

of 3D periodic mesostructured materials without assuming any structural models. The resolution for the structure is primarily limited by the quality of the HREM images, which depends on the long-range mesoscale ordering. Therefore, although further progress may give better resolution, we expect no future change to the present conclusions about the structures of SBA-1, SBA-6 and SBA-16, because the validity of the solutions does not depend on the resolution. This is a characteristic of our method that makes it different from other approaches. We also suggest that the results presented here provide a quantitative topological description of ordered mesostructured composites, and that such descriptions are essential in understanding the properties and possible applications of the composites. The resolution of periodically ordered, 3D arrangements of bimodal (meso-micro) pores in SBA-1 and SBA-6 makes it possible to consider the detailed characterization of the range of complicated porous phases that are now synthetically achievable. □

Methods

Synthesis of SBA-6

3.75 g of tetraethoxysilane (TEOS) was added with magnetic stirring to a clear solution containing 0.5 g of the gemini surfactant 18B_{4,3-1} (N,N,N,N'-pentamethyl-N'-[4-(4-oxa-dodecyloxyphenoxy)-butyl]-propane-1,3-diammonium dibromide, C₁₈H₃₇OC₆H₄OC₆H₄N(CH₃)₂C₃H₇N(CH₃)₃Br₂), 45.4 g of doubly distilled water, and 3.69 g of benzyltrimethylammonium hydroxide at room temperature. Stirring was continued for 20 h after the addition of TEOS at room temperature. The reaction gel mixture was heated for 2 d at 80 °C without stirring. The precipitate was filtered and dried in air at room temperature.

Determination of properties

Ar adsorption and desorption isotherms were measured at 87 K. Pore volumes (cm³ g⁻¹) for SBA-1, SBA-6 and SBA-16 are 0.6, 0.86 and 0.45, respectively, and the ratios of the pore volume to unit cell are respectively 0.57, 0.65 and 0.47. The surface-area/pore-volume ratio (2.26 × 10⁹ m⁻¹) for SBA-1 is nearly three times that of SBA-6 (7.93 × 10⁸ m⁻¹). The silica wall densities determined with an AccPyc 1300 helium pycnometer are also substantially different for SBA-1 (2.00 g cm⁻³) and SBA-6 (2.20 g cm⁻³).

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Improved estimates of global ocean circulation, heat transport and mixing from hydrographic data

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Through its ability to transport large amounts of heat, fresh water and nutrients, the ocean is an essential regulator of climate^{1,2}. The pathways and mechanisms of this transport and its stability are critical issues in understanding the present state of climate and the possibilities of future changes. Recently, global high-quality hydrographic data have been gathered in the World Ocean Circulation Experiment (WOCE), to obtain an accurate picture of the present circulation. Here we combine the new data from high-resolution trans-oceanic sections and current meters with climatological wind fields, biogeochemical balances and improved a priori error estimates in an inverse model, to improve estimates of the global circulation and heat fluxes. Our solution resolves globally vertical mixing across surfaces of equal density, with coefficients in the range (3–12) × 10⁻⁴ m² s⁻¹. Net deep-water production rates amount to (15 ± 12) × 10⁶ m³ s⁻¹ in the North Atlantic Ocean and (21 ± 6) × 10⁶ m³ s⁻¹ in the Southern Ocean. Our estimates provide a new reference state for future climate studies with rigorous estimates of the uncertainties.

