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# Thermodynamically constrained averaging theory approach for modeling flow and transport phenomena in porous medium systems: 2. Foundation

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**Abstract**

This paper is the second in a series that details the thermodynamically constrained averaging theory (TCAT) approach for modeling flow and transport phenomena in porous medium systems. In this work, we provide the mathematical foundation upon which the theory is based. Elements of this foundation include definitions of mathematical properties of the systems of concern, previously available theorems needed to formulate models, and several theorems and corollaries, introduced and proven here. These tools are of use in producing complete, closed-form TCAT models for single- and multiple-fluid-phase porous medium systems. Future work in this series will rely and build upon the foundation laid in this work to detail the development of sets of closed models.


*Keywords:* Porous medium models; Averaging theory; TCAT

## 1. Introduction

The first paper in this series on the thermodynamically constrained averaging theory (TCAT) approach provided a conceptual introduction and established the focus of this research on the production of rigorously-based, closed models [19]. The TCAT approach integrates classic notions of volume averaging with other key concepts such as the need to model interfaces, common curves, and common points in realistic multiphase systems; a rigorous approach for introducing multiscale thermodynamic dependencies of internal energy on other system variables; a formal, systematic approach for constraining the entropy production; and consistent approaches for producing closed models. Each of these steps, and others that are involved, will be fully developed and applied for a variety of systems to produce complete, closed, and well-posed models in this series of papers. A step in facilitating such a development of TCAT-based models is the specification of a mathematical foundation, including necessary notation, definitions, and certain theorems useful for developing such models. That step is the focus of the present paper.

The overall goal of this work is to provide the mathematical foundation upon which TCAT models can be constructed and advanced. The specific objectives of this present paper are: (1) to define carefully the systems and scales of concern; (2) to define the basic properties of these systems; (3) to introduce a compact notation to express common quantities needed in the TCAT approach; (4) to summarize key available theorems for averaging quantities from the microscale to the macroscale; and (5) to advance a set of new theorems and corollaries that

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## Nomenclature

| | |
|---|---|
| $A$ | area measure |
| $\mathbf{d}$ | rate of strain tensor |
| $\mathscr{E}$ | set of all types of entities |
| $\mathbf{e}_{\alpha\beta\gamma}$ | unit vector tangent to the $\alpha\beta\gamma$ common curve and oriented positive outward at the endpoints |
| $f$ | general scalar quantity |
| $\mathbf{f}$ | general vector quantity |
| $\mathbf{f}$ | general second-rank tensor quantity |
| $g$ | general scalar quantity |
| $\mathbf{g}$ | general vector quantity |
| $\mathbf{g}$ | general second-rank tensor quantity |
| $\mathscr{I}$ | index set of all types of entities |
| $\mathbf{I}$ | identity tensor |
| $L$ | length measure |
| $\mathscr{L}$ | measure of entity |
| $\ell$ | length scale |
| $\mathbf{l}_{\alpha\beta\gamma}$ | unit vector tangent to the $\alpha\beta\gamma$ common curve |
| $\mathbf{m}_{\alpha\beta}$ | unit vector orthogonal to $\mathbf{n}_\alpha$ and outward normal from the $\alpha\beta$ interface along the edge of the interface |
| $N$ | number measure |
| $\mathbf{n}$ | outward normal vector |
| $n_{\mathrm{C}}$ | number of common curves |
| $n_{\mathrm{I}}$ | number of interfaces |
| $n_{\mathrm{P}}$ | number of phase volumes |
| $n_{\mathrm{Pt}}$ | number of common points |
| $\mathbf{n}_\alpha$ | outward normal vector from phase volume $\alpha$ |
| $\mathscr{P}$ | set of system properties |
| $t$ | time |
| $\mathbf{t}$ | stress tensor |
| $V$ | volume measure |
| $\mathbf{v}$ | velocity vector |
| $w$ | weighting function for averaged quantity |
| $\mathbf{w}$ | microscale velocity vector of an interface whose tangential components may differ from the tangential velocity of the material in the interface |

*Greeks*

| | |
|---|---|
| $\Gamma$ | boundary |
| $\delta\ell$ | change in length scale |
| $\varepsilon$ | precision estimate for property |
| $\epsilon^\alpha$ | measure of quantity of entity $\alpha$ per system volume |
| $\rho$ | mass density |
| $\tau_{\mathrm{g}}$ | general time scale |
| $\tau_{\mathrm{t}}$ | thermodynamic time scale |
| $\Omega$ | domain |
| $\omega$ | mass fraction |

