Numerical Modeling of Oceanic Crustal Hydrothermal Systems

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Abstract

The oceanic crust is a complex rock-mineral formation which extends up to several kilometers below the sea floor and covers laterally about two thirds of the planet. Hydrothermal circulation within the crust is driven by magmatic sources and carried by the fluid residing in pores and cracks. Hydrothermal advection transfers about one quarter of the Earth's total heat power from the interior.

Marine sediments are believed to be the largest repositories of solid ice-like methane clathrate hydrates. The compliance technique is an important tool for assessment of this resource. It makes use of the oceanic surface gravity waves to induce pressure variations on the sea floor and measure the corresponding vertical deformation.

This thesis deals with the convective heat and mass transfer within the oceanic crust, as a fractured porous medium, and the elastic, quasi-static response of hydrated marine sediments to gravity wave loading. Both generic and site-specific applications are considered. Most applications are tackled numerically in three spatial dimensions.

The major results are as follows. Fractures can trigger and maintain hydrothermal circulation. The permeability-thickness product in the direction of flow is an adequate parameter to represent the fracture if convection is not vigorous. A new temperature homogenization
mechanism for the off-axial convection is proposed which is due to quasi-lateral circulation within a permeable zone between sediment cover and basalt. It explains both the observed correlation between surface heat flux and sediment thickness, as well as regular heat flux variations when no buried topography is present. A hydrothermal model for the CoAxial Segment of the Juan de Fuca Ridge predicts ridge-parallel convection with the low-temperature vents spaced 1 km apart.

The compliance approach is feasible for a non-layered medium. The average compliance response depends on the bulk hydrate content, but not on a particular connectivity pattern. However, the lateral variation in compliance correlates with the size of a typical lateral inhomogeneity.
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Introduction

Chuang-Tzu

Easy is right. Begin right
And you are easy.
Continue easy and you are right.
The right way to go easy
Is to forget the right way
And forget that the going is easy

This thesis deals with topics pertinent to hydrothermal processes in the oceanic crust. Some of the problems addressed are purely mathematical, some generic and some are site-specific applications, stimulated by seismic and heat-flow measurements on the sea floor. The approach is to start with the basic physics of a process, such as the coupled heat and mass transfer in the fully saturated, anisotropic porous Earth structures and the elastic response of hydrated marine sediments to surface gravity waves, and seek solutions to the problems by mainly numerical means. Since the oceanic crust will be our host medium, we outline first the relevant features of this environment.

The oceanic crust

The oceanic crust is a complex rock-mineral formation, extending up to several kilometers below the sea floor. The oceanic floor is associated with a huge area on the globe, as two thirds of the Earth is covered by oceans. Tectonic plate boundaries are the natural divisors of the oceanic crust. New crust is produced at the mid-ocean ridges and spreads out to be consumed under the continents at subduction zones. The annual volume of new sea floor production is about 17 km$^3$/Y.

The spreading rates measure anywhere between 1 – 2 cm/Y for slow spreading centers (e.g. the Mid-Atlantic ridge) and 10 – 15 cm/Y for fast spreading centers (e.g. the East Pacific Rise). The average age of the oceanic crust is about 65 million years (MA). The
younger portions, aged less than 1 MA, are mainly sediment free, while those older than 65 MA are believed to be totally covered by marine sediments.

The newly created crust below the mid-oceanic ridge is heated by 1280°C magma. Thin melt lenses are documented at depth as shallow as ~1.5 km below the sea floor (kmbsf), while the root sits a few kilometers deeper [Sinton and Detrick, 1992]. Magma is injected into cold oceanic crust during dike events, for which the volume fluxes range from $10^2$ to $10^4$ m$^3$/s [Dellane, 1987]. According to Lister [1990], such a dike rises up to the level of neutral buoyancy [Lister, 1990], then propagates subhorizontally with the length-to-height aspect ratio in the range of $10^2$ to $10^4$. Assuming the density of sea floor basalt to be 3000 kg/m$^3$, Schultz and Elderfield [1997] estimate the total mass of newly emplaced magma to be $5.1 \times 10^{13}$ kg/yr.

As can already be inferred, the oceanic crust is often far from being a layered medium, yet its very basic, average geological stratification down from the sea floor features a sediment cover, a layer of volcanic extrusives, dike transitional zone, a sheeted dike complex and a layer of gabbro, which begins at about 2–3 kmbsf - as deep as we would look in this study - and extends to Moho depth at 5–7 kmbsf. In seismic terminology, these layers are numbered as 1, 2a, 2b, 2c and 3, respectively. Note that young oceanic crust often lacks its sediment cover, i.e. layer 1.

One of the most critical parameters of a crustal section from the hydrothermal perspective is its permeability to fluid. We recognize that Earth structures are essentially fractured, porous media. Rocks are naturally porous, but discrete fractures are pervasive in both oceanic crust and in geological sections on land [MacDonald, 1982, Morgan, 1991, Choukroune et al., 1984, Herzog et al., 1989, Pozard et al., 1992]. There are two major types of fractures: planar fractures and pipe-like conduits, often called pipes for simplicity, with typical apertures ranging from a fraction of a millimeter to a few centimeters. The permeability of the oceanic crust is greatly enhanced near the ridges by extensive crustal fissuring and cracking because of mechanical stresses, as the material expands, and cooling by the sea water, whose ambient temperature is close to 0°C. The length of the cracks may reach tens to hundreds of meters, while their orientation is mainly parallel to the ridge axis [Ballard and van Andel, 1977]. Pozard et al., [1992] observe a fine-scaled, of the order of ten meters, horizontally layered volcanic zone, containing both vertical and horizontal fractures. According to Cathles, [1993], some major fractures must extend to Moho depths. Individual fractures are, however, difficult to image, but it may be deduced from ophiolite studies that they should persist through the sheeted dikes [van Everdingen, 1995]. As a rule, the unfractured permeability diminishes with depth and virtually ceases to be significant at depths greater than ~1 kmbsf. On the other hand, as the crust gets older the pores get increasingly
sealed by mineral precipitation in the course of chemical reactions between the fluid and the host rock.

Relatively cold sea water saturates the available permeability through sediment-free sea floor. Upon mixing with dissolved minerals in the host rock it becomes the hydrothermal fluid, which can remain in the liquid state up to the temperatures of ~400°C and pressures of ~300 atm [Bishoff and Pitzer, 1989]. Hydrothermal convection is the mechanism responsible for circulation of hydrothermal fluid, which may persist under certain ambient conditions. A simplified description of this phenomenon is as follows. Portions of hydrothermal fluid heated at depth (e.g. by magmatic sources in close proximity or by ambient heat flux from the interior) would tend to go upwards, being driven by buoyancy force because of a density decrease. These ascending, warmer portions of fluid are replaced by the colder fluids from elsewhere. If the buoyancy force exceeds the counteracting viscous drag force, the medium becomes supercritical and can support convection. The ratio of the buoyancy force to the counteracting viscous drag force evaluated over a typical size of the convection cell is defined as the Rayleigh number [e.g. Turcotte and Schubert, 1982], which is often used for analyzing convection. Jupp and Schultz [2000] extend this approach to a local Rayleigh number which gives the balance at each point within the convection cell. This allows to speak of the precise position at which hydrothermal plumes form. Thus, slightly rephrasing Lowell, [1991], hydrothermal circulation involves interconnected processes of heat, mass and chemical transport, driven by magmatic heat sources and carried by fluid, residing in pores and cracks within the host rock.

We must state here that only a single-phase fluid will be considered in what follows. To model this problem, we solve equations governing conservation of mass, momentum and energy for the fluid. Although clearly a simplification, this is a commonly used approach [e.g. Travis et al, 1991; Fisher and Becker, 1995; Yang, 1996; Yang et al., 1996; Davis, 1997, Schultz and Elderfield, 1997]. A rigorous treatment of the multi-phase convection is outside the scope of this thesis, however, we shall outline briefly how one might approach this problem. One would require in addition equations governing conservation of salinity, composition and relative mass fractions of co-existing vapour and brine phases [Lowell, 1991]. The conservation of momentum and energy equations are written for each respective phase, assuming local thermal equilibrium between the vapour, brine and rock at a point. Generally, the energy conservation equation is formulated for the entropy [Landau and Lifshitz, 1959], but since the latter is a function of temperature and pressure, the resulting governing equations can be written in terms of temperature and pressure as well. The relevant physical properties, such as permeability, viscosity and thermal conductivity are usually assumed to be known functions of the thermodynamic variables and time.
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The actual pattern and scale of the flow depends on the permeability distribution within a specific crustal section of interest, its degree of fracturing and sedimentation, configuration and strength of underlying heat sources, the local sea floor topography and the hydrostatic pressure, including phase effects. Anticipating further development, we hasten to mention now that topography variations and fractures alone can drive steady hydrothermal convection even in a subcritical medium. Given such a variety of geological settings and thermal conditions affecting the circulation, the latter may roughly be classified as on-axial, within a few kilometers around the axis, off-axial, farther away from the axis, high temperature, in which the discharged fluid is heated to a temperature $T_f$ above 200°C, low-temperature with $T_f \leq 50 - 100°C$, deep, reaching depths greater than 1 - 2 kmbsf and shallow, confined mainly within layer $2a$, a few hundred of meters thick. The list is neither exact nor complete. In the absence of sediments, discharge sites on the sea floor are typically either low-temperature diffuse, cellular or high-temperature focused. Figure 1 from Haymon et al., [1991], is an example of inferred hydrothermal flow pattern based on observations with the near-bottom ARGO imaging system along the 200 m-wide axial zone of the East Pacific Rise (EPR) 9°00' - 54°N. The sketch covers a few kilometers along the axis and shows shallow
3D circulation in the permeable volcanic extrusives, 2D ridge-parallel circulation in the less permeable sheeted dikes and high-temperature venting above shallower segments of the axial magma reservoir.

High-temperature venting, discovered about 20 years ago, occurs via discrete pipe-like conduits, extending deep into the crust below the sea floor. An enormous heat power ranging from one megawatt to tens of megawatts is delivered by the so-called black smokers through just a few centimeter wide apertures at temperatures ~ 350°C and velocities of ~ 1 m/s. For example, the group of black smokers in the Southwest Vent Field, 21°N that occupy an area of only ~ 0.1 m² produce up to 300 MW of total hydrothermal power according to Converse et al., [1984]. They further predict that warm springs in that location may discharge a similar amount of heat from an area of ~ 500 m². Black smoker fluids are rich in sulfides which precipitate in the form of chimneys or produce larger sulfide deposits on the sea floor [e.g. Tivey and Delaney, 1986].

Schultz and Elderfield, [1997] point out that low-temperature diffuse hydrothermal circulation is a natural consequence of the cooling of the oceanic lithosphere. Diffuse flow is expected to be ubiquitous both within mid-oceanic ridge crest axial zones of young age (0 – 1 M.A), as well as on the older ridge crest flanks and limbs. Based on the existing global-scale, thermal models, these authors estimate that hydrothermal circulation persists for over half the total area of the ocean basins and that diffuse flow is an intrinsic feature of high-temperature vent fields, taking the dominant share of the total heat and mass flux budget. Although off-axial convection is believed to take place over a vast lateral area, it is hard to detect because most discharge sites have the temperature elevated just a few degrees above the ambient. Fluid flow that can be measured directly with confidence is probably of the order of $10^{-3} - 10^{-4}$ m/s, yet hydrothermal fluids circulating with velocities greater than $10^{-10}$ m/s are already considered geochemically significant and may account e.g. for buffering of Mg and other species in seawater [Mottl & Wheat, 1994]. A typical field example of a low-temperature system is the Galapagos Ridge, where circulation is expected to be normal to axis [Haymon et al., 1991], justified by the existence of continuous diffuse discharge areas along the axis. No high-temperature venting exists today, but there are documented occurrences of inactive chimneys which suggests such an activity must have taken place in the past. At present, we may infer that low-temperature hydrothermal circulation is controlled by the locations of the most recent dike swarms, feeding eruptions along the axial zone. Diffuse venting is probably dominated by sheet-like conduits. It is likely that the upward bending of isotherms above zones of recent shallow dike intrusions thermally drives fluids in the dike complex towards the sea floor [Hyndman et al., 1991]. According to Delaney [1987], the thickness of an individual dike may range between 1 and 10 m, but the variations in...
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thickness should not affect much the rate of heat loss to the host rock. Macdonald, [1995] reports the widest fissures found in the youngest lava fields on EPR 9–10°N to be 5 m wide. He estimates the eruption period of 50–100 Y for fast-spreading ridges and up to 10000 Y for slow-spreading ridges. Adopting a rather ad-hoc relationship that the eruption frequency is inversely proportional to the spreading rate squared [Macdonald, 1995], we estimate that 1000–2000 Y is a timescale for an intermediate spreading ridge such as the Galapagos.

Jeffery et al., [1986] sample a 1 km section through the upper oceanic crust at borehole 504B. The results are that pillows in layers 2A and 2B occupy the upper 600 mbsf. There is a transitional zone between 600 and 800 mbsf. The lower 200 m are occupied by dikes. The level 1350 mbsf marks the 165°C isotherm. An upper boundary value for the permeability of the extrusives is between $10^{-12}$ m² and $10^{-13}$ m², which then grades down to $10^{-16}$ m² towards the dike complex. In many places, heat flow highs tend to elongate parallel to the ridge crest such as near ODP Hole 504 (83°44' W, 1°13' N). The area is blanketed by thick sediments 200 km to the north of the ridge, but these heated patterns co-exist with islands of distinct thermal output. The heat flux varies from 166 mW/m² to 391 mW/m², averaging at 200 mW/m² [Mottl & Wheat, 1994]. In contrast, the Galapagos Mounds area features basal outcrops breaking through a thin sediment cover [Green et al., 1991]. As a result, there is a significant conductive deficit, while the bulk of thermal losses is due to advection from the volcanic crust directly to the overlying ocean. The flux peaks there at 1 W/m², 30 km off the axis.

The heat flux from the Earth's interior is transferred via the oceanic crust by mainly two mechanisms: conduction and advection. The first one is due to the temperature gradient between generally cold sea floor and the lower, heated portions of the oceanic lithosphere. The advective heat transport is caused by hydrothermal circulation. It is responsible for about one quarter of the total heat power released over the globe. Seventy percent of the advective heat flux through oceanic crust is discharged on flanks older than 1 MA [Sclater et al., 1980]. Heat conduction dominates only beyond 65 MA, while highly permeable zones persist up to 100 MA of age. So, in the presence of sediments, heat may still be redistributed within the upper crust advectively to be eventually released through the sea floor by conduction. Earlier thermal models in which the oceanic lithosphere was represented as a cooling plate would necessarily over-estimate the conductive component of heat flux close to the ridge crest [e.g. Parsons and Sclater, 1977], a portion of which is, in fact, carried by advection.
Impact of Hydrothermal Activity

Sea floor hydrothermal activity impacts the Earth system on the global scale, transferring about 25% of the Earth's total heat power from the interior by advection in the upper few kilometers of the lithosphere. The absolute value for the advected heat power is ∼ 11 TW [Stein and Stein, 1994]. Wohletz and Sleep, [1976] estimate that the mass of the oceans is circulated through the crust approximately every 10⁶ years. According to Schultz and Elderfield, [1997], the total water flux due to off-axis flow is 2.4 × 10¹⁸ kg/Y for lithospheric ages of 1–65 MA, while that due to the high temperature axial flow is 2.4 × 10¹⁹ kg/Y for lithospheric ages 0–1 MA, assuming that all off-axis flow takes place at temperature of 8°C and pressure of 250 bar and that all on-axial hydrothermal heat is removed by hydrothermal fluid at 350°C and 250 bar, respectively.

Chemical reactions between the oceanic crust and hydrothermal seawater involve a two-way exchange process that alters both the composition of the crust and the circulating seawater [Lowell et al., 1995]. Hydrothermal effluent acts as both source and sink of many chemical species. Many elements of the Periodic Table are either discharged directly to the ocean or precipitated in the crust. The input is so great, it may exceed that of all the rivers [Edmond et al., 1979]. Water-rock interaction leads, in particular, to the formation of massive sulfide deposits, typically encountered on the sea floor near high temperature vents. Some of formerly submarine mineral deposits, found presently in ophiolites on land, are being mined. Although definitely expensive and technically challenging today, the future mining may be forced to take place below the sea floor off-shore.

Hydrothermal plumes resulting from shallow magmatic diking events may drive mid-depth circulation in the deep ocean, which could play a role in the evolution of the global climate [Owen and Rea, 1985]. Hydrothermal venting on the sea floor is an ecosystem in which chemolithoautotrophs lay the foundation for the carbon cycle.

Methane Clathrate Hydrate

The high-pressure, low-temperature submarine environment is often suitable for the formation of methane hydrates of mainly biogenic origin. Methane hydrates are solid, ice-like mixtures of water and the gas methane. They were first found in permafrost beneath land and shallow sea Arctic regions. Favorable conditions for methane hydrate formation occur naturally a few hundred meters beneath the outer continental margins in the oceans, notably in subduction zones, which are now believed to have the largest occurrences of the resource. Methane is now recognized as a fuel resource and may replace gasoline in the future [S-
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Figure 2: Known and inferred worldwide locations of gas hydrates [Kvenvolden, 1999].

According to various estimates, the amount of "burnable" carbon in methane contained in marine sediments worldwide is in excess of that found on land.

Figure 2 from Kvenvolden, [1999] shows locations of known and inferred gas-hydrate deposits in oceanic sediment and in permafrost regions on land.

Examples of the well-studied submarine hydrate reservoirs include some of the continental slope off Japan, the Blake Ridge area off eastern US, and the northern and southern Cascadia region near Vancouver Island, while global estimates of available gas range from $10^{15}$ m$^3$ [McIver, 1981] to $10^{18}$ m$^3$ [Dobrynin, 1981]. One volume of marine hydrate can yield about 164 volumes of gas, measured at standard conditions [Hyndman, 1995]. So methane hydrates are now recognized as a significant energy resource for the next century, as it may be possible to recover gas from the solid mixture [Sloan, 1990]. On the other hand, it can be a source of hazard, because hydrates may form in water-based drilling fluids in wells, as they do in oil and gas pipelines on land. Another concern is due to the fact that methane is a very strong greenhouse gas, and release of methane to the atmosphere from dissociation of hydrate may contribute to global warming. Unsurprisingly then, methane-hydrate-related studies have taken important positions in geoscience over the last two decades.

Most of deep sea hydrates are generated as a result of hydrothermal activity in which biogenic methane from decaying organic matter percolates upwards, where it is removed from up-welling methane rich fluids, and solidifies with water molecule lattice cages [Hyndman and Davis, 1992]. The resulting white solid clathrate typically contains one methane molecule.
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Figure 3: Fluid expulsion model for gas hydrate formation [Hyndman and Davis, 1992]. Methane is removed from rising pore fluids to form hydrate as the pore fluids move into the hydrate stability field.

per polyhedral cage of hydrogen bounded water molecule. A conceptual diagram illustrating this fluid expulsion mechanism of gas hydrate formation is shown in Fig. 3 [Hyndman and Davis, 1992].

According to [Sloan, 1990], hydrates will likely form at the two-phase (gas-liquid) interface when the residual methane concentration reaches about 10 ml/l of wet sediment. The upward gas motion may be sealed by relatively impermeable sediments or by the methane formation itself. These seals can act to provide traps for free gas from which hydrates may be produced at a later time, building up around an initial hydrate formation as a nucleation site.

The majority of marine seismic sections of hydrate bearing areas feature a bottom simulating reflector (BSR), a seismic reflector with a negative impedance contrast that parallels the sea floor. The BSRS have long been believed to mark the base of hydrate bearing zone, see for example [Stoll and Bryan, 1979] and [Dvorkin and Nur, 1993], however, some controversy does exist among different authors. If the impedance contrast is produced by the seismic velocity contrast between hydrate-bearing sediments above and hydrate-free sediments below, Xu and Ruppel [1998] confirm through modeling that the BSR should indeed lie at the base of the hydrate formation and wholly within the hydrate stability zone. Alternative observations argue that the BSR lies at the top of the free gas zone [Holbrook et al., 1996] in which case the BSR should sometimes occur below the stability zone. According to Finley and Krason, [1986], there are known sites in the Middle America Trench where
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hydrates were recovered, but no BSR was present at all.

Although the presence of BSR is often a sure signature of hydrates, one cannot answer accurately the main prospector's question - how much hydrate is there - based on seismic data alone, because the hydrate bearing zone above the BSR appears to be diffuse on seismograms. Edwards [1997] suggested the use of a time-domain, dipole-dipole electromagnetic system to assess the hydrate content via electrical resistivity of gas hydrate sections. Recent resistivity measurements of Yuan and Edwards [2000] estimate the hydrate content of about 17 - 26% of pore space in the 100 m region above the BSR on the Cascadia margin and predict the hydrate presence in an area to the east of ODP 889B where there is no visible BSR.

Sea Floor Compliance

Sea floor compliance stands out as an independent technique for estimating hydrate concentration. It produces an invertible set of data in terms of the elastic properties of the medium. The elastic moduli, particularly the shear modulus, are increased by the hydrate cementation. To detect these shear property variations, we need a shear source. A conventional seismic vibrator would be problematic to use on soft, mushy sediments, where porosities near the sea floor can reach up to 70% [Webb and Edwards, 1995]. Fortunately, there exists a natural source that can be employed.

Ocean surface gravity waves induce time-varying pressure fields and cause a correlated measurable displacement in the sediment of the order of a few microns at the sea floor level. Differential acceleration and pressure are recorded by a gravimeter and a precision differential pressure gauge, both located at the sea floor. Given the known dispersion relationship for the gravity waves, compliance is calculated as the transfer function between the sea floor displacement and induced pressure. In essence, one probes the stiffness of the sediment that must have been altered by the presence and distribution of methane hydrates using a natural shear source to shake the sea floor laterally. The response is tuned to a specific depth when an appropriate frequency is selected by Fourier-transforming the raw data. This approach resembles magnetotellurics, where natural electromagnetic fields are employed to image structures with depth. Typically, gravity waves can be used to sense structures to several hundreds of meters below the sea floor, with a characteristic wavelength involved being just the depth of the ocean. In this situation, the most useful, measurable frequency spectrum of gravity waves is 0.001 - 0.1 Hz.

The first experimental implementation of this technique is due to Yamamoto and Torii [1986]. They used laterally homogeneous, layered sea floor models to fit compliance measured in shallow water. Crawford et al., [1991] adapted the method for imaging mid-crustal,
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low-velocity zones (LVZ) in the regions of partial melt in good agreement with seismic data. In contrast to the effect of methane hydrates, melts generally decrease the stiffness of the surrounding medium. Later, Crawford et al., [1998] developed a 2-D numerical code to investigate the effect of laterally varying structure in two-dimensional crustal models on the compliance function. The major result of the study was that compliance is significantly modified by lateral variations in crustal elastic properties, while retaining the basic characteristics pertinent to layered models. Willoughby and Edwards [1997] demonstrated that for a simple layered structure, variations in compliance are related to changes in the methane hydrate concentration. Given a compliance measurement accurate to 5%, the total mass of hydrate can be estimated to an accuracy of better than 3% for a typical exploration scenario with the available seismic data. Willoughby et al., [1998] collected a couple of repeatable sets of compliance data at three locations near ODP sites 889/890 in 1998. Later, Willoughby and Edwards, [2000] have measured compliance at eight sites in the Cascadia near ODP 889B and shown that the addition of the known gas hydrate deposit in the upper 200 m to a normal logarithmic velocity model improves the fit to the data in the Kolmogorov-Smirnov sense. Willoughby [personal communication] have pointed out that their method can only resolve the product of the seismic shear velocity and the layer thickness rather than either parameter separately.

Research Objectives

Hydrothermal systems are complicated natural laboratories, but, unfortunately, with no easy access to them. So it is important to back up actual experiments on the sea floor by mathematical modeling. Most phenomena of interest are described by the differential equations which are as hostile towards rigorous analytical development by the theoretician as the submarine environment is to the experimentalist. We tackle their solutions by numerical means. Yet, even with the impressive capacities of modern computers, it is not always possible to incorporate all the desired constraints into a model. Thus, one has to focus on a few essential aspects of a problem.

We consider three applied geophysical problems in three dimensions. None of them, to the best of the author's knowledge, has been addressed before in 3D.

We offer a new explanation for the temperature homogenization mechanism at the base of the sediment cover in the off-axial regions of hydrothermal circulation. It is proposed here that the quasi-horizontal mode of circulation, injected by buried topography, may be responsible for making temperature uniform in the permeable stratum of the rock-sediment interface, so that the heat flux at the sea floor correlates well with the inverse sediment
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thickness, while the basal permeability doesn't exceed reasonable values - in accord with field measurements [e.g. Davis et al., 1992].

Based on a 3D anisotropic permeability structure, inferred from the porosity gradients after a seismic tomographic inversion of P-wave reflection data at the CoAxial Segment of the Juan de Fuca Ridge [Sohn et al., 1997], we built a hydrothermal model and predict the ridge-parallel pattern of circulation in the young (< 0.1 MY) oceanic crust with 1 km vent field spacing along the axis. Besides, we consider the partition of heat and mass fluxes between shallow and deep flow, as well as between high and low-temperature modes.

Modeling the sea floor compliance response of hydrated marine sediments, we again drop the traditional notion of layered medium. Guided by a synthetic model of hydrate concentration profile with depth for the Cascadia region [Willoughby and Edwards, 1997] and the BSR seismic reflection data near ODP 808 [Spence et al., 1996], which suggest lateral variability of the hydrate deposit, we construct a range of generic forward models and examine what happens if the deposit has a finite size and different connectivity pattern. It is shown that the compliance technique in such a situation is still a viable tool for assessing the average bulk content of the resource, regardless of its spatial distribution.

Thesis Structure

It has to be underscored that most of the results of this work follow from numerical experimentation and we must make serious efforts to develop the right software and validate it. We usually begin with the governing equations, formulate the problems mathematically and discuss suitable approximations and limitations of the models. Where possible - but mostly in 2D - analytical solutions are obtained which elucidate the physics and then subsequently used for software validation. Next, we describe numerical algorithms and test them either against the output of the existing software, or against the analytical solutions, if they exist. Then, we follow up with the simplified generic case studies to develop a better understanding of the processes in consideration. Finally, we attempt our major applications. Generic models are typically set up such that the model parameters are within the observable range.

The thesis implicitly contains two parts, each written in the style outlined above. Chapters 1 through 5 deal with the hydrothermal modeling, while the remaining three, 6 through 8, are on the compliance modeling. Let us now take a brief tour over their content.

In Chapter 1, we review the governing equations of energy and momentum conservation in the temperature-streamfunction formalism, required to set up a hydrothermal model and discuss the dependence of viscosity, density, heat capacity and thermal conductivity of sea water on temperature. Two problems are treated analytically in the Rayleigh number
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approximation: the onset of convection in a 2D system with anisotropic permeability and permeable upper boundary and convection around a point source of heat within a porous layer with impermeable lateral boundaries. The first one places constraints on the aspect-ratio of the convection roll at the onset of convection in a system with no sediment cover. We will often use these results as a starting point in setting the model's dimensions, including 3D models, because a 2D roll is often a reasonable initial solution in 3D to start with. The results of the second problem provide some useful conceptual insights on the pattern of flow around concentrated heat sources, such as submarine volcanos or small magmatic intrusions. And, of course, both are used for code testing. We have mentioned that we will be mostly dealing with steady-state applications.

We consider in Chapter 1 one time-dependent problem of propagation of the thermal transient through a typical crustal section, powered by a magmatic intrusion. The reason for it being here is again two-fold: to get an estimate for the time constant of the process and to cross-check the late-time-limit results with the direct steady-state solution.

For modeling in this chapter we use a reputable finite difference package MUDPACK [Adams, 1989] for elliptic differential equations.

In Chapter 2 we recognize that our medium is fractured. Historically, the development here is due to a search for an alternative, steady-state solver, suitable for a medium with a single vertical fracture. Yang, [1996] modified a finite element (FE) code HEATFLOW to make it capable of time-dependent modeling of heat, mass and contaminant transport in a fractured, porous medium and used it for hydrothermal simulation. Most of the results obtained by Yang were in the 2D domain, mainly because of the memory limitations. Also, time-stepping algorithms are heavy on CPU time even for simple problems, while the steady state solution is often all that is desired. Having an economical alternative seemed beneficial in at least two ways: to cross-check the results with the FE code, based on entirely different principles, and to try it out on a variety of single-fractured setting. The basic idea of the algorithm [Dickson et al., 1995; Schultz and Elderfield, 1997] and independently [Latychev and Edwards, 1997] and [Yang et al., 1998] is to iterate the solutions between the fracture and the host unfractured medium until they agree on the interface as required by the conservation laws. In this form, it should work with any pre-programmed algorithm for the unfractured medium; we keep on using MUDPACK. The output of our code compares within a couple of percent with the FE code for the temperature and fluid velocity along the fracture on a benchmark model. In the applications considered in Chapter 2, we vary both depth and extent of the fracture for a typical generic setting with the conditions as near ODP 504. A detailed description of this algorithm can be found in [Yang et al., 1998]. Technically, it could have been also used for a ridge-axis environment where a 2D, ridge-normal circulation
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takes place, but we leave this for a better 3D algorithm to be set up in Chapter 3, where the results for the single-fractured medium will be extended to three dimensions.

In Chapter 3, we develop and test a full 3D solver, capable of handling a multiple-fractured medium with the option to combine high and low resolution within the same model. This double-resolution option was implemented as a natural extension of the 2D, single-fractured algorithm. Now we let a whole subdomain of interest, in which a higher spatial resolution is desired, exchange heat and mass with the rest of the domain in the same way the single fracture did in the 2D algorithm. This feature will be invaluable in Chapter 5 where we model a black-smoker-type system which requires a very fine resolution in the vicinity of the discharge site. The results of our single-fractured modeling in Chapter 2 also suggested a more practical way of mapping fractures, based on the equivalent permeability-thickness product in the direction of flow. We make use of the 2D algorithm here once more to cross-check the results. The point-source model results of Chapter 1 are employed in this chapter as well for validation purposes. At this point we have to desert MUDPACK as the main iterative solver and develop a replacement based on conservative, control volume principles and suitable for modeling of the advection-dominated heat transport. The major 3D applications of hydrothermal modeling are considered in the next two chapters of the thesis.

In Chapter 4, we start with a few basic 3D models, both fractured and unfractured and with the upper boundary (sea floor) permeable or impermeable. We consider two modes of circulation: 2D roll and axisymmetric. Then we construct a model to reproduce small scale sea floor heat flow variations, observed over flat sea floor with no buried sediment topography on the sediment-sealed Eastern flank of the Juan de Fuca Ridge (JdFR). Finally, we propose and demonstrate a mechanism of temperature homogenization at the sediment base of variable thickness to explain the observed correlation between surface heat flux and buried topography.

The modeling in Chapter 5 is based on a crustal permeability structure inferred from 3D seismic tomography studies of Sohn et al., 1997 on the southern portion of the CoAxial Segment of the JdFR. Based on these results, we construct a simple hydrothermal model and simulate temperature field and fluid flow on the scale of 2 km and predict heat and mass budget for the system aged less than 0.1 million years. We also introduce into the model a few features commonly encountered near the ridge axis, such as faults or a pipe-like conduit, to quantify their impact on the flow pattern and heat and mass distribution.

The rest of the thesis deals with forward simulation of the elastic response of hydrated marine sediments, generated by the sea floor palpitations, which are induced by sea surface gravity waves. In Chapter 6, we review the necessary fundamentals (including relevant
elastc properties of marine sediments) behind the compliance technique which measures simultaneously the induced pressure and sea floor deformations. Compliance is the ratio of the two. It assesses the degree of rigidity of the structure beneath the sea floor. Methane hydrates increase the rigidity, thus can be identified. We derive analytically a correction to the standard dispersion relationship for gravity waves that takes into account sea floor deformation.

In Chapter 7, we develop and validate a 3D solver that would suite our needs for the forward compliance modeling, leaving applications to Chapter 8.

The main question addressed in Chapter 8 is: “What happens if a hydrate bearing region is not a simple layered medium?” Many colleagues have expressed their concerns that should a layer-like hydrate deposit lose its integrity, the compliance response of the structure would level with the background value. We consider a number of models in which the deposit’s connectivity and amount of hydrates vary from the simplest hydrated lamella to a random distribution of hydrate-bearing blocks.
Chapter 1

Modeling of Slow Convection in 2D

1.1 Introduction

We are concerned in this chapter with the fundamentals of convection in a porous medium. We shall describe the physics, explain how numerical models are set up, how results are interpreted and how software is tested.

We start off by reviewing the governing equations for convective, coupled mass and heat transfer based on Darcy’s law and momentum and energy conservation equations, respectively, and discuss the constitutive equations of state, relevant to submarine environments. The equations are non-linear and, generally, can only be solved numerically, but when circulation is not vigorous (i.e. velocities are low) an analytical or semi-analytical treatment is often possible in the Rayleigh number ($Ra$) formalism [Turcotte and Schubert, 1982; Kakac and Yen, 1995]. Jupp and Schultz, [2000] adopt the local Rayleigh number approach. Each such an analytical development provides a useful insight into the physics involved and is frequently extendable beyond its strict limitations as an order of magnitude solution to the equations.

The numerical approach is outlined for both the time-dependent and steady-state cases, which are limited here to the two dimensional, unfractured medium and slow convection, where the conductive and advective components of heat transfer are about the same order of magnitude. This allows existing software to be used without reinventing the wheel to examine a number of interesting problems.

The first one is the onset of convection in an anisotropic porous box with the permeable upper boundary. Similar studies have been consistently undertaken for the last half of the century to the present days. Lapwood, [1948] derives the critical $Ra$-number for the onset of convection in a layer with the isothermal and impermeable boundaries. Nield,
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[1968] summarizes the results for a greater variety of boundary conditions. However, several potentially interesting entries appeared to be missing. Beck, [1972] and Zebib and Kasoy, [1976] study the effects of lateral boundaries. Wooding, [1978] and Lowell, [1972] treat anisotropic permeability in a layer. Yang, [1986] considers an anisotropic box with the impermeable and isothermal walls and also proposes a modified definition of Ra-number. Kinura et al., [1995] deal among other issues with the anisotropic porous layer heated from below by a constant heat flux. The anisotropic medium with the permeable upper boundary, directly relevant to a young, unconfirmed oceanic crust, has not received the appropriate attention in literature. We fill this gap in Section 1.6, given the importance of the aspect-ratio of the convection cells to our modeling. A transcendental equation is derived that relates the critical parameters of the cells and the so-called anisotropic coefficient, which is the ratio of the vertical to horizontal permeability. It also provides a simple tool to assess the critical conditions in the setting of interest.

Convection induced by a point heat source, suddenly embedded in a porous medium, is a fundamental problem even with the understanding that the superposition principle can not be used due to non-linearity of the governing equations. Practical applications immediately arise, as volcanic eruptions and magmatic intrusions can be modeled often as concentrated sources of heat. It is also of interest in chemical and mechanical engineering applications [e.g. Minkowycz and Cheng, 1976; Bejan, 1978; Ganapauthy, 1994] where this problem was addressed first. The standard approach here is a power series expansion in Ra. As a starting point, we adopt the first-order Ra-number solution [Bejan, 1978] for fluid flow around a point source of heat in an infinite porous medium and extend it to a layer. The first-order, steady temperature field is then obtained with the Green's function method. We evaluate the time required to reach steady state after the source is "switched on" and the stationary heat flux distribution at the upper boundary. The temperature field itself will be employed mainly for software testing; in this chapter and later, in Chapter 4, where we develop a full 3D solver.

Finally, a conceptual model is set up to estimate typical times for the thermal transient due to a magmatic intrusion to reach the sea floor. Such a time may be generally expected to be a function of the heat content, duration, and depth of the magmatic event, as well as the permeability of the crust as a carrier. Our model will be based on the geological constraints as of near ODP Hole 504B, although we do not intend to target any specific geographical location. We would be rather interested in averaged estimates, as many of the constraints are only good within an order of magnitude.
1.2 Governing Equations

To describe a macroscopic, single-phased flow in a porous medium, we use Darcy's law [Bear, 1972] which relates Darcy's flux, \( \bar{v} \), to the pressure gradient in excess of hydrostatic

\[
\bar{v} = -\frac{K}{\mu} (\nabla p - \rho g).
\]

where \( p \) is the pressure field, \( \rho_f \) and \( \mu \) are the density and dynamic viscosity of the fluid, respectively, \( K \) is the host rock permeability tensor, and \( g \) is the acceleration due to gravity. It is Darcy's flux that should be used in the averaged transport equations, if we want to ignore particular details of the pore geometry and distribution but rather to deal with larger scale changes in permeability. Darcy's flux is related to the actual velocity \( \bar{v} \), where \( \theta \) is the host rock porosity. The permeability is assumed to be heterogeneous and anisotropic along the principal axes. With the vertical \( z \)-axis pointing upwards, we have \( K = (k_x, k_y, k_z) \) and \( \bar{g} = (0, 0, -g) \).

