



AccreDiff v1.0: a modular framework for coupling planetary accretion and core–mantle differentiation

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Abstract. Planetary accretion and core–mantle differentiation are commonly modelled as separate processes, although the chemical evolution of a growing terrestrial planet depends directly on its impact history. We present AccreDiff v1.0, a modular Python framework designed to couple N-body accretion histories with multi-stage metal–silicate differentiation calculations. AccreDiff uses time-ordered collision records and particle histories as input, reconstructs parent–product relationships and source-reservoir contributions, assigns impact-dependent equilibration conditions, and updates mantle and core compositions through event-by-event core–mantle differentiation.

The model workflow consists of four main components. First, initial compositions are assigned using either CI-based refractory-enriched compositions with prescribed oxygen fugacity or reservoir-based meteoritic endmembers. Second, accretion histories are reconstructed from collision records to track planetary growth, parent bodies, and source fractions. Third, impact events are classified into small-impact and large-impact regimes, with corresponding pressure–temperature conditions and magma-ocean effects. Fourth, equilibrating and non-equilibrating material budgets are passed to the differentiation solver, which computes metal–silicate partitioning and records diagnostic quantities such as bulk composition, mantle redox state, and core mass fraction.

The paper documents the governing assumptions, data structures, and reproducible example workflows distributed with the code. The bundled notebooks demonstrate how AccreDiff reads cosmochemical and dynamical inputs, generates intermediate reconstruction products, performs differentiation calculations, and exports outputs for downstream scientific analysis. AccreDiff is intended as a post-processing and coupled geochemical evolution framework rather than as an N-body integrator or hydrodynamic impact model. Its modular structure also supports extensions to alternative gas–disk prescriptions, collision-outcome models, meteoritic reservoir libraries, and sulfur-bearing differentiation chemistry. By providing an explicit and reproducible interface between accretion dynamics and geochemical evolution, AccreDiff offers a flexible platform for investigating how planetary growth histories shape the compositions and internal structures of terrestrial planets.



1 Introduction

Planetary formation involves a complex interplay between dynamical accretion processes and geochemical differentiation.

25 During the early stages of terrestrial planet formation, planetary bodies grow through a sequence of collisions among planetesimals and embryos, while simultaneously undergoing core–mantle differentiation driven by metal–silicate segregation (Righter, 2003; Wood et al., 2006, 2008; Rubie et al., 2011; Fischer et al., 2017; Halliday and Canup, 2023). Understanding how these processes jointly control the final composition of planets remains a fundamental challenge in planetary science.

In recent years, N-body simulations have been widely used to investigate the dynamical evolution of planetary systems and to reproduce the accretion histories and collision sequences of terrestrial planets (Raymond et al., 2004; Hansen, 2009; 30 Nesvorný et al., 2021; Woo et al., 2022; Batygin and Morbidelli, 2023; Kong et al., 2024; Clement et al., 2024). These models track the growth of planetary bodies through gravitational interactions and impacts, but typically do not include chemical differentiation or compositional evolution (Gabriel et al., 2020). In parallel, geochemical models describe core formation and element partitioning under high-pressure and high-temperature conditions, providing constraints on metal–silicate segregation and planetary compositions (Righter, 2003; Wood et al., 2008; Rubie and Jacobson, 2016). However, such models generally 35 rely on simplified or parameterized accretion histories rather than dynamically self-consistent collision sequences.

As a result, dynamical and geochemical approaches are often treated separate modelling components, making it difficult to propagate the consequences of individual collisions into the chemical evolution of growing planets (Mordasini and Burn, 2024). In particular, quantities that are central to core formation, such as equilibration pressure and temperature, redox state, 40 metal–silicate partitioning, mantle composition, and core mass fraction (CMF), depend on the sequence, timing, and mass ratio of impacts (Rubie et al., 2011; Righter et al., 2020; Suer et al., 2021). Without an explicit event-by-event coupling between accretion histories and differentiation calculations, the final chemical state of a planet cannot be directly traced back to its dynamical growth pathway.

Recent studies have made important progress toward coupling accretion histories with core–mantle differentiation processes. 45 Multi-stage differentiation models based on metal–silicate equilibration have been successfully applied to interpret planetary compositions using prescribed accretion scenarios (Rubie et al., 2015; Fischer et al., 2017; Gu et al., 2023; Dale et al., 2025). These studies provide the theoretical basis for linking impact-driven equilibration with planetary chemical evolution. However, many implementations are tailored to specific scientific applications and are not distributed as reusable, documented software packages with standardized input-output interfaces, benchmark cases, and verification tests. This limits reproducibility and 50 makes it difficult to compare different accretion scenarios, compositional reservoirs, or differentiation prescriptions within a common framework.

To address this need, we present **AccreDiff v1.0**, a modular and open-source Python framework for coupling N-body accretion histories with impact-driven core–mantle differentiation. AccreDiff takes collision records and particle histories from dynamical simulations as input, reconstructs the growth and source-material evolution of planetary bodies, classifies impact



55 regimes, assigns pressure–temperature conditions, and updates mantle and core compositions through multi-stage metal–silicate equilibration. The framework is designed around transparent model components, documented parameters, and reproducible workflows, so that users can modify accretion inputs, compositional end-members, partitioning laws, or impact–equilibration assumptions independently.

A central feature of AccreDiff is its event-by-event coupling between collision histories and differentiation calculations. In the framework, each impact can be translated into a chemically meaningful differentiation step, so that the cumulative effects of impact timing, impactor mass, source composition, and equilibration conditions are propagated through the evolving mantle and core reservoirs. This design allows the chemical state of a planet to be traced directly along its dynamical growth history, rather than being evaluated only from an idealized or prescribed accretion sequence. The purpose of this paper is therefore to describe AccreDiff as a reusable model framework. We document its governing equations, software architecture, input-output structure, and benchmark workflows, and we present verification tests for the main numerical components. We further demonstrate the framework using representative terrestrial-planet formation cases, including the Earth-Mars accretion-differentiation problem, thereby providing a reproducible basis for future extensions to additional elements, volatile and sulfur chemistry, alternative impact prescriptions, and different planetary formation scenarios.

The remainder of this paper is organized as follows. Section 2 describes the AccreDiff model formulation and workflow, including the initialization of cosmochemical reservoirs, the reconstruction of accretion histories from collision records, the assignment of impact-dependent equilibration conditions, and the multi-stage core–mantle differentiation calculation. Section 3 presents a reproducible example application based on the bundled notebooks and data products, with emphasis on how the documented workflow can be executed, inspected, and connected to downstream scientific analysis. Section 4 discusses the intended scope of the model, its main assumptions and current limitations, and the extensibility of the code through additional dynamical or impact-physics modules. Section 5 summarizes the main capabilities of AccreDiff and outlines directions for future development.

2 Model description and workflow

2.1 Overview of the AccreDiff workflow

AccreDiff is designed to bridge dynamical accretion simulations and geochemical differentiation models by converting time-ordered collision histories into the compositional and structural evolution of growing terrestrial planets. Rather than treating planetary growth and core formation as separate processes, the framework follows the same planetary bodies through accretion, impact-driven melting, metal–silicate equilibration, and multi-stage core–mantle differentiation. A schematic overview of the AccreDiff workflow, from dynamical inputs to planetary-scale chemical diagnostics, is shown in Fig. 1. In this way, the final bulk composition, mantle redox state, and core mass fraction of a planet are interpreted as outcomes of its full accretion pathway.

The dynamical input to AccreDiff is a collision history derived from N-body simulation. Each collision record contains the time of impact, the identities and masses of the target and impactor, and the identity of the post-collision product. AccreDiff

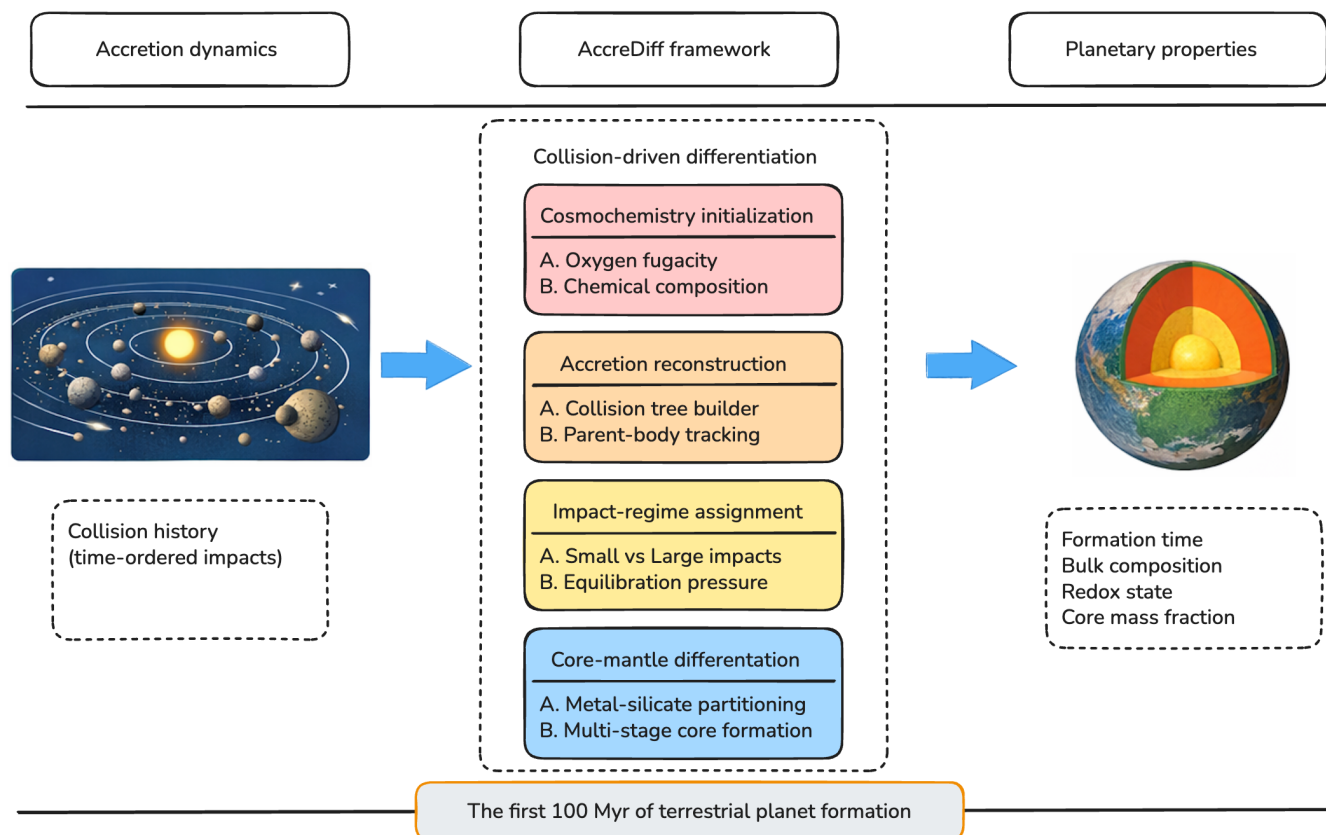


Figure 1. Schematic overview of the AccreDiff workflow. Time-ordered collision histories from N-body accretion simulations provide the dynamical input. AccreDiff first assigns cosmochemical reservoirs and initial redox states to planetary building blocks, then reconstructs collision trees and parent-body contributions, classifies impact regimes and equilibration conditions, and finally solves multi-stage metal–silicate partitioning during core–mantle differentiation. The resulting outputs include formation timescales, source fractions, bulk and mantle/core compositions, redox diagnostics, and core mass fractions over the first 100 Myr of terrestrial planet formation.

does not recompute the N-body dynamics; instead, it uses the dynamical output as the chronological backbone for chemical evolution. At the beginning of the workflow, each planetesimal or embryo is assigned an initial cosmochemical reservoir and redox state according to its source region or a user-defined compositional prescription. In the Earth–Mars benchmark case, these reservoirs correspond to reduced inner-disk and more oxidized outer-disk materials, but the same structure can be generalized to other reservoir definitions.

AccreDiff then reconstructs the accretion history of each final planet from the collision records. A collision-tree builder identifies the parent bodies that contributed to a given planetary product, while parent-body tracking quantifies the mass contribution of different source reservoirs through time. This step converts a purely dynamical history into a chemically labelled accretion sequence. For each impact, the framework also assigns an impact regime according to the timing, mass ratio, and



Table 1. CI-based refractory-enriched bulk elemental inventory used for the prescribed-redox initialization mode. Values follow the Bulk Earth Reference enriched in refractory elements Rubie et al. (2011). Oxygen is not listed because its abundance is determined by matching the prescribed ΔIW value through the oxygen-loss parameter O_L .

Element	Si	Mg	Fe	Al	Ca	Ni
Abundance	10.68	9.61	18.43	1.04	1.14	1.077
Unit	wt%	wt%	wt%	wt%	wt%	wt%
Element	Co	Nb	Ta	V	W	Cr
Abundance	0.0505	300	17.3	60.3	110	2646
Unit	wt%	ppb	ppb	ppm	ppb	ppm

thermal state of the growing body. The impact regime determines the pressure–temperature conditions of metal–silicate equilibration and the fractions of impactor and target material that participate in chemical exchange.

The final stage of the workflow computes collision-driven core–mantle differentiation. For each equilibration event, AccreDiff solves the metal–silicate partitioning of major redox-sensitive elements, including Fe, Ni, Si, and O, while treating Mg, Al, and Ca as lithophile components retained in the silicate mantle. The mantle and core compositions are updated after each event, allowing the model to follow multi-stage core formation along the complete accretion history. The resulting diagnostic quantities include formation timescales, source fractions, bulk composition, mantle and core compositions, redox indicators such as FeO and Mg#, and the core mass fraction.

The following subsections describe the individual components of the workflow in the same order as the central modules in Fig. 1. Section 2.2 presents the cosmochemical initialization of planetary building blocks. Section 2.3 describes the accretion reconstruction procedure used to build collision trees and track parent-body contributions. Section 2.4 defines the impact-regime assignment and the corresponding equilibration conditions. Section 2.5 then presents the core–mantle differentiation model, including metal–silicate partitioning and the multi-stage update of mantle and core compositions.