*Subscripts and superscripts*

| | |
|---|---|
| – | mass average qualifier (superscript) |
| = | specifically defined average (superscript) |
| C | common curve qualifier (subscript) |
| e | external boundary qualifier (subscript) |
| I | interface qualifier (subscript) |
| $i$ | general index (subscript and superscript) |
| i | internal boundary qualifier (subscript) |
| $j$ | general index (subscript) |
| $k$ | general index (subscript and superscript) |
| ma | macroscale qualifier (superscript) |
| me | megascale qualifier (superscript) |
| mi | microscale qualifier (subscript) |
| mo | molecular scale qualifier (subscript) |
| P | qualifier for phases (subscript) |
| Pt | qualifier for points (subscript) |
| r | qualifier for resolution scale (subscript and superscript) |
| T | transpose operator |
| $\alpha$ | entity qualifier for a phase volume (subscript and superscript) |
| $\alpha\beta$ | (or other pair of Greek letters) entity qualifier for an interface between the $\alpha$ and $\beta$ phases (or other pair of phases, subscript and superscript) |
| $\alpha\beta\gamma$ | entity qualifier for a common curve that is on the boundary of the $\alpha$, $\beta$, and $\gamma$ phases (subscript and superscript) |
| $\alpha\beta\gamma\delta$ | entity qualifier for a common point where the boundaries of the $\alpha$, $\beta$, $\gamma$, and $\delta$ phases are in contact (subscript and superscript) |
| $\beta$ | entity qualifier for a phase volume (subscript) |
| $\gamma$ | entity qualifier for a phase volume (subscript) |
| $\delta$ | entity qualifier for a phase volume (subscript) |
| $\iota$ | general entity qualifier which could indicate a phase volume, interface, or common curve (subscript and superscript) |

*Other mathematical symbols*

| | |
|---|---|
| – | closure of set (overline) |
| $\langle\ \rangle$ | averaging operator |
| $\mathrm{D}^{\bar{\iota}}/\mathrm{D}t$ | material derivative as defined by Eq. (15) |
| $\mathrm{D}'^{\bar{\iota}}/\mathrm{D}t$ | material derivative restricted to an interface and defined by Eq. (46) |
| $\mathrm{D}''^{\bar{\iota}}/\mathrm{D}t$ | material derivative restricted to a common curve and defined by Eq. (67) |
| $\mathbb{R}$ | set of real numbers |
| $\partial'/\partial t$ | partial derivative of a point on a potentially moving interface as defined in Eq. (44) |
| $\partial''/\partial t$ | partial derivative of a point on a potentially moving common curve as defined by Eq. (65) |

| | |
|---|---|
| $\nabla'$ | microscale surficial del operator on an interface as defined in Eq. (42) |
| $\nabla''$ | microscale curvilinear del operator on a common curve as defined by Eq. (63) |

*Abbreviations*

| | |
|---|---|
| AO | averaging operator |
| *n* | nonwetting phase |
| *ns* | nonwetting–solid phase interface |
| REV | representative elementary volume |
| RHS | right-hand side |
| *s* | solid phase |
| TCAT | thermodynamically constrained averaging theory |
| *w* | wetting phase |
| *wn* | wetting–nonwetting phase interface |
| *ws* | wetting–solid phase interface |
| *wns* | wetting–nonwetting–solid phase common curve |

will prove useful in producing TCAT-based models of porous medium systems.

## 2. Systems and scales

Fig. 1 shows an example of the physical components of a microscale system composed of a solid phase ($s$), a wetting fluid phase ($w$), and a nonwetting fluid phase ($n$). The figure provides a telescoped view such that the microscale components are seen to be elements within the macroscale averaging volume, which in turn exists in an aquifer. The solid phase is connected and fills a portion of the domain, $\Omega$, and a connected pore space within the solid fills the remaining portion of $\Omega$. The solid phase may be rigid or deform as a function of an applied stress.