Fluid flow must conserve mass in the absence of internal sources or sinks. Following Yang, [1996] and Schultz and Elderfield, [1997], we neglect the inertial term, \( \partial\rho_f/\partial\bar{v} \), assume that the fluid is incompressible, \( \partial\rho_f/\partial\bar{v} = 0 \), and obtain

\[
\nabla \cdot (\rho_f \bar{v}) = 0. \quad (1.2)
\]

Let us now restrict the discussion to two dimensions \( x \) and \( z \), set all the \( y \)-components to zero and introduce a stream function, \( \psi \), defined as

\[
v_x = \frac{1}{\rho_f} \frac{\partial \psi}{\partial z}, \quad v_z = \frac{1}{\rho_f} \frac{\partial \psi}{\partial x},
\]

so that condition (1.2) holds identically. When \( \nabla \rho_f \) is small, \( \bar{v} \nabla \psi = 0 \) which means that contours \( \psi = \text{const} \) are parallel to the stream lines of flow, thus the name. From Darcy's law (1.1), we have

\[
\frac{\mu v_x}{k_x} = -\frac{\partial p}{\partial z} - \frac{\mu v_z}{k_z}, \quad -\frac{\mu v_z}{k_z} = \rho g = \frac{\partial \psi}{\partial z}. \quad (1.4)
\]

Differentiating the first expression above w.r.t. \( z \) and the second one w.r.t. \( x \) and adding, one obtains the fluid flow equation

\[
\frac{\partial}{\partial z} \left( \frac{\mu}{k_x \rho_f} \frac{\partial \psi}{\partial x} \right) + \frac{\partial}{\partial x} \left( \frac{\mu}{k_z \rho_f} \frac{\partial \psi}{\partial z} \right) = -\frac{\partial}{\partial x} (\rho_f g). \quad (1.5)
\]

In setting up the heat transport equation, the assumptions are that both the rock and
Figure 1.1: Fractional density, $\rho_f/\rho_0$, and viscosity, $\mu/\mu_0$, of water as functions of temperature.

The fluid conduct the heat, while only the fluid advects it, and that both are in thermal equilibrium at a specified location

$$\rho_m \frac{\partial T}{\partial t} + \rho_f c_f (\nabla T) - \nabla (\lambda_m \nabla T) = G, \tag{1.6}$$

where $T$ is the temperature, $\rho_m$, $c_m$, and $\lambda_m$ are the density, heat capacity, and thermal conductivity of the medium, respectively, $c_f$ is the heat capacity of the fluid, and $G$ is the volumetric density of heat power due to inner sources. Note that there is no hard limit on the nature of such sources. For example, one can include in $G$ the radioactive heat generation or the latent heat of crystallization. Subscript $m$ stands for medium, so a property $\eta_m = \{c_m, \lambda_m, \rho_m\}$ is calculated as the volumetric average between the corresponding fluid, $\eta_f$, and rock, $\eta_r$, properties as $\eta_m = \eta_f (1 - \theta) + \eta_r \theta$.

Equations (1.5) and (1.6) are the governing equations. To solve them, we must provide the constitutive equations of state. It turns out that the most critical of those are the relationships $\mu(T)$ and $\rho_f(T)$. These functions were communicated to the author by J. Yang and, independently, A. Cherkaoui, but otherwise are found in standard steam tables [e.g. Grigul, 1984]. Both are shown in Fig. (1.1) for pure water as $\mu(T)/\mu_0(T_0)$ and $\rho_f(T)/\rho_0(T_0)$, where $\mu_0 = 1.785 \cdot 10^{-3}$ kg/m/s$^2$ and $\rho_0 = 1000$ kg/m$^3$ are the viscosity and density at $T_0 = 0^\circ C$. In contrast, the thermal conductivity of water is not a strong function of temperature for $T < 300^\circ C$ and pressures about 200 bar and can be approximated as in [Weast, 1981]

$$\lambda_f = 0.5, \quad T < 50^\circ C$$
The specific heat of water varies by only about 4% within the same range, however, we must mention that at the water-vapour boundary, the variability in $c_w$ may be much more noticeable, as $c_{w,vap} \approx 0.5c_f$.

Although the hydrothermal fluid is not pure water, some studies have indicated the average ratios for both the viscosity and density between aqueous solutions of NaCl and pure water are about 0.93 [Yusufova et al., 1978].

1.3 Dimensionless Form

To elucidate the physics, it will be helpful to write the governing equations for $\psi$ and $T$ in terms of non-dimensional variables. Assuming in addition $\lambda_m$ and $c_m$ are constant and no sources of heat present, introduce

$$x = x*H, \quad z = z*H, \quad \psi = \psi \frac{\lambda_m}{c_f}, \quad T = T* \Delta T, \quad t = t \left( \frac{\rho_c H^2}{\lambda_m} \right),$$

where the starred quantities signify non-dimensional values, and $H$ and $\Delta T$ are a typical spatial dimension and a temperature contrast within the model, respectively. Substituting expressions (1.8) into (1.5) and (1.6), we obtain

$$\frac{\partial}{\partial x^*} \left[ \frac{\mu \lambda_m}{k_B c_f H} \frac{\partial \psi^*}{\partial x^*} \right] + \frac{\partial}{\partial z^*} \left[ \frac{\mu \lambda_m}{k_B c_f H} \frac{\partial \psi^*}{\partial z^*} \right] = -g \frac{\partial \theta_f}{\partial z^*}$$

(1.9)

$$\frac{1}{\zeta} \frac{\partial \theta^*}{\partial x^*} + v_2^* \frac{\partial \theta^*}{\partial z^*} + v_z^* \frac{\partial \theta^*}{\partial z^*} - \frac{\partial^2 \theta^*}{\partial z^* \partial z^*} - \frac{\partial T^*}{\partial z^*} = 0,$$

(1.10)

where $\zeta = \zeta(T) = \left( \rho c_f \right) / \left( \rho_w c_w \right)$, $v_2^* = -\left( \partial \phi^* \partial \theta^* \right)$, and $v_z^* = \left( \partial \psi^* \partial \theta^* \right)$. One observes that the flow is driven by the buoyancy term, $-g \left( \partial \theta_f / \partial x \right)$, which is zero in a perfectly stratified medium, but some small perturbations always exist to initiate convection under certain conditions. Generally, no full analytical solution to the system above is possible, so one has to resort to numerical processes.
1.4 Boundary Conditions

For the fluid flow, a boundary may usually be either permeable or impermeable. Along an impermeable boundary in a porous medium, the tangential component of the velocity does not need to be zero, but there is certainly no normal flow. So we assign a constant value to the stream function, which may be conveniently set to zero, $\psi = 0$. The sea floor is often unscouted and permeable, in which case it is approximated as a constant pressure boundary. Since there would be no tangential component in the fluid velocity, we take $\nabla_n \psi = 0$ at the sea floor, where $\nabla_n$ signifies the normal component of the vector gradient.

The temperature conditions may be Dirichlet, a specified heat flux (Neumann), or mixed (Robin). As a rule, the lateral boundaries mark a separation line between adjacent convection cells developed, and thus are adiabatic, $\nabla_x T = 0$. The presence of a permeable sea floor boundary allows to model discharge sites at an elevated temperature, $T_{sf}$, above the ambient, $T_a$, which is typically around $0^\circ C$. The case when $T_{sf}$ is determined in the course of the solution will be referred to as a free-flux boundary condition. If convection is not vigorous, the sea floor is horizontally stratified and there are no oceanic currents above the sea floor, we assume following Yang, [1996] and Molson et al., [1992], that the total convective heat flux carried through the sea floor is proportional to the temperature difference $T_{sf} - T_a$.

$$\lambda_m \frac{\partial T}{\partial z}_{sf} + \rho_f c_f n_z (T_{sf} - T_a) = -w (T_a - T_{sf}),$$

where $w$ is a heat transfer coefficient, typically around 1 W/(m²K). In the high velocity limit, Schultz and Elderfield, [1997] assume $\partial T/\partial z \big|_{sf} \rightarrow 0$ for a zone of hydrothermal discharge and $T = 0$ where cool seawater advects into the top of a permeable region, thus alternating between Dirichlet and Neumann conditions depending on the local behaviour of the solutions. We will describe a similar approach in Chapter 4, allowing in addition for lateral conductive heat losses, as required by the conservative differencing.

1.5 Boussinesq Approximation

One of the rare cases where an analytical answer can be sometimes obtained is the well-known Boussinesq approximation. The basic idea is to allow variations in $\rho_f$ with temperature in the buoyancy term only. As a rule, $\mu$ is set constant. It works when convection is not vigorous and the temperature range is limited to $\sim 30^\circ C$, so that the assumptions above are
reasonable. It is then taken frequently that

\[ \rho_f(T) = \rho_0 (1 - \alpha_f(T - T_0)) \]

(1.12)

with \( \lambda_m, \alpha_f, k_z, \) and \( k_z \) constant, so then the flow equation (1.9) becomes

\[ \frac{\partial \psi^*}{\partial x^2} + \frac{\gamma}{\partial x^2} = Ra \frac{\partial T^*}{\partial z^2} \]

(1.13)

where \( \gamma = k_z/k_x \) is the anisotropic coefficient and \( Ra \) is the Rayleigh number, which is the ratio between the buoyancy force that promotes convection and the viscous drag force that impedes the process

\[ Ra = \frac{k_z \rho_0 \alpha_{f1} \gamma T H}{\mu \lambda_m} \]

(1.14)

This definition is suitable for a cellular convection in a layer of thickness \( H \), with \( \Delta T \) being the temperature difference between the lower and upper boundaries. If the upper boundary, the sea floor, is not isothermal, we can take the ambient temperature \( T_a \) instead. It has been long known [Lapwood, 1948] that for convection to occur within a porous isotropic layer with isothermal and impermeable boundaries, the Rayleigh number must exceed \( 4 \pi^2 \) for a cell aspect ratio of 1. Note that the notion of a local Rayleigh number [Jupp and Schultz, 2000] is more appropriate when considering high-temperature plumes, where convection is generated by a non-uniformly heated lower boundary and where \( \rho_0 = \text{const} \) is clearly invalid an assumption. However, we treat cellular convection here, occasionally resorting to the Boussinesq approximation only to obtain some analytical results.

### 1.6 Onset of Convection in a Permeable Anisotropic Box

What is the critical Rayleigh number and aspect ratio for the onset of convection in a 2D anisotropic box whose upper boundary is permeable? This case is relevant to a young, unseminated oceanic crust that is likely to be anisotropic with \( \gamma > 1 \). For the isotropic case, using formula (1.14) and setting \( k_x = k_z = 10^{-15} \text{ m}^2 \), \( \rho_0 = 10^3 \text{ kg/m}^3 \), \( \alpha = 0.8 \cdot 10^{-4} \text{ K}^{-1} \), \( c_f = 4200 \text{ J/(kg \cdot K)} \), \( \Delta T = 60^\circ \text{C} \), \( H = 500 \text{ m} \) \( \mu = 1.78 \cdot 10^{-3} \text{ kg/(m \cdot s)} \) and \( \lambda_m = 2 \text{ W/(m \cdot K)} \) we obtain \( Ra = 27.7 \). A 2D convection roll is often believed to be the predominant off-axial pattern [Haymon et al., 1991] with the discharge temperatures just a few degrees above the ambient [Lowell et al., 1993], so we may use the Rayleigh number formalism.

Consider a box with the height \( H \) and width \( 2a \), shown in Fig. (1.2) and define \( s = a/H \). The rest of the non-dimensional variables is given in expressions (1.8). Before convection...
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Figure 1.2: Onset of convection in a porous, anisotropic box with the permeable upper boundary.

develops, both horizontal boundaries are isothermal, $\Delta T^* = 1$, the fluid is motionless, $\psi_0^* = 0$, and a linear temperature profile, $T_0^*(z^*) = 1 - z^*$, persists. The lateral walls remain adiabatic at all times. The equations to solve are (1.13) and (1.10).

Consider a first-order perturbation to the steady state, $(T_0^*, \psi_0^*)$, as $T^* = T_0^* + T_1^*$, and $\psi^* = \psi_0^* + \psi_1^*$. The equations on $(T_1^*, \psi_1^*)$ then become

$$
\frac{\partial^2 \psi_1^*}{\partial z^*^2} + \gamma \frac{\partial \psi_1^*}{\partial z^*} = \text{Re} \frac{\partial T_1^*}{\partial z^*},
$$

$$
\frac{\partial^2 T_1^*}{\partial z^*^2} + \frac{\partial^2 T_1^*}{\partial x^*^2} = -\frac{\partial \psi_1^*}{\partial z^*},
$$

and since this is a perturbation, the relevant boundary conditions are all homogeneous

$$
\psi_1^*|_{z^*-s} = 0, \quad \psi_1^*|_{z^*+s} = 0, \quad \frac{\partial \psi_1^*}{\partial z^*}|_{z^*-s} = 0, \quad \frac{\partial T_1^*}{\partial z^*}|_{z^*+s} = 0, \quad T_1^*|_{z^*=0} = 0.
$$

The resulting Sturm-Liouville boundary problem (1.15) - (1.17) admits the solution as a series expansion

$$
\psi_1^* = \varphi(z^*) \sin \left[ \frac{mn}{2} + x^* \Omega \right],
$$

$$
T_1^* = \Theta(z^*) \cos \left[ \frac{mn}{2} + x^* \Omega \right],
$$

where $m = \{1, 2, 3, \ldots\}$ is the number of convection cells that fit within the width $[-s, s]$
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and \( \Omega = (\pi \eta)/(2s) \). Note that \( n/(2s) = \Omega/\pi \) is the height-to-width ratio for a single cell. We will define the inverse quantity as the aspect-ratio and denote it \( O \). Substituting expressions (1.18) and (1.19) into equations (1.15) and (1.16), we get

\[
\gamma \varphi'' - \Omega^2 \varphi = -Ra\Omega \Theta, \tag{1.20}
\]

\[
\Theta'' - \Omega^2 \Theta = -\Omega \varphi, \tag{1.21}
\]

from which we can obtain a single equation on \( \varphi \)

\[
\varphi''' - \Omega^2 \left(1 + \frac{1}{\gamma}\right) \varphi'' + \frac{\Omega^4}{\gamma} \varphi = Ra\frac{\Omega^2}{\gamma} \varphi. \tag{1.22}
\]

To solve the fourth-order equation (1.22), we need four boundary conditions. The first pair is

\[
\varphi(0) = 0, \quad \varphi'(1) = 0, \tag{1.23}
\]

which follows immediately from the second and third conditions (1.17). The remaining pair is obtained by observing that \( T^* \big|_{z^*=0,1} = \text{const} \) and thus its first derivative w.r.t \( z^* \) is zero. Then from the flow equation (1.15) we have \( \frac{\partial^2 \varphi}{\partial z^*^2} \big|_{z^*=0,1} = -\gamma \varphi'' / \varphi^{z^*} \big|_{z^*=0,1} \), which gives rise to

\[
\frac{\Omega^2}{\gamma} \varphi(0) = \varphi''(0), \quad \varphi''(0) = 0, \quad \frac{\Omega^2}{\gamma} \varphi(1) = \varphi''(1), \tag{1.24}
\]

where the second expression above follows from the fact that \( \varphi(0) = 0 \) itself. So the complete set of the boundary conditions is given by expressions (1.23) and the last two expressions in (1.24).

The general solution to equation (1.22) is of the form \( \exp(\xi z^*) \), where \( \xi \) is complex. The auxiliary equation readily gives

\[
2\xi^2 = \Omega^2 \left(1 + \frac{1}{\gamma}\right) \pm \sqrt{\left(\frac{1}{\gamma} - 1\right)^2 + 4Ra \frac{\Omega^2}{\gamma}}. \tag{1.25}
\]

For \( Ra > \Omega^2 \), \( \xi^2 \) will have both signs, therefore the solution should be a mixture of hyperbolic and harmonic functions. The following form identically satisfies both equation (1.22) and the first three boundary conditions for \( Ra > \Omega^2 \)

\[
\varphi'(z^*) = \frac{\sinh \beta z^*}{\beta \cosh \beta} - \frac{\sin \alpha z^*}{\alpha \cos \alpha} \tag{1.26}
\]
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where \( \alpha^2 = -\xi_1^2 \) and \( \beta^2 = \xi_2^2 \) are both positive and real and related to each other through equation (1.25)

\[
\beta^2 = \alpha^2 + \Omega^2 \left( 1 + \frac{1}{\gamma} \right). \tag{1.27}
\]

The remaining boundary condition, the last one in expressions (1.24), requires

\[
\beta \left( \alpha^2 + \Omega^2 \right) \coth \beta = -\alpha \left( \alpha^2 + \Omega^2 \right) \cot \alpha. \tag{1.28}
\]

On the other hand, substituting the solution form (1.26) into the equation on \( \varphi \) (1.22), we obtain the following condition on the Rayleigh number

\[
Ra = \left( \alpha^2 + \Omega^2 \right) \left( 1 + \frac{\alpha^2 \gamma}{\pi^2} \right). \tag{1.29}
\]

It is easy to show that with the choice \( Ra < \Omega^2 \) and \( \xi_{1,z}^2 > 0 \), equation (1.28) would yield \( \cot \beta / \cot \alpha < 0 \) which is inconsistent for any non-trivial positive pair \((\alpha, \beta)\), thus the solution is uniquely given by expression (1.26).

The critical Rayleigh number, \( Ra_{cr} \), is now calculated as follows. Starting with \((\Omega^2, \gamma)\), we solve equation (1.28) for \( \alpha \) on \([0, \pi]\) by the method of bisections, making use of formula (1.27), and obtain \( Ra(\Omega, \gamma) \) straight from expression (1.29).

If we are dealing with a layer, not a box, constrained by \( \Omega^2 = [-s, s] \), the only value of \( \Omega^2 \) that delivers minimum to relationship (1.29), divided by \( \pi \), would be the appropriate critical aspect ratio, \( O_{cr} \), and the corresponding \( Ra_{cr} = Ra(O_{cr}, \gamma) \) be the critical Rayleigh number sought for the particular anisotropic coefficient \( \gamma \). The results for the layer are plotted in Fig. (1.3) as \( Ra_{cr}(\gamma) \) and \( O_{cr}(\gamma) \) for the range of \( \gamma = [0.01, 1.0] \).

For \( \gamma = 1 \) (no anisotropy), we have \( Ra_{cr} = 27.1 \) and \( O_{cr} = 1.38 \), which agrees with the values found in [Nield, 1968], who obtained them in a different way. We observe that \( Ra_{cr} \) is less and the cells are wider for any \( \gamma \) in a layer with the permeable upper boundary, in comparison with that when it is sealed. Yang [1996] found that in the latter case

\[
Ra_{cr} = \pi^2 \left( 1 + \sqrt{\gamma} \right)^2, \quad O_{cr} = \frac{1}{\sqrt{\gamma}}. \tag{1.30}
\]

which we also show in Fig. (1.3). Note that Yang uses \( \sqrt{k_x k_y} \) in the definition of \( Ra \) as opposed to \( k_x \) in formula (1.14), so in order to compare, his original expression for \( Ra_{cr} \) is multiplied by \( \sqrt{\gamma} \) as in equations (1.30).

In modeling convection in a layer numerically, the lateral size of the model is typically an integral multiple of the cell's size. It would then be prudent to stay close to the naturally
1.6. ONSET OF CONVECTION IN A PERMEABLE ANISOTROPIC BOX

Figure 1.3: Critical Ra-number, \( Ra_{cr} \), and the aspect-ratio of the cells, \( O_{cr} \), as functions of the anisotropic coefficient, \( \gamma \), for the onset of convection in a porous box with the isothermal and impermeable lower boundary, adiabatic and impermeable side walls, and both permeable and impermeable upper boundary which is isothermal before convection takes place.
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Figure 1.4: Temperature contours (normalized on \( T_{\infty} = T_0 \)) and streamlines for \( Ra = 1.03 \cdot Ra_{cr} \) and \( k_z/k_y = 10 \) in a layer. Only one cell is shown. The circulation is counter-clockwise.

set aspect ratio, thus minimizing the effect of the boundaries by not forcing \( \psi \) to a favorite number like unity. Figure (1.3) may be consulted as a rough guide in setting up the model's dimensions, while expression (1.26) could serve as an initial guess for the scaled velocity field, which greatly speeds up the steady-state computations. We leave the details of the numerical algorithm for the next section and continue with two examples of its output at the steady state.

Figure (1.4) shows temperature contours and streamlines for \( Ra \) just 3% above the critical and \( \gamma = 10 \) for both types of the upper boundary. The free flux boundary condition is used for the case of permeable sea floor. When it is permeable, we have \( Ra_{cr} = 82 \) and \( O_{cr} = 0.78 \), while when it is impermeable, \( Ra_{cr} = 176 \) and \( O_{cr} = 0.56 \). The rectilinear numerical grid used in both simulations is 65 by 65 nodes, however, very close (within a couple of percent) results are already achieved on a coarser, 33 by 33, grid. We now increase the Rayleigh number by 20% and again compare the two cases in Fig. (1.5). Also plotted there are the heat flux variations through the top of the models. It is apparent, that the permeable-top (Fig. 1.5B) model produces a much more focused discharge sites at the sea floor. We still have \( O = O_{cr} \) for both models. To ensure that, we set the lengths of the domains so that they can accommodate 16 cells on 513 by 33 grid if our initial guess on the aspect ratio is
1.6. ONSET OF CONVECTION IN A PERMEABLE ANISOTROPIC BOX

Figure 1.5: Temperature contours (normalized on $T_{\infty}$), streamlines, and relative heat flux variations at the sea floor for $Ra = 1.2 \cdot Ra_{cr}$ and $k_y/k_x = 10$ in a layer. Four adjacent cells are shown.
1.7. Solution by Finite Differences

A simple and reliable (but, sadly, not the most efficient) way to solve the time-dependent temperature equation (1.6) numerically is the well documented finite difference (FD) Euler scheme [e.g. Wooding, 1976; Ames, 1977; Fehn et al., 1983] on a uniform rectangular grid

\[ x_i = \Delta x(i - 1), \quad i = \{1, nx\}; \quad z_k = \Delta z(k - 1), \quad k = \{1, nz\}; \quad t^n = t^{n-1} + \Delta t_n, \quad (1.31) \]

where \( \Delta x \) and \( \Delta z \) are the spatial increments in the \( x \)- and \( z \)-direction, respectively, and \( \Delta t_n \) is the \( n \)-th time step, \( n = \{1, 2, \ldots\} \). The problem is formulated for a discrete field \( T^n_{i,k} \), which is a projection of \( T(x, z, t) \) on grid \( (x_i, z_k, t^n) \) with spatial dimensions \( (nx, nz) \). In calculating the velocity field, the same convention applies to \( \psi^{n}_{i,k} \). Using explicit forward differencing in time and central differencing for the advective terms, we obtain the following numerical scheme:

\[
\begin{align*}
\frac{1}{\zeta^n} & \left[ T_{i,k}^{n+1} - \frac{T_{i+1,k}^{n+1} + T_{i-1,k}^{n+1}}{2} - \frac{T_{i,k+1}^{n+1} - T_{i,k-1}^{n+1}}{2} \right] \\
& - \frac{T_{i,k}^n - 2T_{i+1,k}^n + T_{i-1,k}^n}{\Delta x^2} - \frac{T_{i,k}^n - 2T_{i,k+1}^n + T_{i,k+2}^n}{\Delta z^2} = 0,
\end{align*}
\]

where \( v_{i,k}^n = -\left(\psi_{i+1,k}^n - \psi_{i-1,k}^n\right)/2\Delta x \) and \( \psi_{i,k}^n = \left(\psi_{i+1,k}^n - \psi_{i-1,k}^n\right)/2\Delta z \) as defined in Section 1.3. This scheme is first order accurate in time and second order accurate in space.

Let \( \widetilde{T}_{i,k}^n \) be a projection of the exact, non-dimensional solution to equation (1.6) on our grid, so that the residual at some point \((x_i, z_k)\) and time \( t_n \) is \( \epsilon_{i,k}^n = \widetilde{T}_{i,k}^n - T_{i,k}^n \). Introduce the following quantities

\[
\begin{align*}
\xi^n_x &= \frac{C^n_x \Delta t^n}{\Delta x^2}, \quad \xi^n_z = \frac{C^n_z \Delta t^n}{\Delta z^2}, \quad \nu_x^n = \frac{C^n_x \Delta t^n \psi_x^n}{2\Delta x^2}, \quad \nu_z^n = \frac{C^n_z \Delta t^n \psi_z^n}{2\Delta z^2},
\end{align*}
\]

(1.33)
then we can re-write equation (1.32) for the residuals as

$$\epsilon_{i,j}^{n+1} = \epsilon_{i,j}^n + \epsilon_{i,j}^n \left( \frac{\epsilon_{i+1,j}^n - 2\epsilon_{i,j}^n + \epsilon_{i-1,j}^n}{\Delta x^2} + \frac{\epsilon_{i,j+1}^n - 2\epsilon_{i,j}^n + \epsilon_{i,j-1}^n}{\Delta y^2} \right)$$

Now let $\eta = \text{Max} \left\{ |\epsilon_i^n| \right\}$ and require $\eta^{n+1} \leq \eta^n$ for convergence, which yields

$$\eta^{n+1} \leq \eta^n \left(1 - 2\xi_1^n - 2\xi_2^n \right) + |\xi_1^n + \xi_2^n| + |\xi_1^n - \xi_2^n| + |\xi_1^n + \xi_2^n| + |\xi_1^n - \xi_2^n|.$$  

Since both $\xi_1^n$ and $\xi_2^n$ are positive, the necessary convergence conditions are $(\xi_1^n + \xi_2^n)_{\max} \leq \frac{1}{2}$, $|\xi_1^n| \leq \xi_1^n$, and $|\xi_2^n| \leq \xi_2^n$. In terms of the grid increments, they give

$$\Delta t^* \leq \frac{\Delta x^2 \Delta y^2}{2v_{\text{max}}^2} \left( \Delta x^2 + \Delta y^2 \right), \quad \Delta t^* \leq \frac{2}{|v_{\text{max}}^*|}, \quad \Delta t^* \leq \frac{2}{|v_{\text{max}}^*|}.$$  

The severe time step limitation is a common problem of most explicit schemes, the price to pay for the simplicity in coding them. However, the last two conditions above are due to the centered difference approximation used for the velocity field. One way to construct the grid is then to choose $\Delta x$ and $\Delta y$ first, based on the maximum anticipated velocity; then select $\Delta t_n$ based on the maximum value of $\xi(T^n)$. The steady-state temperature equation can be solved either as a limiting case of a time-stepping procedure or directly as such, using available iterative solvers. The stationary version of the temperature equation (1.10) as well as the flow equation (1.9) are both elliptic PDEs. We employ a reputable, user-friendly MUDPACK collection of multigrid finite difference solvers, written at NCAR by J. Adams [1989], which handles both general second-order and self-adjoint elliptic forms. The user is required to supply only the coefficients and boundary conditions as external functions. In MUDPACK, the problem is discretized on a rectilinear uniform grid. Advection first-order terms are discretized via centered difference, so the restrictions on the spatial grid spacing as per conditions (1.36) apply. Among other options, we select the default W multigrid cycling, always starting it at the coarsest grid level and Gauss-Seidel line relaxation in both x- and y-directions, chosen for its robustness for the problem at hand. The termination of the iterations is controlled by the maximum norm of the relative difference between the last two computed approximations on the solution grid.

The heat and mass transport equations, as a coupled system, are solved sequentially. A typical cycle is as follows. The latest temperature update is used on the right-hand side of the flow equation in the buoyancy term and on the left-hand side to calculate all temperature
dependent quantities, such as density and viscosity. Then the newly updated velocity field is used in the advective part of the temperature equation, which is a very common approach [e.g. Yang, 1996]. Numerical experiments have revealed that in calculating both the velocity field and buoyancy term, while switching between the two equations, it is best to use the same discretization scheme (particularly near corners and sides) and order of approximation as the solver does.

1.8 Code Testing

The software was tested in a number of ways. First, we verify that both numerical and analytical results for \( Ra_e \) and the aspect ratio, \( O_e \), agree at the onset of convection for both types of the upper boundary within the range of \( \gamma = [0.01 - 100] \). The time-dependent algorithm at the late-time limit produces nearly identical results as the steady-state solver for all runs.

The steady-state temperature equation appears to be more vulnerable to numerical instabilities than are the others, and we validate it, following the procedure suggested by C. Christara [personal communication]. We take an analytical pair, \( (\psi_*, T_*) \), which satisfies all the boundary conditions and operate on it the left-hand side of the temperature equation (1.10) with \( \partial T^*/\partial t = 0 \). As our guess is hardly perfect, a non-zero right-hand side (RHS) usually results. This newly formed equation is solved with MUPDACK for \( T^* \), given \( \psi_* \) and \( RHS \). The process is repeated \( k \) times to obtain \( T^{(k)} \), which ceases to be analytical after \( k = 1 \), and compare it with \( T_* \). Thus, we test how repeated numerical differentiation affects the stability of the solver. We use \( \psi_* \) as in expressions (1.26) and (1.18) for the onset of convection but scale it by a large amplitude so that \( \psi_* \approx \epsilon/\Delta \) and \( \psi_* \approx \epsilon/\Delta \), where \( \epsilon \sim 2 \).

The analytical form for the temperature is

\[
T^* = 1 - z^* - A \left( \frac{\sinh \beta z^*}{\sinh \beta} - \frac{\sin \alpha z^*}{\sin \alpha} \right) \cos \left( \pi \left( \frac{z^*}{O} \right) \right),
\]

where \( A = 50, \alpha = 2.03, \beta = 4.58, \) and \( O = 1.4 \). The maximum relative difference between \( T^{(100)} \) and \( T_* \) on a 65 \times 65 grid is \( \sim 5 \cdot 10^{-3} \) if the relative tolerance is set to \( 10^{-4} \) internally in MUPDACK and \( \epsilon < 3 \).

In the next section, we develop a Green's function solution for the subcritical convection around a point source of heat in a layer which will be compared with the numerical solution. Finally, in Section 1.10 we deal with a time-dependent circulation scenario due to a magmatic intrusion. The late-time and steady-state fields are compared. Both tests are quite satisfactory.
1.9. CONVECTION INDUCED BY A POINT HEAT SOURCE IN A LAYER

Figure 1.6: A point heat source is located at z = h in a porous layer of thickness H. The problem is assumed axi-symmetric.

At the steady state, the software additionally compares the heat flux through the lower and upper boundaries. Ideally, the two should coincide. A typical relative disbalance error is set at about 1% as a complimentary termination criterion.

1.9 Convection Induced by a Point Heat Source in a Layer

Consider an isotropic, subcritical ($Ra < 4\pi^2$) porous layer of thickness H and permeability k with isothermal and impermeable boundaries, kept at temperature $T_b$ at the bottom, $z = 0$, and $T_t$ at the top, $z = H$, respectively. The introduction of a continuous point heat source of power $Q$ at $z = h$, which could well be a small eruption of magmatic matter into otherwise cold sedimentary section, induces an axi-symmetric convection pattern, centered at the source location. The setting is shown in Fig. (1.6) in the cylindrical coordinates $\vec{r} = (\rho, \theta, z)$, $r = (\rho^2 + z^2)^{1/2}$ with the z-axis directed upwards. Note that to distinguish density from the just introduced coordinate $\rho$, there are subscripts attached to the latter; e.g. $\rho_T$ and $\rho_0$. Assuming that $Q$ isn't large, we will solve this in the Boussinesq approximation as an axi-symmetric problem for $\psi(\rho, z)$ and $T(\rho, z)$.

To take advantage of those simplifications, let us slightly modify the definition of the stream function (1.3)

$$\nu_\rho = -\frac{1}{\rho} \frac{\partial \psi}{\partial z}, \quad v_\theta = \frac{1}{\rho} \frac{\partial \psi}{\partial \rho}, \quad v_z = 0, \quad \psi = \psi T_0 = H/\kappa,$$  \quad (1.38)
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which automatically satisfies $\nabla \cdot \vec{v} = 0$, consistent with the Boussinesq approximation. In addition, adopt a different scaling for temperature, based on the source strength and layer thickness, $T^* = T_0 H/Q$, and introduce a source Rayleigh number, $Ra_s$,

$$Ra_s = \frac{k \alpha \rho \varepsilon H Q}{\nu \lambda m}, \quad \eta = \frac{Ra_s}{Ra} = \frac{\Delta TH \lambda m}{Q}. \quad (1.39)$$

Taking curl of Darcy's equation (1.1), we get rid of $\nabla p$ and preserve the $\theta$-component only, because $u_\theta = 0$ and $\partial \theta / \partial \phi = 0$. The non-dimensional flow equation then reads

$$\frac{\partial^2 \psi^*}{\partial \rho^2} - \frac{1}{\rho^2} \frac{\partial \psi^*}{\partial \rho} + \frac{\partial^2 \psi^*}{\partial \phi^2} = Ra_s \frac{\partial \theta^*}{\partial \rho}. \quad (1.40)$$

The appearance of the dimensionless temperature equation as of (1.10) remains intact, but both components of the velocity are now derived from the stream function according to expression (1.38).

It is important to realize that convection will always exist in the close proximity to the true point source, because arbitrary high temperature gradients near it are guaranteed, and the Boussinesq approximation will quite possibly fail. From dimensional analysis and equation (1.40) one may expect $\nu \propto Ra \cdot \kappa_m / r$, where $\kappa_m = \lambda_m / (\rho_0 c_m)$ is the thermal diffusivity of the medium. So we seek the solution as a series expansion, following Bejan, [1978]

$$\psi^* = \psi_0^* + Ra_s \psi_1^* + Ra_s^2 \psi_2^* + ...$$

$$T^* = T_0^* + Ra_s T_1^* + Ra_s^2 T_2^* + ... \quad (1.41)$$

The boundary conditions are $u_\theta |_{\rho = 0} = 0$, $u_\phi |_{\phi = 0} = 0$ and $\partial T^*/\partial \rho |_{\rho = 0} = 0$ because of symmetry, while $\partial \theta^*/\partial \rho |_{\rho = 0} = 0$ follows directly from Darcy's law and the first two conditions. We also have $T_{z = 0} = T_0$ and $T_{z = H} = T_t$, and require both velocity components vanish as $\rho \to \infty$.

When $Ra_s = 0$, there is no flow ($\psi_0 = 0$) and $T_0$ is the solution of the heat diffusion equation with the source term. It can be written as $T_0 = T_{01} + T_{02}$, where $T_{01} = T_s - \Delta T_s / H$, which satisfies the homogeneous version of the temperature equation (1.10), and $T_{02}$ satisfies that equation with the source terms present and the homogeneous (zero) boundary conditions. The solution to the latter problem can be readily obtained from the known whole space solution, $T_{w,sp}$, for a point source located at the origin and switched on at $t = 0$ [Carslaw and Jaeger, 1959]

$$T_{w,sp} = \frac{Q}{4\pi \lambda_m} \exp \left( \frac{r}{\sqrt{4 Ra_s t}} \right). \quad (1.42)$$

We may construct the appropriate layer solution by placing sources and sinks of equal
strength at \( z = \pm h + 2Hn, \ n = \) -\( \infty, +\infty \) and sum up their contributions, so as to secure \( T_{z=\pm H} = 0 \). For convenience, let us introduce a couple of new dimensionless variables

\[
\alpha^*_n = 2n \pm h, \quad \xi^*_n = \sqrt{\frac{\rho^2 + (\alpha^*_n - x^*)^2}{4n}}, \quad \Pi^*_n = \frac{1}{4\pi \xi^*_n \sqrt{4n}},
\]

then we will have for \( T_{z=0} \) in cylindrical coordinates

\[
T_{z=0} = \sum_{n=-\infty}^{n=\infty} (\Pi^*_n - \Pi^*).
\]

Formal substitution of series (1.41) into the governing equations (1.40) and (1.10) gives

\[
\frac{\partial^2 \psi^*_n}{\partial \rho^2} - \frac{1}{\rho} \frac{\partial \psi^*_n}{\partial \rho} + \frac{\partial^2 \psi^*_n}{\partial z^2} = \rho \frac{\partial T^*_n}{\partial \rho^*},
\]

\[
\frac{\partial T^*_n}{\partial \rho^*} + \left( \frac{\partial T^*_n}{\partial \rho^*} + \frac{\partial T^*_n}{\partial z^2} \right) = \frac{1}{\rho} \left( \frac{\partial \psi^*_n}{\partial \rho^*} + \frac{\partial \psi^*_n}{\partial z^2} \right),
\]

to the first order in \( \text{Re}_n \), where \( \partial T^*_n/\partial \rho^* \equiv \partial T^*_n/\partial \rho^* \), and \( \partial T^*_n/\partial z^* = -\eta - \partial T^*_n/\partial z^* \).

Stream Function Equation

We observe that the right-hand side of the flow equation (1.45) contains only derivatives w.r.t. \( \rho^* \), thus it will suffice to solve it for the generic image with fixed \( n \) and then perform the summation over \( \psi^*_n \) as in equation (1.44). Since the following derivation proceeds along the same lines as in [Bojan; 1978], only a brief synopsis is given. Expanding the right-hand side in equation (1.45), we obtain

\[
\frac{\partial^2 \psi^*_n}{\partial \rho^2} - \frac{1}{\rho} \frac{\partial \psi^*_n}{\partial \rho} + \frac{\partial^2 \psi^*_n}{\partial z^2} = -\frac{\rho^2 \phi \xi^*_n \text{erfc}(\xi^*_n) + 2}{\sqrt{\pi} \xi^*_n e^{-\xi^*_n^2}}.
\]

Note that the subscript \( \pm \) is dropped from \( \xi^*_n \) for now, but will be restored later. The solution is guessed in the following form

\[
\psi^*_n = \frac{1}{8\pi \sqrt{\pi}} \int_{\xi^*_n}^{\xi^*_n} \phi^*(\xi^*_n),
\]

which reduces the flow equation to a much simpler, ordinary differential equation on \( \phi^*_n \),

\[
\xi^*_n \phi^*_n - 2 \phi^*_n = \xi^*_n \text{erfc}(\xi^*_n) - \frac{2}{\sqrt{\pi} \xi^*_n} e^{-\xi^*_n^2}.
\]
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Figure 1.7: Dimensionless time to reach steady state in a layer, thickness $H$, with the isothermal and impermeable boundaries and a point heat source as a function of the source elevation, $z = h/H$, for $\rho/H = 0.2$ and $\rho/H = 0.5$.