2.2 Cosmochemistry initialization

2.2.1 CI-based refractory-enriched compositions with prescribed oxygen fugacity

The first cosmochemical initialization mode implemented in AccreDiff follows the CI-based, refractory-enriched approach used in previous accretion-differentiation studies (Rubie et al., 2011; Rubie et al., 2015; Fischer et al., 2017). In this mode, all planetary building blocks are assigned a common bulk elemental inventory derived from CI-like material, but their redox state is prescribed through a target oxygen fugacity relative to the iron–wüstite (IW) buffer. This approach provides a controlled way to generate redox endmembers from the same bulk composition and is therefore useful for testing the sensitivity of metal–silicate differentiation to oxygen fugacity.

The starting bulk composition is based on the Bulk Earth Reference enriched in refractory elements (Rubie et al., 2011). Selected refractory elements, including Al, Ca, Nb, Ta, and W, are enriched relative to CI chondrites, while V is assigned



120 a smaller enrichment. In AccreDiff, this bulk inventory is stored as elemental abundances and converted from mass units to molar amounts before differentiation. The current major-element implementation includes Mg, Al, Ca, Fe, Ni, Si, and O. Mg, Al, and Ca are treated as lithophile components retained in the silicate phase, whereas Fe, Ni, Si, and O are permitted to partition between metallic and silicate reservoirs. The detailed Fe–Ni–Si–O mass-balance equations used during core–mantle differentiation are described in Sect. 2.5.3. In the present section, we focus on how the initial bulk inventory and target redox state are specified. Additional refractory and moderately siderophile elements can be included in future extensions of the same initialization framework. The adopted elemental inventory is summarized in Table 1.

In this initialization mode, the oxygen abundance is not treated as an independently fixed elemental entry. Instead, the redox state is prescribed by a target ΔIW value. AccreDiff searches for the oxygen-loss parameter, O_L , that reproduces the prescribed oxygen fugacity after metal–silicate equilibration. This search is performed together with the mass-balance and partitioning equations, so that the final distribution of Fe, Ni, Si, and O between metal and silicate is consistent with both the bulk elemental inventory and the target redox condition. In the example workflow, endmember compositions are generated for prescribed IW buffers such as $\Delta IW-1.5$ and $\Delta IW-3.5$.

For each target redox state, metal–silicate partition coefficients are evaluated at a reference pressure–temperature condition. In the benchmark notebook, these coefficients are calculated at $P = 0.1 \text{ GPa}$ and $T = 2000 \text{ K}$ using the parameterization of Fischer et al. (2017). AccreDiff then solves the coupled partitioning problem with *OLSolver* and *ForwardKDSolver*. The solution gives the molar abundances of silicate components, including FeO, NiO, SiO₂, and metallic components, including Fe, Ni, Si, and O. These components are then assembled into an MgO-normalized composition together with a scalar core mass fraction. As a verification of this initialization procedure, AccreDiff reproduces the IW-buffered endmember compositions reported by Fischer et al. (2017). Fig. 2 shows the comparison for the $\Delta IW-3.5$ case. The calculated MgO-normalized molar abundances closely match the reference composition for both silicate and metallic components, with small component-wise residuals and a mean absolute percentage error of approximately 2.14%. This agreement verifies that the oxygen-loss search and forward metal–silicate partitioning solver recover the expected redox-calibrated endmember composition.

2.2.2 Reservoir-based meteoritic endmember initialization

The second cosmochemical initialization mode implemented in AccreDiff assigns distinct meteoritic or model-derived endmember compositions to planetary building blocks according to their source regions. Unlike the CI-based prescribed-redox approach described in Sect. 2.2.1, this method allows both the bulk composition and the redox inventory of planetesimals to vary spatially across the initial disk. This reservoir-based initialization follows the approach adopted in recent accretion-differentiation studies, in which radial variations in source materials are used to link planetary feeding zones with final mantle and core compositions (Dale et al., 2025; Kong et al., 2026).

150 In the benchmark workflow, four endmember reservoirs are used: EF, EC, OC, and CI. These reservoirs represent a transition from refractory-rich and highly reduced inner-disk material to more oxidized outer-disk material. The EF reservoir is a model inner-disk component enriched in refractory lithophile elements and depleted in Si-bearing components, whereas EC, OC, and CI represent increasingly oxidized chondritic materials. The endmember reservoirs used in the benchmark workflow are

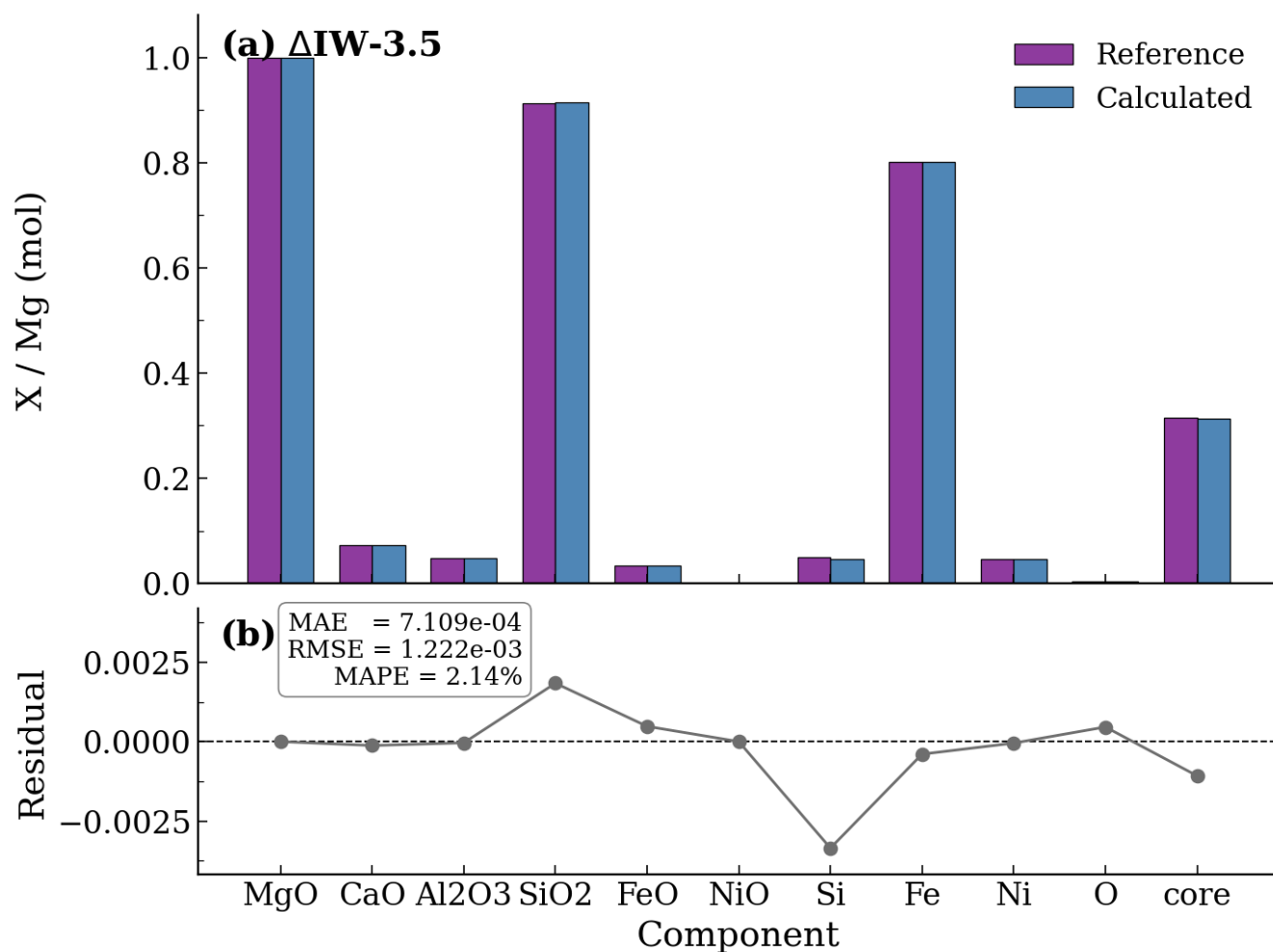


Figure 2. Verification of the CI-based redox initialization against Fischer et al. (2017) for the $\Delta IW - 3.5$ endmember. (a) Comparison between reference and AccreDiff-calculated MgO-normalized molar abundances for silicate components and metallic components. The core entry denotes the CMF and is included as a scalar diagnostic rather than a molar abundance. (b) Component-wise residuals, defined as calculated minus reference values. The error metrics indicate the mean absolute error (MAE), root-mean-square error (RMSE), and mean absolute percentage error (MAPE) across all compared components.



Table 2. Meteoritic and model endmember reservoirs used in the reservoir-based initialization mode. The full oxide and metal component abundances are implemented in AccreDiff as the EF_bulk, EC_bulk, OC_bulk, and CI_bulk dictionaries in `src/accrediff/constant.py`.

Reservoir	Source region	Redox character	Main role
EF	inner disk	highly reduced	refractory-rich, Si-depleted component
EC	inner disk / ring	reduced	enstatite-chondrite-like material
OC	outer ring	moderately oxidized	ordinary-chondrite-like material
CI	outer disk	oxidized / primitive	volatile-rich primitive component

summarized in Table 2. The reservoir definitions and spatial boundaries are user-configurable, so alternative meteoritic or
 155 model-derived compositions can be substituted without modifying the subsequent accretion reconstruction and differentiation modules.

Each reservoir is represented by a set of silicate and metallic components. The silicate inventory includes major oxides such as MgO, Al₂O₃, CaO, FeO, NiO, and SiO₂, while the metallic inventory includes Fe, Ni, Si, and O. The input compositions are specified in weight percent and are converted to molar amounts before being used in the model,

$$160 \quad n_i = \frac{w_i}{M_i}, \quad (1)$$

where w_i is the mass abundance of component i , M_i is its molar mass, and n_i is the corresponding molar amount. Missing components are set to zero. The resulting molar inventories are then normalized to MgO as

$$R_i^{\text{MgO}} = \frac{n_i}{n_{\text{MgO}}}, \quad (2)$$

where R_i^{MgO} is the MgO-normalized molar abundance of component i .

165 For the EF endmember, AccreDiff applies additional corrections to represent a refractory-enriched and Si-depleted inner-disk component. In the benchmark notebook, Al₂O₃ and CaO are enhanced relative to CI by a factor of 1.5, whereas SiO₂ and metallic Si are depleted by a factor of 0.6. This correction reflects the intended role of EF as a highly reduced, high-temperature inner-disk reservoir that can supply refractory-rich material to growing terrestrial planets. These factors are part of the benchmark configuration and can be modified in alternative applications.

170 For diagnostic purposes, the endmember compositions can also be normalized to CI chondrites after MgO normalization. Using the MgO-normalized abundance defined in Eq. (2), the CI-normalized abundance of component i is given by

$$C_i^{\text{CI}} = \frac{R_{i,\text{system}}^{\text{MgO}}}{R_{i,\text{CI}}^{\text{MgO}}}, \quad (3)$$

where $R_{i,\text{system}}^{\text{MgO}}$ and $R_{i,\text{CI}}^{\text{MgO}}$ are the MgO-normalized molar abundances of component i in the target system and in CI chondrites, respectively. This double normalization is used to compare the relative enrichment or depletion patterns of EF, EC, OC,
 175 and CI with planetary reference compositions such as Earth and Mars. In this diagnostic representation, mantle components



are compared using their oxide forms, while metallic Fe, Ni, and Si are mapped to the corresponding CI-normalized oxide components FeO, NiO, and SiO₂. This step is not required for the differentiation calculation itself, but it provides a useful visualization of the compositional contrasts among the reservoirs.

The output of the reservoir-based initialization is a set of MgO-normalized endmember compositions assigned to the initial planetesimal population. Each particle therefore carries both dynamical attributes, such as mass and orbital location, and a chemical reservoir label. During the accretion reconstruction step described in Sect. 2.3, these labelled reservoirs are propagated through the collision tree and mixed according to mass conservation. This initialization mode therefore turns a spatially structured planetesimal disk into a chemically structured disk, allowing final planetary compositions to emerge from the accretional mixing of distinct meteoritic reservoirs rather than from a single prescribed redox state.

185 2.3 Accretion reconstruction and source tracking

The accretion reconstruction module provides the interface between the dynamical simulation output and the chemical differentiation model. In the present AccreDiff implementation, this interface is defined using the output structure of the GENGA N-body code (Grimm and Stadel, 2014; Grimm et al., 2022), which provides orbital-element snapshots and time-ordered collision logs. The snapshots are used to follow particle IDs, masses, and orbital elements through time, whereas the collision logs provide the target and impactor identities, their masses, and the timing of each merger event. Although GENGA is used as the reference format, AccreDiff is not intrinsically tied to a specific N-body integrator. Outputs from other N-body codes can be processed by the same workflow once they are mapped onto the required fields: particle ID, collision time, target ID, impactor ID, target mass, impactor mass, and product ID or sufficient information to determine the surviving product. The subsections below describe how these inputs are converted into gas-phase embryo compositions, post-gas collision trees, source-region fractions, and time-resolved mass and composition histories.

2.3.1 Early-stage reconstruction during the gas disk phase

The first reconstruction step treats the early accretion stage during the lifetime of the gas disk. In the benchmark workflow, this stage is defined as $t \leq t_{\text{gas}}$, with $t_{\text{gas}} = 5$ Myr. During this period, short-lived radionuclides heating is expected to promote extensive silicate melting in growing planetesimals and embryos (Grimm and McSween, 1993; Tang and Dauphas, 2014; McDonough et al., 2020). Following the assumptions used in the coupled accretion-differentiation model of Kong et al. (2026), AccreDiff treats the mantle as efficiently mixed during this early stage (Elkins-Tanton, 2008). As a result, the detailed sequence of individual early equilibration events is not retained. Instead, the early-stage chemical state of each surviving body is reconstructed at t_{gas} from the bulk mixture of its contributing parent bodies.

The reconstruction starts from the initial particle population at $t = 0$, for which each planetesimal has already been assigned a cosmochemical reservoir label as described in Sect. 2.2. AccreDiff then loads all collision records that occur before or at t_{gas} and separates the particles present at t_{gas} into two groups. Particles that did not participate in any recorded collision during the gas-disk phase are treated as original particles and retain their initial reservoir identity. Particles that experienced one or more



mergers are treated as collision products, and their source compositions are reconstructed by tracing their merger histories backward to the initial planetesimal population.