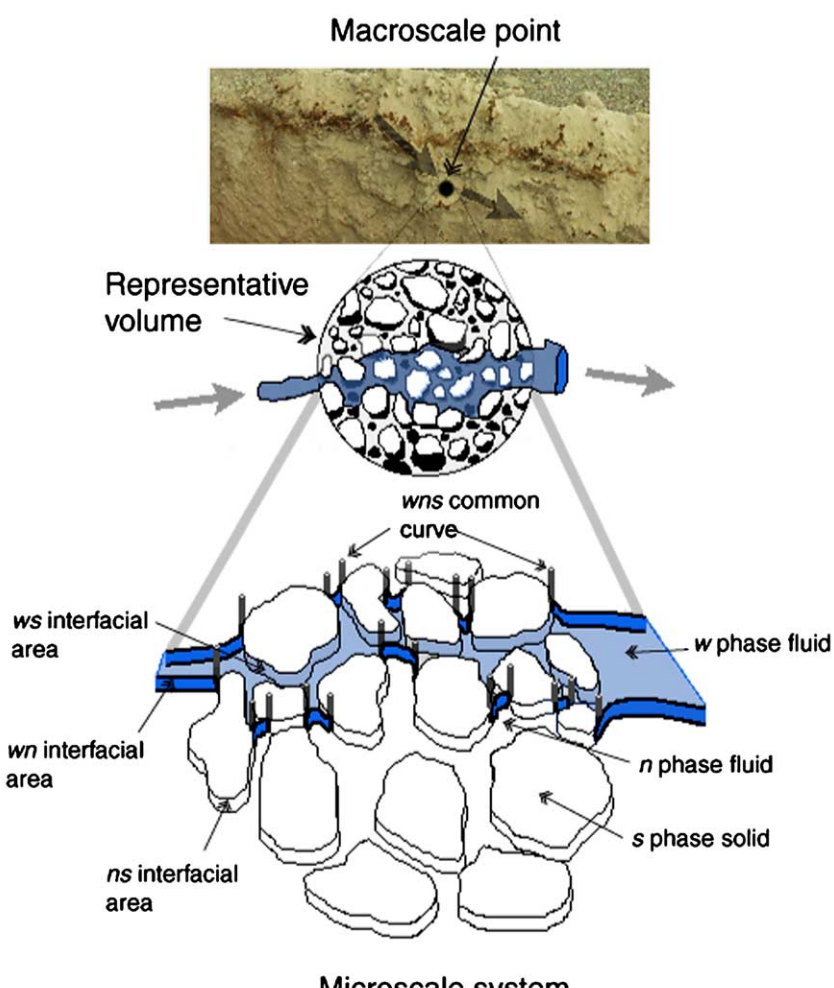


Fig. 1. Physical components of an example three-phase microscale system [14].

In this example, the pore space contains the $w$ and $n$ fluid phases, each of which may be incompressible or compressible. Two-dimensional interfaces within $\Omega$ form the boundaries between pairs of immiscible phases and are denoted as $wn$, $ws$, and $ns$ interfaces with the designations referring to the phases involved. One-dimensional common curves may be identified as the location where three different interfaces or three different phases meet, here denoted as the $wns$ common curve. In general, common curves that could be formed at a juncture of more than three interfaces are not considered in our analysis. Zero-dimensional common points could exist where four common curves, six interfaces, or four phases meet. Common points at the junction of more than four phases are not considered. Since Fig. 1 depicts a system with only three phases, no common points exist. We also exclude from our general discussion common curves and common points that form in foam systems. Interfaces, common curves, and common points are idealizations that account for regions of transition in physicochemical characteristics between or among distinct phases. Transfer of mass, momentum, energy, and entropy between phases occurs at these locations. We refer to the collection of phase volumes, interfaces, common curves, and common points as entities.

We can cast this system description into a more complete, precise set of formal definitions for a domain and the entities within that domain. We identify a domain as a region of study along with its boundary according to the following definition:

**Definition 1** (Domain). The domain of interest is $\Omega \subset \mathbb{R}^3$ with boundary $\Gamma$, and the external closure of the domain is $\overline{\Omega} = \Omega \cup \Gamma$. The extent of $\Omega$ has a measure of volume denoted as $V$.

A phase volume is next defined as occupying a distinct portion of the domain, $\Omega$. The boundary of the phase volume may consist of a portion of the external boundary of the domain along with the interface of the phase with all other phases in the interior of $\Omega$. For a system consisting of only one phase, no internal boundaries exist, and the domain boundary will be the boundary of the phase volume. A phase volume is defined as follows:

**Definition 2** (Phase volume). Phase volumes are regions occupied by a distinct material (either fluid or solid) denoted as $\Omega_\alpha \subset \Omega \subset \mathbb{R}^3$ for material $\alpha$ where $n_\mathrm{P}$ is the number of distinct materials or phase volumes. The set of all types of phase volumes is denoted as $\mathscr{E}_\mathrm{P} = \{\Omega_i \mid i \in \mathscr{I}_\mathrm{P}\}$, and $\mathscr{I}_\mathrm{P}$ is the index set of all types phase of volumes with individual entries consisting of an index corresponding to a phase volume of the form $\alpha$ and having $n_\mathrm{P}$ members. The closure of $\Omega_\alpha$ is denoted as $\overline{\Omega}_\alpha = \Omega_\alpha \cup \Gamma_{\alpha\mathrm{e}} \cup \Gamma_{\alpha\mathrm{i}}$, where the external boundary $\Gamma_{\alpha\mathrm{e}} = \overline{\Omega}_\alpha \cap \Gamma$, and the internal boundary $\Gamma_{\alpha\mathrm{i}} = \bigcup_{\beta\neq\alpha}\overline{\Omega}_\alpha \cap \overline{\Omega}_\beta$. The extent of $\Omega_\alpha$ has a measure of volume denoted as $V^\alpha$ or $\mathscr{L}^\alpha$.