Obtaining a consistent picture of the oceanic circulation requires adjusting thousands of parameters consistently with a priori error estimates. We present here our best estimate from selected hydrographic data (Fig. 1), which will improve with the appearance of new data. Mass flux is the most basic element of the circulation and Fig. 2 shows the best-estimate coast-to-coast integrated water mass transports for selected density classes. A volume of 15 ± 2 Sv (1 sverdrup = 1 × 10⁶ m³ s⁻¹) of North Atlantic Deep Water (NADW) is produced in the northern North Atlantic Ocean and moves southward, entraining Antarctic Bottom Water (AABW) from below, and Antarctic Intermediate Water (AAIW) from above. As a result, the NADW is increased to 23 ± 3 Sv as it exits the South Atlantic at 30° S. In the Southern Ocean, a total of 21 ± 6 Sv of bottom water is formed from lower Circumpolar Deep Water (CDW)—which corresponds approximately to the lower NADW density range. Bottom water inflows (NADW + AABW mixture) to the Atlantic, Indian and Pacific oceans are 6 ± 1.3 Sv, 11 ± 4 Sv and 7 ± 2 Sv, respectively. In the Indian and Pacific oceans, most of this water returns southward at deep and intermediate levels. These net values are the sums of large, strongly spatially varying, flows of opposing sign, and thus oversimplify the actual circulation; a detailed description of the circulation within each ocean basin will be published elsewhere^{3,4}. Our standard model estimate of the inflow in the South Pacific Ocean is in the lower range of previously published values, but it depends directly upon the weight given to the “PO” phosphate–oxygen combination (see Methods^{4,5}) conservation constraints relative to mass conservation³. The deep inflow to the North Pacific Ocean is also weaker than previously found³, as a consequence of our consideration of heat and salt conservation in the northern parts of those basins.

No definition of bottom-water formation can be completely unambiguous because of the entrainment of ambient fluid during the sinking process. In our Southern Ocean definition, the bottom-

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water formation rate corresponds to the total amount of water crossing the neutral surface, $\gamma^n = 28.11 \text{ kg m}^{-3}$ downwards, and subsequently ventilating the deep Atlantic, Indian and Pacific basins. This water is provided primarily from the density range of lower NADW, so that the two sources of deep water are not additive, as is often assumed in qualitative calculations⁶. Consistent with conventional wisdom, no very large amount of deep water forms in the North Pacific or Indian oceans, although intermediate waters are produced there. Transient tracer measurements suggest AABW formation rates of water denser than $\gamma^n = 28.27 \text{ kg m}^{-3}$ at 5 to 8 Sv (ref. 7). Because this density class is almost immediately mixed with CDW above it when exiting the Southern Ocean, it is not separately resolved in our model, and there is no inconsistency. However, there is a contradiction with the suggestion that the current production rate of AABW recently decreased⁶, as we find no inconsistency between the deep, contemporary, geostrophic circulation and the interior tracer field which reflects the circulation integrated over hundreds of years. We believe that the origin of the disagreement is in those authors' *ad hoc* assumptions⁶ about the originating water masses.

The integrated circulation in the upper layers is more uncertain (Fig. 2, red arrows) owing to the enhanced temporal variability known to be present there³. A northward flow of $16 \pm 3 \text{ Sv}$ of thermocline water from the South Atlantic Ocean balances the NADW southward flow; the strength of the Pacific-Indonesian throughflow is estimated at $16 \pm 5 \text{ Sv}$, consistent with the most recent current-meter measurements⁸. This estimate is sensitive to

the use of hydrography at very low latitudes where noise susceptibility and seasonal variability are large.

Vertical exchanges (advection, denoted w^* , and mixing, measured by a diffusion coefficient κ^* across the neutral surfaces⁹ defining the layers) are associated with the general circulation. Both parameters are now the focus of intense research^{10,11} because numerical models are known to be very sensitive to κ^* . Direct measurements have shown little mixing in the ocean interior, while enhanced mixing of order $1,000 \text{ cm}^2 \text{ s}^{-1}$ has been observed in oceanic regions with rough topography¹¹. Table 1 summarizes the abyssal dianeutral (near vertical) exchanges by basin and depth range. Let an overbar denote a basin average. Then, in the deep range ($\approx 2,000\text{--}3,500 \text{ m}$), dianeutral velocities are $\overline{w^*} = (0.1\text{--}0.6) \times 10^{-6} \text{ m s}^{-1}$, and the diffusivities are $\overline{\kappa^*} = (3\text{--}4) \times 10^{-4} \text{ m}^2 \text{ s}^{-1}$ with global averages of $\overline{w^*} = (0.13 \pm 0.03) \times 10^{-6} \text{ m s}^{-1}$ and $\overline{\kappa^*} = (3.7 \pm 0.7) \times 10^{-4} \text{ m}^2 \text{ s}^{-1}$ between 30° S and 47° N . In the bottom layers ($\approx 3,800 \text{ m}$ to the bottom), both means are larger: $\overline{w^*} = (0.4 \pm 0.1) \times 10^{-6} \text{ m s}^{-1}$ and $\overline{\kappa^*} = (9 \pm 2) \times 10^{-4} \text{ m}^2 \text{ s}^{-1}$. Diffusivity values in the deep range are consistent with previous calculations from a crude one-dimensional global balance¹⁰. The largest values are found in the bottom layers although they are correspondingly more uncertain³. The spatial average values that are required by our tracer balance result from all mixing processes, including probable strong mixing generated near topography^{10,11}. We interpret those values¹⁰ as being the basin-average value of a process strongly mixing the ocean at highly localized regions.