210 For each surviving particle p at t_{gas} , AccreDiff reconstructs the set of initial parent bodies that contributed to it, denoted by $\mathcal{A}_p$. Each parent body j has an initial mass M_j and an initial reservoir label. We define

$$I_{j,k} = \begin{cases} 1, & \text{if } \text{reservoir}(j) = k, \\ 0, & \text{otherwise,} \end{cases} \quad (4)$$

where k denotes a cosmochemical reservoir. The mass fraction of reservoir k in particle p is then

$$f_{k,p}(t_{\text{gas}}) = \frac{\sum_{j \in \mathcal{A}_p} M_j I_{j,k}}{\sum_{j \in \mathcal{A}_p} M_j}. \quad (5)$$

215 The numerator is the total initial mass contributed by reservoir k , and the denominator is the total initial mass of all reconstructed ancestors of particle p . If all ancestors are assigned to one of the defined reservoirs, the fractions satisfy $\sum_k f_{k,p} = 1$. For particles that did not collide before t_{gas} , $\mathcal{A}_p = \{p\}$ and the fraction is unity for the particle's initial reservoir.

The reservoir fractions are then converted into bulk elemental compositions using the endmember compositions defined in Sect. 2.2. For each component i , the mixed bulk abundance of particle p is calculated by linear mixing:

$$220 \quad C_{i,p}(t_{\text{gas}}) = \sum_k f_{k,p}(t_{\text{gas}}) C_{i,k}, \quad (6)$$

where $C_{i,k}$ is the abundance of component i in reservoir k . This step transforms the dynamically reconstructed early merger history into a chemically labelled population at the end of the gas-disk phase. Fig. 3 shows an example of the reconstructed compositions of surviving embryos at t_{gas} in the benchmark simulation. The plotted MgO-normalized abundances illustrate how different early merger histories and source-region mixtures produce chemically distinct embryo inventories before the
225 onset of the post-gas accretion stage.

The resulting particle inventory at t_{gas} provides the initial condition for subsequent differentiation calculations. In the benchmark workflow, bodies with masses above an embryo threshold, for example $M_p \geq 0.05 M_{\oplus}$, are identified as early embryos. Their equilibration pressure is assigned by the early-stage prescription introduced in this subsection, while the corresponding equilibration temperature is calculated using the pressure-temperature relation described in Sect. 2.4.4. In particular, because
230 early impacts are assumed to occur under a globally molten mantle regime, AccreDiff evaluates a representative early metal-silicate equilibration step based on the reconstructed bulk composition at t_{gas} , rather than resolving each early collision as an independent preserved chemical event.

2.3.2 Post-gas collision-tree reconstruction

After the gas-disk phase, AccreDiff switches from the early-stage reconstruction mode to an event-resolved accretion mode.

235 The particle inventory reconstructed at t_{gas} provides the initial population for this stage, whereas individual collisions occurring after gas dispersal are retained as discrete events. This distinction reflects the different assumptions adopted for the two

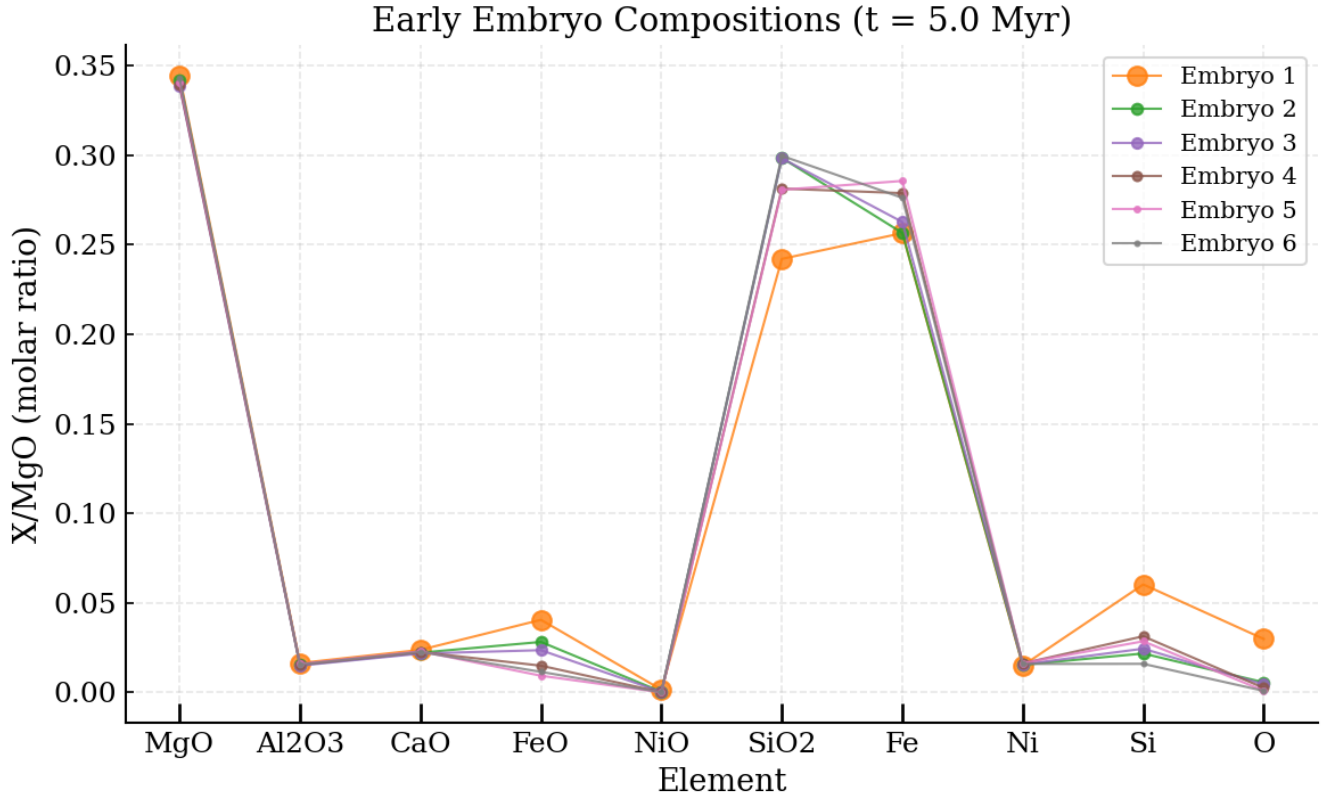


Figure 3. Example of reconstructed early embryo compositions at the end of the gas–disk phase ($t_{\text{gas}} = 5$ Myr). Each curve represents one surviving embryo identified in the benchmark accretion simulation. Component abundances are shown as molar ratios normalized to MgO after reconstructing the mass-weighted source fractions of the embryo’s parent bodies and applying the early-stage chemical update.

phases: early collisions are compressed into the reconstructed embryo inventory at the end of the gas–disk phase, while post-gas collisions are preserved as a time-ordered sequence that controls subsequent impact-regime assignment and multi-stage differentiation.

240 Final planetary products are first identified from the last available snapshot of the N-body simulation. In the benchmark workflow, particles with masses above a prescribed threshold, for example $M_p \geq 0.05M_{\oplus}$, are retained as final planets. The particle IDs of these bodies define the roots of the collision trees to be reconstructed. AccreDiff then filters the collision log to retain only post-gas events,

$$t_{\text{coll}} > t_{\text{gas}}, \quad (7)$$

245 where t_{gas} is taken from the 5 Myr simulation snapshot in the benchmark setup. The filtered collision table contains the collision time, the two colliding particle IDs, and their corresponding masses.



For each retained collision, AccreDiff assigns the surviving product ID using the mass-based survivor rule implemented in the collision tracer. The more massive collision partner is treated as the surviving particle; if the two masses are equal, the smaller particle ID is retained. For the n th collision event, this rule can be written as

$$e_n = (t_n, p_n^i, p_n^j, M_n^i, M_n^j, p_n^{\text{prod}}), \quad (8)$$

where t_n is the collision time, p_n^i and p_n^j are the two colliding bodies, M_n^i and M_n^j are their masses, and p_n^{prod} is the product identifier. This step produces the reduced collision table used by AccreDiff, with the fields `time`, `indexi`, `m_ei`, `indexj`, `m_ej`, and `product_id`. The target and impactor roles used in the later impact-regime calculation are assigned after the product ID has been determined.

For each final planet P , AccreDiff reconstructs the post-gas merger history by recursively tracing the product-ID chain. Starting from the final planet ID, the algorithm searches for all collision events whose product ID is equal to the current particle ID. The two parent IDs in each recovered event are then traced in the same way, until no earlier parent-producing collisions are found. The resulting planet-specific collision history is stored as a time-ordered event set,

$$\mathcal{H}_P = \{e_1, e_2, \dots, e_N\}, \quad t_1 < t_2 < \dots < t_N, \quad (9)$$

where N is the number of post-gas collision events recovered for planet P . This event set preserves the hierarchical structure of accretion: a collision product may participate in later collisions, and the final planet may therefore contain a nested merger tree rather than a simple sequence of independent additions. Fig. 4 illustrates the reconstructed post-gas collision histories for the benchmark simulation. Each coloured sequence corresponds to one final planet, and each marker represents a collision event recovered from the planet-specific history $\mathcal{H}_P$. The marker size scales with the total collision mass, highlighting the transition from frequent lower-mass accretion events to fewer larger impacts during late-stage growth.

The output of this step is a set of collision histories, one for each final planet. Each history records the timing, particle IDs, masses, and surviving product ID for all post-gas mergers in the reconstructed ancestry of the planet. These histories form the central dynamical data structure passed to the following workflow components. Sect. 2.3.3 uses the same collision trees to reconstruct source-region contributions to each final planet, whereas Sect. 2.4 uses the event sequence to assign target–impactor roles, impact regimes, and equilibration conditions for individual post-gas collisions.

2.3.3 Source-region tracking for final planets

The collision histories reconstructed in Sect. 2.3.2 provide the dynamical ancestry of each final planet. AccreDiff uses these histories to determine where the material incorporated into each planet originated in the initial disk. This source-tracking step converts the planet-specific collision history $\mathcal{H}_P$ into a set of reservoir fractions,

$$\mathbf{X}_P = (X_{\text{EF},P}, X_{\text{EC},P}, X_{\text{OC},P}, X_{\text{CI},P}), \quad (10)$$

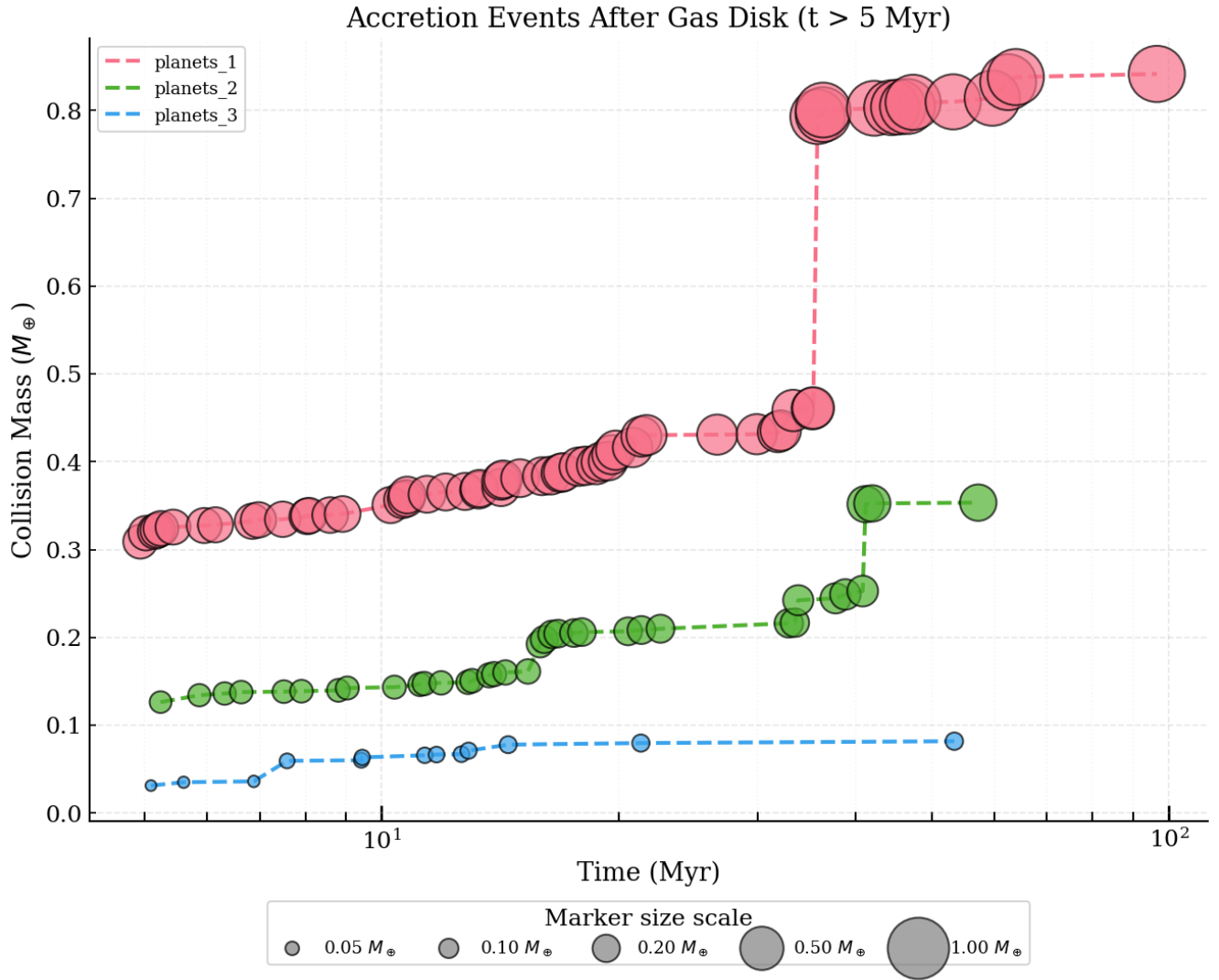


Figure 4. Example of reconstructed post-gas collision histories for final planets in the benchmark simulation. Each colour represents one final planet identified at the final simulation snapshot. Markers denote collision events recovered by the collision-tree reconstruction procedure, with marker size scaled by the total collision mass $M_n^i + M_n^j$. The horizontal axis is shown on a logarithmic time scale to emphasize the concentration of events shortly after gas dispersal.



where EF, EC, OC, and CI denote the four meteoritic source reservoirs defined in Sect. 2.2.2. These fractions provide the dynamical link between the reconstructed accretion history and the reservoir-based cosmochemical initialization.

