. This two-phase model is based on fractional flow theory, which makes it possible to avoid a pressure equation. The solution of the saturation equation is characterized by a dimensionless number, the gravity number, and the 'size' of the capillary forces. When the gravity number is less than 1, buoyancy is less important, while for gravity numbers greater than 1, buoyancy is dominating. We discuss capillary effects, and estimate a Peclet number for the migration process, which shows that capillary forces are less important in this one-lithology model. In the special case of no compaction, negligible capillarity and no generation of pore space due to the kerogen breakdown, we can approximate a solution to the saturation equation by considering Riemann problems. We find that above the source region, we get at least a shock and possibly a rarefaction, too. Below the source region, we have at least a rarefaction wave, and possibly a shock. We present explicit expressions for the shock position, and the characteristics propagating saturations. These solutions enable us to decide if, and when, the shock will reach the top of the basin. If we know the total oil production, we can read off from the flux function curve an approximation of the saturation propagated upwards. Although these solutions apply to the case of no compaction, negligible capillarity and no generation of pore space, they are useful approximations if any of these restrictions is only 'weakly' violated.

Key words: fractional flow theory, hydrocarbon generation, vertical migration.

1 Introduction
Generation, migration and entrapment of hydrocarbons in a real sedimentary basin are complicated processes which involve many geological processes. Generation of hydrocarbons is determined by both the amount, and the type, of organic material (kerogen) deposited, in addition to the temperature history. The movement and entrapment of the hydrocarbons are given by buoyancy, hydrodynamics and rock properties. These processes, the temperature history, the movement and the entrapment of hydrocarbons, are strongly influenced by geological events like sedimentation, erosion, fault activity, diagenesis, hydraulic fracturing and formation of salt diapirs.

In this paper we report the study of a very simple model for generation and migration of hydrocarbons. The model is basically the deposition of one lithology, with kerogen, at a constant rate. The hydrocarbons generated, which are termed oil, form the non-wetting phase. It is assumed that the non-wetting phase is immiscible with the wetting phase water, which is initially present. Both oil and water are assumed incompressible. The two-phase flow of oil and water in a basin during sediment accumulation is modelled by adapting the fractional flow theory of reservoir
simulation (Bear 1972; Aziz & Settari 1979; Peaceman 1977; Marle 1981; Luke 1989). The main differences between the fractional flow theory presented here, compared with reservoir simulation, are that we have a temperature-dependent source term spread out over a certain part of the computational domain, and that the domain is growing with time.

Our model, which is 1-D and of only one lithology, is unable to model the entrapment of oil, which is either a 2-D or 3-D process, or due to lithological contrasts. Anyway, we think that the model presented here captures some of the basic features of the dynamics of the vertical migration process, especially inside a source rock, and in carrier beds above or below a source rock.

The dynamics in this model are caused by constant sedimentation, which assures that the source rock is brought down to depths where kerogen breakdown takes place. The oil generation is assumed to follow the Arrhenius law and first-order kinetics.

The temperature history applied in the kinetic model is the conduction-dominated stationary temperature solution. We discuss the temperature equation (Appendix B) with respect to the moving top boundary and the convection caused by both oil and water flow. We conclude that with reasonable data, both these effects on the temperature solution are negligible.

The model accounts for the volume expansion that may take place when kerogen is transformed to oil, and the increase in pore volume that may result when the solid kerogen disappears. The model does also consider the compaction of the pore space which may result from a large overburden.

The fractional flow approach is used to circumvent a pressure equation. Instead of solving for oil (or water) pressure, which is used to obtain the volumetric flow of oil (or water), we can calculate the total volumetric flow of the phases with the help of the total mass balance.

If the dimensionless saturation equation, there are two dimensionless parameters, a gravity number $\Lambda_\theta$ and a relative capillary pressure $p_c$. The gravity number $\Lambda_\theta = 1$ defines a transition zone for the impact of gravity. For $\Lambda_\theta \gg 1$, gravity is important and the migration process is buoyancy driven, while for $\Lambda_\theta \ll 1$, gravity is negligible and the driving force is oil production. The most sensitive ingredient in the gravity number is the ratio of absolute permeability to the sedimentation rate.

The relative capillary pressure $p_c$ measures the capillary pressure relative to a characteristic pressure given by the model. Since the basin is increasing with time, we will see that the capillary forces become less important with time.

In the absence of capillary forces, the saturation solution above the oil-producing interval is a sharp shock moving upwards. We can estimate when the shock reaches the basin top. In addition to the shock, we might have a rarefaction wave too, if the saturation in the source region is sufficiently high. High saturations in the source region are likely to take place only in the case of 'weak' buoyancy, when $\Lambda_\theta \gg 1$. The saturation in the source region can be approximated by use of the flux function curve for oil and the total volume rate at which oil is generated. Below the oil-producing interval, the saturation tends to the residual oil saturation.

Using a knowledge of the total oil production, we show how to read off the approximate saturation that is propagated upwards. We also discuss conditions for flow, in terms of kerogen concentration, porosity, volume expansion from kerogen to oil, and the residual oil saturation.

We present three pairs of case studies which display various aspects of the model. The first pair is buoyancy-driven migration in the case of no compaction, where we get a breakthrough. The second pair is the same as the first, but now with 'weak' buoyancy. The final pair has moderate buoyancy together with compaction.

The migration process and entrapment of hydrocarbons were studied by Hubbert (1952), and his work has since been the basis for much subsequent work. For instance, He & Lerche (1991) and Lerche (1990a,b) have on this basis tried to estimate the shape of oil stringers in a carrier bed in the presence of water flow. Other authors, like Berg (1975), have studied further how strata with high capillary pressure form traps. England et al. (1987) have discussed the physics of the migration process and the entrapment of hydrocarbons. The method applied by these authors is the force balance of buoyancy, water hydrodynamics and capillarity. Although these works do not consider the dynamics of the combined oil generation and oil flow, they give considerable insight into the nature of the migration process. It should be noted that horizontal migration of oil is far more important than vertical, especially when it comes to long-range petroleum migration (Bethke, Reed & Olitz 1991).

Our model is well suited for making comparisons with more advanced models, which are likely to be based on other kind of numerics (Ungerer et al. 1990; Schneider et al. 1992). This simple model does also throw light on the amount of computational work needed to simulate oil flow on a geological time-scale.

After this introduction, we give a description of the rock and the associated coordinate systems. Then we discuss the porosity functions and present the kinetic model, before we embark on the saturation equation. An important component in the flux function for oil used in the saturation equation is the total volumetric fluid velocity, often termed 'total velocity'. We give expressions for the total velocity in the case of both compaction and no compaction of the pore space. Then we present the relative permeability curves, and the capillary pressure curves, and we discuss capillary effects. We present approximate solutions of the first-order saturation equation, before we present the case studies and give a conclusion.

## 2 ROCK DESCRIPTION AND COORDINATES

The conservation laws for oil and water are first expressed in the real $z$-coordinate which has the basin top as the origin. Any ocean above the basin is ignored. From the $z$-coordinate, the conservation laws are brought to the $\xi$-axis, which measures the height of the non-kerogen part of the completely compacted basin. The $\xi$-axis has the basin bottom as origin. The basin is assumed to be in a state of constant sedimentation, and the sedimentation rate in the $\xi$-space is denoted $\omega$. The height of the basin along the $\xi$-axis is denoted $\xi^+$, and it is given by $\xi^+ = \omega t$. Finally, the $\xi$-axis is scaled down to the unit interval by the transformation $x = \xi/\xi^+$. Note that all three axes have their
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Figure 1. The three coordinate system used: the real z-coordinate, the completely compacted \( \zeta \)-coordinate, and the unit coordinate \( x \).

positive direction pointing upwards, but only the \( z \)-axis has its origin at the basin top (see Fig. 1).

The rock considered here is assumed to consist of three basic parts: pure rocks without any hydrocarbon potential; pure kerogen where all the kerogen may be broken down to oil; and a void part initially filled with water.

The pure rock without any hydrocarbon potential and the kerogen makes up the solid sediment matrix. In a small sediment volume measured to be \( \Delta z \) high, the amount of solid sediment is given by

\[
\Delta \eta = (1 - \phi) \Delta z,
\]

where \( \phi \) is the porosity. \( \Delta \eta \) measures the height of the sediment volume as completely compacted rock.

The kerogen content of the rock is given by the fraction \( C \) of the initial solid part of the rock volume,

\[
C \Delta \eta_0 = C(1 - \phi_0) \Delta z_0,
\]

where \( \phi_0 \) is initial porosity, and \( \Delta z_0 \) is the initial height of the test volume. The height of the volume measured as compacted rock without any kerogen is \( \Delta \zeta \), which is given by

\[
\Delta \zeta = (1 - C_0) \Delta \eta_0,
\]

where \( C_0 \) is the initial kerogen fraction.

Since the \( \zeta \)-height of each sediment grain is a constant when measured from the basement bottom, we choose it as the Lagrangian coordinate in the migration model (see Nakayama 1986). The \( \zeta \)-coordinate is neither influenced by compaction of the sediment column, due to the overburden pressure, nor by the fact that a part of the solid sediment skeleton is transformed to a hydrocarbon fluid.

From the definition of \( \zeta \), we have that

\[
\Delta \eta = \Delta \zeta + C \Delta \eta_0 = \left( 1 + \frac{C}{1 - C_0} \right) \Delta \zeta,
\]

after use of eq. (3). Finally, by use of eq. (1) we can relate the real thickness of test volume to the kerogen-free solid part of it

\[
\Delta z = \frac{\Delta \eta}{1 - \phi} = \frac{(1 - C_0 + C)}{(1 - C_0)(1 - \phi)} \Delta \zeta.
\]

The \( z \)-position of \( \zeta \)-particle is then given by

\[
z(\zeta) = -\int_\zeta^{\zeta'} \frac{[1 - C_0 + C(\zeta')]}{(1 - C_0)[1 - \phi(\zeta')]} d\zeta'.
\]

We have included the minus sign, since the \( z \)-axis has the top of the basin as the origin.

3 POROSITY FUNCTIONS

In case the void generated by kerogen decay adds to the porosity of the rock, under the assumption of no compaction, we use eq. (4) to obtain the increase in porosity. In this case, \( \Delta z \) remains constant from the initial state where \( C = C_0 \) and \( \phi = \phi_0 \). We have from eq. (4) that

\[
\frac{\Delta \eta}{1 - \phi_0} = \frac{1 - C_0 + C}{1 - \phi},
\]

which gives the following porosity relation

\[
\phi = \phi_0 + (1 - \phi_0)(C_0 - C).
\]

If compaction is allowed, the amount of compaction is assumed, given as a porosity function of effective stress. The effective stress is defined to be the overburden pressure (bulk pressure), minus the pore fluid pressure (Terzaghi 1943). The effective stress represents the part of the overburden carried by the sediment skeleton. The porosity is then a volume-pressure relation, which may be considered as a state function for sediments. Most porosity functions are empirical, and the most common ones are given on the functional form

\[
\phi = \phi_0 \exp(-a p_e),
\]

where the two arguments are dimensionless. The parameter \( \phi_0 \) is the initial porosity, \( a \) is a parameter of unit inverse pressure, and \( p_e \) is the effective stress. In Wangen (1992) four different porosity functions on this form are listed, and the one we consider here is

\[
\phi = \phi_0 \exp(-a p_e),
\]

which is a common choice for a porosity function (Bethke & Corbet 1988). This is an adaption of Athy's porosity–depth relationship (Athy 1930) to a porosity function of effective stress. See Bethke & Corbett (1988) and Smith (1971). This porosity function has also been given a theoretical foundation by Korvin (1984). The initial porosity applied in such a porosity function is assumed to be constant.

