Bayesian Modeling of the Equation of State for Liquid Iron in Earth's Outer Core

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Abstract We use Bayesian modeling of the equation of state (EoS) to constrain the density (ρ) and P wave velocity (V_p) of liquid iron under conditions of Earth's outer core. Experiments at such high pressures (P) and temperatures (T) are technically challenging, so there are few data available to use in parameter optimization of the EoS. Our Bayesian inference modeling successfully estimates the posterior probability distribution of the parameters and unobserved data by using the Hamiltonian Monte Carlo method. These posterior probability distributions allow calculation of P-ρ and P-V_p profiles of liquid iron along the adiabatic P-T profile together with the associated credible intervals. Assuming that the temperature at the core-mantle boundary (CMB) is 3,500–4,200 K, the P-ρ and P-V_p profiles show deviations of ρ and V_p from the preliminary reference Earth model of about 8–11% and −3% to −5%, respectively. Deviations of the 95% credible intervals of the P-ρ profile for the CMB and the inner core boundary are 6.9–9.7% and 6.5–9.8%, respectively. Equivalent deviations of the P-V_p profile are −4.8% to −1.5% and −6.0% to −2.3%, respectively. Bayesian modeling of the EoS enables integration of small data sets that include unobserved data and evaluation of uncertainty ranges of physical properties, such as ρ and V_p, which are essential for comparison with seismological properties of the core.

Plain Language Summary Earth's outer core is mainly composed of a liquid iron that is essential in understanding Earth's internal structure. To characterize Earth's outer core, the relation between density, pressure, P wave velocity, and temperature must be known. High-pressure and high-temperature compression experiments provide valuable data to estimate such relation. However, experiments at such high-pressure and high-temperature conditions are technically challenging, so it is difficult to collect an abundant data set covering a sufficiently broad range of pressure and temperature conditions. As it is necessary to estimate the relation using small data set, we performed statistical analysis based on the Bayesian inference that is one of the main probabilistic approaches to data analysis, and the analysis successfully conducted for the small data set. The result of analysis can constrain the pressure-density and pressure-P wave velocity relation of the liquid iron under high-pressure conditions corresponding to Earth's outer core together with associated uncertainties. We conclude that Bayesian inference is a powerful framework for analyzing small data sets from high-pressure and high-temperature experiments.

1. Introduction

High-pressure (P) and high-temperature (T) compression experiments provide valuable information that can constrain estimates of the thermodynamic properties of the deeper parts of Earth's interior (e.g., Poirier, 2000; Stacey & Davis, 2008). Various experiments have paid particular attention to the properties of liquid iron, a major component of Earth's outer core. For example, shock-wave compression experiments have measured the density (ρ) and longitudinal-wave velocity (P wave velocity, V_p) of molten iron at high-P conditions similar to those near the base of the outer core (e.g., Brown & McQueen, 1986). Kuwayama et al. (2020) measured the ρ and V_p of pure liquid iron using X-ray diffraction (XRD) and inelastic X-ray scattering (IXS), respectively, via static compression experiments with a laser-heated diamond-anvil cell (LH-DAC). The resulting data sets facilitate estimation of P-T-ρ and P-T-V_p relations of liquid iron under the high-P and high-T conditions of the outer core by parameter optimization of an equation of state (EoS).
However, such optimization is difficult due to the challenges facing experiments under the high-\(P\) and high-\(T\) conditions of Earth’s core. To obtain a data set covering a sufficiently broad range of \(P\) and \(T\) conditions, it is necessary to integrate different data sets from various experiments, although the type of data observed in each case depends on the experimental procedure. For example, LH-DAC experiments using XRD measurements can simultaneously determine \(P\), \(T\), and \(\rho\), but not \(V_p\) (Kuwayama et al., 2020). In contrast, IXS studies can simultaneously determine \(P\), \(T\), and \(V_p\), but not \(\rho\). Shock compression experiments on liquid iron have provided relations for \(P\)-\(\rho\)-\(V_p\) (Brown & McQueen, 1986), but not direct \(T\) measurements. When parameter optimization is performed for a data set that includes unobserved data, an ordinary brute-force approach is unsuitable because of the enormous computational cost. As a thermal EoS usually contains more than seven parameters (e.g., Ichikawa et al., 2014), \(>10^7\) loss functions have to be evaluated for the EoS optimization even when only 10 test values are assigned for each parameter. The increase in the loss functions requiring evaluation when estimating unobserved data make the computational cost extremely high. Moreover, difficulties in evaluating uncertainties of the estimated parameters prevent determination of the uncertainty of the EoS. Thus, it is difficult to verify plausible ranges of the physical properties derived from the EoS, even though such ranges are required when comparing the EoS and seismological observations.

This study aims to establish an improved procedure for optimization of the parameters of the EoS and for estimation of the uncertainties of the EoS. To achieve this, the optimization procedure must be able to efficiently analyze a data set with the two limitations of having few data points and including unobserved data. These limitations prevent the use of methods that require a large amount of data points, such as deep neural networks.