For a final planet P , AccreDiff first identifies the set of source particles that contributed to its reconstructed collision history. If $\mathcal{H}_P$ is the time-ordered event set defined in Sect. 2.3.2, the corresponding source-particle set is

$$280 \quad \mathcal{S}_P = \{p_n^i, p_n^j \mid e_n \in \mathcal{H}_P\}, \quad (11)$$

where p_n^i and p_n^j are the two colliding particle IDs in event e_n . The IDs in $\mathcal{S}_P$ are then mapped back to the initial N-body snapshot to retrieve their initial orbital elements and masses. In the present implementation, the initial semi-major axis a_s^0 and initial mass M_s^0 of each source particle s are used to reconstruct the orbital source distribution of the final planet.

Each source particle is assigned a normalized mass contribution,

$$285 \quad w_{s,P} = \frac{M_s^0}{\sum_{q \in \mathcal{S}_P} M_q^0}, \quad (12)$$

so that

$$\sum_{s \in \mathcal{S}_P} w_{s,P} = 1. \quad (13)$$

These normalized weights correspond to the mass-fraction column used internally by AccreDiff for source tracking. They ensure that the source distribution of each final planet is evaluated relative to the reconstructed mass of its own contributing particle set, rather than relative to the full initial disk population.

AccreDiff then constructs a weighted empirical cumulative distribution function (ECDF) in initial semi-major axis,

$$F_P(a) = \sum_{s \in \mathcal{S}_P} w_{s,P} \mathbf{1}(a_s^0 \leq a), \quad (14)$$

where $\mathbf{1}$ is the indicator function. The function $F_P(a)$ gives the cumulative fraction of the final planet's reconstructed source material that originated interior to semi-major axis a . This representation is useful because it preserves the continuous orbital information of the contributing material while allowing source fractions to be evaluated at any prescribed radial boundary.

The meteoritic reservoir fractions are obtained by evaluating $F_P(a)$ at the adopted source-region boundaries,

$$a_1 = 1.0 \text{ AU}, \quad a_2 = 1.3 \text{ AU}, \quad a_3 = 3.0 \text{ AU}. \quad (15)$$

The corresponding cumulative fractions are

$$B_1 = F_P(a_1), \quad B_2 = F_P(a_2), \quad B_3 = F_P(a_3). \quad (16)$$

300 Fig. 5 illustrates this weighted-ECDF procedure for representative Earth-like and Mars-like planets in the benchmark simulation. The vertical dashed lines mark the adopted reservoir boundaries, and the cumulative mass fractions evaluated at these

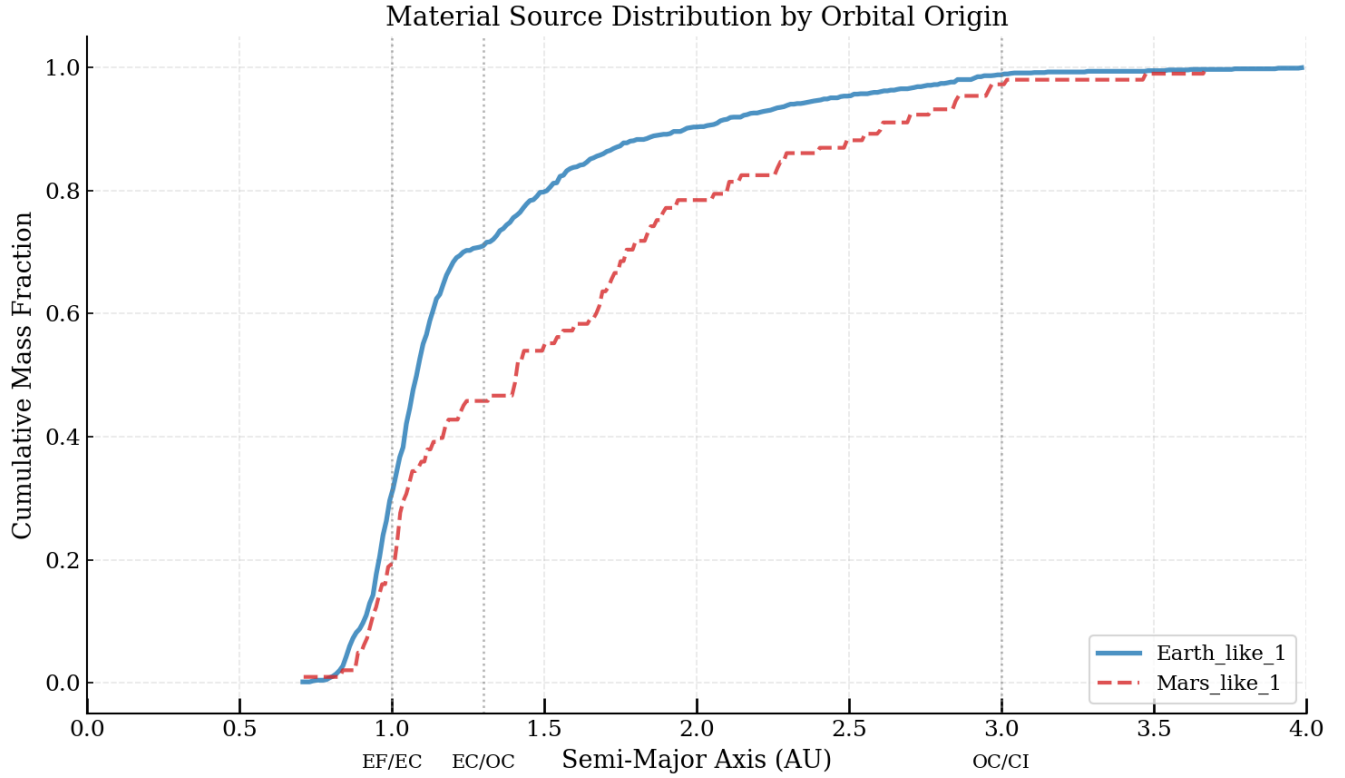


Figure 5. Example of source-region tracking using weighted cumulative mass distributions in initial semi-major axis. The curves show the weighted empirical cumulative distribution functions $F_P(a)$ for representative Earth-like and Mars-like final planets in the benchmark simulation. Vertical dashed lines mark the adopted reservoir boundaries at 1.0, 1.3, and 3.0 AU, corresponding to the EF/EC, EC/OC, and OC/CI transitions. The cumulative values at these boundaries define B_1 , B_2 , and B_3 , which are then converted into EF, EC, OC, and CI source fractions.

boundaries define B_1 , B_2 , and B_3 . These quantities are then converted into absolute reservoir contributions,

$$\begin{aligned}
 X_{\text{EF},P} &= B_1, \\
 X_{\text{EC},P} &= B_2 - B_1, \\
 X_{\text{OC},P} &= B_3 - B_2, \\
 X_{\text{CI},P} &= 1 - B_3.
 \end{aligned} \tag{17}$$

Thus, material initially located at $a \leq 1.0$ AU is assigned to the EF reservoir, material between 1.0 and 1.3 AU to the EC reservoir, material between 1.3 and 3.0 AU to the OC reservoir, and material beyond 3.0 AU to the CI reservoir. The boundary values are configurable and can be modified for simulations that adopt different prescriptions for the radial distribution of cosmochemical reservoirs.



The output of the source-tracking step is a source inventory for each final planet, including its final orbital properties and mass, its cumulative boundary fractions (B_1, B_2, B_3) , and its meteoritic reservoir fractions $(X_{\text{EF}}, X_{\text{EC}}, X_{\text{OC}}, X_{\text{CI}})$. This inventory can be used directly as a diagnostic of accretion provenance, or combined with the endmember compositions described in Sect. 2.2.2 to estimate the bulk cosmochemical mixture associated with each final planet. In the full AccreDiff workflow, these source fractions also provide a compact way to compare the feeding zones of Earth-like and Mars-like planets produced by the same N-body simulation.

2.3.4 Time-resolved growth and composition evolution

The source-tracking procedure described in Sect. 2.3.3 provides the final reservoir fractions of each planet. AccreDiff can also retain the temporal information contained in the reconstructed collision histories and use it to describe how mass and source composition evolve during accretion. This step converts the collision history $\mathcal{H}_P$ into a time-resolved growth path for each final planet. The resulting diagnostics are not used to modify the N-body simulation itself, but provide a reproducible way to compare accretion timing, growth style, and evolving source mixtures among different planetary products.

The procedure starts by assigning a reservoir-composition vector to every initial particle. Using the same radial boundaries as in Sect. 2.3.3, each particle is classified according to its initial semi-major axis. Its initial source vector is then written as

$$\mathbf{x}_p(t_0) = (X_{\text{EF},p}, X_{\text{EC},p}, X_{\text{OC},p}, X_{\text{CI},p})_{t_0}. \quad (18)$$

For an initially unmixed particle, this vector is a one-hot reservoir assignment. For example, a particle assigned to the EF reservoir has $\mathbf{x}_p(t_0) = (1, 0, 0, 0)$, whereas a particle assigned to the OC reservoir has $\mathbf{x}_p(t_0) = (0, 0, 1, 0)$. This representation tracks source ancestry and should be distinguished from the elemental or oxide abundances used in the cosmochemical and differentiation calculations. AccreDiff then processes the reconstructed collision events in chronological order. For a collision between particles p_i and p_j that produces p_{prod} , the product source vector is updated by conservative mass-weighted mixing,

$$\mathbf{x}_{p_{\text{prod}}}(t_n) = \frac{M_n^i \mathbf{x}_{p_i}(t_n^-) + M_n^j \mathbf{x}_{p_j}(t_n^-)}{M_n^i + M_n^j}, \quad (19)$$

where M_n^i and M_n^j are the two colliding masses in event e_n , and t_n^- denotes the state immediately before the collision. The updated vector is assigned to the surviving product ID and is then available for subsequent collisions. In this way, AccreDiff propagates reservoir ancestry through the same collision sequence used for the accretion reconstruction. The update is conservative with respect to source fractions: if both parent vectors sum to unity, the product vector also sums to unity. Fig. 6 illustrates the resulting time-resolved reservoir-fraction evolution for representative Earth-like and Mars-like planets in the benchmark simulation. The stacked areas show how the relative contributions of EF, EC, OC, and CI material change as new collision events are incorporated along the main accretion branch.

For growth diagnostics, AccreDiff extracts the main-branch accretion path of each final planet from the full merger history. In the benchmark workflow, this is done by selecting the subset of events in which the final planet ID is the surviving product. This subset records the direct growth history of the final planetary body, whereas the full collision tree $\mathcal{H}_P$ retains additional

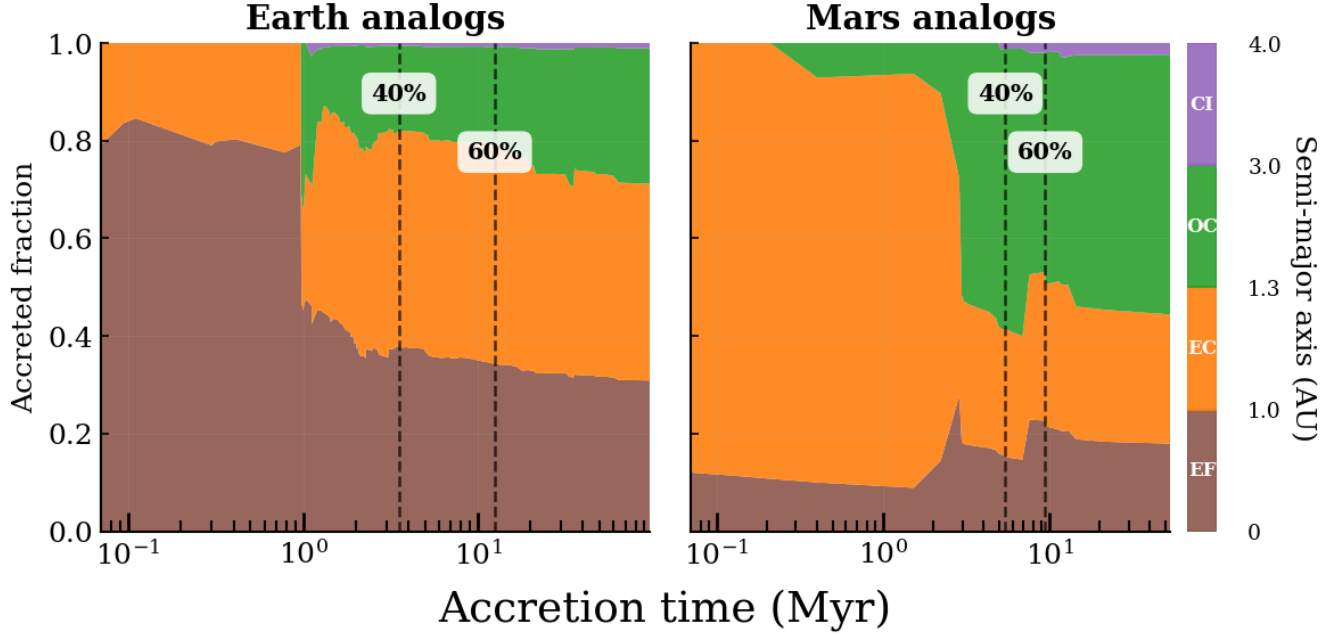


Figure 6. Example of time-resolved source-composition evolution along the main accretion branches of representative Earth-like and Mars-like planets. Stacked areas show the evolving EF, EC, OC, and CI reservoir fractions after sequential mass-weighted composition updates. Vertical dashed lines mark the times at which each planet reaches selected fractions of its final mass. Short ticks along the bottom indicate individual accretion events.

side branches that contributed to its ancestry. At each retained event, the product mass provides a discrete estimate of the planet
 340 mass along the main branch,

$$M_P(t_n) = M_n^i + M_n^j. \quad (20)$$

The corresponding normalized growth curve is

$$\mu_P(t_n) = \frac{M_P(t_n)}{M_{P,\text{final}}}, \quad (21)$$

where $M_{P,\text{final}}$ is the final mass of planet P at the end of the N-body simulation.

345 AccreDiff provides simple diagnostic growth functions to summarize the accretion timescale of different planetary products. For Earth-like planets, the normalized growth curve can be fitted with an exponential form (Yin et al., 2002),

$$g_{\oplus}(t; \tau) = 1 - \exp(-t/\tau), \quad (22)$$

whereas Mars-like growth can be summarized using a rapid-growth form (Chambers, 2006; Dauphas et al., 2011; Tang and Dauphas, 2014),

350 $g_{\text{mars}}(t; \tau) = \tanh^3(t/\tau).$ (23)



Here τ is a fitted timescale parameter. These functions are used as compact diagnostics of growth style and timing, rather than as additional equations of motion or replacements for the N-body accretion histories.