The general solution to the homogeneous portion of the above equation is $A/\xi_n + B\xi_n^2$, where $A$ and $B$ are constants. Both should be discarded, because the $B\xi_n^2$ term generates infinite velocities at $\rho \to \infty$, while the $A/\xi_n$ term doesn't have the right singularity at the source. There we should have $\psi \sim \xi$, to make $v \sim 1/r$ at that limit. The particular solution turns out to be

$$\phi_n = \frac{\xi_n}{2} \operatorname{erfc}(\xi_n) + \frac{1}{4\xi_n} \operatorname{erfc}(\xi_n) - \frac{1}{2\sqrt{\pi}} e^{-\xi_n^2},$$

(1.50)

which may be verified directly. Now we perform the summation over the images to finally obtain

$$\psi(\rho, z, h^*) = \sum_{n=-\infty}^{\infty} \frac{\operatorname{erfc}(\xi_n) + \operatorname{erfc}(\xi_n) - \frac{\xi_n^2}{4\xi_n^2 + (2n + h^* - z^*)^2}}{\sqrt{\rho^2 + (2n + h^* - z^*)^2}} - \frac{\operatorname{erfc}(\xi_n) + \operatorname{erfc}(\xi_n) - \frac{\xi_n^2}{4\xi_n^2 + (2n - h^* - z^*)^2}}{\sqrt{\rho^2 + (2n - h^* - z^*)^2}}.$$ 

(1.51)

It is clear that to the first order in $Ra_n$, the time required to reach the steady state is a function of $\rho^*, z^*, h^*$, and the characteristic time response, $\tau = \rho_0 c_m H^2/\lambda_m$, of the system, but not $\bar{k}$, $\mu$, or $Q$ which only scale the velocity field in the combination $kQ/\mu$.

Define $t_{sl} = t_{sl}(\rho^*, h^*)$ to be a typical time to reach the steady state, if the source, located at $z^* = h^*$, is switched on at $t = 0$, and

$$\frac{\psi(\rho, z = H, t = t_{sl})}{\psi(\rho, z = H, t = \infty)} = 0.7.$$ 

(1.52)

Figure (1.7) displays a plot of $t_{sl}/\tau$ versus $h^*$ for $\rho^* = 0.2$ and $\rho^* = 0.5$, while Fig. (1.8)
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gives an example of \( \psi_t \)-contours as a function of dimensionless time, \( t/\tau \), for \( h = 0.1H \).

At the steady-state limit, \( \xi = 0 \), we have a far simpler formula for \( \psi_t \):

\[
\psi_t(\rho', z', h^*) = \frac{\rho'^2}{4\pi} \sum_{n=-\infty}^{\infty} \left[ \frac{1}{\sqrt{\rho'^2 + (2n + h^* - z^*)^2}} - \frac{1}{\sqrt{\rho'^2 + (2n - h^* - z^*)^2}} \right],
\]

which can be expressed via zero-order Hankel transform [Abramowitz and Stegun, 1968]. Let \( S(\rho', z', h^*) = 8\pi \psi_t / \rho'^2 \), then the sum is

\[
S = 2 \int_0^{\infty} J_0(\rho' x) \sinh(x(1 - h^*)) \sinh(xz^*) dx, \quad 0 \leq z^* \leq h^*;
\]

\[
S = 2 \int_0^{\infty} J_0(\rho' x) \sinh(x(1 - z^*)) \sinh(xh^*) dx, \quad h^* \leq z^* \leq 1.
\]

Temperature Equation

Our attempts to find an analytical solution for the first-order temperature correction were unsuccessful. However, a closed-form expression can easily be derived via the Green's function method [e.g. Carslaw and Jaeger, 1959]. We shall restrict the discussion to the steady-state. Note that equation (1.46) is of the form \( \nabla^2 T_1 = f \), where \( f = (\varepsilon \nabla) I_0 \), and \( T_1 |_{z=h} = 0 \). Thus, the solution is

\[
T_1(\rho, z) = \int G(\rho - \rho_0, z - z_0) f(\rho_0, z_0) d\rho_0 d\theta_0,
\]

where \( G \) is a Green's function, which satisfies the heat conduction equation in a layer with zero temperature on the boundaries and a point heat source of unity strength, located at \( \rho_0 = (\rho_0, z_0, \theta_0) \). Integral (1.55) is a sum of such elementary contributions weighted by the right-hand side \( f \), evaluated at the sources. Starting from the well-known function for the whole space, \( G_{\text{space}} = -1/(4\pi r) \), we construct the required \( G \) using the method of images in the cylindrical coordinates

\[
G(\rho', \rho, z', z, \theta, \theta_0) = \frac{1}{4\pi} \sum_{n=\infty}^{\infty} \left[ \frac{1}{\sqrt{\delta^2 + (2n + z - z_0)^2}} - \frac{1}{\sqrt{\delta^2 + (2n - z - z_0)^2}} \right],
\]

where \( \delta^2 = \rho'^2 + \rho^2 - 2\rho' \rho \cos(\theta - \theta_0) \) and \( \theta \) can be set to zero for convenience. The \( \theta \)-part is integrated out immediately with the help of the identity [Gradshtein and Ryzhik, 1980]

\[
\int_0^{2\pi} \frac{d\theta_0}{\sqrt{1 - b \cos \theta_0}} = \frac{4}{\sqrt{1 + b}} K \left( \frac{2b}{\sqrt{1 + b}} \right),
\]
Figure 1.8: Time sequence of low $Re$-number flow lines developed around a point heat source in a porous subcritical layer for $h^*=0.2$ and $h^*=0.5$. $t^*$ is dimensionless.
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where \( K \) is the elliptic integral of the second kind.

The result is

\[
G(\rho^*, \rho^*, z^*, z^*) = -\frac{1}{\pi} \sum_{n=-\infty}^{\infty} \left\{ \frac{\sqrt{\varepsilon} K\left(\frac{\varepsilon\rho^*}{\sqrt{\varepsilon}}\right)}{\sqrt{3} \rho^*} - \frac{\sqrt{\varepsilon} K\left(\frac{\rho^*}{\sqrt{\varepsilon}}\right)}{\sqrt{3} \rho^*} \right\},
\]

(1.58)

where \( l_0 = 2\rho^* \rho^*/(\rho^*+\rho^*/(2\rho^*+z^*/z^*)^2) \). Proceeding similarly, it is possible to construct the time-dependent Green's function and obtain \( T_0^*(\rho^*, z^*, t^*) \) in closed form. We provide the final answer, leaving off the details

\[
T_0^*(\rho^*, z^*, t^*) = \int_0^t dt^* \int_0^\rho^* d\rho^* \int d^* \int_0^\rho^* d\rho^*/(2\rho^*+z^*/z^*)^2. \]

(1.60)

The first order, steady-state temperature correction, \( T_1^* \), is now evaluated numerically, using expressions (1.55) and (1.58). We calculate the resulting double integral sequentially, performing the finite integration over \( z^* \) first, using 16-point Gauss-Legendre quadratures [Abramowitz and Stegun, 1968]. Eight-point Gauss-Laguerre quadrature, borrowed from the same source, is used to evaluate the remaining semi-infinite integral over \( \rho^* \).

Note that function \( f \) can be conveniently expressed either via infinite sums or suitable Hankel transforms. Chave [1983] provides software to evaluate the latter of any integer order. Let \( \eta = \frac{R_0}{R_0'}, U = \partial S/\partial \rho^* \), and \( W = \partial \rho^*/\partial z^* \), so \( U \) and \( W \) can be obtained from formula (1.54), differentiating under the integral, or series in expression (1.53), then

\[
T_0^* = \frac{1}{4\pi} S + T_0^* - \eta z^*, \quad \frac{\partial T_0^*}{\partial \rho^*} = \frac{1}{4\pi} U, \quad \frac{\partial T_0^*}{\partial z^*} = \frac{1}{4\pi} W - \eta.
\]

(1.61)

Collecting the terms above,

\[
f = (\nabla \nabla) T_0^* = \frac{1}{16\pi^2} WS - \frac{\eta}{8\pi}(2S + \rho^* U).
\]

(1.62)

Calculations reveal that when \( \rho < 2H \), the truncated summation is slightly less accurate, but 2–3 times faster than the Hankel transform. For greater \( \rho \), the transform is absolutely
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Figure 1.9: Convection induced by a point source of heat. Dimensionless temperature contours.

superior. It, however, breaks when \( \rho > 6H \), but the contribution of this region is minimal, so \( \rho' = 6 \) is used as a cut-off value. The overall accuracy of these calculations seems to lie within a couple of percent.

Figure (1.9A) shows a vertical cross-section of the temperature field (first-order \( Ra \)), developed around a point heat source at \( h = 0.2H \), calculated as described above. The Rayleigh numbers are made equal: \( Ra = 10 \) and \( Ra_2 = 10 \). We now cross-check this Green's function solution against the output of the FD solver, shown in Fig. 1.9B. The latter problem is technically discretized for the difference \( T_1 - T_{\text{ref}} \), so that \( T_{\text{ref}} \) is then added back. The two solutions, obtained by clearly distinct methods, agree within a few percent. The maximum difference is observed near the region \( z \sim h \), where the automated Gaussian integration is difficult, because the integrand (1.55) rapidly changes its sign. On the
1.10 Propagation of Thermal Transient Through Oceanic Crust

Our major objective here is to time a thermal transient, as it propagates through a typical crustal section, powered by a time-dependent heat source, such as a cooling magmatic intrusion. Consider a generic model, shown in Fig (1.11). The upper 500 m-thick layer has
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Figure 1.11: Domain geometry, permeability profiles, and ambient temperature and streamlines before intrusion takes place. The sea floor is a permeable, free-flux boundary, and the lateral walls of the model are both impermeable and adiabatic at all times. The difference between Model 1 and Model 2 is the equivalent volume of magma.
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isotropic permeability of $10^{-12}$ m$^2$ which smoothly decreases to the value of $10^{-16}$ m$^2$ towards the base of the model at 1000 mbaf, where $k_x/k_y = 10$. The lower boundary is assumed impermeable and initially isothermal, kept at 100°C. The sea floor, as the upper boundary, is permeable, so that the free flux boundary condition applies. The side boundaries are impermeable and adiabatic to ideally mark the boundaries between adjacent convection cells. Numerical trials show that the cells reside mainly above 500 mbsf. Since the conditions are not much above the critical, we take the aspect-ratio as that for the isotropic layer, $\alpha = 1.4$.

The lateral extent is then fixed at 1400 m to accommodate two convection cells. The initial temperature contours and streamlines are superimposed on the drawing in Fig. (1.11). The ascending limb is right in the middle of the domain, the flanks form the recharge zone. At the discharge site on the sea floor, we have $T_{sf} \approx 6.34^\circ C$ and $V_{sf} \approx 0.56 \text{ m/yr}$, while the ambient sea floor temperature is assumed 4°C.

Now, a magmatic, stock-like intrusion, heated to 1200°C is introduced as a line source, making a small contact area of 60 m at the base of the model, as shown in Fig. (1.11). This contact area cools with time to the ambient 100°C, while the rest of the lower boundary remains isothermal. Although an over-simplification, it looks plausible that the intrusion will likely cause a thin (typically a couple of dozen of meters) conductive boundary layer and much deeper fluid circulation in the regions immediately outside the layer, which will effectively drive upwards the heat flux lost through the sides of the intrusion. In addition, we vary the magmatic content. The equivalent vertical cross-sectional area of the magma is $2 \cdot 10^9 \text{ m}^2$ in Model 1 and half of that in Model 2. Assuming a couple of kilometers extent along the axis and recalling the volumetric rates for magma from the introductory chapter, such volumes could be built up in a matter of a day.

Figure 1.12 shows a few selected snapshots of the temperature field and streamlines developed as time progresses. The accompanying labels contain information about the intrusion temperature, $T_i$, and maximum temperature and fluid velocity discharged at the sea floor, $T_{sf}$ and $V_{sf}$, respectively. For Model 1, there are clearly three stages in the development. The first one lasts approximately 450 Y during which a narrow zone of fluid is formed, featuring deep, focused circulation to the base of the domain. It effectively removes heat from the intrusion and drives strong temperature gradients to the interface with the more permeable upper layer. No significant changes in the latter as yet. Within the next 150 years, the thermal transient makes it to the surface, covering the distance of 500 m. We see that the streamlines pattern resembles that formed around a point heat source (Section 1.9, Fig. 1.8) with the exception that the vortex travels not only outwards but also vertically, along with the heat pulse. It delivers $T_{sf} = 32.5^\circ C$ and $V_{sf} = 4.4 \text{ m/yr}$. Thus, $\xi V_{sf}$, where $\xi \sim 1$, is a typical ascent velocity of the transient. Then the system takes about 1000 Y to
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Figure 1.12: Transient temperature field and streamlines at a few selected times for Model 1.
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Figure 1.13: Temperature of intrusion, $T_i$, maximum temperature and velocity at the discharge site on the sea floor, $T_{sf}$ and $V_{sf}$, respectively, for Model 1 and Model 2 as functions of time. These parameters are normalized on the ambient $T_0 = 1200^\circ C$, $T_{sf0} = 6.34^\circ C$, and $V_{sf0} = 0.56 \text{ m/yr}$. Dimensionless time is based on the thickness of the entire model and provided on a separate axis.

return to the initial conditions we started our simulations from.

The results for Model 2, where the volume of magma is halved, are qualitatively similar, except the transient time through the upper layer is about 2.5 times longer and the time to recover is about twice shorter, in comparison with Model 1. When the transient hits the sea floor in 850 Y since the intrusion, we have $T_{sf} = 11.4^\circ C$ and $V_{sf} = 1.5 \text{ m/yr}$. Again, a typical ascent velocity of the heat pulse in the upper permeable layer is $\sim V_{sf}$. We compare some of the most important temporal characteristics, $T_i$, $T_{sf}$, and $V_{sf}$, between the two models in Fig. 1.13. For both models, there is a nearly perfect correlation between $T_{sf}$ and $V_{sf}$ which supports the earlier assumption in Section 1.2 about local thermal equilibrium between the host rock and fluid. It is also clear that if magmatic events take place with the periodicity of
about 1000 Y, then the elevated temperature and fluid velocity conditions at the discharge sites may be sustained, which would be the case for an intermediate spreading ridge [see introductory chapter].

1.11 Summary

We discussed the governing and constitutive equations for the coupled mass and heat, single-phase transport in unfractured, saturated, anisotropic oceanic crust, including the Rayleigh-number approximation. The latter is limited to low-temperature systems due to the strong temperature dependency of density and especially fluid viscosity.

Analytical expressions for the aspect-ratio of the convection cells and the critical Rayleigh-number at the onset of convection are derived for anisotropic systems with the permeable upper boundary. In comparison with their impermeable counterparts, they feature wider cells and are easier to initiate hydrothermal circulation.

We obtained first-order $Ra$-number streamfunction and temperature fields in closed form for convection initiated by a point source of heat in a porous layer with the impermeable boundaries. The source causes a nearly uniform uplift of isotherms in its vicinity. On the sea floor, the heat flux increase is felt mostly within the radius of half the layer thickness, although it mildly depends on the source altitude. The time to reach the steady state in such a system is about an order of magnitude less than that for a purely conductive regime. The solutions are also useful for software testing.

Based on data from deep oceanic drilling, we set up a permeability model and considered propagation of a hydrothermal transient through the system. For a 1 km-thick section and conditions as of ODP 504B, we expect the transient due to magmatic event to reach the sea floor within a few hundred of years. In the upper, permeable layer of extrusives (2A), the vortex is ascending upwards, while in transit, approximately with the Darcy velocity. Our simulations support the hypothesis that shallow magmatic intrusions at intermediate spreading ridges are able to create low-temperature systems with the discharge temperatures a few dozens of degrees centigrade and exit velocities of a few meters per year.

We fail to produce realistic on-axis hydrothermal diffuse flow velocities here because there was no explicit cracks in the porous medium. In the next two chapters, we shall develop the necessary algorithms to do so.
Chapter 2

Simulating Convection in a 2D, Single-Fractured Medium

2.1 Introduction

We recognize that earth structures are essentially fractured porous media. The potential impact of fractures on hydrothermal circulation has been acknowledged by many [e.g. MacDonald 1982; Choukroune et al., 1984; Herzog et al., 1989; Morgan, 1991; Pezard et al., 1992; Lowell et al., 1995; van Everdingen, 1995], but the vast majority of numerical studies, while employing the notion of fracture, simply replace them with areas of higher permeability. Combined with the usual requirement for the permeability function to be smooth, this approach often results in either inadequate or memory-exhaustive algorithms.

A common starting point is to use the well-known solutions for laminar, 1D flow between two parallel plates or through pipes, derived from simplified Navier-Stokes equations [e.g. Bear, 1972; Turcotte and Schubert, 1982]. Usually, a parabolic velocity profile results, as we now deal with the no-slip conditions at the fracture boundaries for viscous fluid. The average velocity across the aperture is proportional to the applied pressure gradient, therefore by comparison with Darcy’s law, we assign for the planar fractures

$$k_f = \frac{\delta^2}{12},$$

(2.1)

and for the pipes,

$$k_p = \frac{r^2}{8},$$

(2.2)

where $\delta$ is the planar fracture’s aperture and $r$ is the radius of the pipe.

Yang, [1996] undertakes a systematic numerical treatment of the problem of coupled
2.1. INTRODUCTION

Heat and mass transfer in fractured medium, where a separate set of governing equations is used for fractures. They are included explicitly with the permeabilities given by the two expressions above. Edwards [personal communication] suggests the following approach for a single fracture. Exploiting symmetry of the problem, the fracture is moved to a lateral boundary, and its presence is replaced effectively by a special set of boundary conditions.

The original motivation behind this project was to verify the correct operation of the existing finite element (FE) software coded by J.Molson (known as HEATFLOW) and modified by J.Yang to include fractures, as virtually nothing else was available for cross-checks at the time. The idea is to use a proven, reputable code in the main routines and attach to it the fracture part through boundary conditions as standard input. The author has recently become aware that a similar approach was used independently in Dickson et al., [1995] and later appeared in Dickson's PhD thesis, which was not readily available at the time. In what follows, we solve the problem in the unfractured medium with MUDPACk package for the steady state as described in Chapter 1.

Historically, we started off from a conductive plate in electrostatics (or thermostatics up to notations) as a time-dependent problem of the diffusion of charge, but without advective terms, to single out the correct numerical scheme. Upon satisfactory results, the algorithm was subsequently extended to porous medium convection, but the time-dependent part of it was lost, since the main solver was best suited for stationary problems. Although the algorithm we are about to present is definitely limited, it turned out to be highly efficient for what it was designed.

Possible applications include both off-axial and on-axial hydrothermal circulation, enhanced locally by a single major fissure or an equivalent "thin" permeable zone. Another advantage is in that it can be attached to virtually any pre-programmed iterative solver with little effort. To distinguish the proposed algorithm from the FE code mentioned above, we will call it the finite difference method (FD) as it appears in [Yang et al., 1998]. We treat here only a planar vertical fracture, but the extension to a vertical pipe is straightforward.

Section 2.2 explains how the algorithm works, then we show convergence of the scheme analytically on a simplified 1D problem in Section 2.3. Section 2.4 cross-checks the outputs with the FE code on a benchmark problem. Section 2.5 is devoted to applications. We use the algorithm to study the impact of the fracture aperture and extent on hydrothermal circulation in a 2D porous box.
2.2 Numerical Algorithm for a Single-Fractured Medium

Consider steady convection in a 2D domain attached from the right to a vertical fracture of constant aperture $\delta$ as shown in Fig. 2.1. Assume for definiteness the right lateral boundary of the domain is adiabatic and impermeable, the upper and lower boundaries are both isothermal and impermeable, and the fracture extent from the base to the top of the domain, $H$. This set of extra assumptions isn’t mandatory, as we will see soon, however, the solutions sought need to be symmetric about the fracture plane. This symmetry argument, on the other hand, reduces the size of the mathematical problem to half the domain. That’s why the fracture appears on the boundary in Fig. 2.1. We note here at once that the mirror image of the solutions will be appended when displaying temperature, streamlines, heat flux profile, etc., so the fracture will be eventually shown in the middle of the whole domain.

Physics requires that the normal fluxes and tangential fields be continuous at the fracture-medium interface. A suitable procedure is then to compute the normal flux into the fracture from the domain, update the fields in the fracture, and give this update back to the medium as boundary conditions. The numerical process follows this path iteratively until all the boundary conditions are satisfied simultaneously. This is quite contrary to most conventional numerical schemes, where, say, Dirichlet boundary conditions are satisfied automatically by construction. Of course, to terminate the process, the usual convergence criteria for the interior points must also be in place.

Let us derive the fracture boundary conditions starting from the stream function. The
2.2. NUMERICAL ALGORITHM FOR A SINGLE-FRACTURED MEDIUM

notations are consistent with those of Chapter 1. Consider a portion of the fracture stretching from 0 (the base) to \( z \) along the vertical axis, width \( \delta \), and let \( \bar{v}_J \) and \( \bar{u}_J \) be the average vertical component and the horizontal component of the fluid velocity inside the fracture, respectively. The mass conservation equation (1.2) integrated over the specified fracture volume gives

\[
\rho_f \bar{v}_J \mid_{z} - \rho_f \bar{v}_J \mid_{0} = -2 \int_{0}^{\delta} v_x \delta \rho_f dz,
\]

(2.3)

whose right-hand side is the mass influx from the medium, and the factor of two is due to symmetry. We substitute expression (1.3) for \( \sigma \) and use the fact that \( \bar{v}_J \mid_{0} = 0 \) because the lower boundary is impermeable. The answer is simple

\[
\bar{v}_J = \frac{2p(\delta, z)}{\rho_f \delta}.
\]

Further, from Darcy's law (1.1), we have the continuity of \( v_x / k_x \) along the interface \( x = \delta / 2 \), if both pressure and temperature are to be continuous across the interface, thus

\[
\bar{v}_J = \frac{k_x}{k_x} v_x = \frac{k_x}{k_x} \frac{1}{ \rho_f} \frac{\partial \psi}{\partial x} \bigg|_{x=\delta/2}.
\]

(2.5)

The use of the average velocity, \( \bar{v}_J \), is justified, because in deriving \( k_f \) for the fracture in formula (2.1), exactly the same velocity is used. Combining this result with expression (2.4), one obtains

\[
\left( \frac{\partial \psi}{\partial x} - \frac{2 k_x}{k_x} \psi \right)_{x=\delta/2} = 0.
\]

(2.6)

Finally, we non-dimensionalize the last equation according to formulae (1.8) and introduce a fracture factor \( Q \)

\[
\left( \frac{\partial \psi^*}{\partial x^*} - \frac{2}{Q} \psi^* \right)_{x^*=1} = 0; \quad Q = \frac{k_x \delta}{k_x H}.
\]

(2.7)

The stream function boundary condition (2.7) appears to be of mixed type which can be routinely handled by a solver like MUDPACK. The fracture factor \( Q \) is a measure of the impact of the fracture on the convection pattern. If \( Q \) is small, equation (2.7) tends to the impermeable limit, \( \psi = 0 \), conversely, the fracture would "absorb" all the fluid, i.e. \( \partial \psi / \partial n = 0 \). However, condition (2.5) must still hold, and the zero limit is never reached.

To derive the fracture temperature boundary condition, it is helpful to cast the stationary energy conservation equation (1.6) in the divergence form

\[
div(\tilde{\xi}) = 0; \quad \tilde{\xi} = (\rho_f c_f T \bar{v}_J - \lambda_f \nabla T),
\]

(2.8)
2.2. NUMERICAL ALGORITHM FOR A SINGLE-FRACTURED MEDIUM

where \( \vec{\xi} \) will be called the heat transport vector. We integrate this equation over the fracture element \((-\delta/2, \delta/2, z_+, z_-)\), shaded in Fig. (2.1), using Gauss theorem in 2D

\[
\int \int \text{div}(\vec{\xi}) \, ds = \oint \vec{\xi} \cdot d\vec{n},
\]

where \( s \) is the element area and \( \vec{n} \) is the outward vector normal to the area boundary. The result of the integration is

\[
2 \int_{-\delta}^{\delta} \xi_z |_{z=\pm \delta} \, dz + \delta \xi_{\text{av}} = 0,
\]

where, again, \( \xi_{\text{av}} \) stands for the average over the fracture’s aperture, and the factor of 2 is due to symmetry. At the interface, \( x = \pm \delta \), we have continuity of the normal components of both mass and heat fluxes so that

\[
v_{fs} \bigg|_{x=\pm \delta} = v_s \bigg|_{x=\pm \delta} = \left( \lambda_m \frac{\partial T}{\partial x} \right)_{x=\pm \delta} = \left( \lambda_f \frac{\partial T}{\partial x} \right)_{x=\pm \delta}.
\]

The latter condition allows to express \( \partial T/\partial x \) inside the fracture element through that in the medium. We also assume that \( T(\delta/2, z) \) in the medium agrees with \( T(z) \) along the fracture and recall expression (2.5) for \( v_s \). After all this is done, we are now able to express everything in formula (2.10) in terms of the available quantities in the medium

\[
\xi_x |_{x=\pm \delta} = \rho_f c_f T \left( -\frac{1}{\rho_f} \frac{\partial \psi}{\partial x} \right) - \lambda_m \frac{\partial T}{\partial x},
\]

\[
\xi_z = \rho_f c_f T \frac{2\psi}{\rho_f \delta} - \lambda_f \frac{\partial T}{\partial z}.
\]

Substituting these two expressions above into integral (2.10), non-dimensionalizing, and using the identity

\[
(T \psi)_{z=\pm \delta} = 2 \int_{-\delta}^{\delta} (T \frac{\partial \psi}{\partial z} + \psi \frac{\partial T}{\partial z}) |_{z=\pm \delta} \, dz,
\]

we obtain

\[
\int_{-\delta}^{\delta} \left( \psi \frac{\partial T}{\partial z^*} \right) |_{z^*=\pm \delta} = \left( \frac{1}{2} \frac{\lambda_f}{\lambda_m H} \frac{\delta T^*}{\partial z^*} \right) |_{z^*=\pm \delta} = \int_{-\delta}^{\delta} \frac{\partial T^*}{\partial z^*} \, dz^*.
\]

The second term on the left in the above formula can be dropped. It represents heat conduction along the fracture. Typically, we have \( \lambda_f \approx \lambda_m \), but \( \delta/H \approx 10^{-5} \), while \( \psi^*, T^* \), and \( z^* \) are of the order of unity. The temperature boundary condition then reads

\[
\left( \psi^* \frac{\partial T^*}{\partial z^*} \right) |_{z^*=\pm \delta} = \left( \frac{\partial T^*}{\partial z^*} \right) |_{z^*=\pm \delta}.
\]
To begin the algorithm, we require some non-trivial initial approximation, \((\psi, T) \rightarrow (\psi_{ij}, T_{ij}); i = \{1, m\}; j = \{1, n\}\) which may or may not be the true unfractured solution, especially when the medium is subcritical. The only requirement is that the temperature field be different from a stratified distribution. The stationary governing equations to solve on the main domain are (1.9) and (1.10) without the time-dependent term, since we are calculating a steady-state solution. The set of required actions is described in the previous chapter. Now, the outermost iteration loop runs over some index \(n = \{1, N\}\). For each \(n\), there are \(3 - 5\) iterations over the governing equations with the mixed-derivative condition (2.7) and a fixed (Dirichlet) temperature, \(T_{ij}^{(2)}\), along the fracture. The rest of the boundary conditions is as desired. To advance from \(T_{ij}^{(n)}\) to \(T_{ij}^{(n+1)}\), is yet another two-step process. First, heat flux into the fracture is evaluated from the domain temperature via one-sided derivatives (see Fig. 2.1) which are substituted for the right-hand side of equation (2.15). After that, it becomes an ordinary differential equation (ODE) in \(z\). To integrate this ODE, we use the fourth-order Boole quadrature rules [Abramovitz and Stegun, 1968] and denote the resulting temperature values \(T_{ij}^{(n+1)}\). Finally, the boundary temperature is updated according to the following over-relaxation scheme

\[
T_{ij}^{(n+1)} = T_{ij}^{(n)} + E \left( T_{ij}^{(n+1)} - T_{ij}^{(n)} \right),
\]

which is substituted for the right-hand side of equation (2.15). After that, it becomes an ordinary differential equation (ODE) in \(z\). To integrate this ODE, we use the fourth-order Boole quadrature rules [Abramovitz and Stegun, 1968] and denote the resulting temperature values \(T_{ij}^{(n+1)}\). Finally, the boundary temperature is updated according to the following over-relaxation scheme

\[
T_{ij}^{(n+1)} = T_{ij}^{(n)} + E \left( T_{ij}^{(n+1)} - T_{ij}^{(n)} \right),
\]

where \(E\) is an over-relaxation parameter [e.g. Iserles, 1996]. The process is then repeated until either \(n = N\), or

\[
\left| T_{ij}^{(n+1)} - T_{ij}^{(n)} \right| < 0.5E \left| T_{ij}^{(n)} + T_{ij}^{(n+1)} \right|
\]

for all points on the fracture-medium interface, where \(\epsilon\) is a tolerance level. Numerical experiments have revealed that for convergence to occur, \(\epsilon\) should be around 0.1 - 0.2. In most cases, 10 - 30 boundary iterations with this \(E\) is sufficient to achieve \(\epsilon < 0.005\).

It is important to work with the correct value of \(\partial T^*/\partial x^*\) at the base of the fracture when integrating equation (2.15) as an ODE. If the fracture intersects the bottom boundary, this value cannot be obtained from the right-hand side of equation (2.16) because \(\psi(x, 0) = 0\) there. A simple workaround is as follows. If \(T\) is subscripted as in Fig. 2.1, then by analogy with formula (2.17)

\[
\left( \frac{\partial^2 T}{\partial x^2} \right)_{ij} \approx \frac{-3 \left( \frac{\partial \psi}{\partial x} \right)_{61} + 4 \left( \frac{\partial \psi}{\partial x} \right)_{62} - \left( \frac{\partial \psi}{\partial x} \right)_{53}}{2\Delta x}.
\]

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2.3. CONVERGENCE OF BOUNDARY ITERATIONS

On the other hand, from the energy conservation equation (1.10) we have directly

\[
\left( \frac{\partial^2 T}{\partial z^2} \right)_{k_1} = - \left( \frac{\partial^2 T}{\partial z^2} \right)_{k_1}, \tag{2.21}
\]

since \( \partial/\partial t = 0 \), \( (v_3)_{k_1} = 0 \), and \( (\partial T/\partial z)_{k_1} = 0 \). The last statement is based on the plausible assumption that the temperature profile across the fracture (which we have so far ignored while averaging) is a symmetric function for our symmetric problem. Then, \( (\partial T/\partial z)_{k_1} \) can be determined from equations (2.20) and (2.21). Finally, we take \( T_{k_1} \approx T_{k_1} \), and so is then true for the associated tangential derivatives, because the temperature variations across the fracture are small. This completes a basic description of the algorithm, however, we elaborate a bit more on it in the next section.

As a final remark, technically, one can envisage another version of the outlined algorithm that requires the fields in the domain be transferred to the fracture and the normal flux updates returned back to the domain, but this option would far too often lead to a rapid numerical crash. Why this happens is not completely understood, but the fact is the algorithm would diverge after just a few iterations.

2.3 Convergence of Boundary Iterations

The numerical algorithm just described is a sort of an implicit boundary iteration scheme. On some occasions, we found it performs poorly or even fails if \( Q \) is very large, i.e., the fracture has a significant impact globally. The reason for this behaviour is unknown, but it may be a shortcoming of the main solver. A simple replacement of the mixed-derivative condition (2.7) by the following explicit rule which is a classical splitting,

\[
\psi_{i,j}^{(n+1)} = \frac{2}{Q} \left( \psi_{i,j}^{(n)} \right) \left( \psi_{i,j}^{(n)} \right), \tag{2.22}
\]

has turned out to be the universal remedy. The expression above can be rearranged if we use formula (2.7) for \( Q \) and (2.16) for the derivative on the right-hand side

\[
\psi_{i,j}^{(n+1)} = \frac{4\psi_{i,j}^{(n)} - \psi_{i,j}^{(n)}}{R + 3}, \quad R = \frac{4k_1\Delta x}{k_1\delta}. \tag{2.23}
\]

The newly introduced parameter \( R \), unlike \( Q \), contains \( \Delta x \) rather than the thickness of the domain \( H \). It measures the impact of the fracture on a local scale, set by the discretization. If, for example, \( k_1 = 10^{-16} \text{ m}^2 \), \( \Delta x = 30 \text{ cm} \), and \( \delta = 2 \text{ mm} \), then \( R \approx 10^{-7} \), which can be ignored in most practical cases.

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2.3. CONVERGENCE OF BOUNDARY ITERATIONS

We now demonstrate that implementing rule (2.23) for \( R = 0 \) yields a convergent numerical procedure on the following simple example in 1D. Consider a second-order boundary problem

\[
\frac{d^2 f}{dx^2} = g(x); \quad x = [x_{\text{min}}, x_{\text{max}}]; \quad \frac{df}{dx}(x_{\text{min}}) = 0; \quad f(x_{\text{max}}) = f_n x,
\]

(2.24)

which we discretize on a uniform mesh \( x_i : i = \{1, n_x\}; \Delta = (x_{\text{max}} - x_{\text{min}})/(n_x - 1) \) via standard FD rules. The system matrix is tri-diagonal and can be solved even "exactly". We will, however, launch an iterative process, solving with the Dirichlet boundary condition at \( x_{\text{min}} \), whose value is known from the solution at the previous iteration \( n - 1 \)

\[
\begin{align*}
    f(0) &= 0; \quad f(n+1) = \frac{4}{3} f(n) - \frac{1}{3} f(n). \\
\end{align*}
\]

(2.25)

Medvedev [personal communication] suggested to proceed in operator formalism

\[
L f(n) = g(n); \quad f_{n+1} = f_n; \quad \begin{cases} 
    g(n) = M : (f(n), g(n-1)),
\end{cases}
\]

(2.26)

where \( L \) is the system matrix and \( M \) is some operator. In discretized form, we have to the second order in \( \Delta \)

\[
\begin{align*}
    L_{i,i} &= L_{n_x,n_x} = 1, \quad L_{i,i+1} = 1, \quad L_{i,i} = -2, \quad i = \{2, n_x - 1\} \\
    f(n) &= (f_1(n), f_2(n), \ldots, f_{n_x-1}(n), f_{n_x}) \quad g(n) = (\frac{\Delta}{\frac{n_x}{2}} (f(n-1) - f(n)), \Delta^2, \ldots, \Delta^2, \frac{n_x}{2}, f_{n_x}),
\end{align*}
\]

(2.27)

where the rest of the elements in the \((n_x \times n_x)\) matrix \( L \) is zero and the bar sign stands for the transposition operation. For convergence to occur, the error norm must decrease

\[
\|f(n+1) - f(n)\| \leq \|f(n) - f(n-1)\|.
\]

(2.28)

Define for convenience a residual \( e(n+1) = f(n+1) - f(n) \). Then, equation (2.28) can be written as \( \|e(n+1)\| \leq \|e(n)\| \). Further, we observe that

\[
L e(n+1) = g(n+1) - g(n),
\]

(2.29)

where the right-hand side takes a very simple form. We express it as

\[
g(n+1) - g(n) = M e(n),
\]

(2.30)
where matrix $M$ has only two non-zero elements, $M_{1,2} = 4/3$ and $M_{1,3} = -1/3$. Combining (2.29) and (2.30), we obtain

$$L e^{(n+1)} = M e^{(n)}$$

and by induction

$$e^{(n)} = S^n e^{(0)}; \quad S^n = (L^{-1}M)^n; \quad n \geq 1\quad (2.32)$$

Condition (2.28) then requires $S^n \to 0$. With the help of symbolic computation available with Mathematica (if not otherwise by inspection) it is easy to see that $S^n \equiv S$ contains only two columns with non-zero elements

$$S_{i,2} = \frac{4}{3} \frac{n_x - i}{n_x - 1}; \quad S_{i,3} = -\frac{1}{4} S_{i,2}, \quad (2.33)$$

so that the last row, $i = n_x$, contains zeroes only, since we retained the Dirichlet point, $f_{n_x}$, within the matrix. The elements $S_{i,j}$ actually show the impact of the uncertainty in $f$ at $x = x_i$ on the uncertainty in the interior values of $f$. Straightforward multiplication of $S$ by itself $n$ times preserves the original pattern of zeroes; the non-trivial elements are

$$S_{i,2}^n = S_{i,2}(S_{i,2} - \frac{S_{i,3}}{4})^n = S_{i,2}(\frac{n_x - i}{n_x - 1})^n; \quad S_{i,3}^n = -\frac{1}{4} S_{i,2}^n\quad (2.34)$$

We see that for any finite $n$, $S^n \to 0$, although for large $n$ convergence is expected to slow down. This is precisely the behaviour observed both in 1D and 2D. Later, we will employ this approach for a 3D subregion which requires grid refinement.