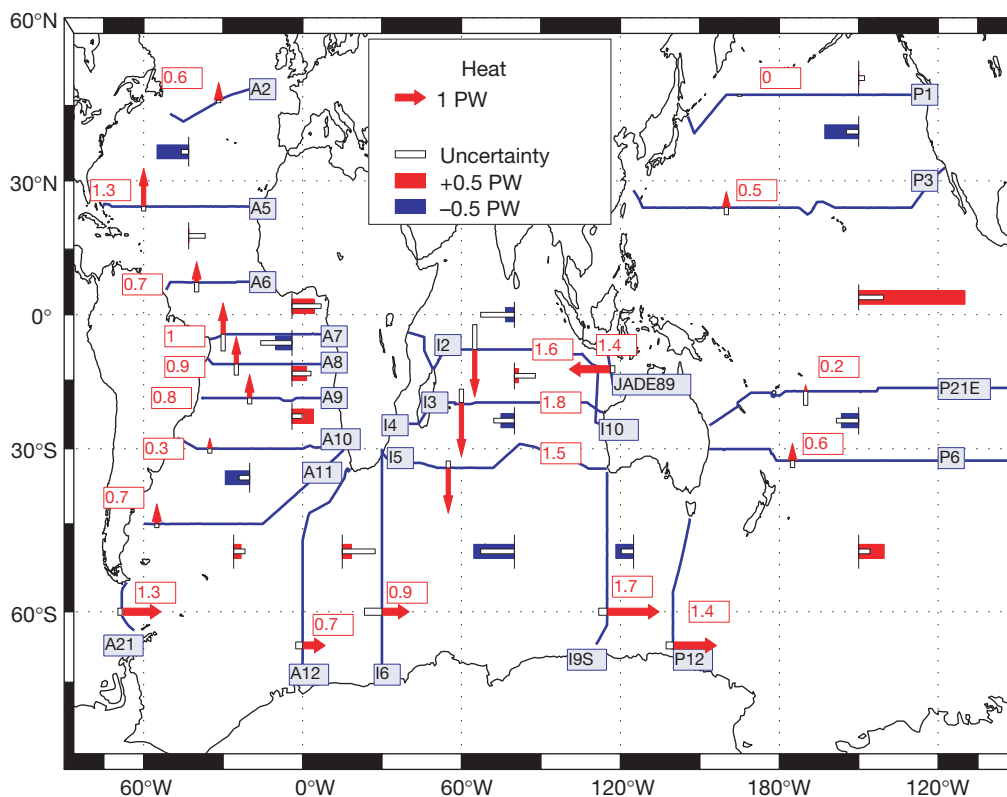


Figure 1 Hydrographic sections and heat fluxes. Transoceanic sections from the WOCE program were selected to ensure a reasonable temporal consistency (1990–1996) and to avoid crossing sections. Between Jakarta and Australia, the 1989 section from the Franco-Indonesian JADE program was used while pre-WOCE sections (1985, 1987)³ were used in the North Pacific and at 32° S in the Indian Ocean. Each section is a collection of high-density temperature, salinity, oxygen and nutrient measurements. From temperature and salinity, a geostrophic velocity field is calculated and adjusted so that mass and other conservative tracers (see Methods) are conserved between sections. The resulting heat (or ‘enthalpy’, where the net mass flux is non-zero) transports are indicated