In addition to the fitted timescale, AccreDiff records the times at which a planet reaches prescribed fractions of its final mass. For a chosen mass fraction f , the threshold-crossing time is defined as

$$t_{f,P} = \min \{ t : M_P(t) \geq f M_{P,\text{final}} \}, \quad (24)$$

with $f = 0.4$, and 0.6 used in the benchmark analysis. Because the reconstructed growth path is discrete, these times are estimated by linear interpolation between adjacent collision records.

The output of this step is a growth-evolution table for each selected final planet. The table includes the planet ID, dynamical class, final mass, fitted growth timescale, number of accretion events, 40, and 60 % accretion times, and final EF, EC, OC, and CI reservoir fractions. These quantities provide a compact summary of the temporal accretion history and the evolution of source composition. They also form a bridge between the dynamical reconstruction presented in Sect. 2.3 and the impact-regime and differentiation calculations described in Sects. 2.4 and 2.5.

2.4 Impact-regime assignment and equilibration conditions

2.4.1 Collision-event preprocessing for impact classification

The impact-regime module takes the collision histories reconstructed in Sect. 2.3 as input and converts each collision record into an impact-event record. For a final planet P , the input is the time-ordered collision history $\mathcal{H}_P$, whose individual collision events have been defined in Eq. (8). The purpose of the preprocessing step is to transform this dynamical event description into the set of quantities required to assign an impact regime and the corresponding metal–silicate equilibration conditions.

AccreDiff first defines the target branch and the impactor for each collision. The surviving product ID is used as the target branch for subsequent chemical updating, while the non-product particle is treated as the impactor. For mass bookkeeping, the target and impactor masses are assigned as

$$M_n^{\text{tar}} = \max(M_n^i, M_n^j), \quad M_n^{\text{imp}} = \min(M_n^i, M_n^j). \quad (25)$$

This convention follows the implementation in AccreDiff, where the larger collision partner defines the surviving body and the smaller partner is treated as the accreted impactor. The target–impactor terminology is therefore a bookkeeping convention used for the chemical model, rather than an independent dynamical classification imposed by the N-body simulation output.

The total colliding mass and the impactor-to-total-mass ratio are then computed as

$$M_n^{\text{tot}} = M_n^{\text{tar}} + M_n^{\text{imp}}, \quad (26)$$

and

$$\gamma_n = \frac{M_n^{\text{imp}}}{M_n^{\text{tot}}}. \quad (27)$$



380 The ratio γ_n is the main scalar quantity used to distinguish different late-stage impact regimes. With the above definition, $0 < \gamma_n \leq 0.5$, where smaller values correspond to planetesimal-like impacts and larger values correspond to more comparable-mass collisions.

The preprocessed information is stored in an impact-event table. For each event, this table contains the collision time, target ID, impactor ID, target mass, impactor mass, total colliding mass, impact ratio, assigned event regime, equilibration pressure, 385 and equilibration temperature, i.e. $(t_n, p_n^{\text{tar}}, p_n^{\text{imp}}, M_n^{\text{tar}}, M_n^{\text{imp}}, M_n^{\text{tot}}, \gamma_n, \text{regime}_n, P_{\text{eq},n}, T_{\text{eq},n})$. The event label is initially set to the small-impact regime and is subsequently updated if the event satisfies the criteria for large-impact or post-impact magma-ocean conditions. This design allows the same table to carry both the original dynamical information and the derived thermodynamic conditions required by the differentiation solver.

As an initial assignment, each event is given the default small-impact equilibration pressure,

$$390 \quad P_{\text{eq},n}^{(0)} = \alpha_{\text{small}} P_{\text{CMB}}(M_n^{\text{tar}}), \quad (28)$$

where P_{CMB} is the core-mantle boundary pressure of the target body and $\alpha_{\text{small}} = 0.6$ in the benchmark workflow. The corresponding equilibration temperature is computed from $P_{\text{eq},n}^{(0)}$ using the pressure–temperature relation described in Sect. 2.4.4. Large-impact events and events occurring during a post-impact magma-ocean interval can overwrite these initial pressure–temperature assignments, as described in the following subsections.

395 The output of this preprocessing step is therefore a planet-specific impact-event table. This table provides the common interface between the accretion reconstruction and the chemical differentiation calculation: Sect. 2.4.2 describes how small impacts retain the default localized-equilibration treatment, Sect. 2.4.3 describes how large impacts modify the pressure conditions and affect subsequent events, and Sect. 2.5 uses the resulting event-by-event conditions to update mantle and core compositions.

2.4.2 Late-phase small impacts

400 After the gas disk has dissipated, short-lived radiogenic heat sources are largely exhausted and the mantles of growing proto-planets are assumed to be predominantly solid. In this late stage, low-mass impactors are not expected to generate long-lived global magma oceans. Instead, they produce localized melt regions in the target mantle. AccreDiff therefore treats late-stage small impacts as local metal–silicate equilibration events, rather than as events that reset the chemical state of the entire target body.

405 Small impacts are identified using the impactor-to-total-mass ratio γ_n defined in Sect. 2.4.1. In the benchmark setup, an event is treated as a small impact when

$$\gamma_n < \gamma_{\text{crit}}, \quad (29)$$

with $\gamma_{\text{crit}} = 0.1$. This threshold separates planetesimal-like impacts from more comparable-mass collisions that can generate extensive mantle melting. The threshold is treated as a configurable parameter in AccreDiff, allowing alternative impact-regime 410 definitions to be tested.

For a small impact, only impactor-derived material is assumed to participate in chemical equilibration. Specifically, 70 % of the impactor core and the entire impactor mantle equilibrate within the localized melt region, whereas the pre-existing



target mantle and target core do not re-equilibrate. The remaining 30 % of the impactor core is assumed to merge directly with the target core. In terms of the material fractions passed to the differentiation solver, the small-impact regime is therefore
415 represented by

$$f_{\text{eq}}^{\text{imp,core}} = 0.7, \quad f_{\text{eq}}^{\text{imp,man}} = 1.0, \quad f_{\text{eq}}^{\text{tar,core}} = 0.0, \quad f_{\text{eq}}^{\text{tar,man}} = 0.0. \quad (30)$$

For these events, AccreDiff retains the default pressure assignment introduced in Sect. 2.4.1. The equilibration pressure is therefore a fixed fraction of the target core-mantle boundary pressure, with $\alpha_{\text{small}} = 0.6$ in the benchmark workflow. This pressure represents equilibration during the descent of impactor metal through a localized molten region in the target mantle,
420 at a depth shallower than the full core-mantle boundary. The corresponding equilibration temperature is calculated from this pressure using the common pressure–temperature relation given in Sect. 2.4.4.

For each small-impact event, AccreDiff records the event label, the retained default equilibration pressure, the corresponding equilibration temperature, and the equilibrating material fractions in the impact-event table. These quantities define the boundary conditions used by the core–mantle differentiation solver in Sect. 2.5. Large impacts, which overwrite this localized-
425 equilibration treatment by generating melt pools or post-impact magma oceans, are described separately in Sect. 2.4.3.

2.4.3 Late-phase large impacts and post-impact magma-ocean stage

Large impacts are treated separately from the late-stage small impacts described in Sect. 2.4.2 because they can generate extensive silicate melting and modify the equilibration conditions of subsequent accretion events. In AccreDiff, the primary classification variable is the impactor-to-total-mass ratio γ_n defined in Sect. 2.4.1. A collision is treated as a large impact when
430

$$\gamma_n \geq \gamma_{\text{crit}}, \quad (31)$$

where $\gamma_{\text{crit}} = 0.1$ in the benchmark workflow. In the implementation, this criterion can be combined with a minimum total-mass threshold and an allowed impact-ratio interval,

$$M_n^{\text{tot}} \geq M_{\text{crit}}, \quad \gamma_{\text{min}} \leq \gamma_n < \gamma_{\text{max}}, \quad (32)$$

435 with benchmark values $M_{\text{crit}} = 0.1M_{\oplus}$, $\gamma_{\text{min}} = 0.1$, and $\gamma_{\text{max}} = 0.5$. These parameters are configurable and are used to identify events for which the default small-impact pressure assignment should be overwritten.

For large impacts, AccreDiff evaluates the geometry and depth of impact-induced melting using the scaling laws of Nakajima et al. (2021). These scaling laws were calibrated against smoothed particle hydrodynamics simulations and describe how impact-induced heat and melt geometry depend on total mass, impactor-to-total-mass ratio, impact velocity, impact angle,
440 and the initial thermal state of the mantle. In AccreDiff, this calculation is implemented through the `MeltScalingModel` module. For each large impact, the model is called with the event total mass, impact ratio, normalized impact velocity, pre-impact mantle entropy, and impact angle. In the benchmark workflow, the normalized impact velocity is set to $v_{\text{imp}}/v_{\text{esc}} = 1$,



the mantle entropy is set to $S_0 = 1100 \text{ J K}^{-1} \text{ kg}^{-1}$, and the impact angle is set to 45° . The output includes the pressure at the base of the melt pool, the pressure associated with an equivalent global magma-ocean geometry, the melt depth, and the mantle melt fraction.

The first stage of a large impact is represented as localized melt-pool equilibration. The metallic core of the large impactor is assumed to emulsify and equilibrate with silicate melt near the base of the impact-generated melt pool. The equilibration pressure for this stage is parameterized as

$$P_{\text{MP},n} = \alpha_{\text{MP}} P_{b,n}, \quad (33)$$

where $P_{b,n}$ is the pressure at the base of the melt pool returned by the melt-scaling model, and α_{MP} is a configurable pressure-scaling factor. Following the physical prescription of Nakajima et al. (2021) and the coupled accretion-differentiation model used here, α_{MP} is typically chosen to be of order unity. In this regime, 30 % of the impactor core, the entire impactor mantle, and a fraction f_{MP} of the target mantle participate in metal–silicate equilibration, while the target core does not re-equilibrate. The fraction f_{MP} is linked to the melt fraction or melt-pool geometry estimated by the scaling-law calculation.

After the initial melt-pool stage, the impact-generated melt region is assumed to evolve into a post-impact magma ocean. This magma-ocean stage is treated as a finite thermal window during which subsequent small bodies accreted by the same target encounter a molten mantle rather than the localized solid-mantle setting described in Sect. 2.4.2. In the benchmark workflow, the magma-ocean lifetime is

$$\Delta t_{\text{MO}} = 5 \text{ Myr}. \quad (34)$$

Thus, a later event e_n is treated as magma-ocean affected if it occurs after a large impact at time t_{GI} and satisfies

$$0 \leq t_n - t_{\text{GI}} \leq \Delta t_{\text{MO}}. \quad (35)$$

For these post-impact magma-ocean events, the equilibration pressure is parameterized as

$$P_{\text{MO},n} = \alpha_{\text{MO}} P_n^{\text{global}}, \quad (36)$$

where P_n^{global} is the pressure associated with the global magma-ocean geometry returned by the melt-scaling model, and $\alpha_{\text{MO}} = 0.5$ in the benchmark workflow. In this regime, 70 % of the impactor core, the entire impactor mantle, and a fixed fraction f_{MO} of the target mantle participate in equilibration. Following the benchmark prescription, $f_{\text{MO}} = 0.05$.

The large-impact processing therefore overwrites the default small-impact conditions assigned during event preprocessing. Events directly associated with melt-pool equilibration and events occurring during the post-impact magma-ocean window are assigned updated event labels, equilibration pressures, temperatures, and mantle melt fractions. The temperature associated with each updated pressure is calculated using the common pressure–temperature relation described in Sect. 2.4.4. The resulting impact-regime prescriptions are summarized in Table 3.



Table 3. Large-impact and post-impact magma-ocean prescriptions used in AccreDiff. The pressure-scaling factors α_{MP} and α_{MO} , the magma-ocean lifetime Δt_{MO} , and the mantle fractions f_{MP} and f_{MO} are configurable model parameters.

Regime	Criterion	Pressure	Impactor core	Target mantle
Melt pool	$\gamma_n \geq \gamma_{crit}$	$\alpha_{MP} P_b$	0.3	f_{MP}
Post-impact magma ocean	$0 \leq t_n - t_{GI} \leq \Delta t_{MO}$	$\alpha_{MO} P^{global}$	0.7	f_{MO}

2.4.4 Equilibration temperature

AccreDiff uses a common pressure–temperature relation to assign equilibration temperatures for all metal–silicate equilibration steps in the workflow. This includes the representative early-stage equilibration applied to embryos at the end of the gas–disk phase (Sect. 2.3.1), the default localized equilibration assigned to late-stage small impacts (Sect. 2.4.2), and the updated pressure conditions associated with large impacts and post-impact magma-ocean events (Sect. 2.4.3). In each case, the relevant model component first defines an equilibration pressure P_{eq} , which is then converted into an equilibration temperature T_{eq} using the same pressure-temperature mapping.

Following Wade and Wade and Wood (2005) and Rubie et al. (2015), the equilibration temperature is parameterized as

$$T_{eq} = \begin{cases} 1874 + 55.43P_{eq} - 1.74P_{eq}^2 + 0.0193P_{eq}^3, & P_{eq} < 24 \text{ GPa}, \\ 1249 + 58.28P_{eq} - 0.395P_{eq}^2 + 0.0011P_{eq}^3, & P_{eq} \geq 24 \text{ GPa}. \end{cases} \quad (37)$$

Here T_{eq} is in Kelvin and P_{eq} is in GPa. Differences in equilibration temperature among early-stage embryos, late-stage small impacts, melt–pool events, and post-impact magma–ocean events therefore arise from their assigned pressure conditions, rather than from separate temperature laws.

In the AccreDiff implementation, this calculation is performed by the pressure–temperature conversion function and the result is stored with each equilibration event as T_{eq} . After this step, each event is associated with a complete set of differentiation boundary conditions: the participating masses or material fractions, the impact or equilibration regime, the equilibration pressure, and the equilibration temperature. These quantities are then passed to the core–mantle differentiation solver described in Sect. 2.5, where they are used to evaluate metal–silicate partition coefficients and update mantle and core inventories.

2.5 Core–mantle differentiation

2.5.1 Event-by-event differentiation workflow

The core–mantle differentiation module takes the chemically initialized body inventory and the impact-event table as input. The initial inventory is provided by the early-stage reconstruction described in Sect. 2.3.1, whereas the post-gas collision histories and their associated equilibration conditions are provided by Sects. 2.3 and 2.4. For each event, the impact-event table specifies



the target ID, impactor ID, event type, equilibration pressure $P_{eq,n}$, and equilibration temperature $T_{eq,n}$. These quantities define the boundary conditions for one step of metal–silicate equilibration.