An interface between phase volumes within the domain will be modeled as a surface between phase volumes. The properties of an interface depend, at least in part, on the chemical constituents making up the phases on each side of the interface. Thus, the different interfaces between a fluid and solid or between a pair of fluids must be stipulated. The boundary of an interface is a common curve on the interior where three phases come together along with the common curve formed by the intersection of the interface with the external boundary of the domain. The interface may be defined as follows:

**Definition 3** (Interface). Interfaces are regions within $\Omega$ formed by the intersection of two distinct phase volumes and denoted as $\Omega_{\alpha\beta} = \overline{\Omega}_\alpha \cap \overline{\Omega}_\beta \subset \mathbb{R}^2$. The set of all types of interfaces is denoted as $\mathscr{E}_\mathrm{I} = \{\Omega_i \mid i \in \mathscr{I}_\mathrm{I}\}$, and $\mathscr{I}_\mathrm{I}$ is the index set of all types of interfaces with individual entries consisting of an index corresponding to a pair of phase volumes of the form $\alpha\beta$ and having $n_\mathrm{I} \leqslant \binom{n_\mathrm{P}}{2}$ members, where the order of the phase volume qualifiers comprising an interface qualifier is irrelevant. The closure of $\Omega_{\alpha\beta}$ is denoted as $\overline{\Omega}_{\alpha\beta} = \Omega_{\alpha\beta} \cup \Gamma_{\alpha\beta\mathrm{e}} \cup \Gamma_{\alpha\beta\mathrm{i}}$, where the external boundary $\Gamma_{\alpha\beta\mathrm{e}} = \overline{\Omega}_\alpha \cap \overline{\Omega}_\beta \cap \Gamma$, and the internal boundary $\Gamma_{\alpha\beta\mathrm{i}} = \bigcup_{\gamma\neq\alpha,\beta}\overline{\Omega}_\alpha \cap \overline{\Omega}_\beta \cap \overline{\Omega}_\gamma$. The extent of $\Omega_{\alpha\beta}$ has a measure of area denoted as $A^{\alpha\beta}$ or $\mathscr{L}^{\alpha\beta}$.

The location where three different phase volumes come together, or three different interfaces have a common boundary, will be modeled as an entity called a common curve. At least three distinct phases must be present if a common curve is to be formed, unless a foam is being considered. The boundary of a common curve is composed of the points at its ends where either a different common curve is encountered or the curve intersects the boundary of the system domain. The common curve is thus defined:

**Definition 4** (Common curve). Common curves are regions within $\Omega$ formed by the intersection of three distinct phase volumes and denoted as $\Omega_{\alpha\beta\gamma} = \overline{\Omega}_\alpha \cap \overline{\Omega}_\beta \cap \overline{\Omega}_\gamma \subset \mathbb{R}^1$. The set of all types of common curves is denoted as $\mathscr{E}_\mathrm{C} = \{\Omega_i \mid i \in \mathscr{I}_\mathrm{C}\}$, and $\mathscr{I}_\mathrm{C}$ is the index set of all types of common curves with individual entries consisting of an index corresponding to a group of three phases of the form $\alpha\beta\gamma$ and having $n_\mathrm{C} \leqslant \binom{n_\mathrm{P}}{3}$ members, where the order of the phase volume qualifiers comprising a common curve qualifier is irrelevant. The closure of $\Omega_{\alpha\beta\gamma}$ is denoted as $\overline{\Omega}_{\alpha\beta\gamma} = \Omega_{\alpha\beta\gamma} \cup \Gamma_{\alpha\beta\gamma\mathrm{e}} \cup \Gamma_{\alpha\beta\gamma\mathrm{i}}$, where the external boundary $\Gamma_{\alpha\beta\gamma\mathrm{e}} = \overline{\Omega}_\alpha \cap \overline{\Omega}_\beta \cap \overline{\Omega}_\gamma \cap \Gamma$, and the internal boundary $\Gamma_{\alpha\beta\gamma\mathrm{i}} = \bigcup_{\delta\neq\alpha,\beta,\gamma}\overline{\Omega}_\alpha \cap \overline{\Omega}_\beta \cap \overline{\Omega}_\gamma \cap \overline{\Omega}_\delta$. The extent of $\Omega_{\alpha\beta\gamma}$ has a measure of length denoted as $L^{\alpha\beta\gamma}$ or $\mathscr{L}^{\alpha\beta\gamma}$.

Those ends of the common curves that are on the interior of the domain of study are referred to as common points. They are the locations where four different phase volumes come together. Their definition is along the same lines as those of phase volumes, interfaces, and common curves except that a common point does not have a boundary:

**Definition 5** (Common points). Common points are regions within $\Omega$ formed by the intersection of four distinct phase volumes and denoted as $\Omega_{\alpha\beta\gamma\delta} = \overline{\Omega}_\alpha \cap \overline{\Omega}_\beta \cap \overline{\Omega}_\gamma \cap \overline{\Omega}_\delta \subset \mathbb{R}^0$. The set of all types of common points is denoted as $\mathscr{E}_{\mathrm{Pt}} = \{\Omega_i \mid i \in \mathscr{I}_{\mathrm{Pt}}\}$, and $\mathscr{I}_{\mathrm{Pt}}$ is the index set of all types of common points with individual entries consisting of an index corresponding to a group of four phases of the form $\alpha\beta\gamma\delta$ and having $n_{\mathrm{Pt}} \leqslant \binom{n_{\mathrm{P}}}{4}$ members, where the order of the phase volume qualifiers comprising a common point qualifier is irrelevant. The extent of $\Omega_{\alpha\beta\gamma\delta}$ has a measure of number denoted as $N^{\alpha\beta\gamma\delta}$ or $\mathscr{L}^{\alpha\beta\gamma\delta}$.