This study focuses on Bayesian inference (e.g., Bishop, 2006; Gelman et al., 2013) as an appropriate method to analyze such a data set. This approach has been applied to classical geophysical tomographic problems in Earth sciences (e.g., Aster et al., 2005; Mosengaard & Sambridge, 2002; Tarantola, 2005), and has recently attracted attention as a framework for data analysis in fields such as geodynamic modeling (e.g., Afonso et al., 2016; Baumann & Kaus, 2015; Kuwatani et al., 2014; Li et al., 2017; Morishige & Kuwatani, 2020; Takeuchi et al., 2019), geochemical data analysis (e.g., Kuwatani et al., 2012, 2018), and seismic data analysis (e.g., de Wit et al., 2013, 2014; Irving et al., 2018). Korenaga & Karato’s (2008) analysis of deformation applied Bayesian inference to over 200 published data on the subsolidus deformation of synthetic olivine aggregates (Hirth & Kohlstedt, 1995; Jung et al., 2006; Karato et al., 1986; Mei & Kohlstedt, 2000a, 2000b) to establish experimental constraints on the rheology of Earth’s upper mantle. Recently, Nakakoji et al. (2018) analyzed over 600 mechanical data under a constant load from 1,054 to 1,370 \(^\circ\)C by using Bayesian inference to obtain the flow-law parameters for interface-controlled and Coble creep. However, the difficulty of obtaining an adequate number of data points under extremely high-\(P\) and high-\(T\) conditions necessitates an investigation using Bayesian inference to assess whether a reasonable EoS can be obtained using these small numbers of experimental data.

This study reports Bayesian modeling of the EoS for liquid iron. The analyzed data set (only 17 data points) is assembled by integrating all available data for liquid iron at high \(P\) from three different experimental procedures. The parameters and unobserved data are estimated using Bayesian inference. This allows us to calculate the \(\rho\) and \(V_p\) of liquid iron at \(P\)-\(T\) conditions corresponding to the outer core, as well as \(P\)-\(\rho\) and \(P\)-\(V_p\) profiles (with associated credible intervals) along the adiabatic \(P\)-\(T\) path. Our work shows that Bayesian inference can provide reasonable results that constrain the thermodynamic properties of the outer core even when using the few available results from various experimental data sets.

2. Overview of the Analysis

Bayesian inference is one of the main probabilistic approaches to data analysis. It involves fitting a probability model to a given data set and summarizing the result with a probability distribution for the parameters of the model (Gelman et al., 2013). The analysis is performed based on the relation \(p(\theta|D) \propto p(D|\theta)p(\theta)\) for the parameter \(\theta\) and given data \(D\), where \(p(D|\theta)\) is the posterior probability distribution, \(p(\theta)\) is the likelihood function, and \(p(\theta)\) is the prior probability distribution. When fitting a model such as an EoS to data, the values of a parameter are estimated by calculating the distribution that maximizes the posterior probability distribution \(p(\theta|D)\). The likelihood function \(p(D|\theta)\) represents the goodness of fit of a model to a given data set for the chosen parameter values, and the prior probability distribution \(p(\theta)\) represents the probability of the parameters before the data are incorporated.
The main basis of our analysis is the use of Bayesian inference assuming that each parameter and unobserved data is a random variable. As this allows the analysis to handle variables indistinguishably, an EoS can be optimized using a single data set compiled by integrating different experimental data sets (Figure 1). The calculation is generally performed using the Markov chain Monte Carlo method (Gelman et al., 2013; McElreath, 2020). This involves randomly collecting samples from a probability distribution and using them to evaluate the characteristics of the distribution, such as the mean and quantiles. Recent developments of this method have enabled the computation of a model with several hundred parameters (Gelman et al., 2013; McElreath, 2020), making it much more efficient than a conventional brute-force approach for the optimization of an EoS. The calculation result is the posterior probability distribution $p(\theta|D)$ (Figure 1). The parameter solution is determined from the mean of the distribution; the distribution's width corresponds to the uncertainty of the solution, and is called the credible interval. The EoS can thus be determined with a credible interval. Consequently, the advantages of the present approach using Bayesian inference for EoS optimization are as follows: (a) each parameter and unobserved data are calculated indistinguishably even when using data integrated from various small data sets; (b) the solution is obtained with its uncertainty (as credible intervals) from the posterior probability distributions; and (c) the obtained EoS can be used to calculate profiles (with credible intervals), such as pressure-density relations along adiabatic temperature profiles (Section 6). The following sections demonstrate the analysis and give explanations of the analyzed data (Section 3), the EoS (Section 4), and the Bayesian modeling (Section 5).