As a final remark, there may be little or no advantage implementing the proposed boundary iteration (2.23) when the problem can be reliably solved by conventional means. However, when the required solution is just a part of some multi-level iterative procedure, including $L f = g$ itself, using scheme (2.23) in place of the mixed-derivative boundary condition is often preferable. At least we found so for our problem.

2.4 Comparison Against FE Method

Now we compare the output of our code against the FE software, mentioned in the introductory section, on the following benchmark model shown in Fig. 2.2. A 2D water-saturated, porous domain with dimensions 20 m by 10 m has all its four boundaries impermeable. The temperatures of the upper and lower boundaries are kept constant at 0°C and 10°C, respectively. The side boundaries are adiabatic. The permeability and the average thermal conductivity of the medium, porosity, and the volumetric coefficient of thermal expansion for
the fluid are assigned the values of $10^{-10}$ m$^2$, 5 W/(m K), 10%, and $0.8 \cdot 10^{-3}$ K$^{-1}$, respectively. We set $\mu = 1.787 \cdot 10^{-3} \text{kg}/(\text{m s})$ which should be good for $T_{\text{max}} < 10^0 \text{C}$. The parameters are so chosen that the Rayleigh number, computed as per expression (1.14), equals to 36, less than the critical value of 47, and convection is inhibited. Now a 3 mm-thick fracture is introduced that rises through the middle from the base to the top of the domain. It helps to maintain a quite vigorous steady convection, as the isotherms are bent strongly near the fracture. It is interesting to note that $Q = 2.223$ for this setting.

Figure 2.3 [Yang et al., 1998] compares the temperature and velocity fields between the FE and FD solutions. Clearly, two distinct numerical techniques, also different in the way the fracture is incorporated, produce very close results. To quantify the differences, we plot the relative temperature and fluid velocity profiles along the fracture, normalized on their corresponding maximum values of $10^0 \text{C}$ and 1.52 mm/s, respectively. These profiles are shown in Fig. 2.4, [Yang et al., 1998], where the solid line denotes the FE solution and the open boxes represent the FD solution. The temperature and fluid velocities along the fracture agree within 5.4% and 4.3%, respectively on a mesh of 40 x 20 elements. The size of the mesh effectively reduces to 21 x 21 for us, since we take advantage of symmetry. The FE algorithm produces time-dependent solutions and takes 6 hours to reach steady state on an IBM RISK 8000 at 166 MHz. Our calculations are done in 15 seconds on the same machine because we solve for the steady state directly. We also repeated them on a number of refined grids (which could take the FE days) to confirm the solutions stay practically intact, and the 41 x 21 grid is adequate.
2.4. COMPARISON AGAINST FE METHOD

Figure 2.3: Temperature and velocity fields for the single-fractured model shown in Fig. (2.2): comparison between the FE and FD solutions [Yang et al., 1998].
2.4. COMPARISON AGAINST FE METHOD

Figure 2.4: Normalized temperature (A) and fluid velocity profiles (B) along the fracture for the model shown in Fig. 2.2: comparison between the FE and FD solutions [Yang et al., 1998].
2.5 IMPACT OF FRACTURE APERTURE AND EXTENT ON STEADY CONVECTION

To quantify the impact of fracture aperture and extent on steady convection, let us consider a generic model, shown in Fig. 2.5. The geometry and boundary conditions are similar to the ones in Fig. 2.2. The size of the model is fixed at 2 km by 1 km, discretized on a uniform 129 x 65 grid, $k_a = k_c = 10^{-13} m^2$, $\mu = \mu(T)$ and $\rho_f = \rho_f(T)$ as discussed in Chapter 1. $c_f = 4174 J/(kgK)$, $\lambda_f = 0.5 W/(mK)$, $\lambda_a = 3 W/(mK)$, and the crustal porosity is assumed 10% everywhere. All boundaries are impermeable, the sides are adiabatic. The base and the top of the model are maintained at constant temperatures of 100°C and 0°C, respectively. In the absence of convection we have a heat flux of 275 mW/m² through the top of the domain (the sea floor), typical of young oceanic crust aged > 0.1 Ma. Circulation, however, does take place, featuring two convection cells. We superimpose the temperature and streamlines contours at this ambient state and show them in Fig. 2.5.

The question we would like to address here is, "What difference does a vertical fracture make?", if we place it in the middle of the domain and allow its aperture and extent vary.

To quantify the anticipated changes, we will look at the following parameters: heat flux through the top boundary, maximum fluid velocity in the fracture, $v_{max}$, mass transport rate through the fracture, $m = \rho u \delta$, and the Nusselt number, $Nu$, defined in Chapter 1 as the ratio of the total heat power transported through the system when convection exists to that when it happens by conduction only. For the unfractured case (Fig. 2.5), we have...
2.5. IMPACT OF FRACTURE APERTURE AND EXTENT ON STEADY CONVECTION

\( Nu = 2.4 \). A few remarks are in order. From the discussion in the previous sections, parameter \( Q = (k_T \delta)/(k_H \ell) \) would seem to be more meaningful as an independent variable than the fracture aperture \( \delta \) itself. Note also that at the steady state and with the adiabatic side walls, the total heat power through any horizontal level should ideally be the same. We carry out the calculations to the point where the relative heat power disbalance is less than 0.5% over all 65 vertical layers. Since we are in 2D, the dimensions of the just introduced mass transport rate are \([kg/(m \cdot s)]\).

The simulations are now run for the following three cases: (A) fracture extends fully across the model from 1000 mbsf to 0 mbsf, (B) from 1000 mbsf to 400 mbsf, and (C) from 800 mbsf to 200 mbsf. The fracture aperture ranges from 0.3 mm to 4 mm in each case, so that the corresponding changes in \( Q \) are 0.0225–53.33. The results for \( T \) and \( \psi \) are displayed in Fig. 2.6 through Fig. 2.8 for a selected subset of apertures, \( \delta = (0.5, 0.7, 1.0, 2.0) \) mm. We observe immediately that the presence of fracture is already felt at \( Q \sim 0.1 \), which corresponds to \( \delta \sim 0.5 \) mm in our example. The distortion from the unfractured case of the temperature and flow lines near the sea floor are most pronounced when the fracture extends fully across the model.

Based on the calculated temperature and stream function values, we plot heat flux profiles through the sea floor in Fig. 2.9, (A) through (C) for the three cases, respectively. Figure 2.10 shows the relationships \( Nu(Q), n\dot{h}(Q), \) and \( v_{max}(Q) \) in sections 1, 2, and 3, respectively. In case A (full extent), increasing the aperture results in the increase of the hydrothermal power through the system and fluid mass transported through the fracture. Heat flux distribution sharpens near the fracture and falls off on flanks. As \( Q \) exceeds a value between 1 and 2, this growth stagnates, and at \( Q \sim 5 (\delta \sim 2 \) mm) saturation occurs. To get a feel for numbers, we compare \( \dot{h} = 11.74 \) kg/(m \cdot s) and \( Nu = 3.04 \) for \( \delta = 3 \) mm versus \( \dot{h} = 0.47 \) kg/(m \cdot s) and \( Nu = 2.43 \) for \( \delta = 0.3 \) mm. As for the maximum velocity in fracture, \( v_{max} \), it takes its highest value of \( \sim 0.8 \text{ cm/s} \) when \( Q \sim 1 \), then drops approximately linearly with \( \delta \) to maintain \( v_{max} \delta \sim \text{const} \). If \( \rho_f \) is not a strong function of local temperature changes, as in our example. Thus, the fracture may greatly impact convection on a local scale, but on the lateral scale of the associated convection cell, its average effect is rather modest, as \( Nu \) increases by just 36% (compare with the corresponding increase of 140%: convection versus conduction in unfractured medium). An explanation to this may be that fluid is supplied by the porous matrix to the fracture. The matrix capacity as a carrier is limited by its permeability and depends on macroscopic thermal conditions. So fracture is there to mainly channel heat and mass.

Qualitatively similar behaviour is exhibited in cases B and C, although all the effects are scaled down somewhat. In case B, the fracture originates right from the base of the
2.5. IMPACT OF FRACTURE APERTURE AND EXTENT ON STEADY CONVECTION

Figure 2.6: Temperature field and stream lines for the model in Fig. 2.5 with a fracture of variable apertures $\delta$, extending fully through the middle of the model (case A).
2.5. IMPACT OF FRACTURE APERTURE AND EXTENT ON STEADY CONVECTION

Figure 2.7: Temperature field and stream lines for the model in Fig. 2.5 with a fracture of variable apertures $\delta$, rising 600m off the base through the middle of the model (case B).
2.5. IMPACT OF FRACTURE APERTURE AND EXTENT ON STEADY CONVECTION

Figure 2.8: Temperature field and stream lines for the model in Fig. 2.5 with a fracture of variable apertures $\delta$, originating 200 m above the base and extending 600 m through the middle of the model (case C).
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Figure 2.9: Lateral heat flux variations on the sea floor for a range of fracture apertures: (A) fracture extends fully across the model, (B) fracture extends from the base (1000 mbsf) to 400 mbsf, (C) fracture extends from 800 mbsf to 200 mbsf. The unfractured model is shown in Fig. 2.8.
2.5. IMPACT OF FRACTURE APERTURE AND EXTENT ON STEADY CONVECTION

Figure 2.10: Nusselt number, $N_u$, mass rate through fracture, $\dot{m}$, and maximum velocity in fracture, $v_{max}$, as functions of parameter $Q$ and fracture aperture $\delta$, shown in sections 1, 2, and 3, respectively for the three fracture locations: (A) fracture extends fully across the model, (B) fracture extends from the base (1000 mbsf) to 400 mbsf, (C) fracture extends from 800 mbsf to 200 mbsf. The unfractured model is shown in Fig. 2.5.
domain and causes more net power through the system than in case C, where both ends of the fracture are in the interior, while the length is kept the same, 600 m. In case C, though, the heat flux profile through the sea floor is affected much stronger. We also note in case B an increase in the heat flux not only near the fracture but on flanks, too. This is because the relatively hot fluid spreads out more uniformly and causes a unilateral uplift of the near-surface isotherms when it leaves the upper portion of the fracture, which is lower on average than in the other two cases where this effect is not observed.

We must say that very similar conclusions regarding the key $Q$ and $N_{t,\text{max}}$ values and the saturation effect in $\nu$ have been drawn from other models with different initial $N_u$ and anisotropic coefficient, $k_f/k_s$, of which the model discussed here is only an example.

2.6 Summary

We have developed an efficient and portable algorithm to handle a vertical fracture or highly permeable zone in modeling of steady hydrothermal circulation in 2D.

The algorithm is successfully tested against the existing FE code on a benchmark model. The results also confirm that a fracture can initiate and maintain convection in a subcritical medium. The addition of the fracture acts to boost the flow rates.

In systems with developed convection, we found a major dimensionless parameter to characterize the impact of the fracture, which is the ratio of the permeability-thickness product of the fracture to that of the host medium. When this parameter is greater than $2 - 5$ (depending on prescribed tolerance), we observe a saturation in the hydrothermal power transported through the system and mass rate through the fracture because flow is medium-limited.

The maximum heat power increase due to the vertical fracture extending fully through the domain is about 1/3 on the lateral scale of one convection cell. Local enhancements for the mass rate and heat flux due to fracture channeling are about an order of magnitude.

For fractures originating and terminating inside the layer, the amount of heat power transported through the system is controlled by the position of the lower end, while the heat flux distribution through the sea floor is mainly determined by the location of the upper end.
Chapter 3

Numerical Algorithm for Modeling Hydrothermal Convection in a 3D Fractured Porous Medium.

3.1 Introduction

The development in this chapter is due to a number of frustrating attempts to tackle one 3D problem (to be dealt with in Chapter 5) with the available software at hand. The software used in Chapters 1 and 2 has appeared to be limited in three ways. It is two dimensional, it deals with a single fracture and is not valid for high fluid velocity. The latter constraint is because the central differencing employed by MUDPACK (as well as many other commercial solvers) is not suitable for advection-dominated transport problems.

To broaden our modeling capabilities, we develop here a more flexible numerical tool, which works in 3D, arbitrary fractured medium with virtually no velocity limitations. We continue to focus on the steady convection and single-phase fluid.

The beginning of this work is dated back to 1998 when the author was aware of only a sparse selection of papers on the true 3D hydrothermal circulation in oceanic crust. Travis et al., [1991] tackle 3D, time-dependent simulations on a larger (10 km) scale in unfractured isotropic medium of rather low permeability. Yang, [1996] models a black smoker discharge site at TAG by actually forcing the upward flow. Lately, Berndt et al., [1998] have started a major project, attempting to incorporate all available data on chemical reactions and phase changes of hydrothermal constituents into their 3D code SalTherm. Berndt indicated [personal communication] that they would not consider fractures, making other issues the top priority.
3.1. INTRODUCTION

Generally speaking, typical actions required to model a physical process involve mathematical formulation of the problem, discretization of the governing equations, numerical solution of the system matrix, and interpretation, linked with the assessment of numerical resolution. Natural convection is described by a coupled system of elliptic PDEs of the second order like (1.5) and (1.6), which upon the discretization becomes a coupled system of algebraic equations of the form $Ax = b$ to solve for the vector $x$. If the coefficients are smooth and the fluid velocity is not very high, most of the common techniques, such as FD or FE, with the central differencing for the advective terms result in very similar system matrices $A$. In an environment like the mid-oceanic ridge, advective heat transfer becomes significant and often dominant. The governing equations then effectively become "parabolic" [Adams, 1989], and the central differencing employed by many solvers ultimately leads to faulty results [Tolstykh, 1994]. This was already recognized by Sharfetter and Gummel, [1969] in their work on semiconductor device simulations, where the ion concentration is analogous to temperature in our case. Heinrich, [1996] constructs an example which shows that in such a situation, even the exact algebraic solution of the system matrix does not converge to the true analytical solution when the discretization step is shrunk to zero. One way to deal with the problem is to use the so-called upstream or upwind discretization for the advective terms [e.g. Tolstykh, 1994], in which they are approximated by one-sided differences in the direction of flow. Having done so, we end up with generally asymmetric and not necessarily diagonally dominant matrix, which presents a challenge for most classical iterative schemes. The popular conjugate gradient method (CG) [e.g. Khosla and Rubin, 1981] is designed for symmetric matrices, but actually it is just one member of the whole family termed Krylov subspace methods [Freund et al., 1992; Meier-Yang, 1992; Tong, 1992] based on the iterative minimization of the residual norm. We chose GMRES (generalized minimal residual) of Saad and Schultz, [1986]. It seems to work correctly and stably for our problem and is recommended by many [e.g. Heinrich, 1996], but is by no means the only possibility, neither is it the "best" compared to its competitive siblings (QMR, BiCGStab, etc.). Before GMRES is applied, the matrix is typically preconditioned to improve its structure, which is achieved by pre-multiplying the system equation by a special matrix. We opted here for the incomplete LU (ILU) preconditioner.

Going back to the discretization itself, many of the upwind schemes are only first order accurate and, worse, non-conservative. This can be easily imagined as the introduction of artificial power sources or sinks, once we have modified the rules to compute advective fluxes. Certainly, a solver that is supposed to be used for assessment of heat and mass fluxes must be at least conservative. So we naturally come to the idea of using the finite volume (FV) , conservative approach that has an excellent reputation in the fields of fluid mechanics,
3.1. INTRODUCTION

electromagnetics and heat transfer [e.g. Patankar, 1980; Arakawa and Lamb, 1977]. Its use here is facilitated by the fact that the governing equations can be put in the divergence form. We require that this divergence vanish (or be equal to the source power density if any) over a control volume around each nodal point, whose faces reside on a staggered grid. It is well known how to construct conservative, mimetic discretization schemes for operators like div and curl on staggered grid of any logically rectangular geometry [e.g. Shashkov and Steinberg, 1996; Hynman and Shashkov, 1996] which mimic the original differential operators in their vector properties. We chose the simple rectilinear grid, and adopted a well-tested, compact, second-order scheme for the temperature equation from [Nogotov, 1978]. The flow equation, on the other hand, has the standard, self-adjoint form, for which the required discretization is immediate.

We find the FV method to handle well step-like, sharp discontinues in permeability, including such extremes as fractures, so that no artificial smoothing over a few nodal points is necessary. Following the results of Chapter 2 that the impact of the fracture is mainly controlled by the permeability-thickness product in the direction of flow, we offer a simple and efficient scheme to explicitly map any desired distribution of fractures by modifying the transport properties within small control volumes. The method is also very flexible when it comes to the inclusion of source terms and specialized boundary conditions.

A couple of words are in order for the defense of simple structured grids and the FV-FD method. There are many encouraging reports on the use of the FV method on rectangular grids with the so-called fictitious domain methods [Bertrand and Tanguy, 1998], where the properties of the continuum are modified to account for the presence of irregularities with complex geometry or even the distinct physics [Ritz and Caltagirone, 1998]. The simplest the grid, the easier it is to find a good conservative scheme without compromising other issues. The computational time savings may be huge, too: 3 hours versus 2 days with nearly identical outputs on the same machine, according to one example of Bertrand and Tanguy [1998] for the 3D Navier-Stokes equation in a visco-elastic medium. And, of course, it is much easier to code and debug. Next, we would like to make a clear distinction between FE, FD, and FV. The latter is rather a strategy which can go together with either FD or FE [Cai et al., 1997]. We use here the FD method to discretize fluxes for its simplicity, however, it would not be correct to always assume FE to be a superior technique. On rectangular grids, there is hardly a difference between the two [Iserles, 1996]. In general, correctly executed, FD performs just fine on arbitrary shaped domains and random, self-adaptive grids [e.g. Karamyshev et al., 1996].

Our programming efforts are mainly concentrated on the discretization, boundary conditions, fracture mapping, matrix assembly, and general drivers. The rest is built of pre-
3.2 GOVERNING EQUATIONS

programmed subroutines, such as format conversion, ILU, and GMRES, coded by Y. Saad and K. Wu. All these modules are part of the SPARSEKIT package [Saad, 1990], available at www.netlib.org. The assembled code is validated on a few selected models and extended to the two-grid case. We will use it in the next two chapters for various 3D applications.

3.2 Governing Equations

Let us express the stationary governing equations in the divergence form. The use of stream-function in 3D is rather cumbersome, so it will be convenient to introduce a pressure variation, $P$, from a reference state of hydrostatic equilibrium

$$P = p - \rho_0 (H - z) - p_e,$$

where $\rho_0$ and $p_e$ are the reference density and pressure at the sea floor. As before, we assume the vertical $z$-axis to be directed upwards, and the sea floor level to be at $z = H$.

Straightforward substitution of both expression (3.1) and the Darcy’s law (1.1) into the mass conservation equation (1.2) with the zero source term gives

$$\frac{\partial}{\partial x} \left( \mu \frac{\partial P}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial P}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial P}{\partial z} \right) = \frac{\partial}{\partial z} \left( \rho \frac{k_z}{\mu} (\rho_0 - \rho_f) y \right).$$

We have introduced the heat flux vector, $\xi$, in Chapter 2, equation (2.8). Define in addition a mass flux vector $f$, so that we have

$$\xi = -\lambda \frac{\partial \rho T}{\partial z} + \rho \nu v \frac{\partial T}{\partial z}, \quad f = -\frac{\partial}{\partial z} \left( \rho_0 \frac{\partial P}{\partial z} + \rho \nu \frac{\partial \rho}{\partial z} \right),$$

where $\nu = \{z, y, z\}$ is a dummy summation index and $\delta_{\nu z}$ is a Kronecker delta. The conservation laws require the divergence of each vector above be equal to zero or to an appropriate source term, which will be retained for generality. It is then customary to integrate the governing equations over a control volume $V$ bounded by a surface $S$ using Gauss theorem

$$\int \int \int \frac{\partial A}{\partial x} dV = \int \int A \nu dS,$$

valid for any vector field $\vec{A}$. Making use of expressions (3.3), the governing equations are now

$$\int \int \xi dS = G, \quad \int \int f dS = M.$$

(3.5)
Figure 3.1: Finite volume discretization near a solution node. The z-direction is highlighted.

where $G$ is the net heat power and $M$ is the net mass rate within volume $V$ due to external sources. In this form, the equations are most suitable for the FV discretization.

### 3.3 FV Discretization

For clarity, we will do the derivations on a uniform grid $(x_i, y_j, z_k)$, where $i = \{1, nz\}$, $j = \{1, ny\}$, and $k = \{1, nz\}$, with equidistant increments $\Delta_x$, $\Delta_y$, and $\Delta_z$, respectively, although in the software they may be variable. Consider a nodal point $(i, j, k)$ and the associated rectilinear control volume $V_{ijk}$ bounded by the six planes $x_{i+1/2} = x_i + \Delta_x/2$, $y_{j+1/2} = y_j + \Delta_y/2$, and $z_{k+1/2} = z_k + \Delta_z/2$, which is shown in Fig. 3.1. Since the permeability tensor is assumed diagonal, all numerical operators on our grid are separable. So we can focus on, say, the $x$-direction, highlighted in the figure. The secondary set of nodes, located half-ways between the solution nodes (shown as squares), form a staggered grid. The following approximations are made. A flux evaluated at a staggered node as per expression (3.3), will be assumed to be the average value over the face. Secondly, all the material properties $\eta = \{\rho_f, \rho, c_f, \lambda_m, k\}$ taken e.g. at staggered node $(i + 1/2, j, k)$ will be the averages over the volume $V_{ijk}$ translated by $\Delta_x/2$ in the $x$-direction. If $n_{ijk}$ and $n_{i+1,j,k}$ are specified at the solution nodes and stand for the representative averages over the volumes $V_{ijk}$ and $V_{i+1,j,k}$.
Section 3.3: FV DISCRETIZATION

Then averaging between the two yields [Patankar, 1980]

\[ \eta_{i,j,k} = \frac{2\eta_{i,j,k} \eta_{i,j+1,k}}{\eta_{i,j,k} + \eta_{i,j+1,k}} \]  

The easiest way to arrive at this expression is via a frequently used analogy with Ohm’s law [e.g. Bear, 1972; Lowell, 1991] in which permeability is the direct analog of conductivity. In our case, two different conductors of the unit cross-section and half the unit length each, connected in series, are to be replaced by the equivalent conductor of the unit volume. In general, the required average for \( \eta \) may be obtained by integration assuming any desired polynomial distribution of the quantity between the solution nodes. We will leave the options open and denote the answers as \( \eta_{i1/2,j,k}, \eta_{i,j,k}, \eta_{i,j+1/2,k} \) for short.

Define fluid transport matrices on the staggered grid

\[
Q_{i+1/2,j,k}^p = -\rho \frac{\partial_\eta \psi \psi}{\psi} \left( \frac{\partial_\eta \psi \psi}{\psi} \right)_{i+1/2,j,k}, \quad Q_{i,j+1/2,k}^p = -\rho \frac{\partial_\eta \psi \psi}{\psi} \left( \frac{\partial_\eta \psi \psi}{\psi} \right)_{i,j+1/2,k}, \quad F_{i,j+1/2,k} = Q_{i,j+1/2,k}^p \left( \Delta \left( \rho \beta - \rho \bar{j} \right) \right),
\]

where \( \beta_x, \beta_y, \) and \( \beta_z \) are geometric factors. If \( i = 1 \) or \( i = nx \), \( \beta_x = 1/2 \), else \( \beta_x = 1 \). Similar statements apply to \( \beta_y \) and \( \beta_z \) with the obvious change of indices. Now we can easily express fluid rate components on the staggered grid, \( \bar{j} = \bar{j}^p \)

\[
q_{i+1/2,j,k}^p = Q_{i+1/2,j,k}^p \left( P_{i+1,j,k} - P_{i,j,k} \right), \quad q_{i,j+1/2,k}^p = Q_{i,j+1/2,k}^p \left( P_{i,j+1,k} - P_{i,j,k} \right), \quad q_{i,j+1/2,k}^p = Q_{i,j+1/2,k}^p \left( P_{i,j+1,k} - P_{i,j,k} \right) - F_{i,j+1/2,k},
\]

With the above definitions, the discretized flow equation (3.5) for the interior nodes becomes

\[
q_{i+1/2,j,k} - q_{i-1/2,j,k} - q_{i,j+1/2,k} - q_{i,j-1/2,k} + q_{i,j+1/2,k} \left( P_{i,j,k+1} - P_{i,j,k} \right) - q_{i,j-1/2,k} \left( P_{i,j,k} - P_{i,j,k-1} \right) = F_{i,j,k+1/2} - F_{i,j,k-1/2} + M_{i,j,k},
\]

It is supposed that the temperature field, \( T_{i,j,k} \), is available to calculate all temperature-dependent coefficients in expression (3.9).

The starting point to discretize the temperature equation is the availability of the fluid rates, \( q_i \), on the staggered grid, whose quick calculation is facilitated by storing and scaling of the transport matrices (3.7). We also need at least an estimate for the temperature field (e.g. from the previous iteration), because the equation is non-linear and coefficients \( \eta \) depend on temperature themselves. We adopt the upwind, conservative scheme from [Nogotov, 1978]
3.4. **BOUNDARY CONDITIONS**

where $D_x$, $D_y$, and $D_z$ are difference operators on the staggered grid for the $x$, $y$, and $z$-direction, respectively. We give the explicit formula for $D_x$ only, as the other two are constructed completely similarly:

$$D_x T_{i,j,k} = a_{i-1/2,j,k} (T_{i+1,j,k} - T_{i,j,k}) + q_{i+1/2,j,k} c_{i+1/2,j,k},$$

$$-a_{i+1/2,j,k} (T_{i-1,j,k} - T_{i,j,k}) - q_{i-1/2,j,k} c_{i-1/2,j,k},$$

where

$$a_{i-1/2,j,k} = \frac{\theta_{i-1/2,j,k}}{1 + \frac{q_{i-1/2,j,k}}{\omega_{i-1/2,j,k}}}$$

and

$$\theta_{i-1/2,j,k} = \lambda_{i-1/2,j,k} \frac{\beta_y \beta_z \Delta x}{\Delta z}.$$  \hfill (3.11)

We see that to be conservative, this upwind discretization requires a correction to the conductive component of flux in the denominator of the first expression in (3.12). We briefly remark that for a non-uniform grid, the only correction to make is e.g. to replace $\beta_y \beta_z \Delta x / \Delta z$ by $(y_{j+1} - y_{j-1})(z_{k+1} - z_{k-1})/4|x_{l+1} - x_l|$ in the expression for $\theta_{i-1/2,j,k}$.

### 3.4 Boundary Conditions

We treat only Neumann and Dirichlet type boundaries. If the function is specified, no action is required. If the flux is specified at the solution nodes on a boundary, neither equation (3.9) nor (3.11) prescribe a rule to evaluate heat power or mass rate through the boundary faces, but they are not necessary. We elect not to enforce the boundary conditions in the strong sense, e.g. via explicit one-sided approximations for the derivatives. The required contributions can be evaluated directly, multiplying the prescribed boundary fluxes by the appropriate face areas. The result is treated as a volumetric source of power or mass and moved to the right-hand side. For example, assuming all outer boundaries impermeable and no sources of mass present, the flow equation produces the following near the corner (1,1,1)

$$2Q_{i-1/2,j,1}^x (P_{1,1,1} - P_{j,1,1}) + Q_{i,1/2,j}^x (P_{1,1,1} - P_{i,1,1}) + Q_{i,j,1}^x (P_{1,1,2} - P_{i,1,1}) = F_{1,1,1}^x.$$ 

\hfill (3.13)
3.5. FRACTURES

In the spirit of FV, this expression secures zero net balance over the entire control volume, which is incidentally \( \frac{1}{2} \Delta x \frac{1}{2} \Delta y \frac{1}{2} \Delta z \), but not \( \vec{q} = 0 \) simultaneously through the three boundary faces.

The case of a permeable sea floor boundary requires some extra care. For the flow equation, we take \( P_{j, \text{sea}} = 0 \), i.e. \( p = p_0 \), which means no tangential mass transport components, and, in turn, \( q_{j, \text{sea}} = q_{j, \text{sea}}-1/2 \). In the recharge zone, where the sea water seeps into the crust from the environment with the ambient temperature \( T_0 \), we take \( T_{i, \text{sea}} = T_0 \). The major assumption is that upon ascent near discharge sites (which tend to be very focused), the hydrothermal effluent is mainly cooled conductively via lateral heat losses. The scheme for \( T_{i, \text{sea}} \) is then

\[
-\theta_{i, j, k, \text{sea}} \frac{T_{i-1, j, k, \text{sea}} - T_{i+1, j, k, \text{sea}}}{\Delta x} + \theta_{i, j, k, \text{sea}} \frac{T_{i, j-1, k, \text{sea}} - T_{i, j+1, k, \text{sea}}}{\Delta y} + \theta_{i, j, k, \text{sea}} \frac{T_{i, j, k-1, \text{sea}} - T_{i, j, k+1, \text{sea}}}{\Delta z} + \frac{(\theta_{i, j, k, \text{sea}} - \theta_{i, j, k, \text{sea}} - \theta_{i+1, j, k, \text{sea}})}{\Delta x} T_{i, j, k, \text{sea}} + \frac{(\theta_{i, j, k, \text{sea}} - \theta_{i, j, k, \text{sea}} - \theta_{i, j+1, k, \text{sea}})}{\Delta y} T_{i, j, k, \text{sea}} + \frac{(\theta_{i, j, k, \text{sea}} - \theta_{i, j, k, \text{sea}} - \theta_{i, j, k+1, \text{sea}})}{\Delta z} T_{i, j, k, \text{sea}} + \frac{Q_{j, \text{sea}, i}}{\Delta x} \left( T_{i, j, k, \text{sea}} - T_{i-1, j, k, \text{sea}} - T_{i+1, j, k, \text{sea}} - T_{i, j, k-1, \text{sea}} - T_{i, j, k+1, \text{sea}} \right)
\]

where the heat source term, \( G_{i, j, k, \text{sea}} \), right on the sea floor is likely to be zero. Numerical tests reveal that in the latter case this scheme would consistently maintain \( \partial T/\partial x \bigg|_{i, j, k, \text{sea}} \approx 0 \) in the core part of the discharge zone, which is consistent with what Schultz and Elderfield [1997] require explicitly. Note that the sign of \( q_{j, \text{sea}} \) dictates what type of the temperature boundary condition (i.e. Dirichlet of Neuman) should be used. We also remark that there is the complete freedom in specifying a Dirichlet or Neuman-type condition along any portion of any boundary in any combination, and that portion may not in general be rectangular.

3.5 Fractures

We have established in Chapter 2 that, numerically, the difference between the fracture and the host rock lies mainly in the permeability-thickness product in the direction of flow. If we assume the local equilibrium condition on the fracture-medium interface, as we did in Chapter 2 following Yang [1996], we observe that the fields and their normal gradients across the face areas of the control volume should be shared by parts of the fractures intersecting these faces. Averaging over the volume makes the transport matrices \( Q^x \), \( Q^y \), and \( Q^z \) the sole holders of the information on fractures. Bear, [1972] uses Ohm's law analogy to average the permeability of layered, porous structures. Lowell, [1991] applies it to analyze pipe models in the oceanic crust. We will follow here this logic, too. In fact, we have used it already discussing formula (3.6). The explanations are easier and the code is more efficient if we assume that the fracture network runs through the solution nodes. However should this be
3.5. FRACTURES

Let us consider then the impact of the smallest possible planar fracture element connecting four nodes on the permeability of one of the control volumes it intersects. For definiteness, we take a horizontal element in the XY-plane connecting the nodes \((i,j,k),\ (i+1,j,k),\ (i+1,j+1,k)\) and \((i,j+1,k)\), shown in Fig. 3.2A. Before the element is introduced, the medium, whose original permeability is \((k_{x0}, k_{y0}, k_{z0})\), may have been already "over-printed" by other fractures, so we start from \(\mathcal{K}_{0}\) and \(\mathcal{Q}^{0}\), \(\nu = (x,y,z)\) and want to update these sets to \(\mathcal{K}\) and \(\mathcal{Q}\). In general, our specific fracture element will be characterized by its thickness, \(\delta\), in the z-direction, the lateral dimensions, \(\Delta_x\) and \(\Delta_y\), and by the three components of permeability, \((k_{i+x}, k_{i+y}, k_{i+z})\). This allows a treatment not only of the "true" fractures, but also of zones with distinct permeability, whose dimensions are beyond our resolution. Note that often cracks get sealed by hydrothermal precipitation, in which case they act as rather impermeable walls, so \(k_{i+x}\) is not necessarily greater than \(k_{x0}\). Further, permeability may depend on temperature [Tivey, 1998], and Darcy's law may not be applicable for high velocities, so explicit formulae like (2.2) may be incorrect.

It is important to realize that in going from \(\mathcal{K}_{0}\) to \(\mathcal{K}\), we first construct an equivalent composite medium with the original permeability \(k_{x0}\) within the region occupied by the fracture and permeability \(\mathcal{K}_{0} = \mathcal{K}_{0}(k_{x0}, k_{y0})\) throughout the rest of the control volume, then
3.5. FRACTURES

replace $k_x$ by $k_{Fr}$ to finally obtain $\tilde{k}_x = \bar{k}_x(k_x, k_{Fr})$. The actual algebra is trivial with the help of the equivalent electrical circuit diagram shown in Fig. 3.2B for $\bar{k}_x$ at $z_{n+1/2}$ and in Fig. 3.2C for $\bar{k}_y$ at $z_{n+1/2}$, respectively. The labels beside each conductor in diagrams B and C indicate, in order, conductivity, cross-sectional area and length of the conductors. The process for $\bar{k}_y$ is

$$\bar{k}_y S = k_y S + \tilde{k}_y (S - S_f), \quad \bar{k}_y S = k_y S + \tilde{k}_y (S - S_f),$$

(3.15)

where $S = \Delta y \Delta x$ and $S_f = \frac{1}{2} \Delta y \delta$. To make it convenient for automated update of the transport matrices, introduce $\eta_1 = S/S_f$, then

$$\frac{\bar{k}_x}{k_x} = 1 + \frac{k_{Fr} - k_x}{k_x} \quad \text{and} \quad \bar{Q}_{i,j,k}^{r} = \frac{\bar{Q}_{i,j,k}^{r}}{\frac{\bar{k}_x}{k_x}}.$$  

(3.16)

The update for $Q_{i,j,k+1/2}^{r}$ is derived completely analogously to that for $Q_{i,j,k+1/2}^{r}$, replacing $x$ by $y$ in all relevant subscripts and superscripts. Proceeding similarly for the $z$-components, we just note that only half the width of the fracture belongs in between nodes $(i, j, k)$ and $(i, j, k + 1)$ and that portion of the fracture is connected in series with the remaining block of the medium having length $\Delta x = \delta/2$ and fractional cross-sectional area $r_1 = 1/4$ (in this example). After some simple manipulations, we obtain

$$\frac{\bar{k}_z}{k_z} = 1 - r_1 + \frac{\gamma_4}{1 + \frac{2\gamma_3}{\Delta x}(\frac{k_x}{k_z} - \frac{k_y}{k_z})}, \quad \text{and} \quad \bar{Q}_{i,j,k+1}^{r} = \frac{\bar{Q}_{i,j,k+1}^{r}}{\frac{\bar{k}_z}{k_z}}.$$  

(3.17)

Any distribution of fractures can now be mapped sequentially, looping over all specified fracture elements (that may comprise any number of nodes within their rectangular areas), then over all control volumes such an element intersects, updating the transport matrices at the faces of each of those affected volumes via expressions (3.16) and (3.17). Pipes are processed in the same fashion if we substitute their cross-sectional areas for $S_f$. To update the transversal components, a pipe may be approximated by the equivalent bar of a rectangular cross-section, but usually we neglect this effect for real pipes of small radii.

The net result of this mapping is that the discretized permeability structure becomes anisotropic. Note that if we specify as many fractures as we have nodal points in any given direction, the original medium can be replaced by its equivalent anisotropic analog because of the resolution limitations. Yang, [1998], whose software operates on entirely different principles, showed through modeling that this replacement is good to within 5% on grids $nx \sim ny \sim 40$. This wouldn’t be quite so in general, if fractures are not forced to connect
3.6 Sparse Matrix Assembly

If we lay out our 3D matrices \( P_{ijk}, T_{ijk}, G_{ijk}, \) and \( M_{ijk} \) as 1D vectors of the dimension \( N = nx \cdot ny \cdot nz \), each of the discretized equations (3.9) and (3.11) can be written in the usual matrix form

\[
A_{mn}x_m = b_l, \tag{3.18}
\]

where \( A \) is a square \( N \times N \) coefficient matrix, \( x \) is the vector to solve for and \( b \) is a vector derived from the known source terms. A common way to unfold a 3D matrix is the so-called natural ordering, \( (k = 1, nz \, (j = 1, ny \,(i = 1, nx)) \) which would map all coefficients of the equation for the volume \( V_{ijkl} \) onto \( l \)-th row of \( A \), where

\[
l(i,j,k) = (k-1) \cdot nx \cdot ny + (j-1) \cdot nx + i. \tag{3.19}
\]

The column index, \( m \), is determined via the same expression (3.19) for the relevant index triplets \( (i-1,j,k), (i,j,k), (i+1,j,k), ... ,(i,j,k+1) \). Matrix \( A \) is sparse, as in it there may be the maximum of 7 non-zero elements per row. The total number of non-zero elements, \( NNZ \), is thus less than \( 7N \). The easiest (but seldom used) scheme to store a sparse matrix is the coordinate format which requires one real array to store all non-zero values of \( A \) and two integer arrays to store their row and column indices, respectively. Denoting these arrays \( V, I \) and \( J \), respectively, we have

\[
A_{mn} = V(n), \quad l = I(n) \quad \text{and} \quad m = J(n), \tag{3.20}
\]

where \( n = \{1, NNZ \} \). To make the storage more efficient and compliant with the solver (to be described), the matrix is re-packed into the compressed sparse row format, where \( V \) contains all non-zeroes of \( A \) row by row, \( I \) contains the pointers to the beginning of each row, and \( J \) still holds the column indices. The required permutations are done with a utility subroutine from SPARSEKIT.