It will prove convenient to have one term that refers to the collection of phase volumes, interfaces, common curves, and common points within the system. These are collectively referred to as entities, which are defined as follows:

**Definition 6** (Entities). The set of all types of entities is denoted as $\mathscr{E} = \mathscr{E}_{\mathrm{P}} \cup \mathscr{E}_{\mathrm{I}} \cup \mathscr{E}_{\mathrm{C}} \cup \mathscr{E}_{\mathrm{Pt}}$, and the index set of all types of entities is $\mathscr{I} = \mathscr{I}_{\mathrm{P}} \cup \mathscr{I}_{\mathrm{I}} \cup \mathscr{I}_{\mathrm{C}} \cup \mathscr{I}_{\mathrm{Pt}}$, giving $\mathscr{E} = \{\mathscr{E}_i \mid i \in \mathscr{I}\} = \{\Omega_i \mid i \in \mathscr{I}\}$.

Many possible types of multiphase systems exist. Variations among these systems include the number of fluid and solid phases as well as the variations in the physicochemical properties of the resulting entities. For example, a strict order of wettability can exist and dictate the type of interfaces, common curves, and common points that may occur in a given system. Not all possible types of interfaces will necessarily form. The physical properties of a specific system under consideration will thus dictate the entities that may exist within that system. The actual number of entities may be less than the maximum possible number of entities that could exist based upon combinatorial considerations alone.

Generally speaking, this work is concerned primarily with two distinct length scales: the microscale, $\ell_{\mathrm{mi}}$, and the macroscale, $\ell^{\mathrm{ma}}$, both of which are much longer than the molecular scale, characterized by the mean free path between molecular collisions. The microscale is often referred to as the pore scale, and it is a scale at which all the entities are resolved and the laws of continuum mechanics apply to an individual entity. An example of the microscale perspective would be the flow of water in a saturated porous medium where individual solid particles are described and resolved. The particle surfaces are treated as boundaries of the fluid phase such that the gradients in fluid velocities between particles can be described.

The macroscale is often referred to as the porous medium continuum scale. It is a scale at which the details of microscale phase boundaries are not explicitly resolved. Rather, descriptions of the system are expressed in terms of entity properties that are averaged over sufficiently large microscale regions pertaining to that entity. The macroscale has also been referred to as the Darcy scale, corresponding to the nature of the scale and intent of the original experiments of Darcy [11,12].

For purposes of this work, we restrict ourselves to deterministic systems for which all entity boundaries are completely described at the microscale $\ell_{\mathrm{mi}}$. At the macroscale, $\ell^{\mathrm{ma}}$, all important properties of the system are well-defined and insensitive with respect to small changes in the length scale. This representation is consistent with the classical definition of a so-called representative elementary volume or REV [5]. The actual physical size of $\ell^{\mathrm{ma}}$, and even the existence of an REV according to the requirements posed above, depends upon the characteristics of the physical system of concern.

We can employ these notions of different spatial scales more completely and precisely by the following:

**Axiom 1** (Hierarchical spatial scales). A clear hierarchy of separate length scales exists and is of the form $\ell_{\mathrm{mo}} \ll \ell_{\mathrm{mi}} \ll \ell_{\mathrm{r}}^{\mathrm{r}} \ll \ell^{\mathrm{ma}} \ll \ell^{\mathrm{me}}$ where the five scales are, respectively, the molecular scale, the microscale, the resolution scale, the macroscale, and the megascale.

Although a clear discrete set of separated length scales has been stipulated, we note that most natural porous medium systems consist of a hierarchy of many different length scales that may not have a clear separation [10]. While such systems occur routinely and are important, these systems are outside the scope of our current focus. However, we believe that the TCAT approach can be employed for the study of such systems. The scales appearing in Axiom 1 have the following definitions:

**Definition 7** (Molecular scale). The molecular length scale, $\ell_{\mathrm{mo}}$, is defined as the length scale for molecular collisions for a phase in a system of concern.

As a point of reference, the length scale of molecular collisions for a gas is the mean free path, which at standard pressure and temperature is approximately $10^{-7}$ m. For a liquid, the scale of molecular collisions is the diameter of the molecule, which is on the order of $3 \times 10^{-10}$ m.

**Definition 8** (Microscale). The microscale, $\ell_{\mathrm{mi}}$, is the smallest length scale at which laws of continuum mechanics can be developed with $\|[\mathscr{P}_i(\ell_{\mathrm{mi}} + \delta\ell_{\mathrm{mi}}) - \mathscr{P}_i(\ell_{\mathrm{mi}})]\| \leqslant \varepsilon_{\mathrm{mi}}$, $\forall i$, where $\mathscr{P}_i(\ell)$ is a microscale property estimated by a well-defined average over length scale $\ell$, $\delta\ell_{\mathrm{mi}}$ is a change in the length scale, and $\epsilon_{\mathrm{mi}}$ is a specified precision of the estimate of $\mathscr{P}_i$.