by the arrows and red numbers (positive northward/eastward). The white box at the tail end of each arrow is the one-standard-deviation uncertainty. Between sections, ocean–atmosphere heat transfers are indicated by the zonal length of the coloured boxes (blue for ocean cooling; red for ocean heating), with the length of the white box inside indicating the uncertainty. (Because the ocean–atmosphere heat transfers are anomaly residuals, that is, corrected for residual mass imbalances, they do not correspond exactly to the differences between net fluxes across sections, for example, in the North Indian Ocean. But this discrepancy is much less than the uncertainties.)

Diffusivities could not be resolved in the Southern Ocean, where many neutral surfaces outcrop. The improved inverse model method has produced the first near-global, resolved estimates of the dianeutral transfers. The overall results are inconsistent with recent suggestions that the ocean mixes primarily at near-surface outcrops of the neutral surfaces, that is, primarily in the Southern Ocean¹². Strong abyssal mixing is required by the observed geostrophically balanced circulation, and its absence is incompatible with the observed property distributions.

Figure 1 shows the heat (actually, enthalpy) transports, across each hydrographic section (arrows) along with the residuals reflecting atmospheric heat exchanges (boxes). Residuals are accurately determined at middle and high latitudes, but are more uncertain at lower latitudes (for example, in the Atlantic Ocean) owing to an enhancement of the geostrophic noise there³. Nevertheless, the total heating over the tropical Atlantic and Pacific oceans are well-determined, respectively 0.7 ± 0.2 PW (1 PW = 10^{15} W) and 1.6 ± 0.4 PW. No significant heat transfers are found in the Indian Ocean because of the large, uncertain, warm water inflow from the Pacific Ocean. This large warm water flux is the main heat escape from the Pacific Ocean, resulting in a northward heat flux in the South Pacific. In the southern Pacific sector, significant heating is found, in contrast with the sparse *in situ* observations¹³, but in qualitative agreement with the recent re-analysis of the European Centre for Medium Range Weather Forecasts¹⁴. Figure 3 shows the globally integrated heat fluxes compared to independent estimates. Most of the cooling occurs in the Northern Hemisphere, at a rate of -1.7 ± 0.2 PW, in balance with the 2.3 ± 0.4 PW heating in the

tropical band and the -0.7 ± 0.3 PW cooling in the Southern Ocean.

Changes in the oceanic heat transport can have a large impact on atmospheric temperature gradients^{15,16} and thus on climate. Previous estimates of the ocean-atmosphere heat exchanges that are based upon purely ocean surface observations are highly uncertain^{17,18}. Analyses from numerical weather prediction centres provide oceanic surface fluxes that are often used as boundary conditions for driving ocean models, but associated uncertainty estimates are not provided. Heuristic calculations suggest uncertainties in their estimates of at least ± 0.6 PW for the meridional oceanic heat transport at most latitudes¹⁹. The present inversion indicates uncertainties that depend on latitude, with a high accuracy of globally integrated heat transfers (Fig. 3). Similar budgets, to be

Table 1 Basin-averaged dianeutral velocities and diffusivities

	\bar{w}^* (10^{-6} m s^{-1})	$\bar{\kappa}^*$ ($10^{-4} \text{ m}^2 \text{ s}^{-1}$)
Atlantic bottom	0.5 ± 0.2	9 ± 4
Indian bottom	0.6 ± 0.3	12 ± 7
Pacific bottom	0.4 ± 0.1	9 ± 2
Southern bottom	-0.25 ± 0.1	-
Atlantic deep	0.1 ± 0.05	3 ± 1.5
Indian deep	0.3 ± 0.15	4 ± 2
Pacific deep	0.1 ± 0.03	4 ± 1
Southern deep	0.1 ± 0.1	-

The average is calculated on neutral surfaces from $\gamma^{\theta} = 28.1 \text{ kg m}^{-3}$ to the bottom (generally 3,800 decibars (or metres) to the bottom) for the 'bottom layers' and from $\gamma^{\theta} = 27.96$ to $\gamma^{\theta} = 28.07$ for the 'deep layers' (generally 2,000 m to 3,500 m).