3. Analyzed Data Set

The analyzed data set comprises 17 experimental data sets from Kuwayama et al. (2020) and Anderson and Ahrens (1994) (Tables S1–S3 in Supporting Information S1). These include $P, T, \rho$, and $V_p$ values obtained by integrating data sets from three different experiments: the $P-T-\rho$ relations of liquid iron determined by XRD measurements (Kuwayama et al., 2020) (run numbers 1–11, Table S1 in Supporting Information S1); the $P-T-V_p$ relations of liquid iron determined by IXS measurements (Kuwayama et al., 2020) (run numbers 12–14, Table

Figure 1. The analytical concept used in this study. We estimate 7 parameters of the equation of state (EoS) and 17 unobserved data using Bayesian inference. The parameters and unobserved data are assumed to be random variables, and the prior probability distributions (red curves)—which are prepared before the calculation—are updated to the posterior probability distributions (blue curves) by Bayesian inference calculations incorporating the data set. Each value of each parameter and of the unobserved data is determined from the mean of each posterior probability distribution. The width of each distribution represents the uncertainty of the values (i.e., the credible intervals). $\rho_0$ and $K_T_0$ are a reference density and the isothermal bulk modulus, respectively.
S2 in Supporting Information S1); and the \( P_p-V_p \) relations with the Grüneisen parameter (\( \gamma \)) of liquid iron from a shock experiment (Brown & McQueen, 1986), which was re-evaluated by Anderson and Ahrens (1994) (run numbers 15–17, Table S3 in Supporting Information S1). We defined these three sets of data as \( D = \{ D_{\text{Vpmiss}}, D_{\text{vp1s}}, D_{\text{vp1sT}} \} \), respectively. The unobserved data of \( V_p, \rho \), and \( T \) in experiment numbers 1–11, 12–14, and 15–17 are labeled \( V_{\text{pmiss}} = \{ V_{\text{p1s}} - V_{\text{p1sT}} \} \), \( \rho_{\text{miss}} = \{ \rho_{\text{p1s}} - \rho_{\text{p1sT}} \} \), and \( T_{\text{miss}} = \{ T_{\text{p1s}} - T_{\text{p1sT}} \} \), respectively. Here, \( m \) means missing. These unobserved data are simultaneously estimated during EoS parameter optimization.

4. Equation of State for Liquid Iron

We employ the EoS based on the Mie-Grüneisen equation, which Ichikawa et al. (2014) previously used for a given atomic volume (\( V \)) and \( T \). In the present study, as \( \rho \) and \( T \) are explanatory variables in the Bayesian model, we rewrite \( V \) to \( \rho \) in the EoSs of \( P \) and \( V_p \). For a given \( \rho \) and \( T \), the EoSs of \( P \) and \( V_p \) are represented as \( P(\rho, T) \) and \( V_p(\rho, T) \), respectively. The analysis uses both EoSs as the response function (see Text S1 in Supporting Information S1 for details). \( P(\rho, T) \) can be expressed as the following sum of the pressure at a reference temperature \( (P_{0}(\rho)) \) and the thermal pressure \((\Delta P_{0}(\rho, T))\):

\[
P(\rho, T) = P_0(\rho) + \Delta P_0(\rho, T),
\]

where

\[
P_0(\rho) = 3K_0\left(\frac{\rho_0}{\rho}\right)^{-\frac{3}{2}} \left\{ 1 - \left(\frac{\rho_0}{\rho}\right)^{\frac{3}{2}} \right\} \exp\left\{ \frac{3}{2} \left( K'_0 - 1 \right) \left[ 1 - \left(\frac{\rho_0}{\rho}\right)^{\frac{3}{2}} \right] \right\},
\]

\[
\Delta P_0(\rho, T) = \frac{\gamma(\rho)}{V} \Delta E_0(\rho, T) = \frac{\gamma(\rho)}{V} [E_0(\rho, T) - E_0(\rho, T_0)],
\]

\[
E_0(\rho, T) = 3nR \left[ T + e_0 \left(\frac{\rho_0}{\rho}\right)^{\frac{3}{2}} T^2 \right],
\]

and

\[
\gamma(\rho) = \gamma_0 \left(\frac{\rho_0}{\rho}\right)^{b},
\]

where \( V \) is the atomic volume, \( K_0 \) is the isothermal bulk modulus, \( K'_0 \) is its pressure derivative, \( \gamma_0 \) is the Grüneisen parameter, \( b \) is a volume-independent adjustable parameter, and \( e_0 \) and \( g \) are constants for the electronic contribution. \( R \) is the gas constant. \( T_0 \) is a reference temperature, and \( \rho_0 \) is a reference density. Subscript 0 denotes zero pressure. Moreover, \( V_p(\rho, T) \) for liquid iron is represented using the adiabatic bulk modulus \( (K_a) \) as follows:

\[
V_p(\rho, T) = \sqrt{\frac{K_a}{\rho}}.
\]

Derivation of \( K_a \) is presented in (Text S2 in Supporting Information S1). Consequently, this study estimates seven parameters: \( \rho_{0p}, K_{0p}, K'_{0p}, \gamma_{0p}, b, e_{0p}, \) and \( g \).