Porosity functions of the form \( \phi = \phi(\phi_0, a p_e) \) are generalized in this paper to handle the case where porosity is generated as a result of kerogen disintegration, by substituting the new uncompacted porosity given by eq. (5)
for \( \phi_0 \). We assume that kerogen behaves like the solid matrix. The extended version of the porosity function is then

\[
\phi = \phi_0 + (1 - \phi_0) (C_0 - C) \exp(-\alpha_p) - (1 - \phi_0) (C_0 - C) \exp(-\alpha_p).
\]

The first term in the sum is the original porosity function, and the second term represents the compaction of the additional porosity generated.

4 THE KINETIC MODEL

The generation of oil is assumed to follow the Arrhenius law for only one activation step, which is only one set of kinetic parameters. Normally, kerogen is subdivided into a range of activation steps (Tissot & Welte 1978), which may be Gaussian distributed. The single step we have selected may be thought of as the mean, in a distribution with a very small standard deviation. In the case studies presented later we have used \( A = 1.0 \times 10^{12} \) s\(^{-1} \) and \( E = 200.0 \) kJ mol\(^{-1} \). The selected step is based on the data given by Burnham et al. (1987) and MacKenzie & Quigley (1988). The kinetic parameters presented by these authors have Gaussian distributed activation energy, with a standard deviation of less than a few per cent of the mean. The spectrum of activation energies shares the same Arrhenius factor. If we had chosen a standard deviation other than zero, we would get very much the same results, except that the regions of oil production would be broader.

As a characteristic time for the migration process we use an estimate for the half-life of kerogen. The estimate, which is denoted \( t_0 \), is given by

\[
t_0 = \frac{t_1}{\log(A t_1)} - t_2,
\]

where times \( t_1 \) and \( t_2 \) are given by

\[
t_1 = \frac{E}{K \Omega} \quad \text{and} \quad t_2 = \frac{T_0}{\Omega}.
\]

The temperature rate \( \Omega \) is related to the burial rate \( \omega \) and the heat flux \( q_h \) by

\[
\Omega = \frac{q_h \omega}{\lambda_b (1 - C_0)(1 - \phi_0)},
\]

where \( \lambda_b \) is the bulk surface heat conductivity. The estimate, which is derived in Appendix A, slightly overestimates the half-life for the activation step used here.

The case studies all have the temperature gradient \( g_h / [\lambda_b (1 - C_0)(1 - \phi_0)] = 0.04 \) K m\(^{-1} \) and the sedimentation rate \( \omega = 100.0 \) m in common. With these data we get \( t_0 = 20.7 \) Myr.

5 THE SATURATION EQUATION

In this section a dimensionless saturation equation is derived from conservation of oil and water. The dimensionless formulation is based on the half-life of kerogen \( t_0 \), subjected to linear growth in temperature as a characteristic time, together with the sedimentation rate \( \omega \) as a characteristic velocity. The saturation equation we arrive at applies only for a basin during constant sediment accumulation.

5.1 The saturation equation in the \( \zeta \)-coordinate

We derive a saturation equation for oil by considering a test volume \( V \) which contains the same 'constant' sediment grains, the kerogen-free grains which do not disintegrate. This volume is, therefore, constant in the \( \zeta \)-space.

The saturation of a phase is defined as the fraction of pore space occupied by the phase. Therefore, oil and water saturations add up to one. The derivation of the saturation equation presented below follows the standard line of reasoning applied in reservoir engineering, in the case of non-compressible fluids. The volumetric flow velocities of either phase will be a function of the total volumetric flow velocity, which may be obtained without solving any pressure equation. This way of circumventing the pressure is called fractional flow theory. See for instance Peaceman (1977), Aziz & Settari (1979) and Lake (1989).

Conservation of oil and water is given by

\[
d \left( S \rho_o \phi \right) + \frac{\partial}{\partial \zeta} (\rho_o u_o) = q_o dz
\]

and

\[
d \left( (1 - S) \rho_w \phi \right) + \frac{\partial}{\partial \zeta} (\rho_w u_w) = 0,
\]

where \( S \) is the oil saturation, \( \rho_o \) and \( \rho_w \) are oil and water densities, and \( u_o \) and \( u_w \) are oil and water volumetric flow velocities. On the right-hand side in eq. (9), \( q_o \) in oil generation in a unit volume. These equations are brought to the \( \zeta \)-space, by use of relation eq. (4) on the differential form, and the related one for partial derivation

\[
dz = \frac{1 - C_0 + C}{(1 - C_0)(1 - \phi)} dz \quad \text{and} \quad \frac{\partial}{\partial \zeta} = \frac{(1 - C_0)(1 - \phi)}{1 - C_0 + C} \frac{\partial}{\partial \zeta}.
\]

Then time derivation goes through the integration sign, and we can drop integrations. In \( \zeta \)-space these equations are

\[
\frac{\partial}{\partial t} \left[ e \left( 1 + \frac{C}{1 - C_0} \right) S \right] + \frac{\partial u_o}{\partial \zeta} = -\frac{1}{1 - C_0} \frac{\partial C \rho_o}{\partial t}
\]

and

\[
\frac{\partial}{\partial t} \left[ e \left( 1 + \frac{C}{1 - C_0} \right) (1 - S) \right] + \frac{\partial u_w}{\partial \zeta} = 0,
\]

where oil and water densities are assumed constant. The void ratio \( e \) is defined as \( e = \phi / (1 - \phi) \), and \( \rho_k \) is the density.
of pure kerogen. The oil source term is obtained from the definition of kerogen content (2), whereby we have

$$q_o dz = -\frac{\partial C}{\partial t} \rho_u d\eta = -\frac{1}{(1-C_0)} \frac{\partial C}{\partial t} \rho_u dz.$$ \hspace{1cm} (14)

The volumetric fluxes of oil and water relative to the sediment particles are related to the pore pressure of oil and water, by Darcy's law.

$$u_o = -\frac{k_{ro} k}{\mu_o} \left( \frac{\partial p_o}{\partial z} - \rho_o g \frac{\partial D}{\partial z} \right),$$ \hspace{1cm} (15)

$$u_w = -\frac{k_{rw} k}{\mu_w} \left( \frac{\partial p_w}{\partial z} - \rho_w g \frac{\partial D}{\partial z} \right).$$ \hspace{1cm} (16)

In these equations, $k_{ro}$ and $k_{rw}$ are the relative permeabilities, while $\mu_o$ and $\mu_w$ are the viscosities of oil and water, respectively. The absolute permeability is denoted $k$, and the constant of gravity $g$. The depth is $D$, which implies $\partial D/\partial z = -1$.

The relative permeabilities $k_{ro}$ and $k_{rw}$ are dimensionless functions of the oil and water saturation, respectively, in the range from zero to one. At a given saturation the relative permeability is a measure of the effective permeability at that saturation relative to the absolute permeability.

The absolute permeability $k = k(\varepsilon)$ is a function of the void ratio of the rock. When it is split into a constant permeability $k_0$ and a dimensionless part $k(\varepsilon)$, we have $k(\varepsilon) = k_0 k(\varepsilon)$. The constant part is chosen to be the permeability at the top of the basin, which implies that $k(\varepsilon_0) = 1$, where $\varepsilon_0 = \phi_0/(1 - \phi_0)$ is the initial void ratio. An example of such a permeability function is the one used by Lerche (1990a).

$$k(\varepsilon) = k_0 \exp[b(\varepsilon - \varepsilon_0)].$$

The dimensionless parameter $b$ in the permeability function controls how fast the permeability will decrease with depth.

The volumetric flow for oil and water is described by Darcy's law (15) and (16) are inverse proportional with the viscosities $\mu_o$ and $\mu_w$, respectively. We will see later that the oil viscosity only enters the model as the relative viscosity $k_{ro}/\mu_o$. Both viscosities depend on temperature, and they decrease with increasing temperature. Since they behave somewhat similarly, we assume that the relative viscosity is constant. The oil is normally more viscous than water, and in the case studies presented later, we have chosen 2 for this number.

The water viscosity will appear in the fraction $k(\varepsilon)/\mu_w$. If initial porosity is large, $0.5 < \phi_0 < 0.75$ and substantial compaction takes place, we can expect $k(\varepsilon)$ to decrease faster than $\mu_w$, and the factor $k(\varepsilon)/\mu_w$ will increase. If the initial porosity is small, or no compaction takes place, or even worse, the porosity increases due to kerogen breakdown, $k(\varepsilon)$ will stay constant or increase, while $\mu_w$ decreases. In this situation, the relation $k(\varepsilon)/\mu_w$ may in the worst case increase by a factor of 1000 from the top of the basin to the bottom. The viscosity decreases from approximately $10^{-3}$ Pa s at $20^\circ$C to approximately $10^{-7}$ Pa s at $150^\circ$C, while we may expect in the worst case of increasing porosity that $k(\varepsilon)$ increases by a factor of 10.

Despite these considerations, we assume a constant relationship $k(\varepsilon)/\mu_w$, which implies that the saturation equation is detached from the temperature equation, except for the oil source term. This assumption is implemented as a constant $\mu_w$ and $k(\varepsilon) = 1$ for all $\varepsilon$.

The mobility of oil and water are defined as

$$\lambda_o = \frac{k_{ro}}{\mu_o}, \text{ and } \lambda_w = \frac{k_{rw}}{\mu_w}.$$  

If we multiply $u_o$ and $u_w$ given by eqs (15) and (16), with $-\lambda_w$ and $\lambda_o$, respectively, we get

$$-\lambda_w u_o + \lambda_o u_w = -\lambda_o u_o - \lambda_w u_w = \lambda_o (\Delta p_g - \frac{\partial p_c}{\partial z}),$$

where $\Delta p = p_o - p_w$ and $p_c = p_o - p_w$. The pressure difference between the oil phase and the water phase is the capillary pressure $p_c = p_c(\delta)$, which is a function of the oil saturation. The last equation is identical to

$$-(\lambda_o + \lambda_w) u_o = -\lambda_o u_o + \lambda_w u_w = \lambda_o (\Delta p_g - \frac{\partial p_c}{\partial z}).$$

which provides the volumetric oil velocity as a function of the total volumetric velocity $u_o = u_o + u_w$. By means of the fractional flow function for oil $f_o$, given by

$$f_o = \frac{\lambda_o}{\lambda_o + \lambda_w} = \frac{1}{1 + (k_{ro}\mu_o)/(k_{rw}\mu_w)},$$

the volumetric oil is

$$u_o = f_o u_o + f_o \lambda_w (\Delta p_g - \frac{\partial p_c}{\partial z}).$$ \hspace{1cm} (17)

Replacing the $\partial p_c/\partial z$ by the corresponding derivation in the $\varepsilon$-coordinate, given by eq. (11), and then substituting the result into the conservation law for oil (12), we have

$$\frac{\partial}{\partial t} \left[ e (1 + C)(1 - C) \frac{C}{1 - C} \right]$$

$$+ \frac{\partial}{\partial \varepsilon} \left[ f_o u_o + f_o \lambda_w \left[ \Delta p_g - \frac{(1 - C) \partial p_c}{(1 + \varepsilon) \partial \varepsilon} \right] \right]$$

$$= -\frac{1}{(1 - C)} \frac{\partial C}{\partial t} \rho_u.$$ \hspace{1cm} (18)

We want to solve this saturation equation for a basin during constant sedimentation, with zero flow into the basin bottom as a boundary condition. The zero flux is accomplished by the Dirichlet boundary condition $S = 0$, because both $f_o = 0$ and $\partial p_c/\partial S = 0$ at zero saturation. At the top we use the Von Neumann boundary condition $\partial S/\partial \xi = 0$. Initial values are zero saturation, and the solution to this equation will not be different from zero, until the hydrocarbon source term starts producing.