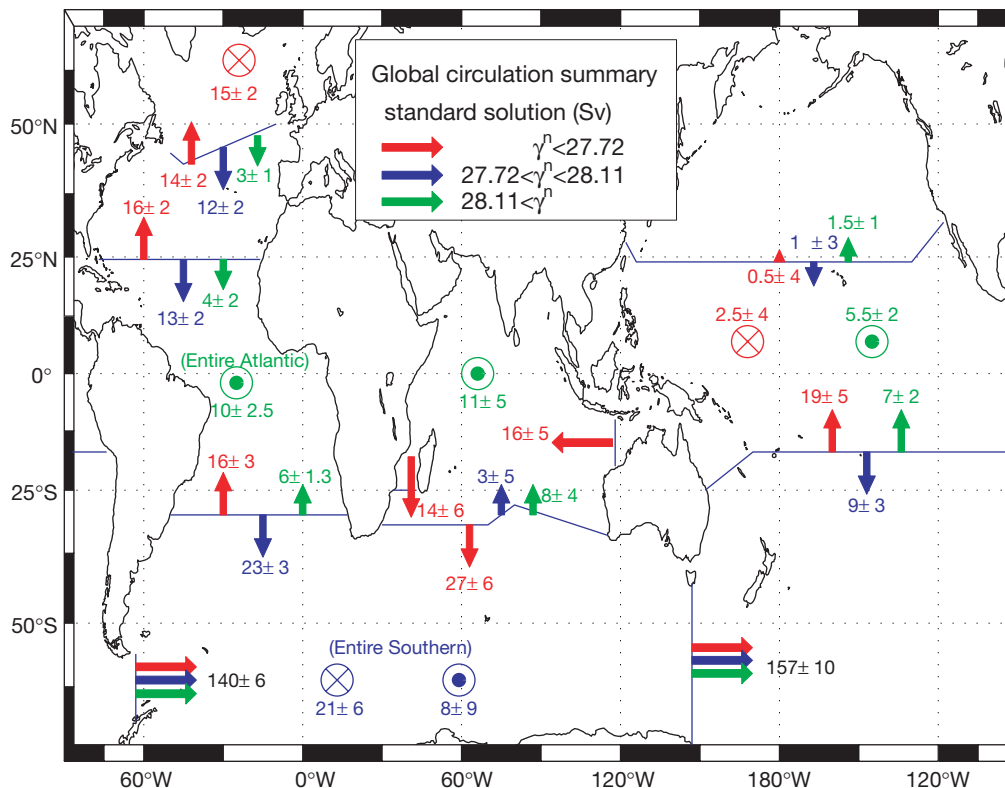


Figure 2 Zonally integrated layer mass transports. The estimated water transports are indicated for the different density classes bounded by neutral surfaces (γ^{θ} , in kg m^{-3}) and across selected hydrographic sections. Neutral surfaces are close to surfaces of constant density, but are chosen so that movement along them minimizes the work done against gravity. The colour of the upwelling or down-welling arrows indicates the layer from which the water is coming. A flux of 0.8 Sv from the Pacific to the Atlantic Ocean through the Bering Strait was taken into account, although it is much smaller than the uncertainties on

the net transports. In the Southern Ocean, the bottom water formation takes place mostly in the Weddell Sea, while the upwelling distribution is uncertain. In the Indian Ocean, most of the upwelling takes place north of 7° S. The South Pacific transports are given at 17° S because of the more complicated structure at 32° S (ref. 3). Note the increase in the Southern Ocean transport south of Australia owing to the recirculation of Indonesian throughflow water.

published elsewhere, of oxygen and nutrients, are important for both climate and biogeochemical processes^{3,20}.