5. Bayesian Modeling of EoS

The set of parameters and unobserved data \( (\theta = \{ \rho_{0p}, K_{0p}, K'_{0p}, \gamma_{0p}, b, e_{0p}, g, V_{\text{pmiss}}, \rho_{\text{miss}}, T_{\text{miss}} \}) \) is estimated by Bayesian modeling. We assume the output \( (y = \{ P, V_p \}) \) to be the sum of the response function \( f(x; \theta) \) for the corresponding input \( (x = \{ \rho, T \}) \) and a noise term \( \epsilon \)

\[
y = f(x; \theta) + \epsilon.
\]

The noise term \( \epsilon \) is a Gaussian random number with zero mean and variance \((\sigma^2)\). The observation can be expressed as follows in terms of the probability density function \( p(y|x, \theta) \)

\[
p(y|x, \theta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( -\frac{1}{2\sigma^2} (y - f(x; \theta))^2 \right).
\]
Bayesian inference assumes the parameters and unobserved data (θ) to be random variables. When the data set \(D = \{X, Y\}\) with \(n\) data \(X = \{x_1, x_2, \ldots, x_n\}, Y = \{y_1, y_2, \ldots, y_n\}\) is obtained, the posterior probability distribution \(p(\theta|D)\) can be expressed as follows using Bayes’ theorem:

\[
p(\theta|D) = \frac{p(Y|X, \theta)p(\theta)}{p(Y|X)} = \frac{1}{Z(D)} \prod_{i=1}^{n} p(y_i|x_i; \theta) = \frac{1}{Z(D)} \exp \left( -\frac{n}{\sigma^2} E(\theta) \right) p(\theta).
\]

\(E(\theta)\) is the mean squared error function (e.g., Nagata et al., 2012), \(p(\theta)\) is the prior probability distribution, and \(Z(D)\) is a normalization constant. The posterior probability distribution \(p(\theta|D)\) represents the conditional probability of the parameters and unobserved data \(\theta\) for the given data set \(D\). We apply the above framework to \(D = \{D_{\text{VP}}^\text{miss}, D_{\text{V}}^\text{miss}, D_{\text{T}}^\text{miss}\}\). Texts S3 and S4 in Supporting Information S1 give details of \(E(\theta)\), \(p(\theta|D)\), and \(q(\theta)\).

The calculation of \(p(\theta|D)\) (Equation S26 in Supporting Information S1) is conducted by the no-U-turn sampler (NUTS) method proposed by Hoffman and Gelman (2014). NUTS is a Hamiltonian Monte Carlo method adopted in the rstan package (https://mc-stan.org/users/interfaces/rstan) for the R language (https://www.r-project.org). The calculation employs 25,000 steps for the warm-up and 5,000 subsequent sampling steps. Tables S1–S3 in Supporting Information S1 list the input data. The initial values of the parameters and unobserved data are randomly generated from each prior probability distribution (Table S4 in Supporting Information S1). Four sets of calculations (Chains 1–4) confirm the stability of calculation.

### 6. Results and Discussion

#### 6.1. Posterior Probability Distribution

The posterior probability distributions of the parameters and unobserved data are obtained. Plots of the parameters’ trajectories during sampling in each chain show convergence to stable distributions (Figures S1–S3 in Supporting Information S1). As the calculation result is a probability distribution, each parameter value, each unobserved data value, and the uncertainties are determined from the mean and quantile of each distribution. The uncertainty of each value is represented here as credible intervals.

Figure 2 shows the posterior probability distributions of the parameters in each chain. Each chain of calculation shows a similar distribution, indicating successful calculation. Compared with the prior probability distribution, the posterior distribution is distributed in a narrower range because it incorporates experimental data into the Bayesian inference framework. The prior and posterior distributions also have different peak positions in the histograms. These differences between the distributions are clear for \(\rho_a\) and \(K_H\). The posterior probability distributions of unobserved data also show narrower distributions than the prior distributions (Figures 3 and 4).