AccreDiff treats core formation as a multi-stage, event-by-event process. Rather than computing the final composition of a planet from a single bulk mixture, the model processes the reconstructed accretion sequence in chronological order. Each collision modifies the mantle and core inventories of the surviving body, and the updated composition is then used as the starting state for subsequent collisions. The final planetary composition is therefore path dependent: two planets with similar final bulk masses and source fractions can acquire different mantle and core compositions if their impact histories and equilibration conditions differ.

For each body p , AccreDiff stores the evolving chemical state as a component vector,

$$\mathbf{C}_p(t) = (\text{MgO}, \text{Al}_2\text{O}_3, \text{CaO}, \text{FeO}, \text{NiO}, \text{SiO}_2, \text{Fe}, \text{Ni}, \text{Si}, \text{O})_p. \quad (38)$$

The first six components describe the silicate inventory in oxide form, whereas the last four components describe the metallic inventory in elemental form. This representation matches the component structure used in the cosmochemical initialization and allows the differentiation solver to transfer Fe, Ni, Si, and O between metal and silicate reservoirs while treating MgO, Al_2O_3 , and CaO as lithophile components.

For each event in the collision history, AccreDiff retrieves the current compositions of the target and impactor from the component library. It then reads the event label and the pressure–temperature pair $(P_{eq,n}, T_{eq,n})$ from the impact-event table. The event label determines which fractions of the impactor core, impactor mantle, and target mantle participate in equilibration. These fractions are used to divide the event inventory into an equilibrating portion and a non-equilibrating portion. The equilibrating portion is passed to the metal–silicate partitioning solver, whereas the non-equilibrating portion is carried forward without re-partitioning during that event.

After the partitioning calculation has been completed, AccreDiff combines the solved equilibrated inventory with the non-equilibrating inventory and normalizes the result by the total post-collision mass. The resulting composition is assigned to the surviving target body and replaces its previous state in the component library. Subsequent events involving the same body therefore use the updated mantle and core inventories. Repeating this procedure through the full collision sequence produces a time-resolved differentiation trajectory for each final planet.

The following subsections describe the internal steps of this event-by-event update. Sect. 2.5.2 defines the equilibrating and non-equilibrating material budgets for different impact regimes. Sect. 2.5.3 describes the pressure- and temperature-dependent partition coefficients and the major-element solver. Sect. 2.5.4 then explains how the solved inventories are merged back into the evolving planetary composition and how the final diagnostic outputs are generated.

2.5.2 Equilibrating and non-equilibrating material budgets

For each differentiation event, AccreDiff separates the collision inventory into material that participates in metal–silicate equilibration and material that is carried forward without re-equilibration during that event. This split is required because the impact regimes described in Sect. 2.4 do not all involve the same fraction of the target and impactor. We write the event inventory



schematically as

$$\mathbf{B}_n = \mathbf{B}_n^{\text{eq}} + \mathbf{B}_n^{\text{neq}}, \quad (39)$$

where $\mathbf{B}_n^{\text{eq}}$ is the equilibrating inventory passed to the partitioning solver, and $\mathbf{B}_n^{\text{neq}}$ is the non-equilibrating inventory that is
530 recombined with the solver output after the event.

In general, the equilibrating inventory contains the entire impactor mantle, a regime-dependent fraction of the impactor core, and, for large-impact regimes, a fraction of the target mantle. This can be written as

$$\mathbf{B}_n^{\text{eq}} = \mathbf{B}_n^{\text{imp,man}} + f_n^{\text{imp,core}} \mathbf{B}_n^{\text{imp,core}} + f_n^{\text{tar,man}} \mathbf{B}_n^{\text{tar,man}}. \quad (40)$$

The complementary inventory,

$$535 \quad \mathbf{B}_n^{\text{neq}} = \mathbf{B}_n - \mathbf{B}_n^{\text{eq}}, \quad (41)$$

is not repartitioned during the event. In the present implementation, the target core does not participate directly in re-equilibration; it is carried forward as part of the non-equilibrating inventory, while any non-emulsified fraction of the impactor core is added directly to the metallic inventory of the surviving body.

For small impacts, the event label is `small`. This regime corresponds to the localized equilibration treatment described in
540 Sect. 2.4.2. The entire impactor mantle and 70 % of the impactor core participate in equilibration, while the pre-existing target mantle and target core remain outside the equilibrating system. Thus,

$$f_n^{\text{imp,core}} = 0.7, \quad f_n^{\text{tar,man}} = 0. \quad (42)$$

The remaining 30 % of the impactor core is added directly to the target core without passing through the partitioning solver.

For melt-pool equilibration associated with large impacts, the event label is `partial`. This label denotes the localized
545 melt-pool stage described in Sect. 2.4.3, not a separate class of N-body collision. In this regime, 30 % of the impactor core, the entire impactor mantle, and a melt-pool-controlled fraction of the target mantle participate in equilibration. The target-mantle fraction is represented by $k_{\text{mantle},n}$, which is derived from the impact-induced melting calculation. The material fractions are therefore

$$f_n^{\text{imp,core}} = 0.3, \quad f_n^{\text{tar,man}} = k_{\text{mantle},n}. \quad (43)$$

550 For post-impact magma-ocean events, the event label is `global`. This label is used for events that occur in the magma-ocean stage following a large impact, or for events whose pressure–temperature conditions have been updated by the post-impact magma-ocean treatment. In this regime, 70 % of the impactor core, the entire impactor mantle, and a smaller fraction of the affected target mantle participate in equilibration. `AccreDiff` parameterizes this target-mantle contribution as

$$f_n^{\text{tar,man}} = k_{\text{mantle},n} f_{\text{MO}}, \quad (44)$$



Table 4. Equilibrating material fractions used by AccreDiff for different event labels. The impactor mantle is fully included in the equilibrating inventory in all regimes. The target core is not re-equilibrated in the current implementation.

Event label	Impactor core	Target mantle	Non-equilibrating material
small	0.7	0.0	target body + 0.3 impactor core
partial	0.3	k_{mantle}	remaining target body + 0.7 impactor core
global	0.7	$k_{\text{mantle}} f_{\text{MO}}$	remaining target body + 0.3 impactor core

555 where $f_{\text{MO}} = 0.05$ in the benchmark workflow. The corresponding impactor-core fraction is

$$f_n^{\text{imp,core}} = 0.7. \quad (45)$$

The event-dependent material budgets are summarized in Table 4.

Only $\mathbf{B}_n^{\text{eq}}$ is passed to the metal–silicate partitioning solver. The non-equilibrating inventory $\mathbf{B}_n^{\text{neq}}$ is stored during the event and recombined with the solved metal and silicate inventories after equilibration. This separation allows AccreDiff to represent
560 incomplete metal emulsification and spatially restricted mantle melting while still updating the full bulk composition of the surviving body after each collision.

2.5.3 Partition coefficients and major-element solver

For each differentiation event, only the equilibrating inventory $\mathbf{B}_n^{\text{eq}}$ defined in Sect. 2.5.2 is passed to the metal–silicate partitioning solver. This inventory is combined with the equilibration pressure and temperature assigned to the event, $(P_{\text{eq},n}, T_{\text{eq},n})$,
565 to determine the distribution of major elements between silicate and metal. From $\mathbf{B}_n^{\text{eq}}$, AccreDiff extracts the total amounts of Fe, Ni, Si, and O involved in the event, together with the lithophile components MgO, $\text{AlO}_{1.5}$, and CaO. These quantities define the mass-balance constraints for the solver.

The pressure- and temperature–dependent partition coefficients are calculated using the parameterized form

$$\log K_D^i = a_i + \frac{b_i}{T_{\text{eq}}} + \frac{c_i P_{\text{eq}}}{T_{\text{eq}}}, \quad (46)$$

570 where i denotes the element, and a_i , b_i , and c_i are experimentally calibrated coefficients (Fischer et al., 2017; Huang et al., 2020, 2021). In the major-element workflow, AccreDiff evaluates K_D^{Ni} , K_D^{Si} , and K_D^{O} for each event. The same partition-coefficient interface can also be extended to additional siderophile elements, but the present multi-stage core-formation calculation focuses on the major Fe–Ni–Si–O system.

The solver represents the silicate and metallic phases using molar variables. In the silicate phase,

$$575 \quad x = n_{\text{FeO}}^{\text{sil}}, \quad y = n_{\text{NiO}}^{\text{sil}}, \quad z = n_{\text{SiO}_2}^{\text{sil}}, \quad (47)$$

whereas in the metallic phase,

$$a = n_{\text{Fe}}^{\text{met}}, \quad b = n_{\text{Ni}}^{\text{met}}, \quad c = n_{\text{Si}}^{\text{met}}, \quad d = n_{\text{O}}^{\text{met}}. \quad (48)$$



The lithophile components are treated as inert with respect to metal–silicate partitioning during the event,

$$u = n_{\text{MgO}}, \quad v = n_{\text{AlO}_{1.5}}, \quad w = n_{\text{CaO}}. \quad (49)$$

580 They remain in the silicate inventory and enter the calculation through the silicate mole-fraction normalization. The major-element mass balance is written as

$$\text{Fe}_t = x + a, \quad \text{Ni}_t = y + b, \quad \text{Si}_t = z + c. \quad (50)$$

The oxygen budget is expressed as

$$O_t = \text{Fe}_t + \text{Ni}_t + 2\text{Si}_t - O_L, \quad (51)$$

585 where O_L represents the oxygen deficit of the equilibrating inventory relative to fully oxidized Fe, Ni, and Si. The amount of oxygen dissolved in the metallic phase is then

$$d = O_t - x - y - 2z. \quad (52)$$

Thus, once the silicate FeO amount x is specified, the remaining variables can be solved sequentially from mass balance and partitioning constraints. The Ni and Si distributions are constrained by their metal–silicate partition coefficients. For Ni,

590 AccreDiff uses

$$K_D^{\text{Ni}} = \frac{X_{\text{Ni}}^{\text{met}} X_{\text{FeO}}^{\text{sil}}}{X_{\text{NiO}}^{\text{sil}} X_{\text{Fe}}^{\text{met}}}, \quad (53)$$

which determines the silicate NiO abundance for a given value of x . For Si, the corresponding relation is

$$K_D^{\text{Si}} = \frac{X_{\text{Si}}^{\text{met}} (X_{\text{FeO}}^{\text{sil}})^2}{X_{\text{SiO}_2}^{\text{sil}} (X_{\text{Fe}}^{\text{met}})^2}. \quad (54)$$

This relation yields a quadratic equation for the silicate SiO_2 abundance z , which is solved internally by selecting the physically
595 admissible root. The metallic Fe, Ni, and Si abundances then follow from the conservation equations above.

The remaining degree of freedom is fixed by matching the oxygen partition coefficient. AccreDiff provides two options for evaluating the oxygen partition coefficient, controlled by the `KD_oxygen` setting in the major-element solver. In both cases, the calculated oxygen exchange coefficient is written as

$$K_{D,\text{calc}}^{\text{O}} = \frac{X_{\text{Fe}}^{\text{met}} X_{\text{O}}^{\text{met}}}{A_{\text{FeO}}^{\text{sil}}}, \quad (55)$$

600 where

$$X_{\text{Fe}}^{\text{met}} = \frac{a}{a + b + c + d}, \quad X_{\text{O}}^{\text{met}} = \frac{d}{a + b + c + d}, \quad (56)$$



and

$$X_{\text{FeO}}^{\text{sil}} = \frac{x}{x + y + z + u + v + w}. \quad (57)$$

The two options differ in the treatment of the FeO term in the silicate liquid. In the `Rubie` option, `AccreDiff` applies the non-ideal FeO activity correction used in the Rubie et al. (2011); Rubie et al. (2015) framework,

$$A_{\text{FeO}}^{\text{sil}} = 1.148 X_{\text{FeO}}^{\text{sil}} + 1.319 (X_{\text{FeO}}^{\text{sil}})^2. \quad (58)$$

In the `Fischer` option, `AccreDiff` follows the idealized form used in the Fischer et al. (2017) major-element calculation and sets $A_{\text{FeO}}^{\text{sil}} = X_{\text{FeO}}^{\text{sil}}$.

Thus, for a trial value of x , the oxygen partition coefficient evaluated by the solver can be written compactly as

$$K_{D,\text{calc}}^{\text{O}}(x) = \frac{ad}{A_{\text{FeO}}^{\text{sil}}(a + b + c + d)^2}. \quad (59)$$

The solution is defined by

$$K_{D,\text{calc}}^{\text{O}}(x) = K_{D,\text{target}}^{\text{O}}, \quad (60)$$

where $K_{D,\text{target}}^{\text{O}}$ is obtained from the same pressure–temperature partitioning relation as the other elements. `AccreDiff` searches for the value of x that satisfies this condition using a grid search to locate a suitable interval followed by bisection. If no sign change is found, the minimum-residual grid point is returned as an approximate solution.

The output of the solver is the equilibrated metal–silicate inventory for the event, (x, y, z, a, b, c, d) , corresponding to silicate FeO, NiO, and SiO₂ and metallic Fe, Ni, Si, and O. These quantities, together with the inert silicate components u, v , and w , define the solved equilibrating inventory. Sect. 2.5.4 describes how this inventory is recombined with the non-equilibrating material and used to update the composition of the surviving body.

2.5.4 Composition update and diagnostic outputs

After the metal–silicate partitioning calculation has been completed for event n , the equilibrating inventory defined in Sect. 2.5.2 is replaced by the solved equilibrated inventory, denoted by $\mathbf{B}_n^{\text{eq,sol}}$. The non-equilibrating inventory $\mathbf{B}_n^{\text{neq}}$ is carried forward unchanged during the event. The updated composition of the surviving product is then obtained by combining these two inventories and normalizing by the post-collision mass,

$$\mathbf{C}_{p_n^{\text{prod}}}(t_n) = \frac{\mathbf{B}_n^{\text{neq}} + \mathbf{B}_n^{\text{eq,sol}}}{M_n^{\text{tar}} + M_n^{\text{imp}}}. \quad (61)$$

This returns the same component vector introduced in Sect. 2.5.1, now updated after the differentiation event. The normalization is applied component by component, so that each entry records the abundance of that component in the surviving body after the collision.