The physical circulation estimated here during WOCE provides a new reference state for climate change studies, and a test—within the estimated uncertainties—of general circulation models of both atmosphere and ocean. The estimated values of κ^* and w^* represent values that models will need to simulate. The high-resolution WOCE data set, the confinement in time, the use of current-meter data as constraints in boundary currents, and the detailed analysis of the uncertainties associated with our method are great improvements in reliability over previous circulation estimates. Within the error estimates, there is no conflict in either transports or heat fluxes with a previous global inversion that was based on a nearly independent and coarser data set^{1,21}, and no statistically significant change in integrated mass transports over the past 30 years was found^{1,22}. This is an important conclusion in its own right.

Improving the accuracy of the estimates made from the present data sets, if interpreted as climatological averages, will not be easy. Although the addition of new data, for example, existing or future meridional sections, will better the spatial resolution, limitations now lie primarily in the uncertainty introduced by true oceanic variability from the daily to the interannual. Significant improvements in the present numbers will occur only through the use of data sets permitting true temporal averaging of the oceanic circulation. For instance, the present solution has large uncertainties due to undersampling of the highly variable Brazil current and Pacific–Indian throughflow. Additional observations there would greatly improve accuracy. Further refinement of the a priori error estimates

by using improved numerical models and other data sets (such as altimetry) is also possible. □

Methods

The method is that of hydrographic inverse box models²³, where the relative, geostrophic velocity field is obtained from temperature and salinity measurements across the sections of Fig. 1. This initial flow is uniformly adjusted at each location so that the flow satisfies near-conservation of mass, anomalies of salt, heat, and the phosphate-oxygen combination (“PO” = $170[PO_4] + [O_2]$)^{24,25} within oceanic layers defined by neutral surfaces (neutral surfaces are densities chosen so that work against gravity is minimized when following the surface, permitting global use of a single density variable²⁶). Silica conservation is also required, top-to-bottom, while heat and PO are conserved only in layers that are not in contact with the surface. The surface layer is directly wind-driven (Ekman transport). Diffusive and advective exchanges between layers are determined by the model. The use of anomaly equations²⁷ permits, through noise subtraction, determination of diffusivities across each interface. Substantial improvements were made to the method, compared to that used in ref. 1, with, in particular, rigorous estimates of uncertainties through a determination of the a priori model error based on a simulation from the output of a quasi eddy-resolving (1/4°) ocean general circulation model²⁸.

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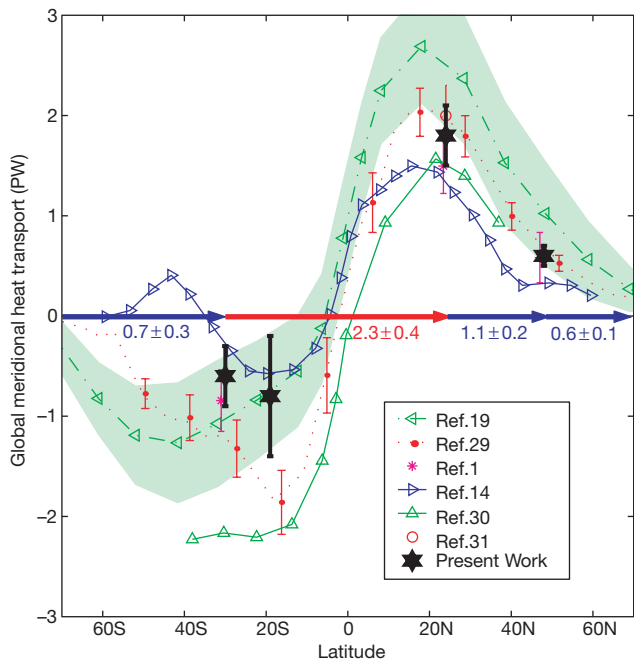


Figure 3 Global meridional heat transports. The black stars with thick error bars indicate the global, zonally integrated heat transports. Ocean–atmosphere heat exchanges between selected latitudes are given by numbers above the northward pointing arrows (positive for oceanic heating). The uncertainties from ref. 19 are indicated by the green band. The previous estimate of ref. 1 is different, but statistically consistent. No incompatibility is found between the estimates by the European Centre for Medium Range Weather Forecasts and US National Center for Environmental Prediction models^{14,19,29} and our new values, owing to their large uncertainties¹⁹. Other climatological estimates^{30,31} were published without error estimates, thus precluding any quantitative comparison. The estimate of ref. 30 is taken from their experiment B. (This figure is adapted and completed from refs 1 and 30.)