### 5.2 The saturation equation in the x-coordinate

Since the basin will be in a state of constant sedimentation, we take eq. (18) from the $\varepsilon$-space to the $x$-axis, where the basin always has the height one. The sedimentation rate measured along the $\varepsilon$-axis is $\omega$, and the transformation from $\varepsilon$ to $x$ is $x = \varepsilon/(\omega)$. This transformation will affect both
time derivations appearing in eq. (12). For instance \( \frac{\partial C}{\partial t} \) will be
\[
\left( \frac{\partial C}{\partial t} \right) = \left( \frac{\partial C}{\partial t} \right)_x + \frac{\partial C}{\partial x} \frac{\partial x}{\partial t} = \frac{x}{\partial t} \frac{\partial C}{\partial x},
\]
where the subscripts \( \xi \) and \( x \) denote that the corresponding variable is kept constant during the derivation. The saturation equation (eq. 18), when expressed in the \( x \)-coordinate, is
\[
\frac{\partial}{\partial t} \left[ \epsilon \left( 1 + \frac{C}{1 - C_0} \right) S \right] - \frac{x}{\partial \xi} \frac{\partial}{\partial \xi} \left[ \epsilon \left( 1 + \frac{C}{1 - C_0} \right) S \right]
+ \frac{1}{\rho_0} \frac{\partial}{\partial x} \left\{ f_u u_x + f_h \lambda \left( \frac{\partial \rho_g}{\partial x} - \frac{(1 - C)}{(1 - C_0 + C)(1 + e)}(\omega t) \frac{\partial \rho_g}{\partial x} \right) \right\} = - \frac{1}{1 - C_0} \left( \frac{\partial C}{\partial t} \right)_x \frac{\rho_x}{\rho_0}. \tag{19}
\]

We still keep the time derivation of \( C \) in the source term at a constant \( \xi \)-position. To bring eq. (19) to a dimensionless form, we introduce the following dimensionless variables
\[
\tau = t/t_0, \tag{20}
\]
\[
\tilde{u}_x = u_x/\omega, \tag{21}
\]
\[
\tilde{\rho}_c = \rho_c/\rho_0, \tag{22}
\]
\[
\tilde{\omega}_n = \omega_n/\omega. \tag{23}
\]
Time is now measured relative to the half-life \( t_0 \) of the kinetic reaction, resulting from the given linear growth in temperature. The burial rate \( \omega \) is the characteristic velocity for the process, and by means of \( t_0 \) and \( \omega \), we obtain a characteristic pressure \( \rho_0 = \Delta p_0 t_0 \omega \). We assume that \( \Delta p = 0 \), which means that buoyancy is always present. With these variables, we are finally ready to write down the saturation equation in dimensionless form:
\[
\frac{\partial}{\partial t} \left[ \epsilon \left( 1 + \frac{C}{1 - C_0} \right) S \right] - \frac{x}{\partial \xi} \frac{\partial}{\partial \xi} \left[ \epsilon \left( 1 + \frac{C}{1 - C_0} \right) S \right]
+ \frac{1}{\rho_0} \frac{\partial}{\partial x} \left\{ f_u u_x + \Lambda_0 f_h \left( \frac{\partial \rho_g}{\partial x} - \frac{(1 - C)}{(1 - C_0 + C)(1 + e)}(\omega t) \frac{\partial \rho_g}{\partial x} \right) \right\} = - \frac{1}{1 - C_0} \left( \frac{\partial C}{\partial t} \right)_x \frac{\rho_x}{\rho_0}. \tag{24}
\]
There is only one explicit parameter left in the model, the gravity number
\[
\Lambda_0 = \frac{k_0 \Delta \rho_g}{\rho_0 \omega},
\]
which controls the amount of the buoyancy. The most important part in \( \Lambda_0 \) is the ratio of the permeability \( k_0 \) and the burial rate \( \omega \). The impact of gravity is to a large extent controlled by this ratio.

The saturation equation (eq. 24) is of second order, since
\[
\frac{\partial \rho_c(S)}{\partial x} = \frac{d \rho_c(S)}{dS} \frac{\partial S}{\partial x}.
\]

In the case where capillary forces are small and can be ignored, the saturation equation is of first order. The first-order term can be expressed as the gradient of a flux function \( F \) defined as
\[
F(S) = f_u(S) \tilde{u}_x + \Lambda_0 f_h(S) \tilde{k}(e) k_{ow}(1 - S). \tag{25}
\]

In the absence of a capillary pressure gradient, \( \omega F(S) \) is the real volumetric flow of oil through a horizontal unit area, when the saturation is \( S \). Although not explicitly given, \( F \) is also a function of \( x \) or \( \xi \), since \( \tilde{u}_x \) is.

## 6 THE TOTAL VELOCITY

So far we have not said anything about how to achieve the total volumetric velocity \( \tilde{u}_x \) in the dimensionless saturation equation (eq. 24). The velocity \( u_x \) is also obtained from the conservation laws, and by adding the eqs (12) and (13) we have
\[
\frac{\partial}{\partial t} \left[ \epsilon \left( 1 + \frac{C}{1 - C_0} \right) S \right] + \frac{\partial u_x}{\partial \xi} = - \frac{1}{1 - C_0} \left( \frac{\partial C}{\partial t} \right)_x \frac{\rho_x}{\rho_0}. \tag{26}
\]

In the rest of this paper we assume that time derivations with respect to \( t \) are done at a constant \( \xi \)-value, and that time derivations with respect to \( \tau \) are done at a constant \( x \)-value. This is the case if nothing else is denoted by a subscript. We get \( u_x \) at \( \xi \), by integrating eq. (26) from 0 to \( \xi \). We have \( u_x = 0 \) at the bottom of the basin, since the boundary conditions yields both \( u_x = 0 \) and \( u_w = 0 \) at the bottom.

\[
u_x = - \int_0^{\xi} \left\{ \frac{1}{1 - C_0} \left( \frac{\partial C}{\partial \xi} \right)_x \frac{\rho_x}{\rho_0} + \frac{\partial}{\partial \xi} \left[ \epsilon \left( 1 + \frac{C}{1 - C_0} \right) \right] \right\} d\xi',
\]

The transformation to the \( x \)-coordinate yields
\[
\tilde{u}_x = - \tau \int_0^x \left\{ \frac{1}{1 - C_0} \left( \frac{\partial C}{\partial \xi} \right)_x \frac{\rho_x}{\rho_0} + \frac{\partial}{\partial \xi} \left[ \epsilon \left( 1 + \frac{C}{1 - C_0} \right) \right] \right\} dx'. \tag{26}
\]

Next we consider the total velocity in the case of no compaction and compaction of the pore space.

### 6.1 No compaction

In the case of no compaction, we can take this equation a step further. There are two situations now, one where the effective pore volume remains constant and independent of kerogen disintegration, and the other one, where removed kerogen volume adds to the porosity. In the first case, we have \( \tilde{u}_x \) given by
\[
\tilde{u}_x = - \tau \int_0^x \left\{ \frac{1}{1 - C_0} \left( \frac{\partial C}{\partial \xi} \right)_x \frac{\rho_x}{\rho_0} + \frac{\partial}{\partial \xi} \left[ \epsilon \left( 1 + \frac{C}{1 - C_0} \right) \right] \right\} dx',
\]

where \( \epsilon_0 = \phi_0/(1 - \phi_0) \).

When the pore volume is increasing according to eq. (5), we have the void ratio given by
\[
\epsilon = \frac{\phi}{1 - \phi} = \frac{\phi_0}{1 - C_0 + C}.
\]

Taking the time derivative of the void ratio \( \epsilon \), and substituting it into eq. (26), we end up with
\[
\tilde{u}_x = - \tau \int_0^x \left\{ \frac{1}{1 - C_0} \left( \frac{\rho_x}{\rho_0} - 1 \right) \right\} dx'. \tag{27}
\]
We see from this equation that \( \rho_k > \rho_o \) is necessary for a positive total volumetric flow. A positive \( u \) implies that the phase moving upwards is of a larger volume than the phase moving downwards.

If \( \rho_k = \rho_o \), and therefore \( u = 0 \), then the volumetric flow of oil is equal to water. If the oil is moving upwards, because of buoyancy, then the same volume of water must move down to replace the oil.

The condition \( u = 0 \) is not sufficient for all the oil generated to stay at rest. The two other conditions needed are \( \partial p_k / \partial S = 0 \) and \( A_o = 0 \). The flow implied by saturation-dependent capillary forces must vanish, together with the gravity term in the flux function. The last condition is met when \( \rho_o = \rho_w \). In this case of no compaction and pore space generation, all oil generated will stay at rest, if \( \partial p_k / \partial S = 0 \) and \( \rho_k = \rho_o = \rho_w \).

### 6.2 Compaction

If compaction takes place, from eq. (26) we have

\[
\hat{u}_t = -\frac{\tau}{1 - C_{\mu,0}} \int_0^1 \left( \frac{\partial C}{\partial \tau} \right) \left( \rho_k + e \right) dx \\
- \tau \int_0^1 \left( 1 - \frac{C}{1 - C_{\mu,0}} \right) \left( \frac{\partial e}{\partial \tau} \right) dx.
\]

The first term is the contribution to the total velocity from the kerogen breakdown, and the second term is the contribution from the compaction. When the pore space is compressed, the pore fluid is forced out.

Since we do not solve any pressure equations, we cannot obtain the exact compaction. Instead, we can approximate the compaction with either of two extremes; no compaction or maximal compaction. No compaction was discussed in the previous section, and maximal compaction is discussed in Appendix D. In Appendix D it is shown that \( \hat{u}_t < 1 \), when \( e_0 < 0.5 \), \( C_{\mu} < 0.1 \) and \( (\rho_k / \rho_o) < 2 \), conditions which are likely to apply in most realistic basins. This upper bound for the total volumetric velocity is also used to show that convection effects in the temperature equation are negligible (see Appendix B).

### 7 RELATIVE PERMEABILITY AND CAPILLARY PRESSURE

The relative permeability curves used in this article are shown in Fig. 2. The curves shown do not pretend to model any specific rock, but they possess the basic properties of all such functions. They are explicitly given by Lake (1989)

\[
k_{ro}(S) = k_{ro} \left( \frac{S - S_{2}}{1 - S_{2}} \right)^{n_o}
\]

\[
k_{rw}(S) = k_{rw} \left( \frac{1 - S - S_{1}}{1 - S_{1} - S_{2}} \right)^{n_w}
\]

where the endpoint values \( k_{ro} \) and \( k_{rw} \), (the maximal relative permeability values), and chosen to be 1. The residual oil saturation and irreducible water saturation, \( S_{1} \) and \( S_{2} \), are both chosen to be 0.2, and the exponents \( n_o \) and \( n_w \) are both taken to be 2.

Both \( S_{1} \) and \( S_{2} \) saturations are due to capillary pressure. During drainage, the oil saturation increases in the water wet rock, and the oil phase enters smaller and smaller pores. This demands an increasing pressure difference between the oil phase and the water phase, due to interface tension and the curvature of the interface. This pressure difference is the capillary pressure. The capillary pressure in a single pore is given by Laplace's equation

\[
p_c = \frac{2\sigma \cos \theta}{R},
\]

where \( \sigma \) is the interface tension, \( R \) is the curvature of the interface and \( \theta \) is the contact angle.

In the reverse process, the imbibition process, the oil saturation decreases, and leaves behind oil globs trapped in the pores. Because of this, the capillary pressure curve followed during imbibition is not the same as that followed during drainage (see Lake 1989). As usual in reservoir simulation, we neglect this hysteresis effect, and the capillary pressure curve applied is shown in Fig. 3. The
Capillary pressure

(dimensionless)

Figure 3. The dimensionless capillary pressure curve. The real capillary pressure curve is obtained by multiplying this dimensionless curve with \( p_{cr} \), a fraction of the characteristic pressure \( p_o \).