Tables 1 and 2 summarize the posterior probability distributions. The listed mean of each distribution (called here the expected posterior, EAP), provides the estimated value of each parameter and unobserved data. The estimates for unobserved data \(V_{\text{VP}}^\text{miss}, \rho_{\text{VP}}^\text{miss},\) and \(T_{\text{VP}}^\text{miss}\) tend to increase with increasing pressure. Those of \(V_{\text{VP}}^\text{miss}\) and \(\rho_{\text{VP}}^\text{miss}\) are comparable to the analyzed data at similar pressures (Tables S1–S3 in Supporting Information S1). In contrast, values of \(T_{\text{VP}}^\text{miss}\) tend to be lower than those estimated by Brown and McQueen (1986). For example, the EAPs of \(T_{10^5}\), \(T_{10^6}\), and \(T_{10^7}\) (5,057.64 K at 278.3 GPa, 5,966.34 K at 331.2 GPa, and 7,047.49 K at 396.7 GPa, respectively) are respectively approximately 1,700, 2,000, and 3,000 lower than the Hugoniot temperature of liquid iron estimated by Brown and McQueen (1986) (Figure 5). These EAPs are, however, in good agreement with those recently calculated using EoS models (Ichikawa et al., 2014; Wagle & Steinele-Neumann, 2019), indicating that Brown and McQueen (1986) may have overestimated temperature. Note that \(T_{\text{VP}}^\text{miss}\) is lower than the melting temperature of iron predicted by Alfè et al. (2009) based on ab initio molecular dynamics (≈6,300–6,400 K at ~330 GPa). However, all three temperatures exceed the melting point of iron reported in recent experiments (e.g., Aquilanti et al., 2015; Basu et al., 2019; Sinmyo et al., 2019; Zhang et al., 2016). For example, Sinmyo et al. (2019) reported a melting temperature of 5,120 K ± 260 K at 285 GPa, which is comparable to \(T_{10^5}\) (5,057.64 K at 278.3 GPa). This seems reasonable, considering that the data at 278.3 GPa were measured just above the condition where the Hugoniot path intersects the melting temperature of iron.
Figure 2. Histogram of each prior (red bar) and posterior (blue bar) probability distribution of the equation of state (EoS) parameter in each chain. Yellow dashed lines show the mean posterior probability distribution for each chain. The posterior distribution is narrower than the prior; the distributions also show different peak positions. The similar convergence achieved by the different chains indicates successful sampling of the posterior distributions.

Figure 3. Histograms of each prior (red bar) and posterior (blue bar) probability distribution of unobservable velocity data ($V_{Pm1} - V_{Pm11}$) in each chain. Yellow dashed lines show the mean posterior probability distribution for each chain. The similar convergence achieved by the different chains indicates successful sampling of the posterior distributions.
Using the obtained posterior probability distributions, we evaluate the credible intervals of the isothermal $P-\rho$ and $P-V_p$ relations of the EoS (Figure 6). These isothermal relations agree well with the experimental data. Moreover, the weak temperature dependence of the $P-V_p$ relations is consistent with theoretical results (e.g.,

### Table 1
**Summary of the Estimated Values of the EoS Parameters**

| Parameter | Estimate | 50% credible interval | 95% credible interval |
|-----------|----------|-----------------------|-----------------------|
|           | Mean     | Lower 50% | Upper 50% | Lower 95% | Upper 95% |
| $\rho_0$  | 7.19     | 7.11       | 7.26       | 6.97      | 7.41      |
| $K_{\text{ij}}$ | 83.12 | 75.40      | 91.02      | 60.12     | 105.52    |
| $K'_{\text{m}}$ | 5.73  | 5.52       | 5.96       | 4.97      | 6.37      |
| $\gamma_0$ | 2.26   | 2.04       | 2.49       | 1.60      | 2.91      |
| $b$        | 0.86     | 0.67       | 1.05       | 0.29      | 1.40      |
| $e_u$      | $1.27 \times 10^{-4}$ | $9.09 \times 10^{-5}$ | $1.62 \times 10^{-4}$ | $2.78 \times 10^{-5}$ | $2.29 \times 10^{-4}$ |
| $g$        | $-1.01$  | $-1.38$    | $-0.58$    | $-2.15$   | $-0.09$   |

*Note.* Upper and lower bounds of credible intervals are derived from the respective posterior probability distributions.
6.3. $P$-$\rho$ and $P$-$V_p$ Profiles Along the Adiabatic $P$-$T$ Profile of Earth’s Outer Core

The posterior density distributions of parameters enable us to calculate $P$-$\rho$ and $P$-$V_p$ profiles along the adiabatic $P$-$T$ profile with credible intervals. As the conventional adiabatic temperature profile in the outer core is not reflected in the parameters’ uncertainties, it is difficult to evaluate the plausible range of the adiabatic temperature profile. In contrast, our analysis based on Bayesian inference successfully provides a plausible range of the profile for constraining the thermal state of Earth’s outer core.

The adiabatic temperature gradient can be calculated by integrating the following thermodynamic relationship:

$$\left(\frac{\partial T}{\partial P}\right)_s = \frac{\gamma T}{K_s}.$$  \hspace{1cm} (10)

Figure 7a shows adiabatic $P$-$T$ profiles calculated for the temperature at the core-mantle boundary (CMB), $T_{\text{CMB}} = 3,500$–4,500 K, by using the values of $T_0$ and $b$ determined in this study. Figures 7b and 7c show equivalent $T$ profiles for $T_{\text{CMB}} = 3,500$ and 4,200 K, respectively, together with the 68% and 95% credible intervals (dashed and dotted curves, respectively). A $T_{\text{CMB}}$ range of 3,500–4,200 K would be reasonably constrained by the melting (solidus) temperature of mantle material at the pressure of the CMB (Andraut et al., 2011, 2014; Boukare et al., 2015; Fiquet et al., 2010; Kato et al., 2016; Nomura et al., 2014; Tateno et al., 2009; Williams & Garner, 1996). Assuming this range for $T_{\text{CMB}}$, the adiabatic $P$-$T$ profiles (Figures 7b and 7c) reveal 4,700–5,700 K as the range for $T_{\text{ICB}}$ considering the 68% credible interval. The adiabatic $P$-$T$ profiles at this $T_{\text{ICB}}$ range do not exceed the melting temperature of pure iron at the ICB pressure extrapolated from recent experiments based on synchrotron Mössbauer spectroscopy measurements (Jackson et al., 2013; Zhang et al., 2016) and a resistance-heated DAC technique (Sinmyo et al., 2019). The Supporting Information S1 presents profiles calculated for other $T_{\text{CMB}}$ values (Figure S8 in Supporting Information S1) and the profiles’ corresponding data sets and 68% and 95% credible intervals (Data Sets S1–S11).