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The use of earthquake rate changes as a stress meter at Kilauea volcano

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Stress changes in the Earth's crust are generally estimated from model calculations that use near-surface deformation as an observational constraint. But the widespread correlation of changes of earthquake activity with stress¹⁻⁵ has led to suggestions that stress changes might be calculated from earthquake occurrence rates obtained from seismicity catalogues. Although this possibility has considerable appeal, because seismicity data are routinely collected and have good spatial and temporal resolution, the method has not yet proven successful, owing to the non-linearity of earthquake rate changes with respect to both stress and time. Here, however, we present two methods for inverting earthquake rate data to infer stress changes, using a formulation for the stress- and time-dependence of earthquake rates⁶. Application of these methods at Kilauea volcano, in Hawaii, yields good agreement with independent estimates, indicating that earthquake rates can provide a practical remote-sensing stress meter.

The inversions use a formulation for earthquake rate changes⁶ derived from laboratory observations of rate- and state-dependent fault strength⁶⁻⁸, which constrain the earthquake nucleation process to be dependent on both time and stress. Previously, this formulation has been applied to model the spatial and temporal characteristics of earthquake clustering phenomena, including foreshocks and aftershocks^{6,7}, and to evaluate earthquake probabilities following large earthquakes⁹. The effectiveness of the formulation for forward modelling of earthquake phenomena, and its derivation from observed fault properties, provide the basis for its use to estimate stress changes from earthquake rate data. This approach yields stresses that drive the earthquake process. As such, it is distinct from other seismological methods that yield measures of stress changes resulting from earthquakes.

The formulation of Dieterich⁶ for rate of earthquake activity R (in a specified magnitude range) can be written in the condensed form

$$R = \frac{r}{\gamma \dot{S}_r}, \text{ where } d\gamma = \frac{1}{A\sigma} [dt - \gamma dS] \quad (1)$$

where γ is a state variable, t is time, and S is a modified Coulomb stress function defined below. The constant r is the steady-state earthquake rate at the reference stressing rate \dot{S}_r . A is a dimensionless fault constitutive parameter with values usually in the range 0.005–0.015 (refs 6–8). The modified Coulomb stress function is defined as

$$S = \tau - [\mu - \alpha]\sigma \quad (2)$$

where τ is the shear stress acting across fault planes that generate earthquakes (positive in the slip direction), σ is the normal stress (less pore fluid pressure), μ is the coefficient of fault friction and α is a constitutive parameter^{6,10} with an assigned value in this study of 0.25 (refs 6, 10). In equation (1), the term $A\sigma$ is a constant (that is, changes in σ are negligible relative to total σ). For a stress step, equation (1) yields the characteristic aftershock sequence, which consists of an immediate jump of seismicity rate followed by decay that obeys the Omori t^{-1} aftershock decay law with aftershock duration $t_a = A\sigma/\dot{S}$ (ref. 6).

We use two methods to estimate stress changes from earthquake rate data. The first gives stress as a function of time in a specified volume. From equation (1), the observed rate R is used to directly calculate γ as a function of time (that is, $\gamma(t) = r/R(t)\dot{S}_r$). This requires an estimate of \dot{S}_r , which can be obtained from independent