8 CAPILLARY EFFECTS

In this section we try to estimate a Peclet number \( Pe_s \) for the saturation equation (eq. 24), when we neglect kerogen concentrations. We carry out the derivations with respect to \( S \), under the assumption of constant void ratio \( \epsilon \), constant permeability \( k(\epsilon) = 1 \) and constant total volumetric flow \( \dot{u}_t \), and get the following first-order and second-order terms.

1st order = \[ -\frac{x}{\tau} \dot{e} + \frac{1}{\tau} (f_{kr} \dot{u}_t \ + \Lambda_o f_{kr}^2 + \Lambda_o f_{kr}') \frac{\partial S}{\partial x}, \]

2nd order = \[ \left( \frac{1}{\tau^2} \Lambda_o f_{kr}^2 \right) \frac{\partial^2 S}{\partial x^2}. \]

We have \( \dot{u}_t < 1 \), \( k_{rw} \leq 1 \), \( f_o \leq 1 \), and for reasonable saturations we can assume \( \dot{\beta}_c < p_{cr} \). We then have a lower bound for \( Pe_s \):

\[ Pe_s > \frac{\dot{e}}{p_{cr}} \left( -\frac{x}{\tau} + f_{kr}^2 + f_{kr}' \right). \] (32)

We do not have any noticeable oil flow until \( \tau > 1 \), and we may assume \( p_{cr} < 1 \). The last inequality applies at least for the case studies presented later, where the characteristic pressure \( p_o \) is of order megaPascals. Since we have the rough estimate \( f_{kr}^2 + f_{kr}' \approx 1.0 \) for saturations in the range 0.35–0.65, we are likely to have \( Pe_s > 1 \). We can, therefore, expect convective transport to dominate, which is precisely what we experience with the case studies presented later.

9 THE FIRST-ORDER SATURATION EQUATION

When capillary forces are weak and can be ignored, the saturation eq. (19) reduces to a first-order equation. By use of the variable

\[ U = \epsilon \left( 1 + \frac{C}{1 - C \alpha} \right) S, \]

the first-order saturation equation is

\[ \frac{\partial U}{\partial \tau} - \frac{x}{\tau} \frac{\partial U}{\partial x} + \frac{1}{\tau} \frac{\partial F}{\partial x} = \dot{\beta}_o. \] (33)

First-order equations are known to admit discontinuous solutions, and we will see that this is the case, in the absence of a capillary pressure gradient.

The smooth solutions for this equation can be found by the method of characteristics. We then seek a one-parameter solution for eq. (33), \( U(s) = U[x(s), \tau(s)] \), where \( s \) is the parameter. By comparing the total derivative of \( U \) with respect to \( s \),

\[ \frac{dU}{ds} = \frac{\partial U}{\partial x} \frac{dx}{ds} + \frac{\partial U}{\partial \tau} \frac{d\tau}{ds} = \dot{\beta}_o, \]

with eq. (33), which may be written

\[ \frac{\partial U}{\partial \tau} + \left( -\frac{x}{\tau} + \frac{\partial \tau}{\partial U} \right) \frac{\partial U}{\partial x} = \dot{\beta}_o. \]
The solution that the plateau saturation in the source region corresponds to an oil flux equal to the total oil production. We can, therefore, use knowledge about the total oil production to read off the plateau saturation from the flux function. The plateau saturation in the source region decides what kind of wave types outside the source region. The wave solutions corresponding to Fig. 4 are shown in Fig. 5. Above the source region, we go from the maximal saturation \( S_0 \), down to zero, and we must have increasing speeds as saturation decreases. If \( S_0 \) is larger than the threshold saturation \( S_1 \), we will first have a rarefaction wave from \( S_0 \) to \( S_1 \), and then a shock wave from \( S_1 \) down to \( S = 0 \). The threshold saturation \( S_1 \) is given by the tangent beginning in the origin (\( S = 0 \)) and touching the flux function. On the other hand if \( S_0 \) is below \( S_1 \), the solution is only one shock from \( S_0 \) down to \( S = 0 \).

Below the source region, we go from the residual oil saturation \( S_1 \), up to \( S_2 \), and as long as \( S_0 \) is less than saturation at the inflection point \( S_1 \), we only get a rarefaction wave. If \( S_2 \) is above \( S_1 \), we will first get a rarefaction wave from \( S_1 \) to \( S_2 \) and then a shock wave from \( S_2 \) to \( S_0 \).

Figure 4. This figure shows a typical flux function curve for buoyancy-drive migration. The flux function shown is divided by \( e[1 + C/(1 - C_0)] \) to make it easy to read off the slope \([F]/[U]\). The saturation \( S_1 \) is given by the point where the tangent from 0 touches the flux function. The inflection point is at saturation \( S_2 \). The plateau saturation in the source region is \( S_0 \).

\[
\frac{\partial \tau}{\partial s} = 1 \quad (34)
\]

\[
\frac{\partial x}{\partial s} = \frac{x}{\tau} + \frac{1}{\tau} \frac{\partial F}{

\]

\[
\frac{\partial U}{\partial s} = \frac{q_v}{\tau} \quad (36)
\]

From eq. (34) we can choose \( s = \tau \). On either side of the oil-producing interval, we have \( dU/d\tau = 0 \). In the case of no compaction, we have on both sides a constant void ratio \( e \), and a constant kerogen concentration \( C \). That is because we have the initial kerogen concentration above the oil-producing region, and zero concentration below. Because of this, \( \bar{u} \), is also constant outside the region of the oil source, and therefore \( \partial F/\partial U \) too. Eq. (35) is then easily integrated in this case, to yield the characteristic of a constant saturation

\[
x(\tau) = \frac{\partial F}{\partial U} \left( 1 - \frac{\tau_0}{\tau} \right) + \frac{\tau_0}{\tau} x_0. \quad (37)
\]

The characteristic passes through the position \( x_0 \) at time \( \tau_0 \). In these regions where \( e \) and \( C \) are constant, \( \partial F/\partial U \) is given by

\[
\frac{\partial F}{\partial U} = \frac{1 - C_0}{e(1 - C_0 + C)} \frac{\partial F}{\partial S}.
\]

If compaction is allowed to take place, neither \( e \) nor \( \bar{u} \) is any longer constant outside the region of the oil source, and the characteristics are not easily found.

Characteristics propagating different saturations may collide in \( x-\tau \)-space, in which case a discontinuous solution is formed. The speed of the discontinuity is given by the Rankine-Hugoniot condition, or the jump condition, which is similar to the equation for the characteristics. It is

\[
\frac{dx}{d\tau} = \frac{x}{\tau} + \frac{1}{\tau} \frac{[F]}{[U]}, \quad (38)
\]

where

\[
\frac{[F]}{[U]} = \frac{F(U_2) - F(U_1)}{U_2 - U_1}
\]

is the jump from the left state \( U_1 \) across the shock to the right state \( U_2 \). A derivation of the Rankine-Hugoniot condition for eq. (33) is given in Appendix E. The shock position is then given by

\[
x(\tau) = \frac{[F]}{[U]} \left( 1 - \frac{\tau_0}{\tau} \right) + \frac{\tau_0}{\tau} x_0. \quad (39)
\]

The time \( \tau_0 \), when the shock reaches the top, is given as a solution of \( x(\tau_0) = 1 \), and we have

\[
\tau_0 = \frac{\left( x_0 - \frac{[F]}{[U]} \right)}{1 - \frac{[F]}{[U]}} \frac{\tau_0}{\tau}. \quad (40)
\]

The solution \( \tau_0 \) makes no sense unless \( [F]/[U] > 1 \). If \( [F]/[U] < 1 \), we either have \( \tau_0 < 0 \) or \( dx/d\tau < 0 \).

In the next section which presents case studies, we will see that the plateau saturation in the source region corresponds...
The volume of kerogen $\Delta V_k$ in the initial amount of solid $\Delta n_0$ is given by eq. (2).

$$\Delta V_k = C_0 \Delta n_0.$$  \hspace{1cm} (41)

The volume of void $\Delta V_\phi$ connected to $\Delta n_0$ is given by

$$\Delta V_\phi = e_{\text{max}} \Delta n_0.$$  \hspace{1cm} (42)

where $e_{\text{max}}$ is either $\epsilon_v$, the initial void, or $(\epsilon_v + C_0)/(1 - C_0)$ in the case of increased pore volume. The last void ratio is given by eq. (28), with $C = 0$.

We will get saturations large enough for oil to flow when

$$S_1 \Delta V_\phi < \frac{\rho_k}{\rho_o} \Delta V_k,$$

where the kerogen volume is multiplied with the volume expansion factor $\rho_k/\rho_o$, for transformation of kerogen to oil. After inserting relation (41) and relation (42) into the inequality above, we get the following two restrictions on the kerogen concentration.

$$\left( \frac{\rho_k}{\rho_o} \frac{C_0}{S_1 \epsilon_v} \right) > 1,$$

$$\left( \frac{\rho_k}{\rho_o} \frac{C_0}{S_1 \epsilon_v} \frac{1 - C_0}{1 + C_0 \epsilon_v} \right) > 1.$$  \hspace{1cm} (43, 44)

The first applies in the case of no increase in pore space, and the second applies when pore space increases due to kerogen breakdown. The last inequality can be factored, to yield a lower bound directly in $C_0$.

**11 CASE STUDIES**

We look at six cases in this section. The first two cases (A) and (B) are both buoyancy driven with $\Lambda_0 = 10$. The first case (A) has no capillary forces, no compaction and no extra pore space generated. In the second case (B), we have turned on capillary forces.

The next two cases (C) and (D) have only weak buoyancy, with $\Lambda_0 = 0.5$. These cases are identical to the previous pair, except for the $\Lambda_0$ parameter.

The last two cases (E) and (F) are moderately buoyancy driven with $\Lambda_0 = 1$. They differ from the first two by hydrostatic compaction and a large initial porosity. The last case (F) also includes generation of pore space.

The most essential parameters in each of the six cases are presented in Table 1.

Common for all six cases are the data given in Table 2. In addition, we have a constant ratio $\mu_\omega/\mu_w = 2$ in the flux function curve. The oil–water density difference $\rho_w - \rho_o$, together with the permeability $k_o$, and the viscosity $\mu_w$, are implicitly given by $\Lambda_0$.