Following Medvedev [personal communication], we scale equation (3.18) by dividing \( l \)-th row of \( A \) as well as \( b_l \) by the diagonal element \( A_{ll} \) to improve the condition number.
3.7 Matrix Inversion

Equation (3.18) is solved iteratively via restarted, preconditioned GMRES(15) algorithm [Saad and Schultz, 1986]. The ILU preconditioner [Van der Vorst, 1981; Barrett et al., 1994] with the maximum of 10 fill elements is applied from the left. Both the GMRES solver and the ILU preconditioner FORTRAN 77 subroutines are adopted from the SPARSEKIT package. We now detail these statements at a conceptual level.

**GMRES solver**

If \( x^{(0)} \) is an initial approximation to the solution of the matrix equation (3.18), we define the residual \( r^{(0)} = b - Ax^{(0)} \) and \( n \)-th Krylov subspace

\[
K_n := \text{span}(r^{(0)}, Ar^{(0)}, A^2r^{(0)}, \ldots, A^{n-1}r^{(0)}).
\]

The GMRES approximation \( x^{(n)} \in x^{(0)} + K_n \) is constructed such that

\[
x^{(n)} = x^{(0)} + \gamma_1 v^{(1)} + \ldots + \gamma_k v^{(k)},
\]

where \( v^{(k)} \), constructed internally in SPARSEKIT via a modified Gramm-Schmidt algorithm, form an orthonormal basis in \( K_n \), and the coefficients \( \gamma_i \) are chosen to minimize the residual norm \( ||b - Ax^{(n)}|| \) [Saad, 1989]. For \( n = N \), the method is exact in exact arithmetic. In practice, \( n \) is restricted anywhere between 5 and 20. If \( x^{(n)} \) is not satisfactory, it is copied into \( x^{(0)} \) and the procedure restarts. Large \( n \) can quickly exhaust the computer memory, while small \( n \) may render the process slow or unsuccessful. As a reasonable compromise, we take \( n = 15 \).

**ILU preconditioner**

The convergence rate of iterative methods depends on spectral properties of the coefficient matrix. Preconditioning is an attempt to improve them. If it is applied from the left, we are solving the following equation

\[
\omega^{-1}Ax = \omega^{-1}b,
\]

where matrix \( \omega \) is the preconditioner. Loosely speaking, we would like the new system matrix \( \omega^{-1}A \) to be as diagonal as possible. It is known that the (complete) LU decomposition [e.g. Iserles, 1996], \( A = LU \), leads to the "exact" solution, but the computational cost involved is roughly the same as that for the direct Gaussian elimination. In the incomplete
3.8. ALGORITHM

implementation, the strategy is to preserve the sparsity structure of \( A \), while building the
LU, perhaps allowing some extra non-zero fill positions in \( w \) that do not exist in \( A \). The
greater the number of fill positions, the more robust the procedure is, however, at some level
the computational expenses outweigh the benefits, both memory- and time-wise. The ILU
preconditioner in SPARSEKIT uses not only the structural control over the fill positions,
but also the so-called drop tolerance. This means that some fill elements which are much less
than the diagonal entry on the same row will be discarded. Experimenting with the solver,
we restrict the number of fill-ins, \( l \), to 10 and use the relative drop tolerance of 1%. With
this choice, the preconditioning operation takes about one quarter of the total time and half
the storage memory to solve for a \((33 \times 33 \times 33)\) matrix.

To implement ILU-GMRES, requires a real storage array with the dimension of at least
\((N + 3)(n + 2) + (n + 1)n/2 + N(2l + 1)\).

3.8. Algorithm

The complete numerical scheme is shown in Fig. 3.3 in a hierarchical form, split between
sections A, B and C of the figure. Each of the governing equations is handled by the same
routine, called algorithm M1 in Fig. 3.3A. To operate, we need both \( P \) and \( T \) fields and
the transport matrices \( Q \) and \( F \) on the staggered grid which are set up first according to
formulae \((3.7)\). For the pressure solver, fractures are mapped at this stage. The coefficient
matrix \( A \) constructed from the transport matrices in the coordinate format is then re-packed
into the compressed sparse row format. After that, it is preconditioned and fed into the
GMRES solver. Upon successful minimization of the residual norm, the solver returns an
approximation to \( x \) from which we recover the original 3D matrix: \( P \) or \( T \), whichever
appropriate.

The coupled heat and mass transport problem is solved with algorithm M2 (see Fig.
3.3B) by iterating between the temperature and pressure equations, each of the equations
being solved with M1. One such an iteration cycle starts from either a reasonable initial
guess or a previously computed pair \((P, T)\)\(^{\text{(m)}}\), where \( m \) is the iteration index. The pressure
field is updated straightforwardly

\[
p^{\text{(m+1)}} = M_{1_{\text{P,\text{m}}}}(p^{\text{(m)}}),
\]

while the temperature update generally requires an over-relaxation step

\[
t^{\text{(m+1)}} = t^{\text{(m)}} + E \left( M_{1_{\text{P,\text{m}}}}(t^{\text{(m)}}) - t^{\text{(m)}} \right),
\]
Figure 3.3: 3D solver in a hierarchical form: (A) single equation solver, (B) coupled heat and mass transport solver on a single grid, (C) two-grid extension.
where $E$ is the over-relaxation parameter, being typically 0.5 on average. It is higher than the one used in our single-fractured algorithm developed in Chapter 2, however, for the process to converge, $E \leq 1$.

**Two-grid extension**

Let us recall the main idea behind the single-fractured algorithm and extend it from a single fracture to a single 3D subdomain of interest, which may be itself multiply fractured, contain sources or other features of interest that require fine resolution. A typical example of where this may be invaluable is the black smoker discharge site transporting \( \sim 350\% \) fluid with the velocity of \( \sim 1 - 2 \) m/s through a pipe-like conduit having the diameter about a couple of centimeters. We will consider this model in Chapter 5.

The approach here will be to use algorithm M2 on the main domain with a coarse grid and a rectilinear subdomain with a fine grid, communicating to each other through boundary conditions along the subdomain boundary. The required boundary conditions to solve in the subdomain are computed from the main domain solutions, while the subdomain solutions are used as inner Dirichlet points for the next iteration on the main domain. Similarly to the single-fractured algorithm, in forming the inner Dirichlet values, we over-relax between the previous solutions in the main domain and the restricted solutions in the subdomain.

The complete process is shown pictorially in Fig.3.3C, where $D_1$ is the main domain, shown in two dimensions for clarity, $D_3 \subset D_1$ is a subdomain of interest, and $D_2$: $D_3 \subset D_2 \subset D_1$ is an auxiliary subdomain with 1–2 extra nodes in each direction comparing to $D_3$ to smoothen the transition between the two grids. This may not be necessary if both $D_1$ and $D_3$ share one or more boundaries with the prescribed conditions. Additional smoothing may be achieved, if desired, by making the grids non-uniform. The degree of mesh refinement for the subdomain is restricted to the powers of two. If it is just 2 as in the figure, the odd-numbered subgrid nodes of $D_2$ will belong to the main staggered grid, while the even-numbered nodes will coincide with the main grid nodes. Good results are obtained with the degrees of 2, 4 and even 8. In projecting or restricting solutions between the grids, we employ the simplest bi-linear or tri-linear interpolation for Dirichlet points. Subdomain $D_2$ is automatically constructed such that its boundary nodes always lie on the main staggered grid, so we have the numerically exact (in exact arithmetic) energy and mass conservation for the Neumann-type boundaries, consistent with the discretization rules. The particular types of the boundaries or their parts, as well as the width of the buffer zone, $D_2 - D_3$, are problem specific and determined experimentally.

3.6. ALGORITHM
3.9 Code Validation

Our earlier testing efforts included solving algebraic equations of the form (3.18) with the strongly asymmetric matrices (up to 100 : 1) with the known answer, as well as solving the temperature equation alone with the forced, cellular flow at nearly sonic velocities. Such high velocities are clearly outside the parameter range for our convection models, but it is a good test on the stability of the upwind scheme and the GMRES solver on a matrix which is not diagonally-dominant. We also cross-checked results for a number of 2D convection models with forced, unidirectional, low-velocity flow against our MUDPACK-based software, which discretizes advective terms and Neuman-type boundary conditions differently. The maximum relative error of 0.3% for the temperature is typically observed near the corners of a domain having 33 x 33 nodes.

The 3D solver usually terminates with a residual norm of $10^{-10} - 10^{-12}$, however, we feel it necessary to perform the direct divergence check for each control volume in the domain. On average, the maximum relative heat disbalance is $10^{-4} - 10^{-7}$, while that for the mass is $10^{-6} - 10^{-9}$. This check is an integral part of the solver; it somewhat degrades the performance, but generally acts as a life insurance, since we have no explicit analysis of convergence conditions to guide us. We stress at this point that our numerical solution is a weak solution, whose differentiability conditions are different from those of the true analytical solution [Iserles, 1996], so cross-checks against any analytical or a proven numerical output are invaluable. And yet, the author must painfully acknowledge the apparent lack of the available 3D models for cross-checks, except the point source model, considered in Chapter 1.

At least we have verified that all steady-state outputs in Chapters 1 and 2 are well reproduced by the 3D solver. Shown below is a selection of those comparisons.

Point Heat Source Model

Let us recall the model of a point heat source within a layer (Chapter 1, Section 1.9, Fig. 1.6). We solve it on a rectilinear domain $(2H, 2H, H)$ with the adiabatic side walls and all six impervious boundaries, shown in Fig. 3.4A; the actual numerical parameters are listed at the end of Section 1.9. Our particular attention will be to a subdomain, lightly shaded in the figure, of which we select an $(H \times H)$ vertical cross-section in the $y = H$ plane, shaded in a darker colour. The solver is used in the two-grid mode: the coarse grid has $(21 \times 21 \times 11)$ nodes over the entire domain, and the fine grid within the subdomain has $(45 \times 45 \times 41)$ nodes. We compare the dimensionless temperature field in the 2D cross-section against the analytical solution derived in Chapter 1. The temperature is normalized on the lower boundary temperature. Note that the Green's function solution is only obtained to
3.9. CODE VALIDATION

Figure 3.4: Point heat source model: (A) full simulation domain, velocity field within the subdomain, and temperature contours within the shaded 2D cross-section in comparison with the analytical solution obtained in Chapter 1, Section 1.9. (B) Temperature solution within the same cross-section obtained on different grids.
the first order in \(Ra\)-number. It is itself good to within 15\%, which is estimated based on the full space third-order solution for \(Ra_n = 10\) [Bejan, 1978]. The comparison with the full numerical solution is within this percentage in the vicinity of the source.

Continuing with this model, we solve the problem on three different grids, using the solver in both the single and two-grid modes and compare in Fig. 3.40 the isotherms within the \(y = H\) plane. The grid parameters are indicated in captions. For the solution on the finest grid, we also detail the temperature field near the source which requires yet finer resolution. We observe an excellent inheritance between the fields obtained on grids with different degree of refinement.

**Single Fractured Models**

In Fig. 3.5, we cross-check the outputs for the velocity field and temperature of the 3D solver (A) and the FD, single fractured software (B) on the benchmark model that contains a single fracture, described in Chapter 2, Section 2.4. To put the 3D solver in the 2D mode, the permeability in the unused dimension is set to a low value of \(10^{-15} m^2\) and the number of nodes in that direction is put to 3. The grid dimensions in the \(x\)– and \(z\)-directions are 41 by 21, respectively. The maximum misfit between the two temperature fields produced by the two pieces of software at the fracture location is about 5\%.

We now set up another 2D test model which features the permeable, free-flux upper boundary. The rest of the boundary condition types is as in the above model and indicated in Fig. 3.6 explicitly. The size of the domain is 600\,m by 400\,m, the size of the grid is 65 \times 65 in the \(x\)-\(z\) plane. A single planar fracture with apertures of 1.5\,mm extends fully across the middle of the domain. The medium is anisotropic: \(k_x = 10^{-15} m^2\), \(k_z/k_x = 5\). The average thermal conductivity is \(3 W/(m\,K)\), the heat capacity of the fluid is 4174\,J/kg/K. A constant temperature of 100\(^\circ\)C is maintained at the lower boundary. Initially, the top
Figure 3.6: A single-fractured model with the permeable, free-flux upper boundary to test the 3D solver against the 2D single-fractured software. Plotted are temperature contours with 5°C increment: (A) 3D solver, (B) 2D solver.

boundary is at the ambient 0°C. We compare the temperature fields produced by the two solvers. Again the maximum difference between the solutions in the fracture is about 5%.

3.10 Summary

We have coded, and tested a 3D solver to model a wide variety of coupled heat and mass transport steady-state problems including advection dominated. The software produces conservative solutions, allows to include fractures and sources of heat and mass.
Chapter 4

Selected 3D Case Studies: Off-Axial Convection in Young Oceanic Crust

4.1 Introduction

Using the stationary solver developed in Chapter 3, we look first at a few simple 3D models. All of them feature isotropic and homogeneous permeability \( k = 10^{-13} m^2 \) within a rectilinear domain whose lower boundary is kept isothermal. The magnitude of \( k \) used is a reasonable approximation for the average permeability of young, off-axial oceanic basalt, at least as the upper bound. For instance, bulk permeability of greater than \( 10^{-14} m^2 \) in the upper 450 m of volcanics is estimated by Green et al., [1981] who conducted a detailed geothermal field study at DSDP Hole 395A. Other relevant parameters are varied so that we can choose between convectively subcritical and supercritical models with either permeable or impermeable sea floor as the upper boundary. The impact of a planar vertical fracture (or equivalent permeable zone) on convection pattern and heat flow is demonstrated next.

With these fundamentals at hand, our attention will then be directed towards a very interesting set of sea floor observations made by Davis et al., [1992]. They reveal regular variations in heat flux at the apparently flat sea floor on the Eastern flank of the Juan de Fuca Ridge (JdFR). The observed heat flux average there of 250 mW/m^2 is modulated by an approximate sinusoid with 40 mW/m^2 peak-to-peak amplitude and a spatial period of a few hundred of meters. The authors link this heat flux pattern to 2D convection rolls. However, later attempts to simulate the process numerically appeared to require a very high bulk permeability of about \( 10^{-11} m^2 \) through the upper 600 m of igneous crust. Although the majority of studies places the upper bound for \( k \) at \( \leq 10^{-12} m^2 \), Davis, [1997] still argues that from geochemical data, fluid discharges above the buried ridge (observed with no sediment...
present) can occur only when \( k \geq 10^{-13} \text{ m}^2 \) and what may make \( k \) even higher is probably the interconnected fractures and extrusive volcanic unit contacts and voids. The latter are allegedly infrequent and can easily go undersampled in borehole measurements. Extensive, high resolution numerical modeling by Wang, He and Davis [1997] shows that no steady-state, large scale convection is possible with this high bulk permeability, which yet again raises concerns as to how good the 2D-roll explanation is for the observed heat flux pattern. Such an explicit concern was already expressed by Davis and Chapman, [1996].

Yang, [1996] reproduced heat flux variations observed by Davis et al. over flat sediment with no basement topography by including randomly distributed vertical and horizontal fractures in the model. However, his most successful model contains one hundred fractures per 200 nodes, which makes the random distribution “dense”. In a later paper, Yang et al., [1998] show that extensively fractured sections can be effectively replaced by an equivalent anisotropic bulk permeability. The 2D solution found by Yang is steady-state.

Fisher and Becker, [1995] proposed a different mechanism that relates heat flux variations observed by Davis et al., [1992] to the buried basement relief of 20 m. High permeability is confined to a much thinner, anisotropic layer, just below the sediment. Although the required topographic perturbations are small, they were ruled out by a high resolution seismic imaging of the area [Davis et al., 1997]. On the other hand, it is very common for the sediment thickness to vary, effecting correlated changes in the surface heat flux carried by conduction. Davis et al., [1997] report variations in sediment thickness by a factor 3: between 200 m and 600 m, found near site 127°45′W and 47°46′N. Moreover, the associated heat flux ranging from 350 mW/m² to 150 mW/m², respectively, is inversely proportional to the thickness of overlying sediment which requires the temperature of the sediment-basement contact to be uniform to within 15% according to the above mentioned authors. Similar conclusions about the degree of the interface temperature homogeneity were drawn by other workers, e.g. [Wang et al., 1997].

Vigorous, unsteady, large scale convection could be a homogenization mechanism, were it not for challenging the magnitude of the bulk permeability, as we mentioned before. Long, stock-like 2D rolls within thin permeable zones of 20 – 40 m proposed by Fisher and Becker are likely to exist only in a 2D medium. Our preliminary simulations in which flow was originally 2D preconditioned have convinced that the rolls may easily be broken by topography along the strike - the dimension missing in 2D models. On the other hand, the existence of thin permeable zones with \( k \sim 10^{-13} \text{ m}^2 \) in the upper oceanic crust is supported experimentally. Drilling at numerous sites has revealed that the upper volcanic crust is highly layered within zones tens of meters thick, both architecturally and w.r.t hydrogeological properties [Pezard et al., 1992]. Usually, anisotropic permeability within these zones is
Inferred; the ratio of the lateral permeability to the vertical one being 100 – 1000 : 1 [Fisher and Becker, 1995]. Baker et al., [1991] provide a geochemical evidence supporting large scale horizontal advection of young seawater through the permeable basement in the equatorial Pacific (110 – 160°W, 5°S – 8°N) based on downdhole pore fluid measurements.

In what follows, we would like to state and support by simulations a simple idea: if these thin, permeable, anisotropic zones exist and follow the basement topography, then fluid may choose to circulate laterally within these zones. First, we construct a model with no buried topography and reproduce the observed heat flux with 40 mW/m² oscillations as a result of convective rolls. Then we let the interface take a simple, sine-like shape and find a circulation pattern that homogenizes basement temperature. Finally, an arbitrary topography model is considered. The reader will notice that he proposed mode of circulation explains equally well the heat flux observations for both flat and rugged basement, covered by sediments.

4.2 Basic 3D Models

Consider two rectangular, isotropic and homogeneous in all geophysical properties domains, 1 and 2, whose dimensions are 400 m x 400 m x 400 m and 600 m x 600 m x 400 m, respectively. Both share the permeability of 10⁻¹³ m², isothermal and impermeable lower boundary and adiabatic and impermeable side walls. The upper boundary (sea floor) is impermeable and isothermal, kept at 0°C for Model 1, while that for Model 2 is a constant pressure, free flux, permeable boundary. Setting the temperature at the base of both models to 100°C makes them supercritical. These basic parameters are chosen such that the Nusselt number doesn’t exceed 3 even if the medium is fractured (to be considered later). According to Lister, [1990], we should be within the steady-state limits for cellular convection in a layer, as long as Nu is less than 6 – 10.

Simulations show that if a 2D roll is an initial approximation, this pattern carries over to the three dimensions as a numerically stable mode, otherwise, an axi-symmetric upwelling, surrounded by a broader recharge zone, is what we often get for both models. This axi-symmetric pattern will be referred to as the 3D mode, although we note right away that the true axial symmetry cannot be reproduced on a rectangular grid and, strictly speaking, we are forcing a lower-order symmetry, compared with, say, triangular grid. Both 2D and 3D modes are shown for each model in Fig.4.1-Fig.4.2. We plot gray-scaled temperature field and Darcy velocity vectors superimposed. Sea floor heat flux map is displayed above each such a figure. Both 2D and 3D modes, once set, are stable with respect to initial perturbations such as point heat sources. Typically, the conservation of mass and heat is maintained to within 10⁻⁸ and 10⁻¹⁰ relative error, respectively. However, the solver is not
Figure 4.1: Model 1 (impermeable sea floor): Temperature and Darcy velocity fields superimposed (bottom) and heat flux (top) for two basic modes of circulation. The medium is unfractured.
4.2. BASIC 3D MODELS

Figure 4.2: Model 2 (permeable sea floor): Temperature and Darcy velocity fields superimposed (bottom) and heat flux (top) for two basic modes of circulation. The medium is unfractured.
4.2. BASIC 3D MODELS

Figure 4.2: Model 2 (permeable sea floor): Temperature and Darcy velocity fields superimposed (bottom) and heat flux (top) for two basic modes of circulation. The medium is unfractured.
designed to perform a rigorous stability analysis.

It is interesting to compare the two models, as well as the two modes within each model, quantitatively. We select for this purpose the following quantities: the total hydrothermal power through the sea floor, $P_t$, root-mean square velocity associated with the mean kinetic energy, $v_{rms}$, maximum heat flux, $q_{max}$, and maximum fluid velocity, $v_{max}$. As expected, axi-symmetric 3D modes feature much more focused discharge sites characterized by higher $v_{max}$ and $q_{max}$, especially when sea floor is permeable, but, surprisingly, there is only marginal difference in $P_t$ and $v_{rms}$ between different modes within each model. So we cannot conclude from these data which mode is more preferential. The numbers for Model 1 are $P_t^{2D} = 0.119 \cdot 10^8 \text{W}$, $P_t^{3D} = 0.114 \cdot 10^8 \text{W}$; $v_{rms}^{2D} = 6.598 \cdot 10^{-9} \text{m/s}$, $v_{rms}^{3D} = 6.602 \cdot 10^{-9} \text{m/s}$; $v_{max}^{2D} = 0.170 \cdot 10^{-7} \text{m/s}$, $v_{max}^{3D} = 0.206 \cdot 10^{-7} \text{m/s}$; $q_{max}^{2D} = 1.29 \text{W/m}^2$, $q_{max}^{3D} = 1.91 \text{W/m}^2$, while those for Model 2 are $P_t^{2D} = 0.304 \cdot 10^8 \text{W}$, $P_t^{3D} = 0.297 \cdot 10^8 \text{W}$; $v_{rms}^{2D} = 7.687 \cdot 10^{-9} \text{m/s}$, $v_{rms}^{3D} = 7.730 \cdot 10^{-9} \text{m/s}$; $v_{max}^{2D} = 0.235 \cdot 10^{-7} \text{m/s}$, $v_{max}^{3D} = 0.448 \cdot 10^{-7} \text{m/s}$; $q_{max}^{2D} = 5.58 \text{W/m}^2$, $q_{max}^{3D} = 13.7 \text{W/m}^2$.

Now, we consider two variants for each model, a and b, respectively. Model 1a contains a planar vertical fracture with the aperture of 0.3 mm, while in Models 2a, 16 and 26, the aperture is increased to 1 mm. The temperature of the lower boundary is set to $70^\circ\text{C}$ for Models 1b and 2b, so that in the absence of fracture, both are subcritical. Solutions are assumed symmetric about the fracture plane. The fracture then is placed on one of the side boundaries, just as we did in Chapter 2. Figures 4.3 through 4.6 show velocity and temperature fields and sea-floor heat flux maps for Models 1a through 2b, respectively. We displayed in these figures 3D fields in the medium (fracture excluded) and selected 2D vertical cross-sections, including one for the fracture. As a rule, velocity vectors in the fracture are scaled down; the coefficient is indicated in white print. One sees from Figures 4.3 through 4.6 that fractures have a strong impact on convection pattern. Similarly to the two-dimensional models, fractures promote convection in subcritical medium. In systems with the permeable sea floor, much of the fracture is occupied by downwelling fluids. They either return to the fracture shortly, if the medium is subcritical or barely supports convection (Model 2b), or may discharge farther away from the fracture as in Model 2a. Flow patterns produced by Models 1a and 1b in the medium resemble axi-symmetric 3D mode of Model 1, considered before. However, the 2D, roll-like signature in the fracture plane is too strong to be missed.
Figure 4.3: Model la: heat flux map at the sea floor, temperature and velocity fields in the medium and selected 2D vertical cross-sections, including fracture plane.
Figure 4.4: Model 1b: heat flux map at the sea floor, temperature and velocity fields in the medium and selected 2D vertical cross-sections, including fracture plane.
4.2 BASIC 3D MODELS

Figure 4.5: Model 2a: heat flux map at the sea floor, temperature and velocity fields in the medium and selected 2D vertical cross-sections, including fracture plane.
4.2. BASIC 3D MODELS

Figure 4.6: Model 2b: heat flux map at the sea floor, temperature and velocity fields in the medium and selected 2D vertical cross-sections, including fracture plane.
4.3. HEAT FLOW VARIATIONS OVER SEDIMENT-SEALED, FLAT SEA FLOOR

Model 3A, shown in Fig. 4.7A, was built with the sole explicit intent to reproduce the observed heat flux variations of 40 mW/m², spaced about half a kilometer apart, over flat, sedimented sea floor [Davis et al., 1992]. Following Yang, [1996], we take the lateral dimension of the model to be ~ 2 km and the depth of 1 km. The actual numbers are 2048 × 2048 × 1140 m³ to fit a numerical grid of 33 × 33 × 20 nodes. The model contains four layers. The uniform thickness of the top sedimentary layer 1 is assumed 240 m and its permeability set to 10⁻¹⁰ m² as in [Davis et al., 1997]. We assume the existence of a highly permeable thin layer with \( k_x = k_y = 10^{-9} \, \text{m}^2 \); \( k_z = 10^{-12} \, \text{m}^2 \) and thickness 40 m just below the sediments [Perez et al., 1992; Fisher and Becker, 1995] which is technically introduced as a horizontal fracture zone with anisotropic permeability. This zone separates the sediment from the permeable basaltic layer 2a whose thickness is set to 480 m and vertical permeability to 10⁻¹⁵ m². Bulk anisotropy is assumed \( k_x/k_z = 10 \) which may be caused by vertical fractures that we can not resolve explicitly, because of computer memory limitations. The lower portion of the model is occupied by essentially impermeable layer 2b, thickness 420 m, \( k = 10^{-17} \, \text{m}^2 \) and \( \lambda = 3 \, \text{W/m/K} \). Note that without the zone, the permeable layer 2a is subcritical. Tests showed that varying the last three parameters liberally has almost no effect on the numerical outputs, so we leave them as stated. All the boundaries are impermeable, the side boundaries are adiabatic, as usual. The base of layer 2b assumes a constant heat flux value of 250 mW/m², in agreement with the observed average.

Figure 4.8 shows the hydrothermal response of the model with the thermal conductivities of the sediment and layer 2a taken as 1.6 W/m/K and 2.1 W/m/K, respectively. In Fig.4.8A,
4.3. HEAT FLOW VARIATIONS OVER SEDIMENT-SEALED, FLAT SEA FLOOR

Figure 4.8: 3D temperature and velocity fields (A), their 2D vertical slice (B) and heat flux variations over flat sediment cover (C) for the model in Fig.4.7A.
4.3. HEAT FLOW VARIATIONS OVER SEDIMENT-SEALED, FLAT SEA FLOOR

We observe a set of regular 2D rolls which cause a sine-like heat flux pattern at the sea floor, as originally proposed by Davis et al., [1992]. The fluid velocity in layer 2a is of the order of $10^{-9}$ m/s, while that within the zone is $\sim 10^{-6}$ m/s. It is interesting to note that the 37°C isotherm in the vicinity of the permeable zone resembles a sinusoid with $\sim 20$ m spatial amplitude - exactly the depth of topography modulations required by Fisher and Becker to explain the same heat flux pattern (see Fig.4.8C).

It is obvious that the average temperature within the zone (or at the sediment base) is directly controlled by the sediment thermal conductivity, $\lambda_1$. What is less obvious is the impact of the thermal conductivities $\lambda_1$ and $\lambda_2$ on the heat flux modulation and flow characteristics. Figure 4.9A displays maximum Darcy velocity in layer 2a, sea floor heat flux variations and the average temperature of the sediment base.

Figure 4.9: The impact of the thermal conductivities of the sediment, $\lambda_1$, and permeable basaltic layer 2a, $\lambda_2$, on the maximum Darcy velocity in layer 2a, sea floor heat flux variations and the average temperature of the sediment base.
4.4 Homogenization Mechanism on Basement Topography

The case of no basement topography is rather too specific and will be now abandoned. To start with, consider a model, shown in Fig.4.7B. It is similar to the one in [Wang et al., 1997] and shares most of the parameters with Model 3a, except the sediment thickness varies sinusoidally with lateral distance and has the quarter period of 2048 m and amplitude of 240 m. The sinusoid is intentionally approximated by a coarse, stair-case segments. The structure is clearly two-dimensional; no changes in the Y-direction (normal to page). The velocity field developed is mainly concentrated within the permeable zone, where it forms a simple vortex to a good approximation, as shown in Fig.4.10A. The maximum Darcy velocity reaches $0.6 \cdot 10^{-5}$ m/s. A typical velocity in the permeable basaltic layer below the zone is $\sim 10^{-5}$ m/s, and the circulation is roughly normal to the interface. We show two typical cross-sections in panels B and C of Fig.4.10. Vigorous (but stable) convection in the quasi-horizontal stratum results in a very efficient temperature stirring within the permeable zone with the average value of 32°C and its standard deviation of 2°C. Thus, the required homogenization is achieved. Note that this stirring is only possible in full 3D models. Panel D of Fig.4.10 shows a heat flux map at the sea floor level which does resemble the buried relief.

It is interesting to see what happens if the buried topography gets a bit more complicated, such as in Fig.4.11B with maximum topography variations of 135 m over a $3 \times 3$ km$^2$ lateral area. The depth of the model is 800 m, and the basic layering is as that in Model 3a. An average vertical section, shown in Fig.4.11A, details the boundary conditions, numerical grid
Figure 4.10: The formation of a vortex within a permeable zone beneath non-flat sediment cover, (A): 3D temperature field for the entire domain and velocity within the zone, (B-C): selected 2D vertical cross-sections, (D): heat flux map at the sea floor.
Figure 4.11: A generic model with buried sediment topography. The domain dimensions are 3 km x 3 km x 800 m. Panel A shows an average vertical cross-section detailing (left to right) boundary conditions, numerical grid and layering. Note that the grid is non-uniform in the vertical direction. For simplicity, the boundary between the sediment and permeable layer 2a is shown flat. The actual topography of the sediment base (top view) is given in Panel B.
4.4. HOMOGENIZATION MECHANISM ON BASEMENT TOPOGRAPHY

and hydrothermal properties of the layers. A uniform heat flux of 300 mW/m² is assumed at the bottom of the model. The average sediment thickness is 230 m. In the sediment layer, \( k = 10^{-16} \text{ m}^2 \) and \( \lambda = 1.5 \text{ W/m/K} \). In layer 2a, \( k = 10^{-13} \text{ m}^2 \) and \( \lambda = 2 \text{ W/m/K} \), while in layer 2b, \( k = 10^{-17} \text{ m}^2 \) and \( \lambda = 2 \text{ W/m/K} \). To follow the relief more closely on our rectilinear grid, we made the grid non-uniform in the vertical direction. In the upper 300 m, the vertical resolution is 15 m; below 300 m, it is 25 m. Lateral resolution is fixed at 50 m everywhere. The sides are impermeable and adiabatic; the sea floor temperature is a 0°C isotherm. We will deal with the following three versions of the model just described. Model 4a has no permeable zone between the sediment and layer 2a. Models 4b and 4c both have it. The permeability-thickness products for the zone across the models are \( 10^{-3} \text{ m}^3 \) and \( 4 \cdot 10^{-8} \text{ m}^3 \), respectively, while the ratio of vertical to horizontal components of the permeability of the zone is taken \( 10^3 \) for Models 4b and 4c.

The hydrothermal output for Model 4a is shown in Fig.4.12. One observes that convection induced by topography is in general three-dimensional. We can identify both 2D rolls and sites with axi-symmetric circulation pattern. The maximum fluid velocity is \( 2 \cdot 10^{-5} \text{ m/s} \). The heat flux map (Fig.4.12 D) and basement relief (Fig.4.11B) have very little in common, since the temperature of the sediment-layer 2a interface is \( 48 \pm 12^\circ \text{C} \); and we can not speak of any homogenization here. The matters change much when the permeable zone is introduced. We observed in Fig.4.13 the fluid ascend at topographic highs and flow downhill to recharge within the valley-like topographic low. A significant fluid exchange exists between the permeable zone and the medium. The sea floor heat flux now follows the topography variations; however, the peak-to-peak amplitude of the heat flux variations is greater than what would be expected of a homogenized interface. Instead, we obtain for the temperature within the permeable zone \( 45 \pm 14^\circ \text{C} \) which implies an overshoot at highs and undershoot at lows. Finally, in Model 4c (see Fig.4.14A) the homogenization takes place when the permeability-thickness product of the zone reaches \( 4 \cdot 10^{-8} \text{ m}^3 \); and we obtain \( 47.8 \pm 3.5^\circ \text{C} \).

Unfortunately, the solutions obtained are only “quasi-steady”. The solver terminates with 10% relative error for the temperature and pressure fields. Iterating any further makes the solutions oscillate about some reference state. So we have exceeded the steady-state limitations set by the solver, but, hopefully, not very much. We plot in Fig.4.14C a sea floor heat flux map which corresponds to conductive heat transport through sediment with the isothermal interface between the sediment and layer 2a as a lower boundary whose temperature is fixed at 47.8°C. This map compares well with Fig.4.14B which shows the heat flux for Model 4c at the sea floor.
4.4. HOMOGENIZATION MECHANISM ON BASEMENT TOPOGRAPHY

Figure 4.12: Model 4a - A: 3D temperature and velocity fields, B and C: selected 2D cross-sections of A, D: heat flux map at the sea floor. No permeable zone exist at the base of sediment.
4.4. HOMOGENIZATION MECHANISM ON BASEMENT TOPOGRAPHY

Figure 4.13: Model 4b - A: 3D temperature and velocity fields, B and C: selected 2D cross-sections of A, D: heat flux map at the sea floor. A permeable zone ($k_b = 10^{-9} m^2$) is introduced just below the sediment base.
4.4. HOMOGENIZATION MECHANISM ON BASEMENT TOPOGRAPHY

Figure 4.14: Model 4c - A: 3D temperature and velocity fields, B: heat flux map at the sea floor, C: heat flux map at the sea floor assuming perfectly homogenized sediment base with $T = 47.8^\circ C$. In this model, we introduce a permeable zone with $k_b = 4 \cdot 10^{-8} m^2$ just below the sediment base.
4.5 Summary

Under certain conditions, steady hydrothermal circulation in a 3D box may feature either a roll or an axi-symmetric pattern. Vertical fractures or equivalent thin permeable zones introduced into such systems result in a mixture of the two patterns in the medium. In the vicinity of fractures, a roll-like circulation in the fracture plane tends to be the preferential mode. The ascending limb of that vortex is typically much narrower than the broader downwelling, sheet-like descending limb. This is especially true for the systems with the permeable sea floor.

Similarly to the case of the two dimensions treated in Chapter 2, fractures induce and maintain hydrothermal convection in a 3D subcritical medium.

We have build a range of models to look at off-axial heat flux variations over a flat, sediment covered sea floor, assuming the presence of a thin permeable anisotropic zone at the base of the sediment. The observed regular heat flux variations of 40 mW/m² when no buried basement relief is present are successfully modeled by a large scale 2D rolls in the subcritical basaltic layer 2a, induced by the permeable zone. The highs in the heat flux at the sea floor are correlated with the ascending limbs of the convection rolls. In the general case of a buried basement topography, the fluid circulates quasi-horizontally. This quasi-horizontal stirring homogenizes the temperature within the permeable zone, so that the surface heat flux is approximately inversely proportional to the sediment thickness above the permeable zone.

Typically, the permeability-thickness product of $4 \times 10^{-8} m^3$ is required for the permeable zone to homogenize the temperature to within 15%. The fluid velocity within the zone is then of the order of $10^{-8} m/s$; the circulation may be unsteady.
Chapter 5

Modeling of Hydrothermal Circulation at the CoAxial Segment of the Juan de Fuca Ridge

5.1 Introduction

It has been generally recognized that multi-dimensional models are necessary to provide a complete picture of accretion and evolution of oceanic crust. Accurate hydrothermal modeling, as an integral part of this activity, requires a comprehensive knowledge of crustal permeability (porosity), fracturing and distribution of heat sources over segment-scale portions of the sea floor. Seismic tomography is one of the few tools suitable for imaging crustal porosity variations with depth.