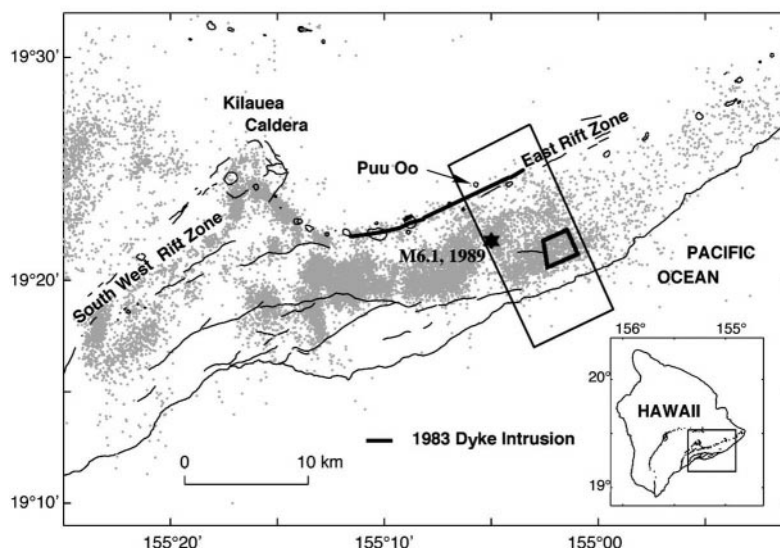


Figure 1 Map of Kilauea volcano showing earthquakes of magnitude $M \approx 1.5$ from 1976 to 1983. Intrusion of magma into the southwest and east rift zones of Kilauea causes rift expansion, and results in motion of the south flank to the SSE. Eruptive fissures initiated

the Puu Oo eruption, which started 1 January 1983 and continues to the present. The small polygon is the region of analysis of Fig. 2; the large rectangle gives the region of analysis of Figs 3 and 4.

is less than 100%). Models for the additional oligonucleotide, GTP molecules and Mg^{2+} ions, have been fitted into electron density maps and refinement of these oligo- Mn^{2+} -polymerase and oligo-GTP-Mg-Mn-polymerase complexes against their data sets, imposing strict threefold NCS constraints, resulted in models with *R* factors of 23.7 and 21.4%, respectively, and good stereochemistry (Table 1).

Figures

Unless otherwise stated figures were drawn using BOBSCRIPT²⁶ and rendered with RASTER3D²⁷.

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Supplementary information is available on Nature's World-Wide Web site (<http://www.nature.com>) or as paper copy from the London editorial office of Nature.

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Correspondence and requests for materials should be addressed to D.I.S. (e-mail: dave@strubi.ox.ac.uk). Coordinates have been deposited in the RCSB Protein database under accession codes: 1HHS, 1HHT, 1HI0, 1HI1, 1HI8.

correction

Improved estimates of global ocean circulation, heat transport and mixing from hydrographic data

Alexandra Ganachaud & Carl Wunsch

Nature **408**, 453–457 (2000).

In this first paragraph of this paper, the uncertainty on the net deep-water production rates in the North Atlantic Ocean was given incorrectly. The correct value should have been $(15 \pm 2) \times 10^6 \text{ m}^3 \text{ s}^{-1}$. □

errata

Changes in Greenland ice sheet elevation attributed primarily to snow accumulation variability

J. R. McConnell, R. J. Arthern, E. Mosley-Thompson, C. H. Davis, R. C. Bales, R. Thomas, J. F. Burkhard & J. D. Kyne

Nature **406**, 877–879 (2000).

As the result of an editing error, the 1993–1998 aircraft-based altimetry surveys of the southern Greenland ice sheet reported by Krabill *et al.* (1999) were erroneously described as satellite-based. □

Genome sequence of enterohaemorrhagic *Escherichia coli* O157:H7

Nicole T. Perna, Guy Plunkett III, Valerie Burland, Bob Mau, Jeremy D. Glasner, Debra J. Rose, George F. Mayhew, Peter S. Evans, Jason Gregor, Heather A. Kirkpatrick, György Pósfai, Jeremiah Hackett, Sara Klink, Adam Boutin, Ying Shao, Leslie Miller, Erik J. Grotbeck, N. Wayne Davis, Alex Lim, Eileen T. Dimalanta, Konstantinos D. Potamouisis, Jennifer Apodaca, Thomas S. Anantharaman, Jieyi Lin, Galex Yen, David C. Schwartz, Rodney A. Welch & Frederick R. Blattner

Nature **409**, 529–533 (2001).

The Genbank accession number for the annotated sequence given in this paper was typeset incorrectly. The correct accession number is AE005174. □