The first four parameters in Table 2 concern the temperature history, and the oil source term. Since these are the same for all cases, they share the characteristic time $t_0 = 20.7 \text{ Myr}$, and the characteristic length $l_0 = \omega t_0 = 2.07 \text{ km}$. The characteristic pressure is given by $p_0 = g(\rho_w - \rho_o)N$. If we can assume anything for the density

**Table 1. Case descriptions.**

<table>
<thead>
<tr>
<th>Case</th>
<th>$\Lambda_0$</th>
<th>$\rho_\omega$</th>
<th>$\rho_w$</th>
<th>$C_0$</th>
<th>Compaction</th>
<th>Extra pore space</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>10.0</td>
<td>0.0</td>
<td>0.1</td>
<td>0.05</td>
<td>no</td>
<td>no</td>
</tr>
<tr>
<td>B</td>
<td>10.0</td>
<td>1.0</td>
<td>0.1</td>
<td>0.05</td>
<td>no</td>
<td>no</td>
</tr>
<tr>
<td>C</td>
<td>0.5</td>
<td>0.0</td>
<td>0.1</td>
<td>0.05</td>
<td>no</td>
<td>no</td>
</tr>
<tr>
<td>D</td>
<td>0.5</td>
<td>1.0</td>
<td>0.1</td>
<td>0.05</td>
<td>no</td>
<td>no</td>
</tr>
<tr>
<td>E</td>
<td>1.0</td>
<td>0.0</td>
<td>0.25</td>
<td>0.05</td>
<td>yes</td>
<td>no</td>
</tr>
<tr>
<td>F</td>
<td>1.0</td>
<td>0.0</td>
<td>0.25</td>
<td>0.05</td>
<td>yes</td>
<td>yes</td>
</tr>
</tbody>
</table>
Table 2. Parameters for all cases.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A (Arrhenius factor)</td>
<td>$1.0 \cdot 10^{12}$ [1/a]</td>
</tr>
<tr>
<td>E (activation energy)</td>
<td>200.0 [kJ/mol]</td>
</tr>
<tr>
<td>$\omega$ (burial rate)</td>
<td>100.0 [m/Myr]</td>
</tr>
<tr>
<td>$\eta_0[\lambda_0(1 - C_0)(1 - \phi_0)]$ (temperature gradient)</td>
<td>0.04 [K/m]</td>
</tr>
<tr>
<td>$\rho_k/\rho_o$ (volume expansion)</td>
<td>1.5</td>
</tr>
<tr>
<td>$S_{o1}$ (residual oil saturation)</td>
<td>0.2</td>
</tr>
<tr>
<td>$S_{w2}$ (irreducible water saturation)</td>
<td>0.2</td>
</tr>
</tbody>
</table>

difference $\Delta \rho = \rho_w - \rho_o$, we can estimate the pressure $p_o$, and the mobility ratio $k_o/\mu_w = (\lambda_0/\rho_0)/(g \Delta \rho)$.

If we let $\Delta \rho = 250.0$ kg m$^{-3}$, we get $p_o = 5.2$ MPa, where the constant of gravity $g$ is taken to be 10 m s$^{-2}$. The relative capillary pressure is taken to be 1.0, if it is non-zero, and at a typical saturation $S = 0.5$ we get the capillary pressure $p_c = 1.0 \rho_o \rho_o (0.5) = 0.6$ MPa. (From Fig. 3 we read of $p_o (0.5) = 0.12$.)

With the same density difference, we get the mobility ratio $\omega (g \Delta \rho) = 1.3 \times 10^{-15}$ m$^2$ Pa$^{-1}$. If $\mu_w = 1.0 \times 10^{-3}$ Pa s and $\lambda_0 = 1$, we get the permeability $k_o = 1.3 \times 10^{-3}$ mD, which may be considered as a characteristic permeability for the given burial rate.

The initial porosity $\phi_0$ is chosen to be 0.1 in the first four cases, and 0.25 in the two last cases. The initial kerogen concentration is $C_0 = 0.05$ in all six cases. A source rock with this kerogen content may be considered rich. As pointed out in the previous section, it is the ratio $(C_0/\rho_k)/(S_{o1}/\rho_o)$ which decides the impact of a kerogen concentration. If real source rocks have much less kerogen than used here, one may expect that effective pore space is less by about the same proportion.

We have chosen the volume expansion factor $\rho_k/\rho_o$, for the transformation of kerogen to oil equal to 1.5. The condition for flow, given by inequalities (43) and (44), are satisfied with a good margin. The volume of oil formed in a test volume of rock relative to the volume of the pore space is $(\rho_k/\rho_o)(C_0/\rho_0)$, and it is 0.83 in the first four cases and 0.38 in the last two. Both these numbers are greater than the residual oil saturation $S_{o1} = 0.2$.

In Appendix C we define a global mass balance criterion $\Delta M$, which is used to check the numerical model. The mass balance in the first four cases was $\Delta M < 0.02$, and $\Delta M < 0.1$ in the last two, for $\tau > 1$. The dimensionless number $\Delta M$ is calculated with the total amount of generated oil as the denominator. We therefore get an improved mass balance measured with $\Delta M$, with increasing amounts of oil in the system. Some details on the numerical methods which were used are given in Appendix F.

11.1 Cases A and B: $\lambda_0 = 10$

Case A is run without capillary pressure, compaction and generation of extra pore space. The temperature history $T(x, \tau)$ is shown in Fig. 6. The oil production $q_o$ and the total volumetric velocity $\bar{u}$, are shown in Figs 7 and 8, respectively. From these figures, we can see the oil production and the total velocity increase through time until all kerogen has been broken at the bottom of the basin. At that time, the oil production and the total velocity have both reached their steady-state levels. Since no compaction takes place and no pore space is generated, the total volumetric flow $\bar{u}$ is entirely due to the breakdown of kerogen, and it is in this case given by eq. (27). At any time, we can see that the total velocity increases in the region of oil production, which is the same as the region of kerogen breakdown.

Figure 9 shows the saturation solution. Until the residual oil saturation $S_{o1} = 0.2$ is reached, the oil is completely immobile. At those positions where $S < S_{o1}$, the saturation is only a result of local breakdown of kerogen.

At the time when the total oil production has reached its steady-state level, the saturation solution is a sharp shock at $S = 0.36$ moving upwards. The shock is plotted at intervals $\Delta \tau = 0.1$, and we can then see from Fig. 9 that the speed along the $x$-axis is approximately 0.8, at time $\tau = 1.80$. If we look at the scaled flux function curve in Fig. 10, we can read off $\bar{u} \equiv 2.2$ at $S = 0.36$. If we insert this factor into eq. (38), with $x_0 = 0.5$ and $\tau_0 = 0.8$, we get the same speed, approximately 0.8.

Figure 11 shows the situation in $x$-$\tau$-space from the time $\tau = 1.8$ to the time $\tau = 2.8$. The shock is shown as the curve crossing upwards between the characteristics. The characteristics above the shock propagate the zero saturation
Oil production

Figure 7. The oil production $q_o$ in case A, plotted from $r = 1.1$ to $r = 2.7$, with the step $\Delta r = 0.1$. We can see from the plot that the source region gets narrower with increasing time. That is because the source region corresponds to a fixed temperature interval, which is approximately $115^\circ$–$145^\circ$. Compare with the temperature shown in Fig. 6.

downwards, as a result of burial. The characteristics below the shock, but above the region of kerogen breakdown, are propagating the saturation $S = 0.36$ upwards. Fig. 11 shows no characteristics in the region of oil production, because they do not propagate constant saturations.

Since $[F]/[U] > 1$, we will get a breakthrough. We can apply eq. (40), with $x_0 = 0.5$, $n = 1.8$ and $[F]/[U] = 2.2$, and we get the breakthrough time $t_n = 2.5$. From Fig. 11 we read off the breakthrough time, the time when the shock reaches the top $x = 1$, to be the same $t_n = 2.5$.

The more towards the bottom of the basin these characteristics start, the more horizontal they get (see Fig. 11). This corresponds to the saturation solution shown in Fig. 9, where the saturation tends down to the residual oil saturation at the bottom of the basin, where all kerogen is broken down.

The total volumetric production after steady-state level is reached is given by $r \int_0^1 q_o \, dx = 0.08$. If we use the flux function to look up the saturation which gives this volumetric oil flow, we find $S = 0.36$. It should be noted that some oil is left behind as residual oil, but this amount is small compared with what is flowing upwards.

Case B is equal to case A except for capillary pressure, which is now given by $p_{cr} = 1$. The resulting capillary pressure gradients give almost the same saturation solution as in case A.

11.2 Cases C and D: $\Lambda_o = 0.5$

In cases C and D, buoyancy is much less important than in the two previous cases, and the driving force is the oil production. When oil is forced into the pore space, both oil and water are forced to move, but the impact of gravity is small due to the low $\Lambda_o$-value. Note that cases C and D differ from A and B, respectively, only by the value of $\Lambda_o$. 

Total velocity

Figure 8. The total volumetric flow $\dot{u}$ in case A, plotted from $r = 1.1$ to $r = 2.7$, with the step $\Delta r = 0.1$. The velocity increases from zero below the source region to its maximal value above the source region.
Figure 9. The saturation solution $S(x, \tau)$ in case A, plotted from $\tau = 1.1$ to $\tau = 2.7$, with the step $\Delta \tau = 0.1$. The solution is a shock moving upwards leaving behind a constant saturation down to the source region. Below the source region there is a rarefaction wave (a smooth wave) down to the residual oil saturation.

The temperature history, oil production and the total volumetric velocity are, therefore, the same.

The saturation solution for $\Lambda_0 = 0.5$ is shown in Fig. 12, which shows considerably higher saturations. The low $\Lambda_0$ value makes the oil more reluctant to flow. This can be seen from the flux function curve 13, where the $\Lambda_0$-peak we saw in Fig. 10 is almost gone at the top of the basin, where $\bar{u}_i$ is maximal. At the bottom of the basin where $\bar{u}_i = 0$, we still have a '{$\Lambda_0$}'-peak. The total volumetric velocity $\bar{u}_i$ is now an important component in the flux function. The total oil production is as before 0.08, and an oil flux of this size takes place at $S \approx 0.62$. We can also notice a small bump in the saturation at the position of maximal oil production.

The expulsion from the source region is low. Since $|F|/|U| < 1$, which can be seen from the flux function curve in Fig. 13, we will not get a saturation front that will reach the basin top.

The saturation solution in case D, with capillary pressure given by $p_c = 1.0$, is very close to the solution in case A shown in Fig. 12, which is without capillary pressure. A visible difference appeared below the source region, where the shock shown in Fig. 12 is smoothed.

11.3 Cases E and F: $\Lambda_0 = 1.0$

In case E we have $\Lambda_0 = 1.0$, which is moderate buoyancy, together with hydrostatic compaction. The porosity is given by eq. (6), where we have approximated the effective stress under hydrostatic conditions by

$$p_s = (\rho_s - \rho_w)g(z^* - \xi) = (\rho_s - \rho_w)g\omega(1 - x)$$

(see Wangen 1992). The pore fluid is assigned the density of water, regardless of any oil saturations. The factor

Figure 10. The flux function divided by $e[1 + C/(1 - C_u)]$ in case A, plotted at time $\tau = 1.80$, at each grid point in the basin. The peak in the middle of the plot is caused by the buoyancy term in the flux function. This is, therefore, a typical flux function for buoyancy-dominated migration.
$x-\tau$-space

**Figure 11.** The characteristics and the shock, plotted from the time $\tau = 1.8$ to the time $\tau = 2.8$, in $x-\tau$-space. We see the shock from Fig. 9 crossing upwards, starting from $x = 0.47$ at time $\tau = 1.8$, and reaching the surface $x = 1$ at breakthrough time $\tau = 2.5$. Below the source region the rarefaction is plotted as a fan of characteristics, which are the space–time curves of constant saturation.

\[ \alpha \left( \rho_s - \rho_w \right) \] is chosen so the characteristic time

\[ t_c = \frac{1}{\alpha \left( \rho_s - \rho_w \right) g \omega} \]

for the compaction process becomes equal to $t_{0i}$. We then have

\[ \alpha p_s = \tau (1 - x), \]

and

\[ \phi = \phi_0 \exp \left[ -\tau (1 - x) \right], \]

when no pore space is generated. The parameter $\alpha$, which may be considered as the compressibility for the rock, is now given by $t_{0i}$.

\[ \alpha = \frac{1}{\left( \rho_s - \rho_w \right) g \omega t_{0i}}. \]

**Figure 12.** The saturation solution $S(x, \tau)$ in case C, plotted from $\tau = 1.1$ to $\tau = 2.5$, with the step $\Delta \tau = 0.1$. Since buoyancy is weak in this case ($\Lambda_{0} = 0.5$) compared with cases A and B ($\Lambda_{0} = 10.0$), the oil is reluctant to move, and we get higher saturations than in cases A and B. Owing to high saturations in the source region, we get a rarefaction wave moving upwards in addition to the shock. Below the source region we get a shock in addition to the rarefaction wave.