Figures 8 and 9 show $P$-$\rho$ and $P$-$V_p$ profiles along the adiabatic $P$-$T$ profiles of liquid iron. They are calculated for comparison with the preliminary reference Earth model (PREM; Dziewonski & Anderson, 1981). The profiles and their associated 68% and 95% credible intervals are for $T_{\text{CMB}} = 3,500$ and 4,200 K. The Supporting Information S1 gives equivalent profiles and credible intervals for all tested $T_{\text{CMB}}$ values (3,500–4,500 K; Figures S9 and S10; Data Sets S1–S11 in Supporting Information S1).

The adiabatic $P$-$\rho$ profiles (Figure 8) show that the density in the PREM is clearly lower than that of liquid iron along the adiabatic temperature profiles calculated for each $T_{\text{CMB}}$, even considering the 95% intervals. Assuming 3,500–4,200 K as an acceptable range for $T_{\text{CMB}}$, the adiabatic $P$-$\rho$ profiles show that the reasonable range of the density deviation in the outer core is 8–11% regardless of pressure. A predicted lower limit of the outer-core density deviation of 8% is consistent with the results of recent thermodynamical and theoretical studies for liquid

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**Table 2**

| Value  | Estimate | 50% credible intervals | 95% credible intervals |
|--------|----------|------------------------|------------------------|
|        | Mean     | Lower 50% | Upper 50% | Lower 95% | Upper 95% |
| $V_{pm1}$ | 5.22    | 5.05      | 5.39     | 4.73     | 5.73     |
| $V_{pm2}$ | 5.59    | 5.42      | 5.76     | 5.11     | 6.08     |
| $V_{pm3}$ | 5.87    | 5.71      | 6.03     | 5.40     | 6.33     |
| $V_{pm4}$ | 5.85    | 5.68      | 6.01     | 5.38     | 6.33     |
| $V_{pm5}$ | 6.24    | 6.08      | 6.40     | 5.78     | 6.71     |
| $V_{pm6}$ | 6.46    | 6.30      | 6.62     | 6.00     | 6.92     |
| $V_{pm7}$ | 6.63    | 6.47      | 6.79     | 6.17     | 7.10     |
| $V_{pm8}$ | 6.63    | 6.47      | 6.79     | 6.16     | 7.09     |
| $V_{pm9}$ | 6.82    | 6.66      | 6.98     | 6.37     | 7.27     |
| $V_{pm10}$ | 7.41   | 7.25      | 7.57     | 6.96     | 7.87     |
| $V_{pm11}$ | 7.51   | 7.35      | 7.67     | 7.05     | 7.97     |
| $\rho_{n12}$ | 8.04  | 7.95      | 8.13     | 7.78     | 8.33     |
| $\rho_{n13}$ | 8.45  | 8.38      | 8.51     | 8.24     | 8.66     |
| $\rho_{n14}$ | 8.94  | 8.86      | 9.01     | 8.74     | 9.19     |
| $T_{m15}$ | 5057.64 | 4816.60   | 5394.90  | 3815.06  | 5785.08  |
| $T_{m16}$ | 5966.34 | 5767.24   | 6188.81  | 5247.76  | 6558.40  |
| $T_{m17}$ | 7047.49 | 6774.18   | 7262.69  | 6377.55  | 7991.90  |

Note: Upper and lower bounds of credible intervals are derived from the respective posterior probability distributions.
iron under high-pressure conditions corresponding to Earth's outer core (Dorogokupets et al., 2017; Ichikawa et al., 2014; Komabayashi, 2014; Wagle & Steinle-Neumann, 2019). Komabayashi, 2014 estimated a density deviation of 8.1% for the ICB, assuming $T_{\text{ICB}} = 4,900$ K. Ichikawa et al. (2014) estimated density deviations of 8.9% and 7.7%, respectively, for the CMB and ICB for $T_{\text{ICB}} = 5,000$ K. Dorogokupets et al. (2017) estimated density deviations of 7.6% and 8.2%, respectively, for the CMB and ICB for $T_{\text{ICB}} = 5,882$ K. Wagle and Steinle-Neumann (2019) estimated density deviations of 8% and 7%, respectively, for the CMB and ICB for $T_{\text{ICB}} = 5,500$ K, respectively.