Sohn et al., [1997] conducted two high resolution seismic P-wave refraction surveys on the CoAxial Segment of the Juan de Fuca Ridge (JdFR); the map of the area is shown in Fig 5.1. JdFR is hydrothermally active and has an intermediate half-spreading rate of 3 cm per annum. The permeability structure for the Southern CoAxial field was derived by Sohn et al. from porosity gradients following van Everdingen, [1995] and constrained by the absolute values of permeability, measured downhole at ODP 504B and 735B. The final permeability structure for that area was communicated to the author by R.A. Sohn [personal communication]. It is assumed symmetric about the ridge axis (X = 0) and constant in properties along the strike (the Y-direction), so we only display one vertical cross-section, normal to the ridge in Fig. 5.2. First 400 m below the sea floor are occupied by isotropic, highly permeable, sediment-free extrusive layer 2a. As we look deeper, both the dike transition zone (layer 2b) and the sheeted dikes (layer 2c) feature strong anisotropy.
5.1. INTRODUCTION

Figure 5.1: Area near CoAxial Segment of the JdFR: seismic survey map [Sohn et al., 1997].
5.1. INTRODUCTION

Figure 5.2: Model 1 setup: A-geometry and basic geological layering, B-permeability structure (vertical component only), C-heat flux distribution and temperature at the lower boundary, used as boundary conditions.
in the proportion $k_2 : k_3 : k_r = 100 : 10 : 1$. The transition zone extends to 1400 mbsf.
The interface between layers 2c and 3e (gabbro) at 2200 mbsf, where seismic velocity suffers
a sharp gradient, is assumed impermeable. No axial magma chamber was detected as of
present. Sohn [personal communication] suggested the maximum temperature at the base
of the model on axis is less than 1000°C and decreases in the normal-to-strike direction.
Using these data, Sohn et al., [1997] argued that circulation must be ridge-parallel with both
discharge and recharge sites located on axis, as opposed to a more traditional 2D model
where fluid circulates normally to the axis.

Based on the results of Sohn et al. we construct a simple hydrothermal model for the
southern, on-axial portion of the segment, aged 0.1 MA to find out primarily what the
circulation pattern is and how much fluid is involved in this circulation. In short, we obtain
a ridge-parallel convection discharging at low temperature. In an attempt to simulate sea
floor discharges at elevated temperatures, often observed, we introduce a couple of additional
features into the model, such as a permeable zone directly on axis and a pipe-like conduit. It
is speculated in Sohn et al., [1997] that along amagmatic, slowly spreading ridges, extensional
faulting (making ~ 30° with the vertical) may locally overprint the background porosity and
create deep, coherent hydrothermal conduits in otherwise hardly permeable crust which may
result in a different circulation pattern. To see the impact of dipping faults, we introduce
one into our permeability structure.

The basic model is labeled as Model 1; the other three, in the order we mentioned them
above, are Model 2, Model 4 and Model 3.

5.2 Model 1: Basic Model

The size of the main simulation domain (Fig.5.2A) conforms with the aspect-ratio of the
developed convection cells (found by the trial-and-error method) and is settled at $2 \times 2 \times
2.2 \text{ km}^2$. Solutions are assumed symmetric w.r.t. the ridge axis which acts here as one of the
lateral boundaries, $X = 0$. The lateral boundaries are impermeable and adiabatic, again by
the symmetry argument. The sea floor (the top) is a constant pressure, permeable sediment
free, free heat flux boundary; so the temperature is not fixed relative to the ambient 0°C.
The heat uptake at the gabbro-dikes interface (the base of the domain) is modeled with
an area of specified heat flux in the first 400 m of the axis, overlayed by a flow zone as in
Lowell, [1991] and Cathles, [1993]. The permeability-thickness product of the flow zone is
$3 \cdot 10^{-12} \text{ m}^2$. For the rest of the lower boundary ($X \geq 400 \text{ m}$), the temperature is specified,
which grades smoothly away from the axis. In constructing the lower boundary, we use the
following two additional constrains. The total hydrothermal power released through the sea
floor aged less than 0.1 MA is about 15 MW per kilometer length along the axis [Schultz and Elderfield, 1997], and the maximum temperature is less than 1000°C in the absence of magma. How well these conditions are obeyed can only be checked after numerical runs. It is, in a sense, an iterative process to satisfy them. The final versions of the flux distribution and temperature tail as functions of the distance normal to axis are both given in Fig.5.2C. In the final model, we specify the heat flux for X ≤ 400 m and temperature for X > 400 m as functions of X for the lower boundary.

The simulation results, showing the temperature field and mass transport vectors for this setting, are presented in Fig.5.3. The upper portion of the figure gives the back and front views of the entire domain. We see that the discharge sides are spaced 1 km apart along the axis, and that the circulation is mainly ridge parallel, extending to the base of the model at 2.2 km below. Thus, the aspect-ratio of the cells is ~ 2.2 which may be explained by high anisotropy. About 200 kg/s of fluid circulates through the system per 1 km length along the axis. The nearly axi-symmetric, shallow (< 400 m b.s.f.) recharge areas form around the upflow zones on axis. They contribute about 70% of the fluid. The remainder comes from the flow circulating in the sheeted dikes.

The maximum temperature and Darcy fluid velocity peak at 20°C and 10^{-6} m/s, respectively. It can be easily estimated that the corresponding advective component of heat flux, carried away upon discharge, is ~ \rho v c T \sim 800 \text{W/m}^3. Fig.5.4A gives the entire heat flux distribution. The pattern is stock-like, ridge-normal. We estimate the square area of the on-axial diffuse venting in Model 1 to be about 5 \times 10^{4} m^2 as simply a region where fluid velocity is directed upwards. Willcock and McNabb, [1996] quote a lower value of 5 \times 10^{4} m^2 for both the Main Vent field and High Rise field on the Endeavor Segment of the JDFR. Their semi-analytical, source-sink model for an axi-symmetric 3D circulation yields \kappa \approx 5 \times 10^{-13} - 6 \times 10^{-12} m^2 for the average permeability. In our case, the permeability of the upper extrusive section, that contributes most to the discharge rate, is much higher, 10^{-9} m^2. That may explain the difference.

Clearly, there exist a set of secondary convection rolls developed in the permeable extrusive layer, some 1 - 1.5 km of axis. We detail one such an area in the lower portion of Fig.5.3. It shows both the front and back views. The site releases \sim 0.15 MW total of hydrothermal power through the sea floor at temperatures 6 - 10°C.

Finally, we display a set of 1D curves in Fig.5.4B which quantify cumulative mass transport rates for different depth and distribution of hydrothermal power through the sea floor - all of them as functions of the distance across the strike per 1 km length along the strike. They are normalized such that the value of unity on the vertical axis corresponds to 200 kg/s for the mass rate and 15 MW for the thermal power contributed by the sea floor region be-
5.2 MODEL 1: BASIC MODEL

Figure 5.3: Hydrothermal output for Model 1. Upper portion shows the temperature and mass transport vectors for the entire domain, while the lower portion details those for an off-axial vent field (Site A).
5.2 MODEL 1: BASIC MODEL

Figure 5.4: Sea floor heat flux (A) and cumulative heat power and mass rate (B) for Model 1.
5.3 Model 2: Permeable Zone on Axis

Let us modify Model 1 and include a vertical fracture (fault) zone directly on axis (see Fig. 5.5A). The zone has its permeability-thickness product $k\delta = 3 \cdot 10^{-12} m^3$ which is equivalent to 0.33 mm planar fracture. In the sheeted dikes complex (below 400 mbsf) we make it anisotropic with the ratio of vertical to across-axis equal to 5.

As seen from Fig. 5.5B, the flow becomes more concentrated around the fracture. Note that for a better view, we have shown a quarter-cut of one discharge site, limiting the lateral dimensions of the box to 500 m each. The maximum temperature at the sea floor reaches 70°C, while the maximum fluid velocity is 1 mm/s. We can magnify this area near the sea floor in Fig. 5.5C. A cell-like, 2D flow pattern exists in lower portion of the fracture (below 1000 mbsf), which is best viewed in Fig. 5.5D. The overall mass rate drops to 150 kg/s down from 200 kg/s comparing to Model 1.

5.4 Model 3: Dipping Fault

An extensional fault, originating at 300 m off the ridge axis and dipping 30°, is added to the previous model (with vertical fracture preserved) as in Fig. 5.6A. The dipping plane is approximated as a stair-case fracture whose aperture decreases form 1 mm at the sea floor to a cut-off value of 0.3 mm, following the permeability changes in the surrounding rock. The 3D numerical output for this model is shown in Fig. 5.6B. Fig. 5.6A also shows an enlarged 2D cross-section, normal to the strike. The presence of the fault in layer 2a is almost “ignored” by the high local permeability, but as the 400 mbsf -boundary is crossed, the fault provides a preferential pathway for the descending fluid in the sheeted dikes off axis. Because of this extra influx of cold water, the maximum temperature at the base of the model becomes less than 700°C. However, the total mass rate remains about the same as that in Model 2, and so are the maximum temperature and Darcy velocity at the discharge sites along the axis.

5.5 Model 4: Pipe-like Conduit

High temperature vents (e.g. black smokers) are often found on the ridge axis. Typical temperatures and fluid velocities associated with black smokers are $T_f \approx 350 - 400°C$.
5.5. MODEL 4: PIPE-LIKE CONDUIT

Figure 5.5: Model 2: A-legend, B-temperature and mass transport vectors, C-discharge site near sea floor, D-circulation in the sheeted dikes.
5.5. MODEL 4: PIPE-LIKE CONDUIT

Figure 5.6: Model 3: A-legend & a cross-section, normal to strike, B-3D temperature and mass transport vectors. Model 4: C-legend, D-temperature and mass transport vectors at the sea floor.
and \( v_x \approx 1 - 2 \text{ m/s} \), respectively, while for the so-called white smokers the corresponding numbers are usually 30% lower. The heat flux density for black smokers can be measured in GW/m² [Lowell et al., 1995]. Many serious attempts have been made to model these events. As mentioned in the Introduction to Chapter 3, Yang, [1996] simulates a TAG-like system where a high temperature discharge takes place through a pipe surrounded by a zone of higher permeability. The sea floor in that model is impermeable except near the pipe, which requires to specify a pressure gradient to drive the flow. Schultz and Elderfield, [1997] solve a similar axi-symmetric problem (in 2.5 D) assuming no sediment cover and assigning the temperature of 350°C all the way along the pipe. Tivey and McDuff, [1990] consider mineral precipitation in the walls of black smoker chimneys. The geochemical part of their model is perhaps the most sophisticated among those known to the author, but the main problem there is the boundary conditions, since the size of the domain is very small comparing to the depth of circulation.

The above papers, except Yang, [1996], recognize that the high temperature venting at the sea floor is turbulent and replace Darcy's law with a semi-empirical relationship for turbulent flow in pipes

\[
\frac{\partial \rho}{\partial z} + \rho g = -\frac{f \rho Q^2}{4\pi r^5},
\]

where \( f \) is a friction (Fanning) factor that is chosen between 0.01 and 0.1, \( Q = \pi r^2 v \) is a volumetric rate, \( v \) is a Darcy velocity and \( r \) is the radius of the pipe. Comparing (5.1) to Darcy law,

\[
v = \frac{k}{\mu} \left( \frac{\partial \rho}{\partial z} + \rho g \right),
\]

we can design an iterative process, making \( k \) a function of \( v \) in order to avoid heavy re-coding. In the subroutine that maps fractures (see Chapter 3) we assign

\[
k^{(n+1)} = \frac{4r \mu}{\rho f v^{(n)}}
\]

where \( n \) is an iteration index. The problem of sharp temperature gradients around the pipe (which is essentially that of numerical resolution) is solved naturally by fitting a suitable subdomain around the pipe and iterating as described in Chapter 3.

Let us start with the setting as in Model 2 and introduce a vertical pipe, \( r = 2 \text{cm} \), extending 1.4 km below the sea floor into one of the discharge sites shown in Fig.6.6C to see what impact it will have. The pipe is surrounded by a 1 m thick cylindrical shell of mineral precipitations with \( k = 10^{-14} \text{ m}^2 \). The pore sealing effect at temperatures 150 – 300°C in the upflow zone (Tivey, [personal communication]; also Tivey, [1998]) is accounted by setting permeability of the outer shell \( k = 10^{-14} \text{ m}^2 \).
We should point out that this is a simple physical model which aims primarily at reproducing high temperatures and high velocities observed at sea floor vents. This model ignores the geochemical processes involved in the rock-fluid interactions. In particular, at temperatures above 150°C, anhydrite, silica and sulphides precipitate, while fresh basalts alter to fine-grained assemblages of clay minerals [Holland, 1967]. However, at $T < 150°C$, anhydrite has retrograde solubility, thereby dissolving. Clearly, a more refined modeling must consider both precipitation and dissolution fronts which regulate the internal permeability structure.

After extensive experimentation, we set $f = 0.02$. Fig. 5.6D shows a temperature field in the vicinity of the pipe, within a $40 m \times 40 m \times 1400 m$ rectilinear subdomain (note huge lateral exaggeration) and mass transport vectors at the sea floor. We note a thin thread of high temperature along the pipe heated to $\sim 400°C$ at the foot. About 280 – 300°C is delivered to the surface with the velocity $u_l - 2$ m/s. Although we were able to model both high mass rate and temperature typical of high-temperature sea floor venting, the accuracy of each of these numbers separately is not expected to be very high. We are rather much more confident in the $T \nu$ product, proportional to the advective heat flux discharging through the pipe, because the code is flux-conservative and the flux is roughly proportional to the product $v_f T_f$. On these grounds, we estimate that the heat power and mass transport via high temperature mode to be 15% and 4% of the totals, respectively. Schultz et al., [1992] suggested that discrete flow only accounts for 10 – 20% of the axial heat flow, while Ginster et al., [1994] give a lower quote of 6%. The rest is discharged via diffuse venting. Since the temperature of the diffuse venting adjacent to the pipe is higher than in Model 2, the total mass rate is 80 kg/s - about twice less than that without the pipe.

5.6 Summary

Based on anisotropic permeability model derived from seismology and constrained by axial heat flux and temperature at the gabbro interface, our simulations indicate that a large scale convective pattern at the CoAxial Segment of the Mid-Atlantic Ridge (MFR) is mainly ridge-parallel with both discharge and recharge on axis and with the venting fields spaced 1 km apart. The nearly axi-symmetric, shallow (400 m) recharge areas form around the upflow zones on axis, contributing $\sim 70\%$ of circulating fluid. The remainder comes from deep-focused flow in the sheeted dikes. A set of secondary convection rolls (also ridge-parallel) may be expected to occur $\sim 1 - 1.5$ km off axis. On average, the maximum temperature of the diffuse venting on axis is 20°C and exit velocity is $10^{-5}$ m/s, however, these may increase to 70°C and $10^{-3}$ m/s, respectively, near cracks with apertures of about 0.3 mm. The net mass rate per one diffuse vent field is about 200 kg/s, assuming no fractures. In the transition zone between
On the on-axial and secondary rolls, there is a signature of a sheet-like, ridge-normal flow due to pressure gradients created by the on-axial circulation. This ridge-normal component would be significantly enhanced, if dipping, extensional faults exist in the system. High temperature venting is possible via pipe-like conduits, but their contributions to the heat and mass budget are expected to be 13% and 4%, respectively.
Chapter 6

Assessment of Marine Gas Hydrates
Through Compliance Modeling:
Fundamentals

At this point, we leave our hydrothermal modeling and consider the second major problem of this thesis - modeling of the compliance response of hydrated marine sediments. To make the transition between the two topics smoother, the reader might find it useful to re-visit the Methane Clathrate Hydrate and the Sea Floor Compliance sections of the introductory chapter.

6.1 Introduction

This chapter is concerned with the necessary groundwork to be done before we attempt modeling of the 3D compliance response. First, we review the physical models of the elastic properties of hydrated marine sediments. Then the governing equations will be set up that describe the response of marine sediments to gravity wave loading. It will be shown that the quasi-static, elastic limit is a completely satisfactory approximation for the problem at hand. Finally, we derive the dispersion relationship for gravity waves, modified by the sea floor motion. The details of the numerical algorithm and applications are left for the next two chapters.

To begin, Fig. 6.1 provides a conceptual view of a submarine hydrate setting, typical of the Cascadia region, near the JdFR. Figure 6.2 gives an example of the depths of hydrate phase stability in oceans. The water depth is assumed 1200 m. The solid curve is the methane hydrate phase equilibrium data, with the pressure converted to depth under hydrostatic
6.2. MODELS OF VARIATION OF ELASTIC PROPERTIES WITH DEPTH IN MARINE HYDRATED SEDIMENTS

Figure 6.1: A typical submarine hydrate setting.

conditions. The dashed curve represents the thermal gradient as a function of depth. Note the discontinuity at the sea floor because of the thermal conductivity contrast. The region bounded by the thermal gradient and methane hydrate phase equilibrium curves gives the range of pressures/depths and temperatures of the hydrate stability fields.

As mentioned in the introductory chapter, the majority of marine seismic sections of hydrate bearing areas feature a bottom simulating reflector (BSR), that parallels the sea floor. Figure 6.3 shows such a BSR in the Cascadia region [Yuan et al., 1996].

6.2 Models of Variation of Elastic Properties with Depth in Marine Hydrated Sediments

As methane hydrates form, they make the sediment behave more rigidly because of cementation and stiffness increase. So the elastic moduli of the medium and the corresponding seismic velocities will change. A few empirical models exist to express the average seismic velocities in a three component medium that comprises porous rock matrix, water, and hydrate. All of those models are power laws in which the compressional velocity, \( V_p \), of porous sea floor sediments is given as a weighted volumetric average between the three phases.

Lee et al. [1993] makes use of the following empirical relationships for effective compressional seismic velocities found by Wood [1941]

\[
\frac{1}{\rho_h (V_p^\text{Wood})^2} = \frac{\phi (1 - \phi)}{\rho_p V_p^2} + \frac{\phi \rho_w V_w^2}{\rho_h V_h^2} + \frac{(1 - \phi)}{\rho_m V_m^2}
\]  

(6.1)
6.2. MODELS OF VARIATION OF ELASTIC PROPERTIES WITH DEPTH IN MARINE HYDRATED SEDIMENTS

Figure 6.2: Methane hydrate phase stability diagram [Kvenvolden, 1988].

Figure 6.3: An example of a bottom simulating reflector on the northern Cascadia continental slope [Yuan et al., 1996].
6.2. Models of Variation of Elastic Properties with Depth in Marine Hydrated Sediments

and Willie et al. [1996]

\[
\frac{1}{V_p^{\text{hyd}}} = \frac{\phi(1-s)}{V_{pf}} + \frac{\phi s}{V_{ph}} + \frac{(1-\phi)}{V_{pm}}, \tag{6.2}
\]

where \(V_{pf}, V_{ph}, \text{ and } V_{pm}\) stand for the compressional seismic velocities in fluid, hydrate and rock matrix, respectively. \(\phi\) is the sediment porosity, and \(s\) is the hydrate concentration. The latter is evaluated as a fraction of the available pore space, determined by the matrix porosity. The bulk density, \(\rho_b\), is calculated as

\[
\rho_b = (1 - \phi)\rho_m + (1 - s)\rho_f + s\rho_h, \tag{6.3}
\]

where the subscripts \(s, b, m, f, \text{ and } h\) stand for the bulk, matrix, fluid, and hydrate properties, respectively. Lee showed that the best fit to the experimental data for the effective compressional velocity, \(V_p\), is achieved using the so-called weighted mean equation

\[
\frac{1}{V_p} = \frac{\phi(1-s)}{V_p^{\text{hyd}}} + \frac{1-\phi}{V_p^{\text{air}}} + \frac{(1-\phi)}{V_p^{\text{air}}}, \tag{6.4}
\]

where \(V_p^{\text{air}}, \text{ and } V_p^{\text{hyd}}\) appear on the left-hand side in expressions (6.1)-(6.2), respectively.

Another empirical formula connects the shear velocity, \(V_s\), to the compressional velocity [Castagna et al., 1985]

\[
V_s(\frac{m}{\lambda}) = \frac{V_p(\frac{n}{2}) - 1360}{1.16}. \tag{6.5}
\]

Now we have a means to relate the hydrate concentration to the compressional and shear elastic moduli, \(\lambda\) and \(\mu\), through the well-known equations [Aki and Richards, 1980]

\[
V_p = \sqrt{\frac{\lambda + 2\mu}{\rho}}, \quad V_s = \sqrt{\frac{\mu}{\rho}}, \tag{6.6}
\]

The concentration of hydrate, \(s\), generally increases with depth and can peak at the value of 20-40% towards the BSR. Past the BSR, it goes back to zero quite sharply. Examples of the inferred concentration profiles from seismic and resistivity data near ODP sites 889/890 are given in Fig. 6.4 [Hyndman et al., 1998]. Both yield average concentration estimates about 20-30% of pore space over the 100 m above the BSR.

Willoughby and Edwards [1997] have constructed a model of hydrate bearing layered sediment, assuming the following typical parameters based on ODP and seismic data: 50% sediment porosity, 400 m water depth, 200 m depth to the BSR. Hydrate concentration increases as a quarter-sine from 0% at 20 mbsf to 40% at the BSR level. The seismic
6.3 Governing Equations

The equation of motion of an elastic solid is Newton's law

$$\rho \ddot{x}_i = \partial_t \tau_{ij},$$  \hspace{1cm} (6.7)$$

where $\tau_{ij}$ is the stress tensor, $x_i$ is the vector displacement, $t$ is the time and $\rho$ is the bulk density of the medium. Indices $i$ and $j$ run from 1 to 3, corresponding to the Cartesian coordinates $x$, $y$ and $z$. Vector $x_i = (U, V, W)$ has three Cartesian components, $U$, $V$ and $W$, which are themselves functions of $x$, $y$ and $z$. Note that $\tau_{ij}$ is read as the $i$-th component.
6.3. GOVERNING EQUATIONS

Figure 6.5: Model M2: profiles of hydrate concentration, seismic velocities, elastic moduli, and density in marine sediment [Willoughby and Edwards, 1997].
of stress acting on a surface whose normal points in the \( j \)-direction.

Applied stress causes material strain which in general a second-order tensor. Hooke's law relates the two through the elastic properties of the medium. If the medium is at least piecewise isotropic and linear, the constitutive equation reduces to [Prager, 1961]

\[
\tau_{ij} = \lambda \delta_{ij} + 2\mu \epsilon_{ij},
\]

(6.8)

where \( \epsilon = \partial_i X_j, \epsilon_{ij} = (\partial_i X_j + \partial_j X_i)/2, \) and \( \delta_{ij} \) is the Kronecker delta. Substitution of \( \tau_{ij} \) from the last expression into Newton’s law (6.7) results in

\[
\rho \partial_t \epsilon_{ij} = \partial_i (\lambda \partial_j X_i) + \partial_j (\mu (\partial_i X_i + \partial_j X_j)).
\]

(6.9)

To derive a couple of useful analytical solutions, assume in addition that the medium is composed of homogeneous layers. This allows to set \( \partial_i \mu = 0 \) and \( \partial_i \lambda = 0 \) in equation (6.9) and write

\[
\rho \partial_t \epsilon_{ij} = (\lambda + \mu) \partial_i (\partial_j X_i) + \mu \partial_j \partial_i X_i,
\]

(6.10)

if we note that \( \partial_i X_i \equiv \partial_j X_j \). In vector notations this becomes

\[
\rho \frac{\partial^2 \vec{\epsilon}}{\partial t^2} = (\lambda + \mu) \nabla (\nabla \cdot \vec{\epsilon}) + \mu \nabla^2 \vec{\epsilon}.
\]

(6.11)

With the help of the well-known vector identity, \( \nabla \times \vec{A} = \nabla (\nabla \cdot \vec{A}) - \nabla \times (\nabla \times \vec{A}) \), we finally obtain the simplified equation of motion

\[
\rho \frac{\partial^2 \vec{\epsilon}}{\partial t^2} = (\lambda + 2\mu) \nabla (\nabla \cdot \vec{\epsilon}) - \mu \nabla \times (\nabla \times \vec{\epsilon}).
\]

(6.12)

Following [Aki and Richards, 1980], vector \( \vec{\epsilon} \) is further decomposed into the compressional and rotational components by virtue of Helmholtz theorem

\[
\vec{\epsilon} = \nabla \varphi + \nabla \times \vec{\psi},
\]

(6.13)

where \( \varphi \) and \( \vec{\psi} \) are a scalar and vector potentials for which we have identically \( \nabla \times (\nabla \varphi) \equiv 0 \) and \( \nabla \cdot (\nabla \times \vec{\psi}) \equiv 0 \). Equations (6.12) and (6.13) then produce

\[
\nabla ((\lambda + 2\mu) \nabla^2 \varphi - \rho \frac{\partial^2 \varphi}{\partial t^2}) = \nabla \times (\mu \nabla \vec{\psi} - \rho \frac{\partial^2 \vec{\epsilon}}{\partial t^2}),
\]

(6.14)
but because the two potentials are independent, both sides must equal to zero. So we have

\[ \frac{\partial^2 \varphi}{\partial t^2} = \frac{\lambda + 2\mu}{\rho} \nabla^2 \varphi, \]  

(6.15)

\[ \frac{\partial^2 \psi}{\partial t^2} = \frac{\mu}{\rho} \nabla^2 \psi. \]  

(6.16)

Equations (6.15) and (6.16) describe a compressional wave, propagating with the velocity \( \sqrt{\frac{\lambda + 2\mu}{\rho}} \), and a shear wave, propagating with the velocity \( \sqrt{\frac{\mu}{\rho}} \), respectively.

Now we demonstrate that the inertial term, \( \rho \partial_t \chi_t \), is actually small in our problem, and the quasi-static limit applies. Let \( H \) be a typical spatial scale, \( \delta \) be a typical scale of the sea floor deformation, and \( \omega \) be the frequency, so that \( \partial_t \propto \omega^2 \) for a harmonic process, then for the \( U \)-component we have

\[ \frac{\partial}{\partial x} (\lambda + 2\mu) \frac{\partial U}{\partial x} \propto \frac{U \delta (\lambda + 2\mu)}{x^2 H^2}, \]  

(6.17)

\[ \rho \frac{\partial^2 U}{\partial t^2} \propto \rho \omega^2 U \delta, \]  

(6.18)

where the starred quantities stand for the non-dimensionalized counterparts of the original variables. Similar relationships can be written out for the other two components, \( V \) and \( W \).

The ratio of the inertial term (6.18) to the diagonally leading compressional term (6.17) is

\[ Q = \frac{\omega^2 \rho H^2}{\lambda + 2\mu}. \]  

(6.19)

The numbers relevant to the gravity waves and marine sediments of interest are \( f \sim 0.04 \) Hz for \( H \sim 1000 \) m and \( \lambda + 2\mu \sim 5 \times 10^6 \) Pa. This yields \( Q \sim 0.01 \) which is of the order of the experimental accuracy. In the course of a numerical solution, \( H \) would rather be the inter-nodal distance, so the estimate for \( Q \) above is very conservative.

It is easy to see that \( Q \) is the squared ratio of the phase velocity, \( \omega/k \), to the compressional velocity, \( V_p = \sqrt{(\lambda + 2\mu)/\rho} \), up to the factor 2\( \pi \) if \( H \) is the wavelength. Typically, \( \omega/k \sim 40 \) m/s, while \( V_p \sim 1500 \) m/s.

The governing equations may then be reduced to the quasi-static limit. This allows us to “freeze” the induced pressure variation at the sea floor, varying the phase if necessary to produce a sequence of snapshots for the deformation field. This is possible physically because the phase velocity of the perturbation due to gravity waves is much less than a typical seismic velocity that propagates the perturbation in the medium. In what follows,
we shall always begin with the full wave equation and apply the quasi-static approximation in the course of the derivations wherever necessary.

6.4 Gravity Waves

Ocean surface gravity waves span a wide wavelength band, ranging from a few hundred meters to a few kilometers with amplitudes \( h \sim 1 - 10 \) cm at the sea surface. The amplitude depends on frequency and decays with depth. The stress variation induced by gravity waves on the sea floor is [Crawford et al., 1998]

\[
\tau_{\text{sea floor}}(\omega) = -\rho_f g h(\omega) / \cosh(k(\omega)H),
\]

where \( g \) is the gravity acceleration, \( k(\omega) \) is the wavenumber and \( H \) is the depth of the ocean. The sea floor displacement under this load is in the micron range. For a reasonable duration, the process may be considered periodic, so we have a plane wave excitation propagating along the sea floor with a slow phase velocity. The geometry of the simplest problem of a gravity wave over a sediment half-space is sketched in Figure 6.6. The direction of propagation of the gravity wave is aligned with the \( x \)-axis, the \( z \)-axis is pointing downwards, and the unperturbed sea surface is at \( z=0 \).

Introduce a scalar potential, \( \Phi(x,y,z,t) \), to generate the required 2D displacements,
6.5 BERNOULLI'S EQUATION

\( \vec{\xi}_f = (U_f, 0, W_f) \) in the fluid. By analogy with equations (6.15) and (6.16)

\[
\frac{\partial^2 \Phi}{\partial t^2} = (\lambda_f + 2\mu_f) \nabla^2 \Phi,
\]

\( \vec{\xi}_f = \nabla \Phi, \) \hspace{1cm} (6.22)

where subscript \( f \) refers to the corresponding fluid entities. No vector potential is needed here, as fluids do not support shear stresses or waves. Also note that \( \mu_f \) is negligible in most practical cases.

6.5 Bernoulli's Equation

The perturbation pressure, \( p' \), from the state of hydrostatic equilibrium on the streamline just below the sea surface is

\[
p'_{z=0} = -\rho g W_f |_{z=0},
\]

where the minus sign is because to create an excess of pressure, the vertical displacement \( W_f \) must be above the sea floor level, i.e., be negative. Edwards [personal communication] noted that Bernoulli's equation [Prager, 1961] for incompressible flow on that streamline can be written for the perturbation propagating in the \( z \)-direction as

\[
(\partial_t \Phi + \frac{1}{2} (\partial_t U_f)^2 + \frac{p'}{\rho_f})_{z=0} = 0.
\]

Note that \( \Phi \) is the displacement (not velocity potential) so an extra differentiation w.r.t. time is required on the left-hand side of the last equation. Now we use the quasi-static approximation, discussed above, drop \( \frac{1}{2} (\partial_t U_f)^2 \) and replace \( \partial_t \) with \( -\omega^2 \) to get the following form of Bernoulli's equation

\[
-\omega^2 \Phi_{z=0} = g W_f |_{z=0}
\]

6.6 Dispersion relationship for Gravity Waves

We must establish the dispersion relationship, \( k(\omega) \), in order to identify the proper wavelengths in the time series of the sea floor displacement. The general solution to the wave equation in the fluid (6.21) in terms of potential \( \Phi \) is

\[
\Phi = (A e^{-\omega t} + B e^{\omega t}) e^{i(kz-\omega t)},
\]

(6.26)
where \( q = \sqrt{k^2 - \omega^2/\alpha_f^2} \) and \( \alpha_f = \sqrt{(\lambda_f + 2\mu_f)/\rho_f} \). Note that as \( \omega/k \ll \alpha_f \), we have \( q \gg 0 \), and the wave is evanescent. Also we can set \( q \approx k \) in the final answer.

The vertical displacement component in the fluid is then

\[
W_f = \frac{\partial \psi}{\partial z} = q(-Ae^{-\nu t} + Be^{\nu t})e^{i(kx - \omega t)}.
\] (6.27)

Substituting expressions (6.26) and (6.27) into (6.25), we obtain a rather generic form for the dispersion relationship

\[
\omega^2 = gq(\frac{A}{B} - 1).
\] (6.28)

Assuming for the moment the sea floor is perfectly rigid, there should be no displacement at \( z = H \), which gives upon setting \( W_f = 0 \) in expression (6.27)

\[
B = Ae^{-2\nu H}.
\] (6.29)

Then from the last two equations, it follows that

\[
\omega^2 = gg \tanh(qH) \approx kg \tanh(kH).
\] (6.30)

This is the most commonly used form for the dispersion relationship (see e.g. [Gill, 1982] or Crawford, [1998]).

Let us now lift the sea floor rigidity assumption and calculate the dispersion relationship taking into account the sea floor deformation. To do that, we will need to solve for the displacements within the sediment as well and link them with those in the fluid at the sea floor boundary to find the required ratio \( A/B \), then use formula (6.28). First, we note that for a layered medium, there should be no \( y \)-displacement, so \( V = 0 \) and \( \partial / \partial y = 0 \). Given the vertical polarization of the gravity wave, we are dealing with the limiting case of the so-called P-SV system [Aki and Richards, 1980], and a further simplification is possible to choose the vector potential in equation (6.16) as

\[
\vec{\psi} = (0, \psi(x, z, t), 0).
\]

Then according to definition (6.13) the \( x \)- and \( z \)-components of the displacement \( \vec{X} \) in the sediment are expressed as

\[
U = \frac{\partial \psi}{\partial x} - \frac{\partial \psi}{\partial z},
\] (6.31)

\[
W = \frac{\partial \psi}{\partial z} + \frac{\partial \psi}{\partial x}.
\] (6.32)
Assuming that the sediment is a half-space, we look for the solutions in the form

\[ \varphi = \alpha_1 e^{\epsilon z} e^{i(kx - \omega t)}, \]
\[ \psi = \beta_1 e^{\epsilon z} e^{i(kx - \omega t)}, \]

where

\[ r = \sqrt{k^2 - \frac{\omega^2}{c^2}}, \quad s = \sqrt{k^2 - \frac{\omega^2}{\beta^2}}, \quad \alpha = \sqrt{\frac{\lambda + 2\mu}{\rho}} \equiv V_p, \quad \beta = \sqrt{\frac{\mu}{\rho}} \equiv V_s, \]

The imaginary unity multiplier, \( i = \sqrt{-1} \), is introduced into expression (6.34) for convenience.

At the sea floor boundary, we have the continuity of both normal stresses and displacements, and no tangential stress condition. The latter can be expressed simply from Hooper's law (6.8)

\[ \epsilon_{xz} \big|_{z=H} = \left( \frac{\partial U}{\partial z} + \frac{\partial W_z}{\partial x} \right)_{z=H} = \left( 2 \frac{\partial \varphi}{\partial z} \frac{\partial \psi}{\partial z} + \frac{\partial^2 \psi}{\partial z^2} \right)_{z=H} = 0. \]  

Substituting for \( \varphi \) and \( \psi \) from expressions (6.33) and (6.34) results in

\[ b_1 = -\frac{2 \epsilon \alpha_1 e^{\epsilon z} e^{i(kx - \omega t)}}{k^2 + s^2}. \]  

The requirement that the vertical displacements, \( W \) and \( W_f \), match at \( z = H \) yields

\[ \left( \frac{\partial \varphi}{\partial z} + \frac{\partial \psi}{\partial z} \right)_{z=H} = \left( \frac{\partial \Phi}{\partial z} \right)_{z=H}, \]

from which it follows that

\[ -q A e^{-\epsilon z} H + q B e^{\epsilon z} H = -r_1 e^{-\epsilon z} H - k b_1 e^{\epsilon z} H. \]  

Now the term \( r_1 e^{-\epsilon z} H \) can be conveniently expressed from equations (6.37) and (6.39) as

\[ r_1 e^{-\epsilon z} H = \frac{(q B e^{\epsilon z} H - q A e^{-\epsilon z} H)(k^2 + s^2)}{(k^2 + s^2)}. \]  

The remaining boundary condition is that the normal stress components across the sea floor must be continuous. In the fluid, we evaluate the normal component of stress at the sea floor from expression (6.20), setting \( h(w) = \frac{\partial \Phi}{\partial z} \big|_{z=0} \). In the sediment, it is obtained from
6.6. Dispersion Relationship For Gravity Waves

equations (6.8) and (6.13). The stress continuity condition then reads

\[-\frac{\rho g}{\cosh (kH)} \frac{\partial \phi}{\partial z} \bigg|_{z=0} = (\lambda + 2\mu) \frac{\partial \psi}{\partial z} + \lambda \frac{\partial \phi}{\partial x} = \frac{\partial \psi}{\partial x} = \text{right side of equation (6.41)} \]

Substituting for \( \psi, \psi, \) and \( \Phi \) from expressions (6.33), (6.34), and (6.26), respectively, we obtain after some straightforward algebra from equation (6.41)

\[ \frac{\rho g [A - B]}{\cosh (kH)} = \left( \lambda \frac{\omega^2}{k^2 + \sigma^2} + (\lambda + 2\mu) \frac{\sigma^2}{k^2 + \sigma^2} - 4\mu \frac{k^2 \sigma}{r^2} \right) \left(r \sigma, e^{-rH} \right). \]

On the right-hand side of the last statement, we express \( r^2 \) and \( \sigma^2 \) in terms of \( \omega, k, \alpha, \) and \( \beta \) via formulae (6.35), approximate the \( sr \)-product to the second order as

\[ sr \approx k^2 \left( 1 - \frac{\omega^2}{2\sigma^2 k^2} \right) \left( 1 - \frac{\omega^2}{2\beta^2 k^2} \right), \]

and substitute expression (6.46) for the rightmost bracket. Then the normal stress continuity condition (6.39) takes the following form

\[ \frac{\rho g [A - B]}{\cosh (kH)} = -2(\lambda + \mu) k^2 \frac{[B e^{kH} - A e^{-\sigma H}]}{r (\lambda + 2\mu)} \left( 1 - \frac{\omega^2}{2\beta^2 k^2} \right). \]

Again, as \( \omega^2 / 2\sigma^2 k^2 \ll 1 \), we can drop the rightmost term in brackets in the last equation, and by the same token set \( r \approx k \). Now ratio \( A/B \) is finally calculated from equation (6.43), and we get the desired dispersion relationship for ocean gravity waves from equation (6.28)

\[ \omega^2 = g k \frac{\sinh (kH)}{\cosh (kH) - 1} \]

where \( \Gamma = \rho g \zeta / \cosh (kH) \) and \( \zeta = (\lambda + 2\mu)/(2\kappa \mu (\lambda + \mu)) \). Incidentally, \( \zeta \) turns out to be the sea floor compliance, which will be formally defined in the next section.