If we let $\rho_s - \rho_w = 1000.0 \text{ kg m}^{-3}$, we get $\alpha = 5.0 \times 10^{-8} \text{ Pa}^{-1}$, which is a typical number for this parameter.

The porosity is shown in Fig. 14, and we see that the initial porosity is 25 per cent, while the porosity at the bottom decreases to below 2.5 per cent. The flux function in this case is shown in Fig. 15, where we can see how the buoyancy effect is diminished by the compaction flow as we approach the basin top. The compaction flow dominates the total volumetric velocity. The saturation solution is shown in Fig. 16, which has the same characteristic features as in the earlier cases. We have a shock in the front and a rarefaction behind.

In case F we have allowed the pore volume to increase due to kerogen breakdown, at the same time as we have compaction. The resulting porosity is shown in Fig. 17. The
Scaled flux function

![Scaled flux function graph](image)

**Figure 13.** The flux function divided by \( e^{1 + C/(1 - C)} \) in case C, plotted at time \( \tau = 2.0 \), at each grid point in the basin. Above the source region, the 'peak' caused by bouyancy which dominated the flux function in cases A and B (see Fig. 10) is now almost gone. In this region the flux function is dominated by the \( \tilde{a}_t \)-term. Below the source region, where \( \tilde{a}_t = 0 \), we still have a 'peak', which means that bouyancy is the only force acting in this region, even if it is weak. Note that the shape of the flux function only changes in the source region, due to a non-constant \( \tilde{a}_t \) in that region.

Porosity

![Porosity graph](image)

**Figure 14.** The porosity \( \phi(x, \tau) \) in case E, plotted from \( \tau = 1.0 \) to \( \tau = 2.5 \), with the step \( \Delta \tau = 0.1 \). The figure shows the porosity decreasing with time and depth.

Oil saturation

![Oil saturation graph](image)

**Figure 13.** The flux function divided by \( e^{1 + C/(1 - C)} \) in case C, plotted at time \( \tau = 2.0 \), at each grid point in the basin. Above the source region, the 'peak' caused by bouyancy which dominated the flux function in cases A and B (see Fig. 10) is now almost gone. In this region the flux function is dominated by the \( \tilde{a}_t \)-term. Below the source region, where \( \tilde{a}_t = 0 \), we still have a 'peak', which means that bouyancy is the only force acting in this region, even if it is weak. Note that the shape of the flux function only changes in the source region, due to a non-constant \( \tilde{a}_t \) in that region.

12 CONCLUSION

We have presented a simple 1-D and one-lithology model for integrated hydrocarbon generation and vertical migration. Even if the model is simple, we think that some of the most basic features of the migration process are captured; especially the vertical flow in the source rock and the carrier beds. The dynamics in the model are caused by sedimentation, which occurs at a constant rate. Because of this, we get an almost linear growth in the temperature, and we will always reach the temperature interval where oil is generated. The temperature equation is discussed with respect to both the moving boundary and convection caused by both oil and water flow.

The saturation equation is formulated by means of fractional flow theory, where oil and water pressure gradients are replaced by the total volumetric velocity \( \tilde{a}_t \). This velocity is obtained from the total mass balance of water and oil, and we give exact expressions for it. The saturation equation is derived with respect to both compaction of pore space and generation of pore space due to kerogen breakdown.

The solution of the saturation equation is characterized by a gravity number and a dimensionless capillary pressure number. We can see from the flux functions that bouyancy-driven migration corresponds to gravity numbers larger than one. If the gravity number is less than one, bouyancy is negligible. We discuss capillary pressure effects, and give an estimate for the Peclet number. With the basin data applied here, we get negligible smoothing due to capillarity. Be aware that we do not consider capillarity contrasts, which are an important mechanism for entrapment of oil.

In the case of no pore compaction, and negligible capillarity, we can approximate a saturation solution on the
Figure 15. The flux function in case E, plotted at time $\tau = 2.0$ for each grid point in the basin. Since compaction flow contributes to $\mu$, this flux function of moderate buoyancy ($\Lambda_B = 1.0$) changes shape more smoothly from the bottom to the top of the basin. Compare this flux function with the flux function of weak buoyancy shown in Fig. 13 in the case of constant porosity, which is plotted with the same number of grid points.

Figure 16. The saturation solution $S(x, \tau)$ in case E, plotted from $\tau = 1.0$ to $\tau = 2.5$, with the step $\Delta \tau = 0.1$. This is a saturation solution in the case of decreasing porosity and moderate buoyancy ($\Lambda_B = 1.0$), and it has the same features as the saturation solution with constant porosity and dominating buoyancy. Compare this solution with the saturation solutions of cases A and B shown in Fig. 9.
basis of Riemann problems. The region where oil is generated, where we find the highest saturations, is taken as one of the two states in the Riemann problem. The other state is zero above the source region, and is the residual oil saturation below the source region. When capillary forces are 'weak', we show that we have at least a shock above the source region, and possibly a smooth rarefaction wave also. This is opposite below the source region, where we have at least a rarefaction wave, and possibly a shock too. We give explicit expressions for the shock moving upwards, and for the characteristics outside the source region, which propagate constant saturations. By means of these solutions, we can decide both if and when the shock will reach the basin top.

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**REFERENCES**

APPENDIX A: ESTIMATION OF KEROGEN HALF-LIFE

The half-life $t_0$ of an activation step subjected to linear growth in temperature is given as the solution to the equation

$$\log (2) = \int_0^{t_0} K(t') \, dt' \quad \text{and} \quad K(t) = A \exp \left( -\frac{t_1}{t + t_2} \right),$$

where the times $t_1$ and $t_2$ are given by eq. (8). By changing the variable to

$$y = \frac{t_1}{t + t_2},$$

the same equation is expressed as

$$\log (2) = A t_1 \int_{-t_2/t_1}^{-t_1/(t_0 + t_2)} \frac{1}{y} e^y \, dy + 2 \int_{-t_2/t_1}^{-t_1/(t_0 + t_2)} \frac{1}{y} e^y \, dy.$$

From the definition of $t_1$ and $t_2$ given by eq. (8) we have

$$t_1 = \frac{E}{t_2} = \frac{E}{RT_0},$$

and as long as $E \gg RT_0 = 2.29 \, \text{kJ mol}^{-1}$, which applies for the activation energy used in this article, we have $t_1 \gg t_2$. If we assume $t_1 \gg t_0 + t_2$, we can make the following approximation

$$\log (2) \approx A t_1 \left[ \left( \frac{t_0 + t_2}{t_1} \right)^2 \exp \left( -t_1/(t_0 + t_2) \right) \right] - \left( \frac{t_2}{t_1} \right)^2 \exp \left( -t_1/(t_0 + t_2) \right).$$

The first of the two terms inside the parentheses dominate, and we have

$$\log [\log (2)] \approx \log (A t_1) - 2 \log \left( \frac{t_1}{t_0 + t_2} \right) - \frac{t_1}{t_0 + t_2}.$$

By taking into account the two dominating terms, we are left with

$$\frac{t_0 \approx t_1}{t_0 + t_2} \log (A t_1),$$

and we finally have

$$t_0 \approx \frac{t_1}{t_0 + t_2}.$$

Note that this estimate is only valid for a limited range of activation steps. From eq. (A1), we see that the assumption $t_1 \gg t_0 + t_2$ is met when $\log (A t_1) \gg 1$.

The hydrocarbon source term in a test volume is proportional to

$$\frac{dC}{dt} = -K(t) \exp \left[ \int_0^t K(t') \, dt' \right].$$

If we try to estimate at what time the oil production reaches its maximum, when $K(t) = A \exp \left( -t_1/(t + t_2) \right)$, we will once more estimate the time $t_0$. From $d^2C/dt^2 = 0$, we get

$$\frac{dK}{dt} (t_0) = [K(t_0)]^2,$$

independent of the choice of $K(t)$. With our choice of $K(t)$, we have

$$\left( \frac{t_1}{t_0 + t_2} \right)^2 = A t_1 \exp \left( -\frac{t_1}{t_0 + t_2} \right),$$

which is identical to

$$2 \log \left( \frac{t_1}{t_0 + t_2} \right) = \log (A t_1) - \frac{t_1}{t_0 + t_2}.$$

Under the same assumptions as above, we have

$$t_0 \approx \frac{t_1}{\log (A t_1) - t_2}.$$

APPENDIX B: THE TEMPERATURE EQUATION

The temperature history applied in the kinetic model is the conduction dominated stationary solution. During stationary conditions, the heat flux $q_h$ through the entire basin is constant. The temperature is then given by

$$T(z) = \int_0^z \frac{q_h}{\lambda (\phi, S)} \, dz,$$

or when expressed in the $x$-coordinate

$$T(x) = \int_x^1 \left[ \frac{t_0 \log_h}{\lambda_h (\phi, S)} \right] \frac{1 - C_0 + C}{(1 - C_0)(1 - \phi)} \, dx,$$

where $\lambda_h (\phi, S)$ is the bulk heat conductivity. This function is dependent both on the porosity and the saturation, since the heat conductivity of the sediment matrix $\lambda_S$, the oil $\lambda_O$, and the water $\lambda_w$ are quite different. (Note that heat conductivities are denoted by capital subscripts on the $\lambda$, to differentiate them from the mobilities.) We have used the following formula for the bulk heat conductivity

$$\lambda_h (\phi, S) = \lambda_S \left[ \frac{\lambda_O S + \lambda_w (1 - S)}{\lambda_S} \right] \phi,$$

which is commonly used in basin modelling (Ungerer et al. 1990; Bethke et al. 1991). The formula is adapted to two-phase flow by assigning the heat conductivity $\lambda_O S + \lambda_w (1 - S)$ to the pore fluid.

We now justify the solution (B1) or (B2), by considering the time dependence caused by the moving top boundary, and the influence of the convection term.
The basin is fed with a constant heat flux into the basin bottom, and until a certain time \( t_{mb} \), the heat flux will maintain stationary conditions. At time \( t \), when stationary conditions still persist, the temperature at depth \( z \) may be approximated by

\[
T(z) = -\frac{q_h}{\lambda_A} z,
\]

where \( \lambda_A \) is some average bulk heat conductivity. The temperature at the top of the basin is assumed to be 0°C. Recall that the \( z \)-axis has its origin at the basin top, and a \( z \) position in the basin is, therefore, a negative number. The energy stored in the basin at time \( t \) is then

\[
E_b(t) = c_b\rho_b\Lambda_0 \int_0^{h(t)} T(z) \, dz
\]

where \( c_b \) is some average bulk heat capacity, \( \rho_b \) is some average bulk density, and \( \Lambda_0 \) is the unit area. We can estimate the height of the basin by

\[
h(t) = \frac{q_h}{\lambda_A (1 - \phi_h)},
\]

where \( \phi_h \) is some average porosity. The kerogen concentration is assumed to be small and is left out. The energy stored in the basin at time \( t \) is

\[
E_b(t) = \frac{1}{2}c_b\rho_b\Lambda_0 \left( \frac{q_h}{\lambda_A} \right)^2 h^2(t).
\]

The given heat flux \( q_h \) can support stationary conditions as long as

\[
\frac{1}{A_0} \frac{dE_b}{dt} < q_h.
\]

At break even, which occurs at time \( t_{mb} \), we have equality in eq. (B4). By use of eq. (B3), we have

\[
\frac{1}{A_0} \frac{dE_b}{dt} = q_h,
\]

which is easily solved with respect to \( t_{mb} \):

\[
t_{mb} = \frac{q_h\Lambda_0}{c_b\rho_b} \frac{\lambda_A (1 - \phi_h)^2}{\omega}.
\]

The only sensitive parameter in \( t_{mb} \) is the sedimentation rate \( \omega \), which appears in the power of 2. In the section presenting case studies, we have taken \( \omega \) to be 100 m Myr\(^{-1}\), and with a typical value for the diffusivity \( \lambda_A/(c_b\rho_b) \) equal to 1.0 \times 10^{-5} \text{ m}^2 \text{ s}^{-1} = 3.2 \times 10^7 \text{ m}^2 \text{ Myr}^{-1}, \) and \( \phi_h = 0.25 \), we get \( t_{mb} = 1.8 \times 10^3 \text{ Myr}. \) The activation step we have chosen has \( t_0 \ll t_{mb} \), for the same burial rate, and we are well inside the region of stationary temperature conditions.