The obtained $P-\rho$ profiles (Figure 8) suggest that the deviation between liquid iron and the PREM is almost constant through the entire depth of Earth's outer core in terms of relative values at each $T_{\text{CMB}}$, even considering the credible intervals. For $T_{\text{CMB}} = 3,500$ K, the 95% credible interval of the adiabatic bulk modulus for the CMB is 597.1–713.2 GPa. For $T_{\text{CMB}} = 4,200$ K, this interval becomes 624.6–685.4 GPa. Given that the adiabatic bulk modulus at the CMB reported in the PREM is 644 GPa, the difference is <10% when considering the 95% credible interval for $T_{\text{CMB}} = 3,500$ K and <6% for $T_{\text{CMB}} = 4,200$ K, providing tight constraints on the chemical composition of the outer core. For example, incorporation of silicon and carbon substantially changes the compressibility (inverse of the bulk modulus) of liquid iron (e.g., Badro et al., 2014; Morard et al., 2013; Nakajima et al., 2015). The small deviation of the adiabatic bulk modulus between liquid iron and the PREM indicates either that silicon and carbon cannot be the predominant light elements in Earth's core or, if the core does contain large amounts of silicon and/or carbon, that the core must contain other light elements that cancel out their effect on compressibility.

The $P-V_p$ profiles in Figure 9 reveal that $V_p$ in the PREM is higher than that in the profiles calculated for each $T_{\text{CMB}}$ even considering the 95% intervals. As these results show that the deviation of $V_p$ between liquid iron and the PREM increases by <1.5% with increasing pressure from the CMB to the ICB, the deviation of $V_p$ displays a slight dependence on pressure. Assuming that the acceptable range of $T_{\text{CMB}}$ is 3,500–4,200 K, the reasonable
Figure 6. Isothermal (a), (c) $P-\rho$ and (b), (d) $P-V_p$ relations of the equation of state (EoS) of liquid iron obtained from Bayesian inference. (a), (b) Red to yellow solid curves show estimated isothermal relations at $T = 2,000$ to $9,000$ K at 1,000 K intervals. These relations are calculated from the means of the respective posterior probability distributions of the parameters, called the expected a posteriori (EAP). The unobserved and experimental data (Tables S1–S3 in Supporting Information S1) are shown as diamonds (blue) and circles (black). These symbols are colored according to the relevant $T$ of the solid curves. (c), (d) Obtained $P-\rho$ and $P-V_p$ relations with associated credible intervals at $T = 5,000$ K. The credible intervals for other temperatures are in the Supporting Information (Figures S8 and S9 in Supporting Information S1). Dashed and dotted curves show 68% and 95% credible intervals, respectively, obtained from the respective posterior probability distributions. Light-blue curves are relations calculated using 5,000 sets of parameters in the posterior probability distributions (Chain 1).

Figure 7. (a) Calculated adiabatic $P-T$ profiles for $T_{\text{CMB}} = 3,500$–4,500 K at 100 K intervals (purple to yellow). The profiles for $T_{\text{CMB}}$ values of (b) 3,500 and (c) 4,200 K. The Supporting Information S1 present profiles for other core-mantle boundary (CMB) temperatures (Figure S10 in Supporting Information S1). Dashed and dotted curves represent the 68% and 95% credible intervals, respectively, obtained from the posterior probability distributions. Light-blue curves are profiles calculated using 5,000 sets of parameters in the posterior probability distributions (Chain 1).
range of the deviation of \( V_P \) in the outer core is \(-3\% \) to \(-5\% \) regardless of \( T_{CMB} \), and the deviation of \( V_P \) increases slightly with increasing pressure. Such deviations of \( V_P \) and \( \rho \) are attributable to light-element impurities in the core (Badro et al., 2014; Umemoto & Hirose, 2020).

We compare the \( P-\rho \) and \( P-V_P \) profiles with those determined by Ichikawa et al. (2014) and Wagle and Steinle-Neumann (2019) (Figures 8 and 9). Ichikawa’s profiles are determined here using the same EoS model as used in this study, although the parameters’ values are different. Wagle and Steinle-Neumann’s profiles are determined by using two EoS models different from ours: one of them contains a correction term for Helmholtz energy formulated by French and Mattsson (2014), the other EoS model does not. Figure 8 shows that Ichikawa’s and Wagle and Steinle-Neumann’s \( P-\rho \) profiles lie within the 95% credible intervals of our \( P-\rho \) profiles at \( T_{CMB}=3,500 \) and 4,200 K. The differences among the profiles tend to be small at high \( T_{CMB} \). Thus, our \( P-\rho \) profiles do not differ significantly from theirs at any given \( T_{CMB} \) (see also Figure S9 in Supporting Information S1).