Figure 6.7 displays the dispersion relationship, \( \omega(k) \), calculated from formula (6.44) for the two ocean depths, \( H=400 \text{ m} \) and \( H=1000 \text{ m} \). It follows that \( \Gamma \) is less than a percent for \( H \sim 1 \text{ km} \) and \( \lambda, \mu \sim 10^9 \text{ Pa} \), so we are justified in using the simplified formula (6.30). However, some compliance applications require large wavelengths (up to 30 km) [Crawford et al., 1998] to image deep crustal structures. In such a situation, the correction may be of the order of several percent, and should be included into data analysis.
Sea Floor Compliance and Stiffness

The sea floor compliance, $\zeta(\omega)$, is defined as the ratio of the vertical component of the sea floor displacement to the vertical component of stress induced by a periodic shear loading, acting on the sea floor

$$\zeta(\omega) = \frac{W(\omega)}{\tau_{xx}(\omega)_{\text{sea floor}}}.$$  \hspace{1cm} (6.45)

It is easy to work out this expression for the half space, using equations (6.38), (6.41), (6.33), (6.34), and (6.37) from the previous section. The answer is

$$\zeta(\omega) = \frac{\lambda + 2\mu}{2k(\omega)\mu(\lambda + \mu)},$$ \hspace{1cm} (6.46)

obtained first by [Sorrels and Coforth, 1973] in this form. It is convenient to work with the normalized compliance [Crawford, et al., 1998] which is the modulus of the last expression, multiplied by $k(\omega)$, however, since hydrates result in sediment stiffening, the reciprocal of the normalized compliance will be a better choice. We will denote it $\xi$ and refer to as stiffness

$$\xi = \frac{1}{k(\omega)W(\omega)}.$$ \hspace{1cm} (6.47)
6.8. PORO-ELASTICITY CONSIDERATIONS

which for the half-space obviously becomes

\[ \xi_{S,EP} = \frac{2\mu(\lambda + \mu)}{\lambda + 2\mu}. \] (6.48)

If \( \lambda \gg \mu \), stiffness is directly proportional to the shear modulus. Differentiating expression (6.48) w.r.t. \( \mu \) and \( \lambda \) and taking the ratio, we find that stiffness of the half space is much more sensitive to changes in \( \mu \) than those in \( \lambda \)

\[ \left( \frac{\partial \xi}{\partial \mu} \right)_{S,EP} \left( \frac{\partial \xi}{\partial \lambda} \right)_{S,EP} = \left( \frac{\lambda}{\mu} \right)^2 + 2 \left( \frac{\lambda}{\mu} \right) + 3. \] (6.49)

6.8 Poro-Elasticity Considerations

We must recognize that the oceanic crust in which methane hydrates are formed is actually a porous medium, and that surface loading due to gravity waves causes over-pressures which may drive fluid flow. Thus, the structure's response is, generally speaking, visco-elastic, and the following question naturally arises: will this fluid flow have a serious impact?

Wang and Davis [1996] show that the response of a poro-elastic half space to a harmonic surface loading of the form \( p_b \cos(\omega t) \) is a sum of the diffusive (viscous) and instantaneous (elastic) components

\[ p(z, \omega) = p_b \cos(\omega t) \left[ (1 - \gamma) e^{-\eta z^*} + \gamma \right], \] (6.50)

where \( p_b \) is the amplitude of the pressure variation at the sea floor, \( \gamma \) is the loading efficiency, \( \omega \) is the circular frequency, so that the frequency is \( f = \omega / (2\pi) \) and the period is \( T = 1 / f \), and \( z^* \) is the dimensionless depth, given by the expression below

\[ z^* = \frac{z}{\sqrt{\pi \eta f^2}}. \] (6.51)

In expression (6.51), \( \eta \) is the so-called hydraulic diffusivity, defined as [Wang and Davis, 1996]

\[ \eta = \frac{k}{\mu S}. \] (6.52)

where \( k \) is the host rock permeability, \( \mu \) is the dynamic viscosity of the fluid, and \( S \) is the storage coefficient. There are a few models, reviewed in the cited above paper that relate \( S \) to the elastic moduli and porosity of the medium. They calculate from expression (6.51) that for a typical marine sediment, having \( k = 10^{-18} \text{ m}^2 \), \( \gamma = 0.5 \), and the loading period of 12 hours due to tides, the dimensionless depth of unity, \( z^* = 1 \), corresponds to the depth \( z_1 = 10 \text{ m} \). At such a depth, the ratio of the diffusive response to elastic response...
amplitudes is \((1 - \gamma)e^{-x}/\gamma\) from formula (6.50). If \(\gamma \approx 0.5\), we obtain that at \(z^* = 1\), the ratio is approximately 0.043. It follows from formulae (6.50) and (6.51) that \(z_1 = z_1\left(1/\sqrt{E_T}\right)\), so, say, for a highly permeable sedimentary section with \(k = 10^{-11}\) m\(^2\) and a typical compliance frequency of 0.05 Hz (\(T = 20\) s) \(z_1 \approx 20\) m. Below this depth, the medium may be treated as an elastic solid for our purposes.

6.9 Summary

The compliance technique is a suitable tool for detecting changes in the elastic properties. It makes use of the ocean surface gravity waves as a natural shear source to shake the sea floor laterally. We have derived the dispersion relationship between the wavelength of the gravity wave and its frequency, and demonstrated that for relatively short wavelengths, it is a function of the ocean depth only. To a good approximation, the forward compliance modeling can be set up as a quasi-static, elastic problem.
Chapter 7

Assessment of Marine Gas Hydrates
Through Compliance Modeling:
Numerical Algorithm

7.1 Introduction

How do we model the compliance problem? We can turn first to the available literature and software. Seismologists treat the Earth as an elastic medium and compute the response to P- and S-waves both analytically and numerically [e.g. Aki and Richards, 1980], whereas hydrologists model the process of settlement in a saturated porous medium under the time-dependent surface loading [e.g. Bear, 1972]. The compliance problem is simpler. The spatial scale of our problem (a couple of kilometers) allows one to neglect the Earth curvature. The inertial terms can be dropped and a quasi-static approximation used. So adapting seismic software would not be the most efficient approach, except for the layered medium [Gomberg and Masters, 1988]. The effects of poro-elasticity, often significant for the hydrologist, are also negligible here for the frequencies involved, as shown in the last section of the previous chapter.

Compliance calculations using modified seismic codes have been published by Crawford et al., [1998]. They use a 2D finite difference code and apply it to estimate oceanic crustal velocities, focusing in particular on low-velocity zones (LVZ), such as magma chambers. The problem of spatial resolution becomes very acute, because in their modeling, numerical stability concerns, inherited from seismic software, require an artificial transition zone of 12 -- 15 nodes to connect discrete areas of constant elastic parameters on a uniform grid. According to Fig. 6.4 (Chapter 6) which gives a field example of hydrate distribution, we
7.2. QUASI-STATIC EQUATIONS IN 3D

We elect to develop here a simple, economic, full 3D numerical algorithm to model the compliance response of an arbitrary, possibly random, distribution of hydrate bearing volumes, within a rectangular domain, using the quasi-static governing equations. They are formulated for the displacement components in the medium under periodic surface loading. The governing equations can be put in a self-adjoint form naturally. We use the control volume discretization, which is good at handling discontinuities in the coefficients and accurate treatment of the boundary conditions.

Our work on hydrothermal modeling (Chapter 3) suggested that solving coupled systems of PDEs sequentially isn’t the most efficient approach. So we apply a simple Jacobi over-relaxation iterative point scheme to all three displacement components simultaneously. Large values of the over-relaxation parameter may then be used to speed-up iterations. In contrast, for the sequential iterations, the over-relaxation parameter should by typically much smaller than unity, rendering the iterations slow.

In this chapter, we describe the numerical algorithm, test it against analytical and numerical solutions, and run a few simplified models to elucidate the physics involved and to work out the criteria for the optimal domain dimensions and number of nodal points per loading wave cycle.

7.2 Quasi-Static Equations in 3D

Expanding the equation of motion (6.9) in Cartesian coordinates and keeping with the same notations, we obtain in the quasi-static limit

\[
\frac{\partial}{\partial x}((\lambda+2\mu)\frac{\partial U}{\partial x}) + \frac{\partial}{\partial y}((\lambda+2\mu)\frac{\partial U}{\partial y}) + \frac{\partial}{\partial z}((\lambda+2\mu)\frac{\partial U}{\partial z}) = -\left[ \frac{\partial}{\partial x}(\mu\frac{\partial V}{\partial y}) + \frac{\partial}{\partial y}(\mu\frac{\partial V}{\partial z}) + \frac{\partial}{\partial z}(\mu\frac{\partial V}{\partial x}) \right],
\]

\[
\frac{\partial}{\partial x}((\lambda+2\mu)\frac{\partial V}{\partial x}) + \frac{\partial}{\partial y}((\lambda+2\mu)\frac{\partial V}{\partial y}) + \frac{\partial}{\partial z}((\lambda+2\mu)\frac{\partial V}{\partial z}) = -\left[ \frac{\partial}{\partial x}(\mu\frac{\partial U}{\partial y}) + \frac{\partial}{\partial y}(\mu\frac{\partial U}{\partial z}) + \frac{\partial}{\partial z}(\mu\frac{\partial U}{\partial x}) \right],
\]

\[
\frac{\partial}{\partial x}((\lambda+2\mu)\frac{\partial W}{\partial x}) + \frac{\partial}{\partial y}((\lambda+2\mu)\frac{\partial W}{\partial y}) + \frac{\partial}{\partial z}((\lambda+2\mu)\frac{\partial W}{\partial z}) = -\left[ \frac{\partial}{\partial x}(\mu\frac{\partial U}{\partial y}) + \frac{\partial}{\partial y}(\mu\frac{\partial U}{\partial z}) + \frac{\partial}{\partial z}(\mu\frac{\partial U}{\partial x}) \right].
\]

These equations are to be solved for the three displacement components, U, V, and W. We have split the equations (7.1) in such a way that the left-hand side (LHS) operates on a single scalar field, while the other two components are collected on the right-hand side.
7.3. BOUNDARY CONDITIONS

Figure 7.1: Solution domain and boundary conditions

(RHS). We will refer to these equations as the U-, V- and W-equation, respectively.

Each term on either the LHS or RHS of equations (7.1) fits the following generic description

\[ L(f) = \alpha(\partial_m f), \]  

(7.2)

where \( i, m = \{x, y, z\}, f = \{U, V, W\}, \) and \( \alpha = \{\lambda, \mu, \lambda + 2\mu\}. \) The Lame parameters \( \lambda \) and \( \mu \) are functions of position. The spatial scale of their variations can easily be smaller than the grid step size we can afford. Consequently, we leave the Lame parameters inside the brackets in the terms like (7.2). The equations are then suitable for the control volume discretization, which can handle rapid variations in the self-adjoint coefficients.

The coupling terms appear on the RHS of the governing equation (7.1). Physically, when an elastic volume gets deformed in one of its principal directions, deformations will develop in the other two directions. The RHS does not contain real source terms explicitly. The loading force is part of the boundary condition on the normal stress at the sea floor, i.e. the top of the model.

7.3 Boundary Conditions

The governing equations are solved in a rectilinear domain, shown in Fig. 7.1, with the dimensions \( X_{\text{max}}, Y_{\text{max}} \) and \( Z_{\text{max}}. \) The z-axis is directed upwards. The sea floor makes the
upper boundary, \( z = Z_{\text{max}} \). Assume that the vertical component of stress at the sea floor, \( \tau_{zz} \), is a known periodic function due to plane wave loading. The algebra is simplified if we align one of the lateral axes, say the \( x \)-axis, with the direction of propagation of the gravity wave. Then we can write

\[
\tau_{zz}|_{z = Z_{\text{max}}}(x) = \Xi \sin \left( \frac{2\pi x}{\Lambda} + \nu \right),
\]

where \( \Xi \) is the amplitude, \( \nu \) is the phase, and \( \Lambda \) is the integral number of forcing wavelengths that must fit within the domain boundaries in the direction of strike. By inspection, \( X_{\text{max}}/\Lambda \) is the wavelength which we will denote as \( \Lambda \), lest it be confused with the compressional elastic modulus. The following expression, obtained straight from Hooke's law (6.8)

\[
\tau_{zz}|_{z = Z_{\text{max}}} = \left[ \lambda \left( \frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} + \frac{\partial W}{\partial z} \right) + 2\mu \left( \frac{\partial W}{\partial x} \right) \right]_{z = Z_{\text{max}}},
\]

will serve as the stress boundary condition at \( z = Z_{\text{max}} \) for the \( W \)-equation. Note that because the problem is linear, the magnitudes of both stresses and displacements are proportional to the amplitude of the loading force, \( \Xi \). Therefore, compliance (or stiffness), as the stress-displacement ratio, will be independent of \( \Xi \), and we can set the latter at will to any convenient number.

Another pair of boundary conditions is obtained from the no-shear-stress condition at \( z = Z_{\text{max}} \), because it is in contact with fluid. So we have from equation (6.8)

\[
\tau_{zz}|_{z = Z_{\text{max}}} = 2\mu \left( \frac{\partial U}{\partial x} + \frac{\partial W}{\partial z} \right)_{z = Z_{\text{max}}} = 0,
\]

\[
\tau_{ss}|_{z = Z_{\text{max}}} = 2\mu \left( \frac{\partial V}{\partial y} + \frac{\partial W}{\partial z} \right)_{z = Z_{\text{max}}} = 0.
\]

Expressions (7.5) and (7.6) will be used as the stress boundary conditions at \( z = Z_{\text{max}} \) for the \( U \)- and \( V \)-equation, respectively.

As it is not possible to solve for the infinite medium, we need to make an assumption about the lateral boundaries. There may be two sensible choices: no-displacement or periodic boundaries. Following [Crawford et al., 1998], we use the latter which implies that the elastic moduli \( \lambda \) and \( \mu \) as well as the solutions must be periodic functions, too. In reality they are not, so the region of interest must be well within the interior of the domain, unless we are dealing with a layered medium. It turns out that isolated 3D features are resolved reasonably well if they are located within a centered rectilinear region, whose size is about half of the main simulation domain. On the other hand, the consequences of the periodicity assumption
7.4 Control Volume Discretization

are mitigated if \( \lambda \) and \( \mu \) are randomly distributed. The situation is similar to that when one is computing a 2D Fourier transform of a function, defined on \([-\infty, +\infty]\). Given the evanescent nature of the induced displacement fields, we take

\[
U_0 = 0, \quad V_0 = 0, \quad W_0 = 0
\]

(7.7)

at the bottom of the domain. As we will see later, it is sufficient to have \( Z_{\text{max}} \) to be just one wavelength of the forcing gravity wave for condition (7.7) to work properly. This completes the description of the boundary conditions. For a brief summary, see Fig. 7.1.

7.4 Control Volume Discretization

Define the main computational rectilinear grid, \((x_i, y_j, z_k)\),

\[
\begin{align*}
\alpha_i &: i = \{1, nx\}, \quad \alpha = 0, \quad \alpha_{max} = X_{\text{max}} \\
\beta_j &: j = \{1, ny\}, \quad \beta = 0, \quad \beta_{max} = Y_{\text{max}} \\
\gamma_k &: k = \{1, nz\}, \quad \gamma = 0, \quad \gamma_{max} = Z_{\text{max}}
\end{align*}
\]

(7.8)

and the auxiliary staggered grid, \((\alpha'_i, \beta'_j, \gamma'_k)\),

\[
\begin{align*}
\alpha'_i &: i = \{1, nx + 1\}; \quad \alpha_i = x_i; \quad \alpha_i = \frac{1}{2}(x_i + x_{i+1}) : i = \{2, nx\}; \quad \alpha_{i+1} = x_{\alpha}\, x_{\alpha}, \\
\beta'_j &: j = \{1, ny + 1\}; \quad \beta_j = y_j; \quad \beta_j = \frac{1}{2}(y_j + y_{j+1}) : j = \{2, ny\}; \quad \beta_{j+1} = x_{\beta}\, x_{\beta}, \\
\gamma'_k &: k = \{1, nz + 1\}; \quad \gamma_k = z_k; \quad \gamma_k = \frac{1}{2}(z_k + z_{k+1}) : k = \{2, nz\}; \quad \gamma_{k+1} = x_{\gamma}\, x_{\gamma}.
\end{align*}
\]

(7.9)

Note that the grids are allowed to be non-uniform for greater generality, but the staggered nodal points are always located half-way between the major nodes. The following notation will be often employed

\[
t_{l+1} = t_{l+\frac{1}{2}} : l = \{1, nl - 1\},
\]

(7.10)

where \( t = \{x, y, z\} \) and \( l = \{i, j, k\} \).

A rectilinear control volume, \( V_{ijk} \), around a node \((i, j, k)\) is formed by the intersection of the following six planes \( x_{ij\frac{1}{2}}, y_{ij\frac{1}{2}}, z_{ij\frac{1}{2}} \). There are three principal faces associated with \( V_{ijk} \), whose normals point in the \( x-, y-, \) and \( z-\) direction, respectively

\[
\begin{align*}
s_{ik} &= (y_{ij} - y_{ij}) (x_{ij} - x_{ij}), \\
s_{ik} &= (x_{ij} - x_{ij}) (x_{ij} - x_{ij}), \\
s_{ij} &= (x_{ij} - x_{ij}) (y_{ij} - y_{ij}).
\end{align*}
\]

(7.11)
7.4. CONTROL VOLUME DISCRETIZATION

Figure 7.2: Computational grid in the vicinity of nodal point \((i, j, k)\). Shaded region makes up control volume \(V_{ijk}\). Nodes on the main grid are shown as stars. Staggered grid nodes are shown as opaque squares and circles.

Figure 7.2 displays the computational stencil centered around a nodal point \((i, j, k)\). The main nodal points are shown as stars, the staggered grid nodes are shown as opaque squares and circles. Control volume \(V_{ijk}\) is shaded for clarity.

If a property \(\alpha\) such as \(\lambda\), \(\mu\), or \(\lambda + 2\mu\) that enters relationship (7.2) is to be evaluated on the staggered grid, the following notations will be helpful

\[
\alpha(x_i, y_j, z_k) = \alpha_{i, j, k} ; \quad \alpha(x_{i+1/2}, y_j, z_k) = \alpha_{i+1/2, j, k} ; \quad \alpha(x_i, y_j, z_{k+1/2}) = \alpha_{i, j, k+1/2} \quad (7.12)
\]

Assuming that \(\alpha\) is defined at the major grid points, we can approximate its value on face
7.4. CONTROL VOLUME DISCRETIZATION

\[ s_{ijk} \text{ in one of the two ways} \]
\[ a_{ij,k} = \frac{2a_{i,j,k} + a_{i+1,j,k}}{a_{i,j,k} + a_{i+1,j,k}}; \quad a_{i+1,j,k} = \frac{1}{2}(a_{i,j,k} + a_{i+1,j,k}). \]  
(7.13)

called the geometric and algebraic average, respectively. Similar relationships can be written by inspection for \(a_{i,j+k}\) and \(a_{i,j+k+1}\) on faces \(s_{ik}\) and \(s_{ij}\). The geometric averaging is what most texts would recommend [Patankar, 1980]. In practice, however, the difference is often negligible, unless the grid is very coarse. Other approximations are possible, but they usually result in computationally expensive algorithms.

Having set up the grids and the rules for calculating the coefficients, the next step is to integrate the discretized governing equations (7.1) over the control volume at each (non-Dirichlet) node, thus effectively reducing the order of the derivatives to approximate. Note that we have conveniently defined the staggered grid arrays in a way that no special adjustments are required for the boundary points.

The following generalization of the Gauss theorem due to Ostrogradsky will help to perform the integration

\[ \int \int \int \left( \frac{\partial F_1}{\partial x} + \frac{\partial F_2}{\partial y} + \frac{\partial F_3}{\partial z} \right) dV = \int \int \left( F_1 \cos(n_x) + F_2 \cos(n_y) + F_3 \cos(n_z) \right) dS, \]  
(7.14)

valid for any smooth functions \(F_1\), \(F_2\), and \(F_3\) with continuous first derivatives within volume \(V\), bounded by surface \(S\). Here \(\cos(n_x)\), \(\cos(n_y)\), and \(\cos(n_z)\) are the directional cosines made by the outer surface normal with the coordinate axes. The first-order derivatives are discretized via standard finite difference formulae. As an example, we integrate the terms \(\frac{\partial W}{\partial y}\) and \(\frac{\partial W}{\partial z}\) that appear on the LHS and RHS of the U-equation in (7.1), respectively

\[ \int \int \int_{V_{ijk}} \left( \frac{\partial W}{\partial y} \right) dxdydz = \int \int_{S_{ijk}} \left( \frac{\partial W}{\partial y} \right)_{\frac{1}{2}} dS; \quad \int \int \int_{V_{ijk}} \left( \frac{\partial W}{\partial z} \right) dxdydz = \int \int_{S_{ijk}} \left( \frac{\partial W}{\partial z} \right)_{\frac{1}{2}} dS. \]  
(7.15)

In the last expression, \(W\) is approximated at the staggered nodal points, shown as circles in
7.5. ITERATIVE SCHEME

Fig. 7.2, as

\[ W_{i,j,k} \approx \frac{1}{4} \left( W_{i-1,j,k} + W_{i,j+1,k} + W_{i-1,j+1,k} + W_{i,j,k+1} \right). \]  (7.17)

Note that similar arguments are used in analytical derivations, involving stress tensors [Boley and Weiner, 1988]. Then it follows from the formulae (7.17), (7.16), and (7.10)

\[ \int \int \int \frac{\partial}{\partial x} \left( \frac{\partial W}{\partial x} \right) dx dy dz \approx \frac{1}{4} \left( \lambda_{i+1,j,k} (W_{i+1,j,k} + W_{i+1,j+1,k} + W_{i+1,j,k-1} - W_{i,j,k-1}) - \right. \\

\left. \lambda_{i,j+1,k} (W_{i,j+1,k} + W_{i,j+1,k} + W_{i,j+1,k} - W_{i,j,k-1}) \right) \left( y_{j+1} - y_{j-1} \right). \]  (7.18)

The rest of the discretization is performed similarly by cyclic permutation of the indices, coordinates, and displacement components in equations (7.15) and (7.18).

Since we have assumed the solution to be periodic w.r.t the lateral boundaries, a simple translation rule is used, should a node \((i,j,k)\) belong to the domain boundary

\[ f_{i-1,j,k}^{\text{left}} = f_{i+1,j,k}^{\text{right}} ; \quad f_{i,j+1,k}^{\text{up}} = f_{i,j,k}^{\text{down}} \]

\[ f_{i,j-1,k}^{\text{down}} = f_{i,j+1,k}^{\text{up}} ; \quad f_{i,j+1,k}^{\text{right}} = f_{i,j,k}^{\text{left}}, \]  (7.19)

where \( f = \{ U, V, W \} \). At the lower boundary where \( k = 1 \), the displacements are known (zeroes), so no actions are necessary. Integrating the terms of the form \( \int \int \frac{\partial}{\partial x} \left( \frac{\partial \tau_{ij}}{\partial x} \right) dx dy dz \) in equation (7.1), we use boundary conditions (7.4) - (7.6) to evaluate the resulting surface integrals over a portion of the sea floor. The result is forced to zero for the \( U \) - and \( V \) -equations because of the free-slip conditions (7.5) and (7.6), while for the \( W \)-equation it is exactly \( \int \int \tau_{ij} \left|_{x=x_{\text{lower}}} \right. \approx 0 \), according to condition (7.4).

Note that in the development above, \( \lambda \) and \( \mu \) need only be evaluated on the staggered grid, at the nodes shown as squares in Fig. 7.2. This allows to lock up discontinuities in the elastic moduli in the major grid nodes.

7.5 Iterative scheme

Each of the discretized governing equations (7.1) is now put in the following form

\[ \mathcal{G}(f_{i,j,k}) = c_1 f_{i-1,j,k} + c_2 f_{i+1,j,k} + c_3 f_{i,j-1,k} + c_4 f_{i,j+1,k} + c_5 f_{i-1,j,k} + c_6 f_{i,j,k+1} - c_7 f_{i,j,k} = R_{i,j,k}, \]  (7.20)

where coefficients \( c_i \) are functions of the elastic moduli and geometry, \( f \) stands for one of the displacement components \( \{ U, V, W \} \), and \( R_{i,j,k} \) is not a function of that particular \( f \). The
LHS operator $\mathfrak{S}(f)$ is diagonally dominant and positive definite by construction, so that $c_0 = \sum_{i=1}^{n} z_i > 0$. We split it into the diagonal and off-diagonal parts

$$\mathfrak{S}(f_{i,j,k}) = \mathfrak{S}(f_{i,j,k}) - c_0 f_{i,j,k}. \tag{7.21}$$

The Jacobi over-relaxation method (JOR) [Serles, 1996] was elected to solve system (7.20) for its simplicity, robustness, and low memory requirement. It is a two-step process. A standard Jacobi point iteration is performed first

$$f_{i,j,k}^{\text{new}} = \frac{-\mathfrak{S}(f_{i,j,k}) + R_{i,j,k}^{(n)}}{c_0}. \tag{7.22}$$

Note that it is an explicit scheme, so the result depends on the previously computed values at the nodes, neighboring $(i,j,k)$ only. The solution is advanced from iteration level $(n)$ to an intermediate level $(n+\frac{1}{2})$ at each node. Then the process is accelerated by an over-relaxation step

$$f_{i,j,k}^{(n+1)} = f_{i,j,k}^{(n+\frac{1}{2})} E + f_{i,j,k}^{(n)} (1 - E), \tag{7.23}$$

where $E$ is the so-called over-relaxation parameter. The value of $E$ is normally chosen between 1 and 2, the particular value being adjusted experimentally. For the current problem, we use $E = 1.8$. Higher values may cause divergence, while lower values slow down the computations.

The diagram below describes the algorithm schematically

$$V(i,j,k) : \begin{array}{c} \left( U_{i,j,k}^{(n)}, V_{i,j,k}^{(n)}, W_{i,j,k}^{(n)} \right) \rightarrow \left( U_{i,j,k}^{(n+1)}, V_{i,j,k}^{(n+1)}, W_{i,j,k}^{(n+1)} \right) \rightarrow \\
\left( U_{i,j,k}^{(n+1)}, V_{i,j,k}^{(n+1)}, W_{i,j,k}^{(n+1)} \right) \rightarrow \left( U_{i,j,k}^{(n+2)}, V_{i,j,k}^{(n+2)}, W_{i,j,k}^{(n+2)} \right) \end{array} \tag{7.24}$$

where the starting value, $(U^{(0)}, V^{(0)}, W^{(0)})$, can be a previously computed iterate on the same grid or just zero if nothing better is available. The details of going from $f^{(n)}$ to $f^{(n+1)}$ are given in equations (7.22) and (7.23).

The convergence rate of scheme (7.24) depends strongly on the order in which the nodal points are visited. The schedule, found empirically to perform substantially better than any other, is shown below in a rather compact, FORTRAN-like notations

$$\begin{array}{c} (i = 1, 8, \ (k = nz - k_l(i), 2, -2, \ (j = j_l(i), ny, 2, \ (i = i_l(i), nx, 2))), \\
i_u = /1, 2, 2, 1, 2, 1, 2, 1/, \ j_u = /1, 2, 2, 1, 2, 1, 2/, \ k_u = /0, 0, 1, 1, 1, 0, 0/, \\
i_l = /1, 2, 2, 1, 2, 1, 2, 1/, \ j_l = /1, 2, 2, 1, 2, 1, 2/, \ k_l = /0, 0, 1, 1, 1, 0, 0/ \end{array} \tag{7.25}$$
7.6. CONVERGENCE CRITERIA

where, for example, \( i_a(l = 1) = 1 \), \( i_a(l = 2) = 2 \), \( i_a(l = 3) = 2 \), etc. It loops over the entire domain, picking up nodes to be used by algorithm (7.24). First, the solution is updated at the "skeleton" nodes, skipping every second point in \( i, j \) and \( k \) upon descend from the upper boundary, where the loading force acts. This provides the maximum decoupling between the updates \( U^{(\alpha+1)}, V^{(\alpha+1)} \), and \( W^{(\alpha+1)} \) at the neighbouring nodes. The remaining part of the schedule is less critical, but, loosely speaking, resembles the sequence of wheel alignment in the car. Note that overall, it is not the Red-and-Black ordering [Iserles, 1996], which is rather of the chess-board type. The latter was tried as well, but appeared to be less successful.

These peculiarities of the nodal ordering suggested a way of constructing the initial approximation by linearly interpolating solutions from coarser grids, often starting from as coarse a grid as, say, \( 3 \times 3 \times 3 \). This was implemented and found to speed up the convergence rate by the factor of 10 comparing to the single grid version, other conditions being equal.

Should the JOR method be appropriate for the use with a full multi grid algorithm as a smoother, far richer rewards might be expected, however, the initial desire to experiment with it was eventually arrested. Newton's method was tried in place of JOR with the algorithm described above, where the error vector \( \{ \Delta U^{(\alpha+1)}, \Delta V^{(\alpha+1)}, \Delta W^{(\alpha+1)} \} \), was minimized. It does work but proved to be slower than JOR for problem (7.1). Also it requires twice as much memory for storage.

7.6 Convergence criteria

Both absolute, \( \varepsilon_{abs} \), and relative, \( \varepsilon_{rel} \), errors are used in the convergence criteria, defined in the usual way

\[
\text{Max}\left\{ \left| U^{(n)} - U^{(n-1)} \right|_{l,j,k}, \left| V^{(n)} - V^{(n-1)} \right|_{l,j,k}, \left| W^{(n)} - W^{(n-1)} \right|_{l,j,k} \right\} \leq \varepsilon_{abs}, \quad (7.26)
\]

\[
\text{Max}\left\{ \left| \frac{U^{(n)} - U^{(n-1)}}{U^{(n)}} \right|_{l,j,k}, \left| \frac{V^{(n)} - V^{(n-1)}}{V^{(n)}} \right|_{l,j,k}, \left| \frac{W^{(n)} - W^{(n-1)}}{W^{(n)}} \right|_{l,j,k} \right\} \leq \varepsilon_{rel}. \quad (7.27)
\]

The relative errors are generally more informative, as they are scale-independent, but make little sense if the magnitude of the displacement itself is zero or very small. To avoid a \( \frac{1}{l} \) possibility, the absolute values of \( U^{(n)}_{l,j,k}, V^{(n)}_{l,j,k} \), and \( W^{(n)}_{l,j,k} \) are calculated first and compared to a prescribed cut-off value, for example \( 10^{-3} \) - \( 10^{-4} \) of the maximum. The relative errors are then evaluated only for those displacement components whose moduli exceed the cut-off level.

The software is coded in portable ANSI FORTRAN77 in double precision and has been tested to compile (with all levels of optimization) and run well on SUN, SGI and IBM.
RISC6000 workstations, and on P-II generation of PCs. Typical CPU times are about 4 hours on IBM RISC6000 at 166 MHz and under 2 hours on P-II at 400 MHz for a 3D model, having 100 nodes in each dimension and for $\varepsilon_{nl} \sim 10^{-4} - 10^{-5}$. The CPU time increases substantially if a higher precision is desired. This behavior is typical for classical iterative schemes. On the practical side, though, compliance is hardly measured better than 0.1%.

For a given accuracy, the CPU time is proportional to the number of nodes.

7.7 Code Validation. Simplified Case Studies

We start off with a uniform sediment half-space setting for which an analytical solution is known. For definiteness, let $V_p = 1800 \text{ m/s}$, $V_s = 400 \text{ m/s}$, and $\rho = 2000 \text{ kg/m}^3$

Subscript zero will be added to all the notations relevant to this test case. Consider a harmonic pressure perturbation at the sea floor in the form $\Xi_0 \sin(k_0 x - \omega t)$ and let $\Xi_0 = 10 \text{ Pa}$, $\lambda_0 = 2\pi/k_0 = 500 \text{ m}$. Using formulae (6.6) and (6.7), we calculate the elastic moduli $\lambda_0 = 5.84 \times 10^6 \text{ Pa}$ and $\mu_0 = 0.32 \times 10^6 \text{ Pa}$. The stiffness is then determined from formula (6.48) to be $\xi_0 = 0.6084 \times 10^6 \text{ Pa}$.

Figure 7.3 shows a vertical $(x-z)$ cross-section of the vector-displacement field in the sediment and, separately, contours of the vertical and horizontal displacement components, $W_0$ and $U_0$, which are in the micron range for the parameters above. The pattern shown corresponds to the zero phase case, $\nu_0 = 0$ as in expression (7.3). The complete picture in the time domain can be obtained by translation. The maximum amplitude is attained at the sea floor $|W_{\text{max}}| = 1.28 \mu m$. Note that it can also be calculated straightforwardly from compliance, wavelength, and perturbation amplitude as

$$|W_{\text{max}}| = \frac{\Xi A}{2\pi \xi^2} \quad (7.28)$$

according to formula (6.47).

Calculations are carried for two spatial periods of the forcing gravity wave with the relative error tolerance set at $10^{-5}$ for the cut-off value of $10^{-3}$, as described in Section 7.6, and a variable depth of the model. The number of nodal points per wavelength is 81, which amounts to 6.25 m of spatial resolution, maintained constant in all three dimensions. For this 2D problem, varying the number of nodes in the p-dimension (across the strike) has, as it should, no effect, and is set to 2. It was found experimentally that setting the depth of the model to one wavelength, $Z_{\text{max}} = \lambda$, is a safe choice, so that compliance is virtually unaffected by assigning any greater value, given the evanescent nature of the induced displacement field. Similar checks were performed for all other models with the
Horizontal component of the displacement.
$\varepsilon_0=0.44 \, \mu m$.

Lateral extent (m)

Depth (mbsf)

Figure 7.3: Half space test model. Displacement in the sedimentary section.
same success. This is in complete agreement with [Crawford et al., 1998] who also restrict the depth of the model to one wavelength. Thus, the size of the half-space model will be $101 \times 2 \times 81$ nodes.

Numerically, we obtain for stiffness $\xi_{0}^{\text{num}} = 0.613 \cdot 10^{9} Pa$, some 0.8% greater than the analytical answer. Similarly, Crawford et al., [1998] observed that numerically obtained compliance is always smaller than that given by formula (6.46) by 0.01 – 5%. It may be of interest to shed some light on what contributes to this bias.

According to expressions (6.47) and (6.48), the sea floor stiffness (as well as compliance) is a function of the following parameters $\xi = \xi(\Lambda, \mu, \lambda)$, in which $\Lambda$ and $\mu$ enter as scaling factors only. Thus, it is prudent to find out how the ratio $\lambda/\mu$ and the spatial resolution influence the accuracy of the calculations. Let us note at once that since $\Lambda$ is the only meaningful spatial scale of the problem, the spatial resolution makes sense only as a fraction of the wavelength. So it is more appropriate to speak of the number of nodal points per wavelength. Figure 7.4 shows a family of curves, each drawn for the fixed ratio $\lambda/\mu = \{1, 10, 100\}$, which gives the error of the generic half-space model, $|\xi_{0}^{\text{num}} - \xi|/\xi$ as a function of the number of nodal points per cycle, $n_x$. The accuracy of 1% is attained if $n_x \geq 65$ and $\lambda/\mu \leq 20$. One percent can be considered an adequate accuracy, because the actual field accuracy of the compliance measurements is not much higher than that. The results in Fig. 7.4 are for the case of a uniform grid and identical grid size in all three dimensions, $\Delta_x = \Delta_y = \Delta_z$. If, for example, $\lambda/\mu = 20$ and $n_x = 65$, making $\Delta_x/\Delta_x = 2$ results in an
7.7. CODE VALIDATION. SIMPLIFIED CASE STUDIES

Figure 7.5: A second test model: a layer over a half space.

A piece of software [provided by W. Crawford], that will be called the 1D code is available for compliance calculations in a layered medium. Our second test model is then a "soft" layer, with a rather elevated ratio $\frac{\lambda}{\mu} \approx 70$, over a half space. The model is sketched in Fig. 7.5. The density of 2000 $kg/m^3$ is assumed constant throughout the model. In the layer, we have $V_p = 1700 m/s$, $V_s = 200 m/s$, thus $\lambda = 5.62 \cdot 10^9 Pa$ and $\mu = 0.08 \cdot 10^9 Pa$, while in the lower half space $V_p = 2000 m/s$ and $V_s = 600 m/s$, so that $\lambda = 6.56 \cdot 10^8 Pa$ and $\mu = 0.72 \cdot 10^9 Pa$. The depth of the ocean is assumed 2000 m. Because the output of the 1D code is the normalized compliance vs. frequency, we plot exactly that for the sake of comparison in Fig. 7.6. The solid line [computed by E. Willoughby] is produced by the 1D code, the data points shown as circles are obtained with our 3D code for 120 nodes per cycle spatial resolution. Also shown in the figure are the upper and lower compliance bounds calculated analytically from formula (6.46). The two calculations agree within 3%.