The temperature equation, expressed in the \( \xi \)-coordinate with the energy storage term left out, is

\[
(c_d\rho_uu_o + c_w\rho_wu_w) \frac{\partial T}{\partial \xi} - \frac{\partial}{\partial \xi} \left[ \lambda_u(e, S) \left( 1 + \frac{C}{1 - C/M} \right) \frac{\partial T}{\partial \xi} \right] = 0.
\]

To make the equation more amenable to analytical considerations, we approximate the factor inside the square brackets by some average constant conductivity \( \lambda_A \), and we have

\[
(c_d\rho_uu_o + c_w\rho_wu_w) \frac{\partial T}{\partial \xi} - \lambda_A \frac{\partial^2 T}{\partial \xi^2} = 0.
\]

For a typical oil we have \( c_o\rho_o < c_w\rho_w \), which means that water is more able to store and convect heat than oil. We also have \( u_o \geq 0 \) and \( u_w > 0 \), which means that there is never a total volumetric flow downwards, and that the volumetric flow of oil is always upwards.

If the convection factor \( c_d\rho_uu_o + c_w\rho_wu_w \) is positive, we can add the positive number \( c_d\rho_uu_o + c_w\rho_wu_w \), and we have the following upper bound,

\[
(c_d\rho_uu_o + c_w\rho_wu_w) < (c_d\rho_uu_o + c_w\rho_wu_w)u_o < 2c_w\rho_wu_w < 2c_w\rho_ww_0.
\]

The last inequality follows from \( u_o < 1 \), which is the same as \( u_o < 0 \) (see Appendix D). Although we have \( u_o > 1 \) and \( u_w > 0 \), we may have a negative convection factor \( c_d\rho_uu_o + c_w\rho_wu_w < 0 \). In the case of no compaction, we have \( u_o = 0 \) below the oil-producing layer. If pore space is fixed and no oil is generated, then the volume of oil moving upwards must be compensated by an equal volume of water flowing down. Since water convects heat better than oil, we get convection overturned. In this situation we can at least assume the weak inequality

\[
-2c_w\rho_ww_0 < (c_d\rho_uu_o + c_w\rho_wu_w)u_o < 2c_w\rho_ww_0
\]

and thereby bound the convection factor below.

If this bound for the convection term is inserted into the temperature eq. (B6), and the resulting equation brought to the \( x \)-space, we have

\[
\frac{\partial u}{\partial x} = \frac{\lambda_A}{2\omega^2 c_b\rho_b u_o} \frac{\partial^2 u}{\partial x^2} = 0.
\]

An estimate for \( c_w\rho_w \) in terms of \( c_b\rho_b \) is \( c_w\rho_w = 2c_b\rho_b \), and we have

\[
\frac{\lambda_A}{2\omega^2 c_w\rho_w u_o} = \frac{\lambda_A}{4\omega^2 c_b\rho_b u_o} \frac{1}{4} \frac{t_{mb}}{t_0} \frac{1}{1 - \phi_h}.
\]

An estimate for the Peclet number \( Pe_T \) is then

\[
Pe_T = 4(1 - \phi_h)^2 \frac{t_0}{t_{mb}}
\]

With characteristic time (half-life) \( t_o < t_{mb}/6 \), \( \phi_h = 0.25 \), and time spans for the migration process \( t_{max} < 3.0 \), we get \( Pe_T < 1 \). With the data applied in the case studies, we have \( t_o < 25 \text{ Myr} \), \( t_{mb} > 180 \text{ Myr} \), and \( t_{max} < 3.0 \), so we can safely neglect convection effects.

Note that the heat conduction term dies out with the
factor $1/t$, which implies that convection gets more important with time.

APPENDIX C: MASS BALANCE

The mass balance check is important for validating the numerical methods applied. Global mass balance is formulated as

$$M_{\text{gen}} = M_{\text{present}} + M_{\text{out}},$$

where $M_{\text{gen}}$ is the mass of all oil generated, $M_{\text{present}}$ is the mass of all oil present in the basin, and $M_{\text{out}}$ is mass of all oil having left the basin at the top. From eq. (14), we have

$$M_{\text{gen}} = \int_0^h (C_0 - C)(1 - \phi_0)\rho_k \, dz_0 = \int_0^{\zeta_0} \left( \frac{C_0 - C}{1 - C_0} \right) \rho_k \, d\zeta = \omega t \int_0^h \left( \frac{C_0 - C}{1 - C_0} \right) \rho_k \, dx,$$

where $h$ is the height of the basin. A similar calculation leads to

$$M_{\text{present}} = \int_0^h \phi S\rho_o \, dz = \int_0^{\zeta_0} S e \left( 1 + \frac{C}{1 - C_0} \right) \rho_o \, d\zeta = \omega t \int_0^h S e \left( 1 + \frac{C}{1 - C_0} \right) \rho_o \, dx,$$

where the program measures the mass balance by the

$$\Delta M = 1 - \frac{M_{\text{present}}}{M_{\text{gen}}} - \frac{M_{\text{out}}}{M_{\text{gen}}}.$$ (53)

The amount of oil that has left the system so far, is given by

$$M_{\text{out}} = \omega t \int_0^h F(S)\rho_o \, dt,$$

where $F$ is the flux function given by eq. (25).

The program measures the mass balance by the dimensionless number $\Delta M$,

$$\Delta M = 1 - \frac{M_{\text{present}}}{M_{\text{gen}}} - \frac{M_{\text{out}}}{M_{\text{gen}}}.$$ (53)

which measures missing mass relative to the total mass generated.

APPENDIX D: AN UPPER BOUND FOR THE TOTAL VELOCITY

In this appendix we derive an upper bound for $u_t$ given by eq. (30). In the last two parts of this appendix the following two expressions are derived:

$$-\tau \int_0^1 \left( \frac{\partial e}{\partial \xi} \right)_\xi \, dx < 2C_0,$$ (D1)

and

$$-\tau \int_0^1 \left( \frac{\partial e}{\partial \xi} \right)_\xi \, dx = e(0) - e(c\zeta^*) < e_{\text{max}}.$$ (D2)

By application of the estimates (D1) and (D2), we get

$$u_t < 2 \left( \frac{C_0}{1 - C_0} \right) \left( \frac{\rho_k}{\rho_o} + e_{\text{max}} + \left( 1 + \frac{C_0}{1 - C_0} \right) e_{\text{max}} \right) = e_{\text{max}} + \left( \frac{C_0}{1 - C_0} \right) \left( 2 \frac{\rho_k}{\rho_o} + 3e_{\text{max}} \right).$$

With the reasonable assumptions, $e_{\text{max}} < 0.5$, $C_0 < 0.1$ and $\left( \rho_k/\rho_o \right) < 2$, we have $u_t < 1$, which means that total velocity $u_t$ is less than the sedimentation rate $\omega$.

D1 The volumetric flow due to hydrostatic compaction and the inequality (D2)

The volumetric flow due to maximal compaction takes place under almost hydrostatic conditions, which are often found in sand lithologies. We then have the following upper bound for the effective stress $\rho_s$,

$$\rho_s = (\xi^* - \zeta)(\rho_0 - \rho_o)g,$$

(see Wangen 1992). The pore fluid density is approximated by the density of the water, since we expect water to be more dense than oil. If we, for the time being, neglect the effect of kerogen concentration, the pore volume $V_\phi(\zeta)$ of the basin up to height $\zeta$, is given by

$$V_\phi(\zeta) = \int_0^\zeta \phi e(\zeta^* - \zeta')d\zeta' = \int_0^\zeta e(\zeta^* - \zeta')d\zeta',$$ (D3)

where the constant $c$ is given by $c = a(\rho_0 - \rho_o)g$. With the choice of porosity function given by eq. (6), $V_\phi$ is explicitly given by

$$V_\phi(\zeta) = \frac{1}{c} \log \left( \frac{1 - \phi_0 e(\zeta^* - \zeta)}{1 - \phi_0 e(c\zeta^* - c\zeta)} \right).$$

Note that the pore volume $V_\phi(\zeta)$, up to the height $\zeta$, is also a function of the total height of the basin, $\xi^*$. By use of eq. (D3), the volumetric flow of pore fluid $u_t$ at position $\zeta$ is

$$u_t = -\frac{\partial V_\phi}{\partial \zeta} = -\int_0^\zeta \frac{\partial e}{\partial \zeta} \, d\zeta' = -\int_0^\zeta \frac{\partial e}{\partial \zeta} \, dy = \omega \int e(c\zeta^* - c\zeta) \, dy,$$ (D4)

where $y = c(\zeta^* - \zeta)$. By changing the variable to $y$, we get

$$u_t = \omega \int_{c\zeta^*}^{c(\zeta^* - \zeta)} \frac{de}{dy} \, dy = \omega [e(c\zeta^* - c\zeta) - e(c\zeta^*)].$$ (D5)

independent of choice of porosity function. Eq. (D5) says that the maximal volumetric flow at position $\zeta$, measured relative to the sedimentation rate, is equal to the difference in void ratio at height $\zeta$ and height $0$. This result applies only to an almost hydrostatic basin during constant sedimentation. If the sedimentation process is stopped, the compaction process is almost stopped too. In the presence of kerogen, we cannot obtain any exact flow rates, but at least we have

$$\frac{u_t}{\omega} \leq \left( 1 + \frac{C_0}{1 - C_0} \right) \left( e(c\zeta^* - c\zeta) - e(c\zeta^*) \right).$$

With small kerogen concentrations, eq. (D5) is a fairly good estimate.
From eq. (D4), we have
\[ u_t = -\int_0^\tau \left( \frac{\partial C}{\partial t} \right)_\zeta \, d\zeta = -\omega \tau \int_0^1 \left( \frac{\partial e}{\partial \tau} \right)_\zeta \, dx, \]
which implies the inequality (D2).
\[ -\tau \int_0^1 \left( \frac{\partial e}{\partial \tau} \right)_\zeta \, dx = e(0) - e(c^*) < e_{\text{max}}. \]

The maximal void ratio \( e_{\text{max}} \) is provided by maximal porosity, \( \phi_{\text{max}} = \phi_0 + C_0(1 - \phi_0) \), given by eq. (5). Eq. (D2) facilitates an upper bound for the second term in eq. (30) for \( \tilde{u}_i \).