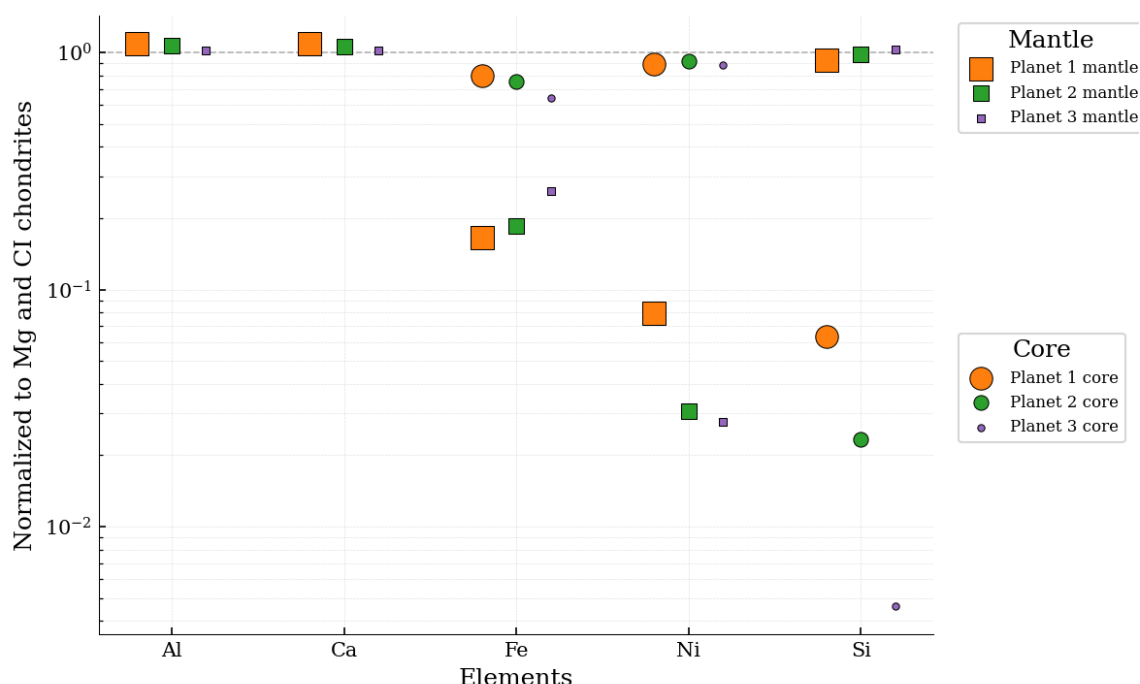


Figure 7. Example of final composition diagnostics produced by the multi-stage differentiation workflow. The plotted values are normalized first to Mg and then to CI chondritic abundances. Square symbols denote silicate mantle components represented by oxides, whereas circular symbols denote metallic core components represented by elemental abundances. Marker size scales with final planet mass.

The updated composition replaces the previous state of the surviving target in the component library. Subsequent collisions
 630 involving the same body therefore use this new mantle and core inventory as their starting condition. This recursive update is the step that makes the multi-stage differentiation calculation path dependent: the outcome of each later event depends not only on the new impactor and pressure–temperature conditions, but also on the chemical state inherited from all earlier events.

For each final planet or collision scenario, AccreDiff stores the resulting event-by-event composition history as a time series. Each row records the model time, the target ID, and the updated component abundances after a differentiation event.
 635 The corresponding impact–event table can be used to link each composition update to the event type, equilibration pressure, equilibration temperature, and mantle fraction used in that step. The last row of the time series represents the final modeled mantle-core inventory of the planet and is used for comparison with planetary and meteoritic reference compositions.

AccreDiff also provides diagnostic visualizations of the modeled compositions. These include MgO-normalized molar abundance diagrams and CI-normalized comparison plots that separate silicate and metallic inventories. An example of the CI-
 640 normalized diagnostic output is shown in Fig. 7. Such plots are intended as model diagnostics: they allow the user to inspect whether the event-by-event differentiation sequence produces coherent mantle and core abundance patterns, and to compare the modeled planets against chondritic or planetary reference compositions.



The full event-level output is exported as a multi-sheet table, with one sheet for each modeled collision scenario or final planet. These tables provide transparent records of the differentiation calculation and allow individual events to be inspected
645 or reproduced. Together with the accretion and impact-event tables described in Sects. 2.3 and 2.4, they form the complete AccreDiff record linking N-body accretion histories to final mantle and core compositions.

2.6 Diagnostic analysis and post-processing

In addition to the core accretion-differentiation workflow described above, AccreDiff provides post-processing notebooks for diagnostic analysis of the model outputs. These tools take the event-level and final composition tables produced by the
650 differentiation module as input. For each modeled planet or collision scenario, the final row of the composition history is extracted as the final planetary state. The post-processing routines do not modify the model calculation itself; instead, they provide a reproducible pathway for comparing, aggregating, and visualizing the resulting planetary compositions.

The first group of diagnostics compares final modeled compositions with planetary and meteoritic reference values. AccreDiff supports MgO-normalized abundance comparisons, Earth- and Mars-normalized ratios, and CI- or meteorite-normalized
655 composition diagrams. These comparisons can be applied to bulk compositions or to separated mantle and core inventories, allowing the user to inspect which elements or reservoirs drive differences among final planets. The resulting plots are intended for both model verification and scientific interpretation of the simulated planetary analogs.

A second group of routines aggregates outputs from multiple N-body simulations or model realizations. Final bodies can be classified as Earth-like or Mars-like according to their masses, and derived quantities such as CMF, mantle Mg number, and
660 final planetary mass can be summarized across each population. These multi-run diagnostics provide mean values, scatter, and uncertainty estimates that are useful for comparing modeled analogs with Solar System reference values.

Finally, AccreDiff includes source-composition diagnostics that summarize the EF, EC, OC, and CI reservoir fractions of final planets. These tools connect the source-tracking outputs described in Sect. 2.3.3 with the final differentiated compositions described in Sect. 2.5. All post-processing results can be exported as CSV or spreadsheet tables, providing transparent data
665 products for result interpretation, figure generation, and reproducibility checks. The corresponding example workflows are provided in the `examples/Outcome_analysis/` directory of the AccreDiff repository.

3 Example application and reproducibility

Sect. 2 described the model structure, data flow, and main physical assumptions implemented in AccreDiff. The purpose of this section is not to interpret a specific planetary system, but to demonstrate that the complete AccreDiff workflow can be executed
670 reproducibly from cosmochemical initialization to final composition diagnostics. We therefore focus on the organization of the example workflow, the intermediate data products produced by each step, and the diagnostic outputs that allow users to inspect the calculation.

The example application is based on the executable notebooks provided in the `examples/quickstart/` directory of the AccreDiff repository. These notebooks are designed to be run sequentially, with each step producing explicit intermediate



Table 5. Quickstart benchmark workflow provided with AccreDiff. Each step is implemented as an executable notebook and produces intermediate data products used by later steps.

Step	Workflow component	Role	Main output
01	Constants and setup	Load constants and references	Reference tables
02	Meteorite composition	Process reservoir endmembers	Endmember composition table
03	Embryo composition	Reconstruct t_{gas} bodies	Embryo composition table
04	Accretion history	Trace post-gas collisions	Collision-history workbook
05	Impact events	Classify impacts and assign P_{eq}	Impact-event workbook
06	Differentiation	Run multi-stage core formation	Differentiation history workbook
07	Bulk comparison	Compare final compositions	Normalized composition table

675 tables that are used as input by later steps. This design exposes the state of the calculation at each stage, rather than hiding the complete workflow inside a single monolithic script. It also allows users to replace individual inputs, such as the N-body collision history, reservoir compositions, or impact-regime parameters, while retaining the same overall workflow.

3.1 Benchmark quickstart workflow

The quickstart workflow provides an end-to-end benchmark application of AccreDiff. It starts from constants, reference compositions, and cosmochemical endmembers, proceeds through embryo reconstruction, post-gas accretion tracking, impact-event classification, and multi-stage core–mantle differentiation, and ends with reference-normalized composition diagnostics. The workflow does not introduce additional model assumptions beyond those described in Sect. 2; instead, it demonstrates how the individual modules are assembled into a reproducible calculation.

685 Table 5 summarizes the seven steps of the benchmark workflow. Each step corresponds to one executable notebook and produces data products that can be inspected independently. The outputs are intentionally saved as human-readable tables or spreadsheets, so that users can verify intermediate results before proceeding to the next stage of the calculation.

The sequential structure of the quickstart workflow is useful for reproducibility because each notebook can be rerun from the stored output of the previous step. For example, the embryo composition table generated at the end of the gas–disk stage is used by the differentiation workflow, while the collision-history workbook is used to construct the impact-event table. The final 690 bulk-comparison notebook then reads the differentiation output and compares the modeled final compositions with planetary reference compositions. This chain of explicit inputs and outputs makes it possible to identify where a change in assumptions, parameters, or input data affects the final result.

Although the quickstart notebooks provide a benchmark example, the same workflow can be applied to other simulations. Users may replace the supplied N-body output with their own collision histories, modify the cosmochemical reservoir definitions, adjust the impact-regime thresholds, or change the partitioning parameters. Provided that the required input fields 695 are supplied in the expected format, the downstream reconstruction, impact classification, differentiation, and diagnostic steps

**Table 6.** Main intermediate data products generated by the AccreDiff quickstart workflow.

Data product	Workflow stage	Contents	Downstream use
Reservoir composition table	Cosmochemistry	MgO-normalized endmembers	Embryo initialization
Early composition table	Gas-disk reconstruction	t_{gas} body compositions	Differentiation input
Collision-history workbook	Accretion reconstruction	Per-planet merger histories	Impact classification
Impact-event workbook	Impact assignment	Regime, P_{eq} , T_{eq}	Differentiation input
Differentiation-history workbook	Core formation	Event-by-event compositions	Final diagnostics
Bulk-comparison table	Post-processing	Reference-normalized outputs	Figures and statistics

can be reused without changing the overall structure of the workflow. The main intermediate data products generated by this workflow are described in the following subsection.

3.2 Reproducible intermediate data products

700 A central design principle of the AccreDiff example workflow is that intermediate outputs are written explicitly at each major stage of the calculation. These data products serve as checkpoints between modules. They allow users to inspect the state of the workflow after cosmochemical initialization, accretion reconstruction, impact classification, and differentiation, rather than relying only on the final modeled composition. This design is intended to support reproducibility, debugging, and sensitivity testing.

705 Table 6 summarizes the main classes of intermediate data products generated by the quickstart workflow. File names may differ between the quickstart notebooks and the extended example folders, but the same data-product classes are used throughout the repository.

Because these products are stored separately, downstream stages can be rerun without repeating the entire workflow. For example, a user can modify the impact-regime thresholds and regenerate the impact-event workbook while retaining the same reconstructed collision histories. Similarly, alternative partitioning parameters can be tested by rerunning the differentiation step from the same early-composition and impact-event inputs. This modular restart capability makes it easier to identify which assumptions control a given final composition.

715 The intermediate products are written as human-readable CSV or spreadsheet files. This format is intentionally simple: it allows users and reviewers to open the outputs directly, verify the contents of individual rows, and compare results across parameter choices or simulation runs. These tables can also be archived together with the code release and benchmark input data, providing a transparent record of the calculation used to generate the diagnostic figures and statistical summaries.

The final comparison tables generated from these intermediate products are used by the diagnostic analysis routines described in Sect. 3.3. They provide the link between the event-by-event model outputs and the composition, source-region, and planetary-analog statistics used for interpretation.



720 3.3 Connection to downstream scientific analysis

The diagnostic routines provided with AccreDiff are designed to connect the event-by-event model outputs to downstream planetary-formation analyses. They correspond to the post-processing logic used to interpret Earth–Mars analogue systems in Kong et al. (2026), where final planetary compositions, source-region contributions, and derived planetary properties were analysed across an ensemble of N-body simulations. In the present article, we do not repeat the ensemble figures or scientific interpretation from that study. Instead, we document how the AccreDiff outputs can be converted into reproducible diagnostic quantities.

The main diagnostic quantities are derived from the final composition and source-tracking tables described in Sects. 2.3, 2.5, and 3.2. These include final bulk, mantle, and core compositions; MgO-normalized and reference-normalized abundance ratios; core mass fraction; mantle Mg number; CMF; and EF, EC, OC, and CI source fractions. Final bodies can also be classified as Earth-like or Mars-like according to their mass ranges, allowing the same workflow to be applied to single benchmark simulations or to multi-run ensembles.

The example workflows in the `examples/Outcome_analysis/` directory provide reproducible implementations of these post-processing steps. They include routines for comparing final modeled compositions with Earth, Mars, and meteoritic reference compositions, aggregating multiple simulation outputs, calculating derived quantities such as core mass fraction and Mg number, and summarizing source-reservoir fractions. These routines operate on the exported AccreDiff tables and therefore do not modify the underlying accretion or differentiation calculation.

This separation between model execution and diagnostic analysis is useful for both reproducibility and reuse. The same post-processing routines can be applied to new N-body simulations, alternative cosmochemical endmember choices, modified impact-regime parameters, or different partitioning assumptions. In this way, AccreDiff provides not only the physical workflow for coupling accretion and differentiation, but also the data products needed for transparent comparison with planetary and meteoritic reference constraints.

4 Discussion

4.1 Model scope and intended use

AccreDiff is designed as a coupling framework between dynamical accretion simulations and geochemical core–mantle differentiation calculations. It is not intend to replace N-body integrators, impact hydrodynamics models, or mantle convection models. Instead, it provides a reproducible interface that converts externally generated accretion histories into event-by-event chemical evolution histories. In this sense, AccreDiff occupies the workflow layer between dynamical simulations and geochemical interpretation.

The primary input to AccreDiff is a time-ordered accretion history, including particle IDs, collision times, target and impactor masses, and information needed to identify the surviving product. From this input, the model reconstructs collision trees, tracks source-region contributions, assigns impact-dependent equilibration conditions, and updates mantle and core compositions



through multi-stage metal–silicate partitioning. The framework is therefore most suitable for studies in which the dynamical growth history is already available and the scientific question concerns how that history maps onto planetary bulk composition, redox state, source provenance, or core–mantle partitioning.

755 The intended applications are terrestrial planet formation problems, especially those involving comparisons among Earth and Mars analogues. AccreDiff can be used to test how different source-region assignments, accretion histories, impact-regime parameters, or partitioning laws affect final mantle and core compositions. Because the workflow stores intermediate tables at each stage, it is also well suited for sensitivity analyses in which one module is modified while the others are held fixed.