The maximum absolute discrepancy occurs at the high frequency end (short wavelength, resolving shallow structure), as expected, because there we have a big $\lambda/\mu$ ratio. A rather specific discretization problem takes place at the low frequencies (large wavelength that sees deep into the lower half space). That is the layer is represented by only a couple of nodal points in the z-direction, and so its width is accounted less accurately. On the other hand, the influence of the layer on the compliance at large wavelengths isn't great. The balance between the two effects explains the slight scatter in the compliance response at the low frequencies. According to Crawford et al., [1998] for a given wavelength $\Lambda$, the half-space compliance is the most sensitive to the perturbation in elastic parameters within the region $z = \left[ \frac{\Lambda/4 - \Lambda/6}{} \right]$. As follows from Fig. 7.6, the maximum slope on the compliance-wavelength graph is observed at $\Lambda = 1000 m$, so that the interface between the layer and
7.8. Obtaining Stiffness Map

Experimentalists calculate compliance as a transfer function from power spectra of the induced pressure variation and sea floor vertical acceleration. The latter is easier to measure than the vertical displacement, $W$. In the frequency domain we just divide the acceleration spectrum, $S_a$, by $\omega^2$ to convert it to the displacement spectrum, $S_W$. Thus for noise-free data, the normalized compliance is

$$|\zeta(\omega)| = k(\omega) \frac{|S_W|}{|S_p|},$$

(7.29)

where $S_p$ is the induced pressure spectrum. In practice, each $S_W$ and $S_p$ is estimated from finite-length records. 

Figure 7.6. Cross-check of the compliance calculations with the 1D code on the model shown in Fig. 7.5.

the half spacings at $z = \lambda_m/5$. Note also that the graph is smooth even though we have constructed the interface as a perfect step function.

7.8 Obtaining Stiffness Map

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Trevorrow et al., [1988] calculate both power spectra in the time domain, on Fourier-filtered data, averaging over all such records that show high coherence between $S_W$ and $S_p$. Willoughby and Edwards, [2000] work in the frequency domain and use
7.8. OBTAINING STIFFNESS MAP

the best estimator for expression (7.29)

\[ |\zeta(\omega)| = k(\omega) \frac{< W(\omega)P(\omega)^* >}{< P(\omega)P(\omega)^* >}, \quad (7.30) \]

where the angular brackets signify averaging over all available records, the tilde sign refers to a Fourier-transformed quantity and the star stands for a complex conjugate. The latter expression may be recognized as the regression of \( W \) on \( P \) in the frequency domain.

In the forward modeling considered here, the loading pressure is controlled. Bailey [personal communication] then suggested to use formula (7.29) and proceed as follows. Consider a harmonic pressure perturbation on the sea floor in the form of a travelling wave in the positive \( x \)-direction with amplitude \( P_0 \), frequency \( \omega \) and wavenumber \( k = k(\omega) \)

\[ P_0 \cos(kx - \omega t) = P_0 \cos(kx) \cos(\omega t) + P_0 \sin(kx) \sin(\omega t). \quad (7.31) \]

Let \( W_c \) be the vertical component of the sea floor displacement under the load \( P_0 \cos(kx) \) and \( W_s \) be that due to \( P_0 \sin(kx) \). Then the full vertical component of the sea floor deformation at a point \( (x, y) \) and time \( t \) can be written as

\[ W(x, y, t) = W_c(x, y, t) \cos(\omega t) + W_s(x, y, t) \sin(\omega t). \quad (7.32) \]

From the definition of power spectrum,

\[ S_r(\omega) = \lim_{T \to \infty} \frac{1}{T} \left| \int_{-\frac{T}{2}}^{\frac{T}{2}} r(t) e^{-i\omega t} dt \right|^2, \quad (7.33) \]

where \( r = \{ W, P \} \), we obtain after some straightforward algebra

\[ \zeta(\omega) = k(\omega) \sqrt{\frac{W_c W_c + W_s W_s}{P_0^2}}. \quad (7.34) \]

So we have to run the software twice to obtain two complimentary deformation fields, \( W_c \) and \( W_s \), and then use the above expression.

As explained in Chapter 6, the reciprocal of the normalized compliance, stiffness, will be more convenient to use. We will be dealing with stiffness contours over the lateral area of the simulation domain, as opposed to just a number in layered models. For better viewing, the contours are plotted as 3D surfaces. A hydrate deposit will feature a convex surface on the map - another reason to use stiffness - as compliance would produce a concave surface, which is more difficult to display.
7.9 Summary

We have coded an algorithm to do forward modeling of the compliance response in a variety of elastic earth structures. Based on a conservative finite-volume difference discretization, we solve a set of full 3D, quasi-static governing equations, formulated for the displacement components in the elastic medium. The Jacobi over-relaxation iterative scheme is applied simultaneously to all the displacement components on a set of progressively refined grids to accelerate convergence. Among the features of the algorithm are the ability to handle sharp contrasts in elastic moduli with no artificial smoothing and the low computer memory usage. This makes it suitable for modeling compliance response of randomly hydrated, realistic marine sediments. The software is tested against some simplified 2D models. Recommendations are given on the required spatial resolution to achieve the prescribed accuracy. Overall, if we allow about 65 nodal points per forcing wavelength, the minimum of 1% accuracy may be expected for an equidistant or mildly distorted grid spacing for $\lambda/\mu \leq 20$. 
Chapter 8

Assessment of Marine Gas Hydrates Through Compliance Modeling: Forward 3D Modeling Results

8.1 Introduction

Let us assume we know how to assess the amount of methane hydrate in a layered sedimentary section from sea floor compliance measurements. One of the corner stones of such an assessment is the direct connection between compliance and hydrate content. The problem we would like to address here through forward modeling is roughly how much a non-layered hydrate deposit may complicate the matter. An example of a realistic structure is shown in Figure 8.1 [Spence et al., 1996]. It contains lateral maps of seismic reflection coefficients of the sea floor and BSR (left to right, respectively) obtained in a survey near ODP 898. The changes in the response are attributed to the lateral variations in methane hydrate concentration, featured on both large and small scales (100 m - 2 km). Clearly, the structure is de-facto three-dimensional, and not a simple layered medium.

We will demonstrate that, at least qualitatively, the 1D approach is still viable with a few corrections. This is encouraging, since the full 3D inversion results in increased cost for both fieldwork and analysis. Specifically, we look at the response of heterogeneous hydrate structures on scales both large and small (comparing to the wavelength) and consider lateral compliance variations due to the bulk hydrate content and its connectivity using the software, described in Chapter 7.

The effect of finite dimensions of the deposit is examined in Section 8.2 on the simplest 3D model, a lamella, subjected to gravity waves within the compliance frequency band.
Figure 8.1: Lateral maps of seismic reflection coefficients near ODP 898 [Spence et al., 1996].

Divided plate model is generated from the lamella in Section 8.3 by breaking it into four equal plates. The response of this structure is simulated for two different spacings between the plates. Then we simulate randomly distributed hydrated structures in Section 8.5 using a heuristic, Monte-Carlo approach and calculate the responses of two models which produce different clumping patterns. A possible effect of anisotropy in the compliance response is considered in Section 8.6. Finally, in Section 8.7, we compare the responses of two layers with different hydrate connectivity patterns and variable hydrate content. Section 8.8 is a compilation of the above results, where we produce a cumulative plot of the compliance spread versus a typical size of lateral inhomogeneity. In Section 8.9, we palpitate the sea floor with two mutually orthogonal gravity waves with an arbitrary relative phase shift between them. It is demonstrated on an example that the resulting stiffness map is almost identical with that produced by a single wave if we eliminate the areas of induced pressure lows in the power spectrum.

Speaking of the modeling domain dimensions, the vertical extent of all models is kept equal to one gravity wave length, while the lateral size is maintained to be an integral number of the wavelength, often one of two. For a finite-sized deposit, the lateral extent of the modeling domain is at least twice that of the deposit size in the corresponding direction. The latter requirement was established experimentally. It reduces the effect of the periodic boundaries to the numerical precision level. Also, with this choice, the calculated compliance (or stiffness) assumes its ambient value on the lateral boundaries, which is used for calibration.
purposes and often as a complimentary convergence indicator.

The number of nodal points per one wavelength is 65+, as discussed in Chapter 7; the upper bound is mainly limited by computer RAM. It is not possible to keep this number constant for all wavelengths, because we must secure a reasonable resolution for the hydrate deposit itself, which is “thin” in comparison with the typical domain dimension, and will be effectively scaled down by larger wavelengths. For all runs, nevertheless, there are at least 11 nodal points per vertical extent of the deposit, yielding 15 m or better of physical resolution.

8.2 Basic Models

Consider the following three simple elastic models of marine sediment, based on model M2, described in Chapter 6, Section 6.2. They will be called the Base model, the Layer model, and the Plate model.

The Base model features some ambient 1D elastic structure with no hydrates present. The seismic velocities increase from $V_p = 400 \text{ m/s}$ and $V_p = 1223 \text{ m/s}$ at the sea floor level to $V_p = 714 \text{ m/s}$ and $V_p = 2187 \text{ m/s}$ at depth of 1000 mbaf. The host matrix is assumed to have a constant density of 2670 kg/m$^3$ and to be saturated with 50% of water with density 1000 kg/m$^3$. All the properties are constant below 1000 mbaf.

The Layer model is derived from the above setting, as a background, by superimposing a 150-m-thick layer, bearing methane hydrates between 50 and 200 mbaf. The hydrate concentration within the layer increases as a quarter-sine wave from 0% at 50 mbaf to 40% at 200 mbaf, away from the sea floor. This amounts to 20% of maximum hydrate content, given 50% porosity. The hydrate density is 915 kg/m$^3$. For definiteness, assume the water depth of 400 m in accord with model M2, although changing this value to, say, 1000 m will only affect the wavelength-frequency conversion (6.44). Our treatment will be wavelength-based. In Fig. 8.2 we show the profiles of the Lamé parameters for these models, calculated from expressions (6.6) and (6.3) of Chapter 6, as well as the concentration profile for the Layer model.

A first 3D model is derived from the Layer model by restricting the lateral size of the hydrate deposit to a 500 x 500 m$^2$, retaining all other properties of the Layer model intact. This would represent a stand-alone, finite-size hydrated portion of the sediment, shown in Fig. 8.3, which we will call the Plate model. It can be anticipated that wavelengths of the order of a few hundred of meters should be able to sense such a formation, buried on average 100 m below the surface. Thus, restricting the lateral size of the plate to 500 m would cover the complete set of interesting possibilities: the wavelength being smaller, equal, or greater than the size of the deposit.
8.2. BASIC MODELS

Figure 8.2: Profiles of hydrate concentration and elastic moduli for the Base and Layer models.

Figure 8.3: Plate model.
8.3 DIVIDED PLATE MODEL

Now we palpitate the Plate model by gravity waves in the range 300 m - 2000 m, corresponding to the frequency range of 0.072 Hz - 0.026 Hz for water depth of 400 m. The stiffness contours are shown in Fig. 8.4. Each of them looks like a bell-shaped body, whose volume may be thought of as the increase of the local rigidity due to the plate as “seen” by the gravity wave of a particular length. One observes from the figure a transitional zone, outside the lateral location of the plate, over which the stiffness contours level smoothly with their half-space values (the Base model). Paying respect to the tradition, we also plot in Fig. 8.5 the average compliance response over the plate versus frequency and compare it with the response of the other two models. As might be expected, the plate behaves at high frequencies in nearly the same way as the layer. The response picks up at about \( \Lambda = 500 \) m, which is the size of the plate. This is where the maximum compliance (or stiffness) contrast between the plate and the half-space occurs, or, alternatively, where the volume, bordered by the stiffness surface above the background level, reaches maximum. Numerically, this maximum difference is about 30\% in absolute values. We also see that the maximum difference between the plate and the layer response is about 1/3 of that between the layer and the half-space, i.e. \( \sim 10\% \). Note that the numerical accuracy of our calculations in that region is about 1\%, as can be expected from Fig. 7.4.

Finally, we present in Fig. 8.6 a sample of a 3D deformation field, developed around the plate at \( \Lambda = 1000 \) m and \( \nu_e = \pi/2 \) in the Plate model, so that underpressure is created directly above the plate. The gravity wave is traveling in the \( x \)-direction. The entire simulation domain for this calculations is \( 1000 \times 1000 \times 1000 \) m\(^3\) and the grid used consists of \( 129 \times 129 \times 129 \) nodal points, but for clarity, only a subset of the displacement vectors is shown within a region \( x = [0, 1000] \) m, \( y = [0, 1000] \) m, and \( z = [0, 375] \) mbsf. The body of the plate is marked as a semi-transparent shade. The figure also contains two orthogonal vertical cross-sections of the displacement vectors, intersecting along the vertical through the center of the plate. The maximum vertical rate of the sea floor displacement is 0.2 \( \mu \)m/Pa in this example. On average, the rate of the lateral displacement at the same location is roughly ten times less. Fig. 8.7 displays separately the lateral \( (x - y) \) displacement components at the following three depths: the sea floor above the plate, \( z = 0 \) mbsf, close to the top of the plate, \( z = 60 \) mbsf, and close to the bottom of the plate, \( z = 190 \) mbsf, respectively.

8.3 Divided Plate Model

The plate is now broken down into four equal blocks of the same vertical extent as the original plate. We fix the wavelength at 500 m which generates the maximum response for the Plate model and vary the spacing between these four blocks to quantify smaller scale
8.3. DIVIDED PLATE MODEL

Figure 8.4: Normalized stiffness contours $\xi = \xi(x, y)$ for the Plate model.
8.4 Simulation of Heterogeneous Structures

We have considered thus far a couple of deterministic models, featuring hydrate deposits of rectilinear shapes, which may not be always so. Now we lift this restriction. The following conventions will be used throughout the remainder of this chapter.

A hydrate bearing block will be defined as an elementary rectangular region which spans one or more computational nodes, including the associated control volumes around each node, and contains some hydrates. For example, both Divided plate models set up in Section 8.3 consist of four hydrate bearing blocks in this terminology. We will adopt the hydrate...
Figure 8.6: Plate model: Deformation field around the plate for $\Lambda = 1000 \, \text{m}$. 
8.4. SIMULATION OF HETEROGENEOUS STRUCTURES

Figure 8.7: Plate model: horizontal components of the deformation within the lateral plate location at different depth for $\Lambda = 1000\text{m}$. 
8.4. SIMULATION OF HETEROGENEOUS STRUCTURES

Figure 8.8: Divided plate model response. The top portion is reproduced from Fig. 8.4 for comparison.
8.5. EFFECT OF CLUMPING

concentration profile from the Layer model to use within each block, so the concentration will be the known function of depth only, regardless of the block's lateral location. Note that this choice eases the interpretation and is mainly due to the lack of real data, not the code limitations.

Now, hydrate deposits will be simulated numerically using these blocks as building bricks by placing them at random within a prescribed rectilinear deposit zone. The depth range of the zone will be that used for the Layer model, i.e. [50, 200] mbsf for consistency with the adopted concentration profile. The blocks are allowed to overlap, so the resulting deposit can develop quite complex a shape, but no part of them may reside outside of the prescribed depth range.

The ratio of the total hydrate content within the blocks to the total hydrate content within the deposit zone will be defined as the hydrate bearing volume and denoted as $u_{\text{hydr}}$. If, as in our case, the hydrate concentration is a function of depth only and the distribution of the blocks within the zone is perfectly random, then $u_{\text{hydr}}$ is just the ratio of the total volume of the blocks, less overlaps, to the volume of the deposit zone.

The lateral dimensions of the deposit zone have to be less by, say, 1 block size, than those of the whole simulation domain to maintain periodicity in the elastic moduli on the side boundaries, required by the software (see previous chapter). The side boundaries will be then hydrate-free and produce lows on stiffness maps, but we will take these areas out of consideration when analyzing the maps. Apart from that, setting $u_{\text{hydr}} = 0$ results in the Base model, while $u_{\text{hydr}} = 1$ takes us back to the Layer model.

In setting up a less trivial hydrate distribution, $0 < u_{\text{hydr}} < 1$, on the solution grid, we mark the control volume around each nodal point within the block as black and the rest of them, outside the blocks, as white. The Lamé parameters within each such a control volume will assume constant values, equal to those at the nodal location. Algebraic averaging (7.13) is used to approximate $\lambda$ and $\mu$ on the staggered grid. The need to map the properties onto a series of different grids in the course of the numerical solution, calls for the extension of this black/white-type logic to a grey-scale scheme, in which a grey volume is the result of a simple volumetric averaging between the black and white contributions. Fig. 8.9 shows an example of this type of mapping. The original distribution is generated on a grid of $15 \times 19 \times 17$ nodes and mapped onto a grid of $27 \times 17 \times 31$ nodes.

8.5 Effect of Clumping

We compare in this section the responses of two different randomly generated hydrate formations. The first one is made up of $60 m \times 60 m \times 120 m$ blocks, while the other is built from
Figure 8.9: An example of a heterogeneous hydrate deposit generation and its mapping onto a different numerical grid.

larger 200 m × 200 m × 120 m blocks. The lateral area of the hydrate zone is 1 km × 1 km, and the depth range is [50, 200] mbsf. Both formations are shown in the top portion of Fig. 8.10. The hydrate bearing volume is fixed for both models at 50% level. If the average hydrate concentration over all hydrate bearing blocks is $n \approx 20\%$ and porosity, $\phi$, is 58%, then we are dealing with $n_{\text{avg}} \phi m \approx 5\%$ of volumetric hydrate content within the zone. Thus, we can estimate from the known volume of the zone and hydrate density ($\sim 1 \text{g/cm}^3$) the column mass of methane hydrate to be $\sim 0.75 \cdot 10^8 \text{kg}$ per square kilometer of sea floor area with these settings. The rest of Fig. 8.10 shows in comparison stiffness contours for the two formations, produced by gravity waves of $A = 500 \text{m}$ and $A = 1000 \text{m}$. Consider the following quantities, defined in the usual way. They are

$$\text{Average stiffness: } \bar{\xi} = \frac{\sum_{i}^{n_{\text{dx}}} \sum_{j}^{n_{\text{dy}}} \xi_{ij}}{(i_e - i_e + 1)(j_e - j_e + 1)}, \quad (8.1)$$

where $i = (i_x, i_y)$ and $j = (j_x, j_y)$ are the lateral nodal coordinates of the hydrate zone, and

$$\text{Standard deviation: } \sigma = \sqrt{\frac{\sum_{i}^{n_{\text{dx}}} \sum_{j}^{n_{\text{dy}}} (\xi_{ij} - \bar{\xi})^2}{(i_e - i_e + 1)(j_e - j_e + 1) - 1}}. \quad (8.2)$$

Note again that, as discussed in the previous section, if $\delta_x$ and $\delta_y$ are the lateral dimensions of the hydrate bearing block and $\Delta_x$ and $\Delta_y$ are the grid increments in the $X-$ and $Y-$dimensions, respectively, we take

$$\delta_x = (i_e - 1)\Delta_x = (n_x - i_e)\Delta_x, \quad \delta_y = (j_e - 1)\Delta_y = (n_y - j_e)\Delta_y. \quad (8.3)$$
8.5. EFFECT OF CLUMPING

Figure 8.10: Effect of clumping: Response of two different random hydrate deposits.
Simple evaluation of expressions (8.1) and (8.2) reveals that the two formations yield nearly identical stiffness averages, $\xi$, for a given wavelength and hydrate bearing volume, however, the one that is composed of larger blocks has higher statistical scatter, $\sigma$. We have $\sigma = 8.8\%$ versus $\sigma = 4.4\%$ for $\Lambda = 1000\, m$ and $\sigma = 13.3\%$ versus $\sigma = 6.5\%$ for $\Lambda = 500\, m$, respectively, where we normalize $\sigma$, defined by expression (8.2), on the stiffness contrast between the Base and Layer models. As we move away from the best resolving frequency, $\Lambda = 500\, m$, the amplitude of these fluctuations decays. The average stiffness, $\xi$, is bounded by its limits at $v_{\text{hyd}} = 0$ and $v_{\text{hyd}} = 1$ and follows the general trend set by the background profile of the elastic moduli, as per the Base model.

It is then argued that in the long-wavelength limit or, alternatively, when the size of the blocks is much smaller than the average thickness of the zone, the Plate model can be used to simulate the response of the structure. For the blocks of larger size (i.e. rough structure on macroscopic scale) or in the short-wavelength limit, we can use the Divided plate model as a starting point to simulate local compliance variations on the scale of a single block.

### 8.6 Anisotropy

One would wonder whether an arbitrary hydrate deposit produces the same response if the loading gravity wave changes its direction. We build our deposit from sets of parallel thin plates $120\, m \times 30\, m \times 150\, m$ in size that randomly occupy 50% of the hydrate zone, described in the previous section. Intuitively, this structure could feature anisotropy in the response, depending on the direction in which the loading gravity wave travels. The two models, corresponding to the $x$ and $y$ directions of strike, are shown in Fig. 8.11. The wavelength is fixed at $500\, m$. The average stiffness values and relative standard deviations are indicated beside each model. The average stiffness and degree of fluctuations for these two scenarios show very little difference: $0.871 \cdot 10^9\, Pa$ versus $0.864 \cdot 10^9\, Pa$ and $6\%$ versus $6.3\%$, respectively.

### 8.7 Compliance and Bulk Hydrate Content

The next series of simulations is concerned with finding a relationship between the compliance (stiffness) response and the content and connectivity pattern of hydrate within the deposit zone. We start from the Base model that contains no hydrates, $v_{\text{hyd}} = 0$, and randomly deposit increasing amounts of hydrate, eventually transforming it into the Layer model. The layer is located between $50\, mbsf$ and $200\, mbsf$. As $v_{\text{hyd}}$ is varied between 0 and 1, we compute the response of that structure for two cases, referred further as Model 1 and Model
8.7. COMPLIANCE AND BULK HYDRATE CONTENT

Figure 8.11: Response of a structure made of a set of parallel plates to two loading gravity waves travelling in the mutually perpendicular directions.
2. The dimensions of the hydrate bearing block in Model 1 are 20 m x 20 m x 120 m, while those in Model 2 are 40 m x 40 m x 40 m. The wavelength is fixed at 500 m, and so are both the lateral extent (in x and y) and vertical extent of the simulation domain.

If \( \xi_0 = \xi_0(\lambda, \lambda, \mu) \) is the stiffness of the unhydrated section, \( \xi = \xi(\lambda, \lambda, \mu) \) is the stiffness of the Layer model, and \( \xi \) is the average stiffness of a hydrated model with a given hydrate bearing block geometry and distribution of the blocks, define the fractional change in stiffness, \( \xi_f \), as

\[
\xi_f = \frac{\bar{\xi} - \xi_0}{\bar{\xi} - \xi_0}.
\]

The relationship between \( \xi_f \) and \( \sigma_{\text{std}} \) is displayed in Fig. 8.12 for both models. As seen from the figure, a straight line can be fitted to the numerical data. Since the two lines nearly coincide, it may be concluded that the average stiffness is sensitive only to the bulk hydrate content and not to its particular distribution within the deposit zone, as Models 1 and 2 clearly generate distinct connectivity patterns.

In interpreting compliance, the following uncertainty might be anticipated, that is likely to arise from insufficient experimental data, as to what is mainly responsible for the lateral variations in the response: connectivity (voids) or local fluctuations in the concentration profile. On the positive side, a simple linear perturbation theory can be adopted to facilitate the inversion process.

### 8.8 Lateral Variations in Compliance

Although the average stiffness over a representative area (greater than the size of a typical inhomogeneity) seems to depend only on the bulk hydrate content, the lateral spread of stiffness definitely correlates with the size of the hydrate bearing block. To quantify this statement, we compile the results over all the models for \( \Lambda = 500 \) m and plot in Fig. 8.13 the normalized standard deviation of stiffness, \( \sigma/(\xi - \xi_0) \), versus the cube root of the hydrate bearing block, which would stand for the characteristic size of a typical inhomogeneity involved. Note that these estimates are identical for both stiffness and compliance.

For example, if this size is about the thickness of the deposit zone (150 m), then we should observe \( \sim 15\% \) of the lateral variations in \( \xi \). These numbers are for the best resolving frequency (\( \Lambda = 500 \) m); for other frequencies, the effect is less pronounced.
8.8. LATERAL VARIATIONS IN COMPLIANCE

Figure 8.12: Fractional change in stiffness versus fractional volume occupied by hydrates within the deposit zone for two different connectivity patterns, samples of which at $v_{\text{hyd}} = 50\%$ are shown in the top portion of the figure.
8.9 Loading of Sea Floor by two Plane Waves

In all the models above, the sea floor has been loaded by a single gravity wave, traveling in one direction, as we have demonstrated changing orientation has little effect. Nevertheless, Trevorro et al., [1988] argue that in reality many surface gravity waves interact randomly, propagating in several directions over the observation point. What difference does it make?

Let us consider the case when two gravity waves travel in the mutually orthogonal directions, so that the loading term at the sea floor becomes

\[ P(x, y) = P_0 \cos(kx - \omega t) + P_0 \cos(ky + \nu_{xy} - \omega t), \]

where \( \nu_{xy} \) is an arbitrary phase shift. Proceeding as described in Chapter 7, Section 7.7, we compute the responses, \( W_x \) and \( W_y \), to the following loading configurations \( P_0 \cos(kx) + \cos(ky + \nu_{xy}) \) and \( P_0 [\sin(kx) + \sin(ky + \nu_{xy})] \), respectively and calculate the normalized stiffness from

\[ \xi = \frac{1}{k(\omega)} \frac{\sqrt{2(1 + \cos(k(x - y) - \nu_{xy})}}{\sqrt{W_x^2 + W_y^2}}. \]  

In Figure 8.14 A we show stiffness maps for the Plate Model loaded by two orthogonal waves with \( \Lambda = 500 \text{ m} \) each, and for \( \nu_{xy} \) varying from 0 to \( \pi \) with the increment of \( \pi/4 \). The white lines on these maps correspond to the nodes in the pressure power spectra which occur where the numerator of the expression above takes its zeroes

\[ \frac{2\pi}{\Lambda}(x - y) - \nu_{xy} = \pi(2n + 1), \text{ where } n = \pm1, \pm2, \pm3 \ldots \]  

Figure 8.13: Normalized lateral compliance variations versus a typical size of inhomogeneity in hydrate deposit for the best resolving frequency.
8.9. LOADING OF SEA FLOOR BY TWO PLANE WAVES

Figure 8.14: A: Stiffness maps for a range of $\nu_{xy}$, B: stiffness map compiled from the areas of maxima in pressure power spectra.
It is obvious that such areas produce grossly erroneous stiffness values and therefore should be avoided. For the field work this means to use data records corresponding to as high values of the pressure spectrum as possible. This recommendation is consistent with the averaging procedure \((7.30)\) according to Edwards [personal communication]. Panel B of Fig. 8.14 shows the “best” stiffness map compiled from the areas where the pressure spectrum is maximum (between the white lines). We replotted it in Fig. 8.15 and compare with the stiffness map produced by a single plane wave. The two are nearly identical.

### 8.10 Summary

The average compliance response is sensitive to the bulk hydrate content but not its connectivity pattern. Thus, most qualitative 1D assessment considerations should remain in place as we go to 3D. Lateral variations in compliance correlate with the characteristic size of the inhomogeneities in the deposit.

To estimate the correct average in processing sea floor compliance data, it seems prudent in the ideal case to collect the data at a few locations, including the deposit’s center and margins. At each such a location, a few measurements might be necessary, spaced laterally about half of the deposit’s thickness. The fragments of data with weak pressure signals should be excluded from interpretation.
Conclusion

Let us summarize and discuss the results of this study.

Hydrothermal Modeling

We considered natural hydrothermal convection in typical oceanic crustal sections, both in two and three dimensions with the host matrix fractured and unfractured and with the sea floor permeable and impermeable. It is described by a coupled, second-order, highly nonlinear system of partial differential equations of heat and mass transfer in a porous medium. Full analytical solutions are unlikely to exist, unless certain approximations are made, such as the well-known Re-number approximation. We derived analytical expressions for the aspect-ratio of the convection cells and the critical Re-number at the onset of convection for anisotropic systems with the permeable upper boundary. Such systems feature wider convection cells and lower critical Re-number compared with systems whose upper boundary is impermeable. The increase in vertical anisotropy results in the increase of the height-to-width ratio of the cells. These results are useful for the assessment of the critical conditions for the onset of convection in sediment-free, young oceanic crust. They can also serve as a starting point in constraining the geometry and initial solutions of hydrothermal models with the finite-amplitude convection.

In Chapter 1, in the small Re-number limit, we obtained closed-form solutions for the velocity and temperature fields, generated by a point source of heat, embedded in a subcritical porous layer with the impermeable and isothermal boundaries. The steady-state results show that the upward flow is very intense above the source. This region receives additional heating from natural convection. In the vicinity of the source, a nearly uniform uplift of isotherms is observed. On the sea floor, the heat flux increase is felt within a radius of approximately half the layer thickness. This model can simulate the hydrothermal convection induced by a small magmatic intrusion or volcanic eruption. It is also used here for software testing, given an apparent lack of analytical solutions available for cross-checks, especially in 3D.
We set up a simple numerical model to time a thermal transient, propagating through a crustal section, powered by a magmatic intrusion as a line heat source. For a 1 km-thick permeable section as of ODP 804B, the transient reaches the sea floor within a few hundred million of years and produces a low-temperature venting. In the most permeable, shallow layer 2a, the vortex is ascending approximately with the Darcy velocity, determined largely by the crustal permeability. Thus, at intermediate spreading centers, which have the eruption period of a few hundred thousand of years, shallow magmatic intrusions may be able to produce a quasi-steady, low-temperature venting.

In Chapter 2, we considered convection in a fractured medium, starting with the case of a single fracture. An efficient and portable numerical algorithm was developed to treat a single vertical fracture or a permeable zone in both on-axial systems, symmetric about the ridge, and hydrothermal circulation on the flanks, enhanced by a major fissure of fault, around which the solution is symmetric. The algorithm generates solutions by iterating between the fields within the fracture and the host rock until the two agree on the fracture boundary. We successfully tested this scheme against the existing FE code on a benchmark problem.

The 2D algorithm is now used to perform a number of case studies to quantify the impact of fracture on natural convection. The results confirm that a fracture can initiate and maintain convection in a subcritical medium. In systems with the developed convection, we found a major dimensionless parameter to characterize the impact of the fracture. It is the ratio of the permeability-thickness product of the fracture to that of the medium, where for the latter, the size of the convection cell acts as the required dimension of length. A single vertical fracture, extending fully across the layer, increases the heat power discharged through the system by about one-third, measured over the lateral size of the convection cell. However, the local channeling of heat and mass by the fracture is much more pronounced. For fractures originating and terminating inside the layer, the amount of heat power transported is controlled by the position of the lower end of the fracture, while the heat flux distribution at the upper boundary is controlled by the position of the upper end.

In Chapter 3, we developed and validated a 3D numerical code, suitable for modeling of vigorous convection in a multiple-fractured medium. To eliminate costly time-stepping, we compute the steady-state directly. The upwind, finite-volume discretization scheme used allows to overcome the usual limitation on the fluid velocity, common among the solvers that employ central differencing for advective fluxes. The resulting matrices for the temperature and momentum equations are inverted separately, using a GMRES solver with ILU preconditioning from the SPARSEKIT package. The final solutions are obtained by iterating between the governing equations. We offer a simple algorithm for the inclusion of any number of discrete fractures into the modeling domain. The averaging process follows from the
CONCLUSION

results of the single-fractured 2D modeling and based on the permeability-thickness product in the direction of flow. Our 3D solver permits us to have low and high spatial resolutions in two different subdomains within the same model. This is achieved by iterating between the solutions in the two subdomains until they agree on their common inner boundary - a natural extension of the 2D single-fractured algorithm. Such a feature is useful e.g. in modeling of high temperature venting. The upwelling hot fluid is confined to a narrow limb with high temperature and pressure gradients and generally requires high resolution, preferably of the order of tens of centimeters. For the rest of the medium a 20 - 50 m spatial resolution may be adequate, but we must have a representative portion of it in our model to minimize the effect of the external boundary conditions on the high-temperature conduit. The solution we offer is definitely less expensive compared with the alternative to generate an adaptive, heterogeneous grid in 3D.

Next, we tackle 3D applications, starting from a few simple generic models in Chapter 4. We found two basic configurations in convection patterns in unfractured medium: a 2D-like, cellular and an axi-symmetric, but it is not clear which mode is preferred. One may expect to see a mixture of the two, since the actual flow pattern may be influenced by fractures, heat sources and topography. In 3D steady convection in the vicinity of the fracture, fluid would tend to circulate within the fracture (fault) plane if the sea floor has a sediment cover. If there is no cover, a sheet-like downflow zone occupies most of the fracture. This creates underpressure and heat flux deficit over a large lateral area with dimensions comparable to the depth of circulation. This picture is consistent with the 2D observations that in sediment-free systems upflow zones are much more narrow than in those with the sediment cover on.

Explanations for the observed, regular heat flux variations over flat, sediment-covered sea floor, as well as for the temperature homogenization mechanism at the sediment-basalt interface have been a subject of ongoing debates for the last twenty years. We demonstrate in Chapter 4 that both off-axial heat flux variations over flat, sedimented sea floor with or without buried sediment topography may be well explained by the presence of a thin, permeable anisotropic zone at the sediment base in which fluid circulates laterally, quasi-horizontal. In the case of topography driven circulation, the temperature at the sediment base homogenizes by lateral stirring to within 15%, in accord with observations, if the permeability-thickness product of the permeable zone is \( \sim 4 \times 10^{-9} \text{m}^3 \). Only if the basalt-sediment interface is flat, do we observe cellular convection, so that the horizontal mode is not excited and homogenisation is not achieved. In the latter case, the cellular convection is maintained by the permeable zone, otherwise the conditions within the permeable basalt are below critical. So our model does not require vigorous convection, neither does it support
high permeability figures in the buried basalt for convection to occur, but it relies heavily on the existence of the permeable zone. Such formations have been observed, but it is not known how widespread they are.

In Chapter 5, we constructed a hydrothermal model for the southern portion of the CoAxial Segment, JdFR, based on a permeability structure provided by seismologists and additional heat flux constraints for the intermediate-spreading ridge. We also introduced in this basic model a few features, commonly encountered in the young oceanic crust, such as a permeable zone on axis, a dipping fault and a pipe-like conduit to see their impact. For the basic model, we predict both recharge and discharge on axis with ridge-parallel convection cells, extending to the gabbro layer at 2.2 kmbsf. Given high degree of permeability anisotropy, the aspect ratio of the cells is approximately 2.2, and on-axial vent field spacing is $\sim 1$ km. The nearly axi-symmetric, shallow (400 m) recharge areas form around the upflow zones on axis, contributing $\sim 70\%$ of circulating fluid. The remainder comes from deep-focused flow in the sheeted dikes which seem to determine the vent field spacing on axis. A set of secondary convection rolls (also ridge-parallel) may be expected to occur $\sim 1 - 1.5$ km off axis. The maximum temperature of the diffuse venting on axis is 20$^\circ$C and exit velocity is $10^{-5}$ m/s, however, these may increase to 70$^\circ$C and $10^{-4}$ m/s, respectively, near cracks with apertures of about 0.3 mm. The net mass rate per one diffuse vent field is about 200 kg/s, assuming no fractures. In the transition zone between the on-axial and secondary rolls, there is a signature of a sheet-like, ridge-normal flow due to pressure gradients created by the on-axial circulation. This ridge-normal component would be significantly enhanced, if dipping, extensional faults exist in the system. High temperature venting is possible via pipe-like conduits, but their contributions to the heat and mass budget are expected to be 15% and 4%, respectively.

**Compliance Modeling**

In Chapter 6, we start with the seismic wave equation and Hooke's law, but demonstrate using dimensional analysis that the time-dependent, inertia terms are small in our compliance problem. Small is also the viscous component of the response of a typical marine sediment to gravity wave at the frequencies of interest. So the compliance problem we are solving is static and elastic. The governing equations are formulated for the displacement components under plane wave load. We have derived analytically the dispersion relationship between the wavelength of the gravity wave and its frequency, taking into account the sea floor movements, which are routinely neglected elsewhere. We calculate a correction due to the sea floor rigidity and show that this correction becomes important in some compliance...
applications which require wavelength as large as ~ 30 km, e.g. in deep crustal imaging. For methane hydrate applications, we are justified in using the simplified dispersion relationship.

In Chapter 7, we develop a numerical algorithm to do forward compliance modeling in three dimensions. The governing equations are solved simultaneously with an iterative Jacoby over-relaxation scheme. We test the software against the analytical solution for the half-space and a numerical solution for a test layered model. Since the problem is entirely scaled by the wavelength, one of the major considerations in choosing the numerical grid is the number of nodes per wavelength. For a given number of nodes per wavelength, the expected accuracy is a function of $\lambda/\mu$.

Applications are considered in Chapter 8. We examine the effect of finite dimensions of the hydrate deposit on a plate model, subjecting it to gravity waves within the compliance frequency band. Then we simulate randomly distributed hydrated structures and calculate their compliance response. We demonstrate that the compliance technique is viable in three dimensions, with most qualitative 1D assessment considerations in place. The average compliance response is sensitive to the bulk hydrate content but not its connectivity pattern. Lateral variations in compliance correlate with the characteristic size of the inhomogeneities in the deposit. Thus, we recommend (if possible) to collect data at a few locations, including the deposits center and margins, spacing measurements stations laterally about half the deposits thickness.
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