According to this definition, quantities appearing in microscale continuum equations involve a length scale large enough that averages over molecular interactions are stable with respect to perturbations in the size of the averaging region. A minimum length scale for such an average is typically an order of magnitude larger than the molecular interaction scale. Thus, for a gas the microscale is larger than $10^{-6}$ m (1 μm), while a liquid microscale is roughly 2.5 orders of magnitude smaller.

**Definition 9** (Resolution scale). The resolution scale, $\ell_{\mathrm{r}}^{\mathrm{r}}$, is the length scale needed to resolve features related to transport phenomena for the system of concern.

The resolution scale is particularly important for porous media as it relates to the natural length scales of the system. For a natural system, the average diameter of a sand grain is typically on the order of $10^2$ μm. If the grains are well sorted, this would be the resolution scale. However, granular porous systems may contain solid particles ranging in size from approximately 1 μm to $10^{-1}$ m or larger. The features of a general porous system may include small pores, fractures that are evident on a larger scale, boulders, and, perhaps, caves formed by a karstification process. Thus, although the molecular scale and the microscale can be defined within an easily reasoned length, identification of the resolution scale is complicated by the features one wishes to study. The resolution scale will vary widely depending on the problem of interest.

**Definition 10** (Macroscale). The macroscale, $\ell^{\mathrm{ma}}$, is the length scale at which the set of averaged properties of concern for the system can be rigorously defined and $|[\mathscr{P}^i(\ell^{\mathrm{ma}}+\delta\ell^{\mathrm{ma}})-\mathscr{P}^i(\ell^{\mathrm{ma}})]|\leqslant\varepsilon^{\mathrm{ma}}$, $\forall i$, where $\mathscr{P}^i(\ell)$ is a macroscale property estimated by a well-defined average over length scale $\ell$, $\delta\ell^{\mathrm{ma}}$ is a change in the length scale, and $\epsilon^{\mathrm{ma}}$ is a specified precision of the estimate of $\mathscr{P}^i$.

The macroscale is implicitly employed for the description of porous medium systems in defining average geometric properties such as the fractional volume of the porous medium occupied by each phase volume or the amount of interfacial area between phases per volume. These quantities do not exist at the microscale but become important at the macroscale in much the same way that mass densities do not exist at the molecular scale but become important at the microscale. The macroscale must be larger than the resolution scale to incorporate a region of the porous medium large enough that the volume fractions will be insensitive to small perturbations in the size of the length scale. At a minimum, the macroscale should be roughly 10 times the resolution scale with more stable averages obtained if the macroscale is on the order of $10^2$ times the resolution scale. For a well-sorted sample with grain sizes on the order of $10^2$ μm, these considerations seem to result in a macroscale of approximately $10^{-2}$ m. However, depending upon how the fluids are distributed within the porous medium system, the macroscopic length scale might have to be increased to obtain stable values of interfacial areas per volume [23]. Within the mathematical framework to be developed here, we implicitly assume that all macroscale variables are specified at the same macroscopic length scale. This assumption, of course, raises concerns about the stability of all macroscale quantities with respect to changes in length scale. Additionally, in some systems there will be more than one identifiable macroscopic length scale. For example, in a system composed of a fractured porous medium, one macroscale may be employed relative to the pore diameter or grain size while a larger macroscale can be identified relative to the fractures. Modeling of the whole system requires that techniques be employed that couple these two domains.

**Definition 11** (Megascale). The megascale, $\ell^{\mathrm{me}}$, is the length scale corresponding to the domain of interest $\Omega$.

This scale must be much larger than $\ell^{\mathrm{ma}}$ because macroscale quantities may be defined only at points farther than half $\ell^{\mathrm{ma}}$ from the boundary of the domain. Therefore, if variations in properties and gradients of variables are to be defined meaningfully in most of the domain, its length scale must be much larger than the macroscale. Note that in some cases, it is useful to average from the microscale over a full system dimension. In that case, it is not possible to account for variations over that dimension. For example, in modeling nearly horizontal flow in an aquifer, it may be possible to neglect vertical gradients of properties. Thus the averaging employed might be macroscopic in the lateral direction (i.e., using a length scale $\ell^{\mathrm{ma}}$ such that $\ell_{\mathrm{r}}^{\mathrm{r}}\ll\ell^{\mathrm{ma}}\ll\ell^{\mathrm{me}}$), whereas the averaging would be over the full vertical length scale of the system. Such a description can also be obtained by three-dimensional averaging to the macroscale followed by integration over the vertical. In our exposition, we will be concerned only with averaging to obtain the macroscale equations.