A central design goal of AccreDiff is transparency rather than maximal automation. The example workflows retain intermediate data products such as embryo composition tables, collision-history workbooks, impact-event tables, and event-by-event differentiation histories. These files allow users to inspect how final compositions arise from earlier model stages and make it easier to identify which assumptions control a given outcome. This structure is particularly useful for code comparison, benchmark testing, and reproducible analysis across multiple N-body simulations.

760 The current implementation focuses on major-element core formation and source-composition tracking. It provides built-in examples for CI-based redox initialization, meteoritic reservoir initialization, GENGA-style accretion histories, impact-regime assignment, and Fe–Ni–Si–O metal–silicate differentiation. The same modular structure, however, is intended to support alternative input formats, cosmochemical reservoirs, impact prescriptions, and partitioning models, as discussed in Sect. 4.3.

4.2 Key assumptions and current limitations

770 AccreDiff relies on several simplifying assumptions that define the current scope of the model. The first concerns the dynamical input. The code does not compute the N-body evolution internally, but instead uses externally generated accretion histories as prescribed input. In the benchmark workflow, these histories are based on GENGA-style collision outputs, and the reconstruction assumes that each collision can be represented by a time, two colliding bodies, their masses, and a surviving product. This treatment is appropriate for perfect-merger accretion histories, but it does not explicitly represent hit-and-run outcomes, erosive impacts, fragmentation, or the reaccretion of debris unless these processes are already encoded in the input data.

775 A second assumption concerns the treatment of early accretion during the gas–disk phase. In the current workflow, collisions before the selected gas–dispersal time are reconstructed as mass-weighted source mixtures and converted into initial embryo compositions. This approach is motivated by the expectation that early bodies are likely to experience extensive melting and efficient chemical mixing. However, it compresses the detailed sequence of early impacts into a single reconstructed state at t_{gas} . As a result, AccreDiff does not currently resolve the individual thermal and chemical consequences of each pre-gas-dispersal collision.

780 The impact-regime model is also parameterized. Late-stage impacts are divided into small impacts, large impacts that generate localized melt pools, and subsequent events occurring during a post-impact magma-ocean interval. These regimes are assigned using impactor-to-total mass ratios, total collision mass, and prescribed timescales or scaling-law outputs. The resulting equilibration pressures and participating material fractions should therefore be interpreted as physically motivated parameterizations rather than direct hydrodynamic calculations. In particular, AccreDiff does not solve impact-induced melt geometry,



Table 7. Representative extension modules distributed with AccreDiff.

Extension axis	Module or example	Main purpose
Gas–disk prescription	<code>gas_migration.py</code> ; <code>gas_disk/</code>	GENGA-compatible gas–disk setup
Collision outcome model	<code>collision_outcomes.py</code> ; <code>collision_detail/</code>	EDACM-style impact diagnostics
Differentiation chemistry	<code>differentiation_sulfur.py</code> ; <code>Fe_Ni_S_ternary/</code>	Fe–Ni–S partitioning extension

metal diapir descent, or magma-ocean cooling self-consistently; instead, it imports scaling-law information and user-defined parameters to provide event-level boundary conditions for chemical differentiation.

The metal–silicate differentiation calculation is similarly focused on a restricted chemical system. The current implementation tracks major oxide and metallic components relevant to Fe–Ni–Si–O partitioning and core formation. This design is sufficient for modelling bulk redox evolution, core mass fraction, mantle FeO, and related major-element diagnostics. However, trace elements, volatile species, isotope systems, sulfide partitioning, and explicit mantle crystallization are not yet included as dynamic components of the calculation. These processes may be important for specific geochemical applications and should be added as separate modules or extensions if they are central to the scientific question.

Another limitation is that several parameters are currently prescribed rather than inferred. Examples include reservoir boundaries, endmember compositions, oxygen fugacity or oxygen-loss settings, impact-regime thresholds, equilibration pressure scaling factors, magma-ocean lifetimes, and metal–silicate partitioning parameter choices. AccreDiff exposes these quantities so that they can be modified and tested, but the benchmark workflow should not be interpreted as a unique solution. Instead, it provides one internally consistent implementation that can be used for sensitivity tests and comparison among alternative assumptions.

Finally, AccreDiff is intended for comparative and mechanistic studies rather than for producing a single deterministic reconstruction of terrestrial planet formation. The final compositions depend on the input N-body simulations, the assumed cosmochemical reservoirs, and the adopted differentiation parameters. The strength of the framework is that these dependencies are made explicit through intermediate tables and modular workflows. The current limitations therefore also define natural directions for future development, including support for non-perfect-merger collision outcomes, additional chemical systems, alternative impact prescriptions, and broader ensemble-based uncertainty analysis.

4.3 Extensibility and future development

AccreDiff is designed as a modular workflow rather than a single monolithic model. Its main components, including cosmochemical initialization, accretion-history reconstruction, impact-regime assignment, core–mantle differentiation, and post-processing diagnostics, communicate through explicit tabular data products and documented module interfaces. This structure allows individual physical assumptions to be replaced or extended without rewriting the full workflow. In practice, extension modules can target at least three different levels of the calculation: the upstream dynamical forcing, the interpretation of collision outcomes, and the chemical formulation of metal–silicate differentiation (Table 7).



One example of this extensibility is the gas-disk module implemented in `src/accrediff/gas_migration.py` and demonstrated in `examples/Expansion_module/gas_disk/`. This module provides a Python-side implementation and validation interface for a modified GENGA gas-disk prescription. The corresponding CUDA source file is distributed as `examples/dataset/gas_config/gas.cu`, which can be used to replace the original gas-disk configuration file in GENGA. The modified prescription implements the gas-disk setup described in Sect. 2.2 of Nesvorny et al. (2025), including the radial gas surface-density structure and associated type-I migration torques (Paardekooper et al., 2010, 2011). The example notebook evaluates gas surface-density profiles, torque components, torque zero-crossing locations, and analytic migration tracks, and compares them with bundled GENGA-style test outputs. This example therefore illustrates how AccreDiff can support upstream dynamical-model development and validation, rather than only post-processing completed N-body simulations.

A second example is the EDACM-style collision-outcome classifier implemented in `src/accrediff/collision_outcomes.py` and demonstrated in `examples/Expansion_module/collision_detail/`. The example workflow reads a real N-body collision file, converts the stored GENGA-like quantities to SI units, derives impact velocity, impact angle, and impact parameter from the relative position and velocity vectors, and classifies each event using an analytic collision-outcome model based on Leinhardt and Stewart (2012), which predicts the largest-remnant mass and uses it, together with the relevant impact-energy regime, to classify each collision outcome. The resulting event table includes outcomes such as perfect merger, hit-and-run, partial accretion, erosion, and super-catastrophic disruption, together with diagnostic quantities such as the interacting projectile fraction, specific impact energy, disruption threshold, and largest-remnant mass fraction. Here the catastrophic-disruption threshold denotes the specific impact energy required to disperse half of the total colliding mass. This module was originally developed for applications to episodic planetesimal disruption during gas-disk dispersal (Shuai et al., 2026) and is included here as an example of how external collision-outcome prescriptions can be exposed through the AccreDiff workflow interface. This extension demonstrates how the impact-regime layer of AccreDiff can be enriched by more detailed collision physics before the resulting event properties are mapped onto equilibration pressures, material budgets, volatile-retention rules or debris-production prescription.

A third example extends the chemical differentiation calculation itself. The standalone Fe–Ni–S metal–silicate differentiation module, implemented in `src/accrediff/differentiation_sulfur.py` and demonstrated in `examples/Expansion_module/Fe_Ni_S_ternary/`, expands the default Fe–Ni–Si–O formulation to include sulfur-bearing metal–silicate partitioning. The module follows the staged treatment adopted in the supplementary methods of Brennan et al. (2020), in which the first differentiation event uses the sulfur-partitioning relation of Rose-Weston et al. (2009), corresponding to Eq. S8 in Brennan et al. (2020), whereas later differentiation events use the composition-dependent sulfur relation of Boujibar et al. (2014), corresponding to Eq. S7. The module also incorporates Fe–Ni–S ternary metal activity corrections based on the interaction model of Ma (2001). Baseline Ni, Si, and O partition coefficients are evaluated using the parameterizations adopted by Brennan et al. (2020), with Ni following Siebert et al. (2011) and Si and O following Fischer et al. (2015). The silicate FeO activity coefficient is fixed following the supplementary treatment of Brennan et al. (2020), based on Holzheid and Palme (1996) and O'Neill and Eggins (2002).



The two Fe–Ni–S example notebooks separate primordial differentiation from later collision-driven re-equilibration. `Initial_Differentiation_S8.ipynb` applies the initial Rose-Weston et al. (2009) sulfur-partitioning prescription to a homogeneous bulk composition, whereas `Subsequent_Differentiation_S7.ipynb` constructs a later event from pre-existing target and impactor reservoirs and applies the Boujibar et al. (2014) composition-dependent sulfur prescription only to the equilibrating subsystem. The module returns sulfur-bearing core and mantle inventories, solver diagnostics, ΔIW matching information, and explicit mass-conservation checks. This example shows that the differentiation chemistry in AccreDiff can be extended beyond the default major-element system while preserving the same reservoir-bookkeeping and input–output logic used by the main workflow.

These examples illustrate the intended extension pattern for AccreDiff. Extension modules do not need to modify every part of the codebase. Instead, they should expose their results as standardized table columns, phase-resolved inventories, or reproducible diagnostic outputs that can be inspected, archived, and passed to later workflow stages. In the gas–disk example, the module provides a transparent way to inspect and validate a modified GENGA gas–force prescription. In the EDACM example, the output is an enriched collision-event table that can be mapped in future work onto modified impact-regime and material-budget rules. In the Fe–Ni–S example, the output is a sulfur-bearing core–mantle differentiation state that follows the same reservoir bookkeeping principles as the default solver. This interface keeps the coupling transparent and makes it possible to test new assumptions one module at a time.

Several future developments follow naturally from this structure. The most immediate extension is to couple non-perfect-merger collision outcomes directly to the mantle and core material budgets used by the differentiation module. This would require explicit rules for hit-and-run events, erosion, largest-remnant growth, debris loss, and possible reaccretion. A second direction is to integrate sulfur-bearing and volatile-bearing differentiation more tightly into the main accretion workflow, including upstream sulfur inventories, volatile-delivery prescriptions, and calibration-range checks for empirical partitioning laws. Other directions include support for additional N-body output formats, alternative gas–disk prescriptions, expanded meteoritic reservoir libraries, trace-element partitioning, and ensemble-level uncertainty analysis. The current expansion-module examples are therefore best viewed as prototype demonstrations of the interface design: they show how new physical components can be added to AccreDiff while preserving the reproducible workflow structure described in this paper.

5 Conclusions

This paper presents AccreDiff v1.0, a modular framework for coupling planetary accretion histories with multi-stage core–mantle differentiation calculations. The model is designed to translate the dynamical information recorded by N-body simulations into chemically meaningful planetary growth histories. Rather than treating accretion and differentiation as separate modelling problems, AccreDiff provides a workflow in which time-ordered collision records, source-reservoir information, impact-regime assignments, and metal–silicate equilibration calculations are combined within a single reproducible framework.



The model description in this paper defines the main components of the AccreDiff workflow. Cosmochemical initial conditions can be assigned either from CI-based refractory-enriched compositions with prescribed oxygen fugacity or from reservoir-based meteoritic endmembers. Dynamical histories are then reconstructed from collision records by tracking parent–product relationships, source fractions, and planetary growth paths. For each differentiation event, AccreDiff assigns an impact regime and corresponding equilibration conditions, including localized small-impact equilibration and large-impact magma-ocean effects. These event-level conditions are then passed to the core–mantle differentiation solver, which updates mantle and core inventories through metal–silicate partitioning and records diagnostic quantities such as bulk composition, redox state, and core mass fraction.

The accompanying example notebooks and bundled data products demonstrate how the documented workflow can be executed and inspected in practice. These examples are intended to support reproducibility and workflow transparency in the context of a model-description paper. They show how AccreDiff reads accretion and cosmochemical inputs, generates intermediate reconstruction products, performs differentiation calculations, and exports diagnostic outputs for downstream analysis. The ensemble-scale scientific interpretation of such outputs, including their implications for terrestrial planet formation, is presented in the companion application study of Kong et al. (2026), while the present paper focuses on the structure, implementation, and reproducibility of the code itself.

AccreDiff is intended as a post-processing and coupled geochemical evolution framework rather than as an N-body integrator or a hydrodynamic impact model. Its current version relies on parameterized prescriptions for impact regimes, equilibration pressure and temperature, and metal–silicate partitioning, and it is primarily targeted at terrestrial planet formation scenarios involving chondritic or meteoritic source reservoirs. These assumptions define the present scope of the model and should be considered when applying the code to different dynamical architectures, volatile-rich systems, or impact regimes outside the calibration range of the adopted prescriptions.

The modular structure of AccreDiff provides a basis for future extensions. Potential developments include support for additional N-body output formats, expanded meteoritic reservoir libraries, alternative gas–disk and migration prescriptions, updated collision-outcome models, and new metal–silicate partitioning parameterizations. Further benchmark cases and automated tests will also strengthen the long-term reproducibility of the framework. By separating the major steps of accretion reconstruction, impact-regime assignment, and chemical differentiation into documented and extensible modules, AccreDiff provides an open platform for investigating how planetary growth histories shape the chemical evolution of terrestrial planets.

Code and data availability. The source code of AccreDiff v1.0.0 is available from GitHub at <https://github.com/kong996/AccreDiff>. The archived version corresponding to this paper is available on Zenodo at <https://doi.org/10.5281/zenodo.21591695> (Kong, 2026). The archive contains the model source code, example notebooks, bundled input data, tests, and documentation used to reproduce the workflows presented here. AccreDiff is released under the MIT License.



- 910 *Author contributions.* Zhihui Kong and Beibei Liu made the primary contributions to the conception, design, and implementation of Ac-
creDiff. Zhihui Kong led the development of the main codebase, including the accretion-reconstruction, impact-regime assignment, and
core–mantle differentiation workflows, prepared the example notebooks, carried out the verification tests, and wrote the initial manuscript
draft. Beibei Liu co-designed the model framework, contributed to the implementation strategy and scientific formulation, supervised the
code organization, and revised the manuscript. Ke Chen and Qiyu Wang contributed the Fe–Ni–S extension module and its documentation.
- 915 Kang Shuai contributed the EDACM-based collision-outcome extension module and its demonstration workflow. All authors contributed to
discussion of the model structure, reviewed the manuscript, and approved the submitted version.

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