**D2 The inequality (D1)**

To bound the first term in eq. (30) for \( \tilde{u}_i \), we must make an upper bound for
\[ \int_0^1 \left( \frac{\partial C}{\partial \tau} \right)_\zeta \, dx. \]
To do so, we assume stationary conditions in the sense that kerogen breakdown takes place in a fixed area from the top of the basin down to the depth \( \Delta \zeta \). Above this depth we assume that the kerogen concentration is \( C = C_0 \), and below this depth that it is zero. In \( x \)-space, the boundary for the area of non-zero kerogen concentration is
\[ x(t) = 1 - \frac{\Delta \zeta}{\omega t}. \]
Let \( t_1 \) be the time when \( \Delta \zeta \) is the height of the entire basin, which means that \( \Delta \zeta = \omega t_1 \). We then have
\[ x(\tau) = 1 - \frac{\tau_1}{\tau}, \]
where \( \tau_1 = t_1 / t_0 \). By means of the interval \( [x(\tau), 1] \), we have
\[ \int_0^1 \left( \frac{\partial C}{\partial \tau} \right)_\zeta \, dx = \left( \frac{\partial}{\partial \tau} \right)_\zeta \left( \int_0^1 C \, dx \right) \]
\[ \leq - \left( \frac{\partial}{\partial \tau} \right)_\zeta C_0 [1 - x(\tau)] = -C_0 \frac{\tau_1}{\tau}. \]

Note that any \( \zeta \) dependence is removed from the integral, so a time derivation with respect to \( x \) or \( \zeta \) is indifferent. At time \( \tau > \tau_1 \) we have oil generation at full height, and it is reasonable to assume that \( \tau_1 \) is only slightly larger than \( \tau = 1 \), the half-life. We therefore have
\[ -\tau \int_0^1 \left( \frac{\partial C}{\partial \tau} \right)_\zeta \, dx < 2C_0, \]
which is the estimate wanted.

**APPENDIX E: THE RANKINE-HUGONIOT CONDITION**

The first-order eq. (33) may be expressed as
\[ \partial U / \partial \tau - x \partial U / \partial x + \partial F / \partial x = 0, \tag{E1} \]
to avoid a singularity at \( \tau = 0 \). If \( U \) has a discontinuous solution, then \( \partial U / \partial x \) is not defined, and eq. (E1) does not make sense at the discontinuity. In order to obtain a solution, which may be discontinuous, we will make a 'weak' formulation of eq. (E1). See, for example, Smoller (1983) for more details.

To do so, we multiply eq. (E1) by a \( C^1 \) function \( \psi(x, \tau) \), which vanishes on the boundary of the domain \([0, 1] \times [0, \infty] \). We integrate over the entire domain, and after integration by parts, we are left with
\[ \int_0^1 \int_0^1 \left( \partial U / \partial \tau - U \partial \psi / \partial x + F \partial \psi / \partial x \right) \, dx \, d\tau = 0. \tag{E2} \]
This is the weak formulation, and \( U \) is a weak solution provided that eq. (E2) holds for all \( C^1 \) functions \( \psi \) which are zero on the boundary.

We now assume that \( U \) has a discontinuity across the \( \Gamma \) given by \( x = x(\tau) \) in \( x-\tau \)-space. Let \( D \) be a small disc centred at \( P \) (Fig. E1), and \( D_1 \) and \( D_2 \) are the two parts of \( D \) on each side of \( \Gamma \). Let \( \psi \) be a \( C^1 \)-function that vanishes on the boundary of \( D \), and from eq. (E2) we have
\[ \sum_{i=1}^2 \int_{D_i} \left[ \partial \psi / \partial \tau - (U \partial \psi / \partial x + F \partial \psi / \partial x) \right] \, dx = 0. \]
Since \( U \) is continuous in \( D_1 \), we have
\[ \int_{D_1} \left[ \partial \psi / \partial \tau - (U \partial \psi / \partial x + F \partial \psi / \partial x) \right] \, dx = \int_{D_1} \left[ \partial \psi / \partial \tau (U \psi) - \partial \psi / \partial x (U \psi - F \psi) \right] \, dx = \int_{\partial D_1} \psi | -U \, dx - (U \psi - F \psi) \, d\tau = 0. \]
by use of the divergence theorem. Since \( \psi = 0 \) along the boundary of \( D \), these line integrals are non-zero only along...
\( \Gamma \) If \( U_1 = U[x(\tau) - 0, \tau] \) and \( U_2 = U[x(\tau) + 0, \tau] \), we have
\[
\int_{\partial D} \psi[-U \tau dx - (Ux - F) dt] = \int_{\partial D} \psi[-U_1 \tau dx - (U_1x - F(U_1)) dt],
\]
\[
\int_{\partial D} \psi[-U \tau dx - (Ux - F) dt] = \int_{\partial D} \psi[-U_2 \tau dx - (U_2x - F(U_2))] dt.
\]
We therefore have
\[
\int_{\partial D} \psi(-U \tau dx - (Ux - F(U)) dt) = 0,
\]
where \([U] = U_x - U_t\) and \([Ux - F(U)] = [U_x - F(U_x)] - [Ux = F(U_x)]\). The speed of the discontinuity is then given by
\[
dx = \frac{x}{\tau + \tau[U]}.
\]

**APPENDIX F: NUMERICAL METHODS**

Each time step is started by a calculation of the new temperatures, the kerogen concentrations, and the new porosity. Since the new porosity is calculated after the temperatures, the temperature solution is based on the porosity from the previous time step. The porosity is a slowly changing parameter, if changing at all, so we do not expect any significant error from this. In addition, the time steps are usually small due to the Lax–Friedrich–Courant conditions applied to the saturation equation. The last variable calculated during the time step is the saturation.

The first order-Arrhenius kinetics are given by
\[
\left( \frac{\partial C}{\partial t} \right)_\ell = -KC,
\]
which is
\[
\frac{\partial C}{\partial \tau} \frac{x}{\tau} + \frac{C}{\tau x} = -\tau_0 KC,
\]
when expressed in the \(x\)-space. This equation is solved numerically by the following explicit scheme
\[
C^n_{i+1} = exp(-\tau_0 K \Delta \tau) C^n_i + \frac{\Delta \tau}{\Delta x} \left( C^n_{i+1} - C^n_i \right).
\]

The saturation equation is solved with the first-order term explicitly and the second-order term implicitly or explicitly depending on the capillary pressure gradient. The non-linearities in the implicit treatment of the second-order term are done by a two-step predictor–corrector scheme.

The first step yields a solution at \( \tau^n + \Delta \tau/2 \), which is then used to evaluate the non-linear coefficients for the entire step (see Meek & Norbury 1982).

The first-order saturation equation (33) is solved numerically by the explicit upstream or Lax–Friedrich schemes. The upstream scheme is implemented as follows
\[
U^n_{i+1} = U^n_i + \frac{\Delta \tau}{\Delta x} \left[ -\frac{x}{\tau_n} (U^n_{i+1} - U^n_i) + \frac{1}{\tau_n} \Delta F \right],
\]
where
\[
\frac{\partial F}{\partial U} > 0 \text{ then } \Delta F = F(U^n_{i+1}) - F(U^n_{i-1})
\]
else
\[
\Delta F = F(U^n_{i+1}) - F(U^n_i)
\]
end,
and the Lax–Friedrich scheme is implemented as
\[
U^n_{i+1} = \frac{1}{2} (U^n_{i+1} + U^n_{i-1}) + \frac{\Delta \tau}{2 \Delta x} \left[ -\frac{x}{\tau_n} (U^n_{i+1} - U^n_{i-1}) + \frac{1}{\tau_n} \Delta F(U^n_{i+1}) - F(U^n_{i-1}) \right].
\]

The subscript \(i\) denotes grid position \(i\), and the superscript \(n\) denotes the time step \(\tau_n\).

In order to have stable explicit schemes, the time step must obey the Courant–Friedrich–Lewy condition, which is implemented as
\[
\frac{\Delta \tau}{\Delta x} \frac{1}{1 + \max \left( \frac{[F(S)]}{e} \right)} < 1.
\]

**APPENDIX G: NOTATION**

\( A_0 \) Unit areal
\( A \) Arrhenius factor
\( c \) \( = \alpha (\rho_s - \rho_w) g \)
\( c_s \) Heat capacity sediment
\( c_w \) Heat capacity water
\( C \) Kerogen concentration
\( C_0 \) Initial kerogen concentration
\( D \) Depth
\( dF \) Either \( \partial F / \partial U \) or \([F]/[U]\)
\( e \) Void ratio
\( e_0 \) Void ratio at the basin top
\( e_{\text{max}} \) Maximal void ratio
\( E \) Activation energy
\( E_n \) The energy stored in the basin
\( E_0 \) Constant relating the energy stored in the basin to time \( t \)
\( f_0 \) Fractional flow function
\( F \) Flux function for oil
\( k(e) \) The permeability as function of void ratio
\( k(e) \) Dimensionless permeability as function of void ratio
\( k_0 \) The permeability at the basin top
\( k_{ol} \) Endpoint relative permeability for oil
\( k_{ro} \) Relative permeability for oil
\( k_{ow} \) Relative permeability for water
\( k_{rw} \) Endpoint relative permeability for water
\( g \) Constant of gravity
\( h \) The real height (or depth) of the basin
\( l_p \) Characteristic length \( \omega_l n \)
\( \Delta M \) Mass missing relative to mass generated
\( M_{\text{gen}} \) Mass of all generated oil
\( M_{\text{out}} \) Mass of all oil having left the basin
\( M_{\text{present}} \) Mass of all oil present in the basin
\( n_o \) Exponent in oil relative permeability function
\( n_w \) Exponent in water relative permeability function
Vertical migration of hydrocarbons

\[ p_c \] Capillary pressure
\[ p_0 \] Characteristic pressure
\[ \bar{p}_c \] Dimensionless capillary pressure
\[ \bar{p}_{cr} \] Relative capillary pressure
\[ p_o \] Oil pressure
\[ \rho_s \] Effective vertical stress
\[ \rho_w \] Water pressure
\[ Pe_S \] Peclet number for saturation equation
\[ Pe_T \] Peclet number for temperature equation
\[ q_h \] Heat flux into the basin bottom
\[ q_o \] Oil source term
\[ q_w \] Dimensionless oil source term
\[ R \] Interface curvature
\[ S \] Oil saturation
\[ S_o \] The saturation corresponding to the total oil production
\[ S_{11} \] Residual oil saturation
\[ S_{22} \] Irreducible water saturation
\[ t \] Time
\[ t_0 \] Characteristic time for the migration process
\[ t_{mb} \] Characteristic time for temperature moving boundary effects
\[ T \] Temperature
\[ u \] Dimensionless excess pressure
\[ u_o \] The volumetric flux of oil relative to matrix
\[ u_i \] Total volumetric flux of pore fluid
\[ u_w \] The volumetric flux of water relative to matrix
\[ U = e[1 + C/(1 - C_o)]S \]
\[ \bar{u} \] Dimensionless temperature
\[ V \] A test volume that follows the compaction
\[ x \] Sediment height on the unit interval
\[ z \] z-coordinate

Greek symbols
\[ \alpha \] Scaling factor in porosity (void ratio) functions
\[ \zeta * \] The height of the basin in \( \zeta \)-coordinate
\[ \lambda_o \] Oil mobility
\[ \lambda_w \] Water mobility
\[ \lambda_A \] An average bulk heat conductivity
\[ \lambda_B \] The bulk heat conductivity
\[ \lambda_O \] The oil heat conductivity
\[ \lambda_S \] The sediment matrix heat conductivity
\[ \lambda_W \] The water heat conductivity
\[ \lambda_0 \] Gravity number
\[ \mu_o \] Oil viscosity
\[ \mu_w \] Water viscosity
\[ \rho_b \] Bulk sediment density
\[ \rho_k \] Kerogen density
\[ \rho_o \] Oil density
\[ \rho_s \] Matrix sediment density
\[ \rho_w \] Water density
\[ \phi \] Porosity
\[ \phi_o \] Porosity at the basin top
\[ \phi_b \] Average bulk porosity
\[ \tau \] Dimensionless time
\[ \theta \] Contact angle
\[ \sigma \] Interface tension
\[ \omega \] The sedimentation rate

Subscripts
0 Reference point, usually at the top of the basin
b Bulk
i Grid point number
k Kerogen
o Oil
s Sediment
w Water

Superscripts
n Time step number