A wide range of temporal scales occur in porous medium systems, just as is the case for spatial scales. The temporal scales of concern are related to the spatial scale of concern and to the particular phenomena to be modeled. For example, one can consider the time required for equilibrium to be obtained for various physical and chemical processes, such as thermal equilibrium or equilibrium of chemical potentials. In addition, time scales are often described relative to certain physicochemical characteristics of a system, such as advection, diffusion, dispersion, a chemical or biological reaction rate, or a rate of mass exchange between phases. Elucidation of time scales and comparison of time scales are valuable approaches from which considerable insight can be obtained about a given problem. We define two types of time scales, a thermodynamic equilibrium time scale and a general time scale. The former is related to a thermodynamic property of the system and the latter is related to a transport or reaction property of the system, which may be described by a parameter used to characterize a conservation equation or a closure relation.

**Definition 12** (General time scale). The general time scale $\tau_g = \tau_g(\ell; \mathscr{P}_i)$ is the time scale related to a general property $\mathscr{P}_i$ with respect to length scale $\ell$.

**Definition 13** (Thermodynamic time scale). The thermodynamic time scale $\tau_t = \tau_t(\ell; \mathscr{P}_i)$ is the time scale needed to approach the equilibrium value of thermodynamic property $\mathscr{P}_i$ for a system of length scale $\ell$ within some small measure of distance of equilibrium.

Difficulties in defining precisely when an equilibrium state is reached motivates the definition of thermodynamic time scale as, essentially, a measure of the time to reach equilibrium for practical purposes. If rates of evolution of a system are to be considered, a general time scale must be chosen that is less than the equilibrium time scale. Many interesting and useful time scales exist when one considers porous medium systems. For example, recharge to the subsurface may be modeled in terms of decades if one is interested in long-term groundwater depletion. Annual models are of interest if the infiltration is related to recent trends. Monthly values can be important for crop growth. Daily or hourly values of infiltration in response to a storm event are modeled when one considers watershed response. In laboratory studies or in consideration of the initiation of infiltration into a dry soil, a time scale on the order of minutes or seconds may be appropriate. Studies of unsaturated flow often involve column studies in which small changes in pressure are imposed on the system sequentially, with the system relaxing to equilibrium between each step (e.g. [25]). In such cases, the dynamics within a step occur at a smaller interval than the time required for equilibrium to be achieved.

In the study of porous medium systems, it is interesting to note that length scales relate to the physical properties of the system. Selection of various length scales can result in the system being modeled as heterogeneous, for example, with flow in pores within the solid, or as homogeneous, for example, with the system being viewed with all entities existing at a point but with different densities. The boundaries between entities must be accounted for. Conversely, the time domain is continuous without heterogeneities. There are no boundaries in the time domain. Therefore, averaging over time as well as space does not alter the form of the equations in comparison to averaging only over space, although it does alter the meaning of the terms that appear in the equation. For this reason, time averaging is not explicitly applied in the subsequent formulations; but one must consider the meanings of the various terms as averages over space and time when employing the resulting formulas.

## 3. Macroscale properties

System properties are members of the set $\mathscr{P}$, with members of the set denoted as $\mathscr{P}^i$. Macroscale system properties are obtained as averages of microscale properties or as averages of combinations of microscale properties. The macroscale properties are constructed using a variety of averaging approaches. In some instances, a macroscale property is conveniently expressed as a combination of other macroscale properties that have been obtained directly from averaging. Of course, these combination properties may also be obtained as averages of combinations involving microscale variables. Considerable relevant foundational effort has been invested in the development of macroscale averaging theory for multiphase porous medium systems (e.g. [1,3,4,6,7,9,13,15–18,20–22,24,26]). Rather than reproducing these notions in detail, we summarize briefly in this section a few key definitions needed to establish our notation and to develop the theorems that follow.

We define an averaging operator (AO):

**Definition 14** (Averaging operator).

$$\langle \mathscr{P}_i \rangle_{\Omega_j,\Omega_k,w} = \frac{\int_{\Omega_j} w \mathscr{P}_i \,\mathrm{d}\mathfrak{r}}{\int_{\Omega_k} w \,\mathrm{d}\mathfrak{r}}, \tag{1}$$

where $\mathscr{P}_i$ is a property to be averaged to the macroscale, and the subscripts on the operator correspond, respectively, to the domain of integration of the numerator, the domain of integration of the denominator, and a weighting function applied to the integrands in the definition of the averaging process. Omission of the third subscript on the averaging operator implies a weighting of unity. If the domain over which the averaging is being performed is a set of common points, the integral is replaced by a discrete summation over all points in the specified entity set.

The averaged quantity on the left-hand side of Eq. (1) is a member of $\mathscr{P}$. Because of the variety of ways that averaging of a microscale quantity may be performed through selection of averaging regions and weighting functions (i.e., through selection of $\Omega_j$, $\Omega_k$, and $w$), a number of different averages of a single microscale quantity or combination of microscale quantities may be defined.