In contrast to the \( P-\rho \) profiles, the \( P-V_P \) profiles show appreciable differences. Of note, Ichikawa’s profile tends to overestimate \( V_P \) even when compared with the 95% credible interval of ours (Figure 9). The difference is particularly remarkable near the CMB pressure; Ichikawa’s profile shows larger \( V_P \) than the upper bound of our 95% credible interval, and the value of \( V_P \) is almost the same as the PREM data (see also Figure S10 in Supporting Information S1). Wagle and Steinle-Neumann’s \( P-V_P \) profile using the uncorrected EoS also overestimates \( V_P \) relative to our profile for \( T_{CMB}=3,500 \) K, while the deviation from our profile becomes smaller at high \( T_{CMB} \). For example, their profile is within our 95% credible interval for \( T_{CMB}=4,200 \) K. Their profiles using the corrected EoS are consistent with our results, being within 95% of our credible intervals for both \( T_{CMB}=3,500 \) and 4,200 K (Figure 9), suggesting the importance of the correction term. Although their corrected \( P-V_P \) profiles look similar to our results, the slopes are steeper. The gradients indicate that the deviation from our profile becomes large in the high-pressure region for low \( T_{CMB} \) and in the low-pressure region for high \( T_{CMB} \).

As Ichikawa’s and our profiles are determined using the same EoS, any differences arise from the different data sets used for optimization of the EoS. Ichikawa used a \( P-\rho-T \) data set obtained by ab initio molecular dynamics.
calculations. However, it is difficult to obtain an absolute value of the density of iron via ab initio calculations regardless of the choice of commonly used exchange-correlation functionals, as noted by Wagle and Steinle-Neumann (2019). For example, Ichikawa et al. (2014) underestimated the density of iron at ambient pressure. In fact, Wagle and Steinle-Neumann’s corrected profiles show much better agreement with our results compared with their uncorrected ones. Furthermore, our profiles were obtained from a $P$-$\rho$-$V_p$ data set compiled by integrating results obtained using three experimental approaches. As our EoS reflects $V_p$ data—which are strongly related to, e.g., compressibility and thermal expansivity—our profile seems to be more reasonable than Ichikawa’s profile that was obtained without $V_p$ data. Similarly, our profile may be more reasonable than Wagle and Steinle-Neumann’s profile determined from a $P$-$\rho$-$T$ data set (and an EoS model differing from that used in this study). To clarify the differences among the EoS models used by Wagle and Steinle-Neumann (2019) and by us and Ichikawa et al. (2014), it is necessary to derive a new Bayesian model for optimizing Wagle and Steinle-Neumann’s EoS model, which is more complicated than that optimized here. Such optimization requires further extension of the analysis procedure demonstrated here. Further study is required to analyze the various EoS models based on Bayesian inference.

Previous studies have proposed $\rho$ and $V_p$ profiles as a function of $P$ for iron and iron alloys at high pressures, although did not evaluate the profiles’ uncertainties, despite this being indispensable for investigating and understanding the thermal state and chemical composition of Earth’s core. This study demonstrates that Bayesian inference works well for analyzing a small data set that includes unobserved data. Moreover, Bayesian inference is advantageous over other approaches in that it can evaluate unobserved data as well as the credible intervals of the EoS. Here, we report an EoS for liquid iron obtained from all available experimental data at high pressures together with its associated credible intervals; our results show small uncertainties in the calculated $\rho$ and $V_p$ along the adiabatic temperature profiles.
7. Conclusions

We conducted Bayesian modeling of the EoS for the thermodynamic properties of pure liquid iron under high-P and high-T conditions corresponding to Earth's outer core. To cover a broad range of P and T conditions, the analyzed data set was collated by integrating three data sets obtained from different experimental procedures: an LH-DAC experiment using XRD measurements, an LH-DAC experiment using IXS measurements, and a shock experiment. However, as \( V_p \), \( \rho \), and \( T \) were technically unobservable in each respective experimental procedure, the analyzed data set includes unobserved data. Our analysis based on Bayesian inference successfully estimated the parameters of the EoS and the unobserved data for the small data set used, thus enabling calculation of \( P-V_p \) profiles for liquid iron along the adiabatic \( P-T \) path together with associated credible intervals for Earth's outer-core conditions. The profiles show that \( \rho \) and \( V_p \) of liquid iron deviate from those of the PREM by about 8–10% and −3% to −5%, respectively, when the temperature at the CMB is assumed to be 3,500–4,200 K. Deviations of the 95% credible interval of \( P-V_p \) profiles for the CMB and ICB are −4.8% to −1.5% and −6.0% to −2.3%, respectively, and those of \( P-V_p \) profiles for the CMB and ICB are 6.9–9.7% and 6.5–9.8%, respectively. We conclude that Bayesian inference provides a powerful framework for analyzing small data sets that include unobserved data from high-P and high-T experiments, and that the resultant analysis can constrain the thermodynamic properties of the deeper part of Earth's interior.

Conflict of Interest

The authors declare no conflicts of interest relevant to this study.

Data Availability Statement

Input data for this paper are available in Zenodo (https://doi.org/10.5281/zenodo.4034164).

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