This averaging operator provides an unambiguous notation for defining many macroscale variables that will be important for model description. However, use of this notation for all variables for purposes such as specifying conservation-equation-based models is cumbersome. Because of this, we will rely upon a shorthand notation for commonly used quantities, which is much more compact than the fully specified averaging operator. In doing so, we will be careful to identify macroscale variables not readily defined unambiguously using an abbreviated notation, since our ultimate objective is to define complete, consistent models of multiphase porous medium systems.

Some specific and common examples of the application of Eq. (1) can be shown to connect to common notions. As a first case, consider the notation that will be employed for the various geometric densities. Define these densities, $\epsilon^{\iota}$, as averages by setting $\mathscr{P}_i = 1$ according to

$$\epsilon^{\iota} = \langle 1 \rangle_{\Omega_\iota,\Omega} = \frac{\int_{\Omega_\iota} \mathrm{d}\mathbf{r}}{\int_{\Omega} \mathrm{d}\mathbf{r}} = \frac{\mathscr{L}^{\iota}}{V}. \tag{2}$$

Specification of values of $\iota$ that correspond to common entity types, such as phase volumes, interfaces, or common curves, leads to the common geometric quantities of $\epsilon^{\alpha}$, the volume fraction of the $\alpha$ phase volume; $\epsilon^{\alpha\beta}$, the specific interfacial area of the $\alpha\beta$ interface; and $\epsilon^{\alpha\beta\gamma}$, the specific common curve length of the $\alpha\beta\gamma$ common curve. None of these common geometric quantities exists at the microscale.

A second example is an entity average of a microscale variable, an average that has traditionally been referred to as an intrinsic average. Let $\mathscr{P}_i = f_\iota$, where the subscript $\iota$ denotes that the variable is a microscale property of entity $\iota$. The intrinsic average, $f^{\iota}$ is given by

$$f^{\iota} = \langle f_\iota \rangle_{\Omega_\iota,\Omega_\iota} = \frac{\int_{\Omega_\iota} f_\iota \, \mathrm{d}\mathbf{r}}{\int_{\Omega_\iota} \mathrm{d}\mathbf{r}} = \frac{1}{\mathscr{L}^{\iota}} \int_{\Omega_\iota} f_\iota \, \mathrm{d}\mathbf{r}. \tag{3}$$

The macroscale variables of the form $f^{\iota}$ are routinely used for all entity types, leading to phase volume intrinsic averages $f^{\alpha}$, interface intrinsic averages $f^{\alpha\beta}$, and common curve intrinsic averages $f^{\alpha\beta\gamma}$.

A third average that is often employed is that obtained by using the microscale density as the weighting function. This intrinsic mass average for the case where the microscale property of interest in entity $\iota$ is the member of $\mathscr{P}$ denoted as $\mathscr{P}_i = f_\iota$ is indicated as $f^{\bar{\iota}}$ and is defined according to

$$f^{\bar{\iota}} = \langle f_\iota \rangle_{\Omega_\iota,\Omega_\iota,\rho_\iota} = \frac{\int_{\Omega_\iota} \rho_\iota f_\iota \, \mathrm{d}\mathbf{r}}{\int_{\Omega_\iota} \rho_\iota \, \mathrm{d}\mathbf{r}} = \frac{1}{\rho^{\iota}\mathscr{L}^{\iota}} \int_{\Omega_\iota} \rho_\iota f_\iota \, \mathrm{d}\mathbf{r}, \tag{4}$$

where $\rho_\iota$ is the microscale mass density of entity $\iota$, and $\rho^{\iota}$ is the intrinsic average mass density in the entity domain $\Omega_\iota$. When the entity is a phase volume, $\rho_\iota$ has the standard meaning of mass per volume. The generalization of this notion leads to mass per area and mass per length for interfaces and common curves, respectively. These quantities have been previously used in multiphase model formulation work [15,16]. The following identities may also be shown to apply:

$$\rho^{\iota} f^{\bar{\iota}} = \rho^{\iota} \langle f_\iota \rangle_{\Omega_\iota,\Omega_\iota,\rho_\iota} = \langle \rho_\iota f_\iota \rangle_{\Omega_\iota,\Omega_\iota} = (\rho_\iota f_\iota)^{\iota}, \tag{5}$$

where the last expression on the RHS of Eq. (5) is a short-hand notation that implies the averaging domains.

In some cases, the averaging that is performed is done with a weighting that involves the properties of a chemical species, $k$. For example, if the microscale mass fraction of species $k$ in entity $\iota$ is denoted as $\omega_{k\iota}$, the species weighted average of the velocity of species $k$ in entity $\iota$ is

$$\begin{aligned}\langle \mathbf{v}_{k\iota} \rangle_{\Omega_\iota,\Omega_\iota,\rho_\iota\omega_{k\iota}} &= \frac{\int_{\Omega_\iota} \rho_\iota \omega_{k\iota} \mathbf{v}_{k\iota} \, \mathrm{d}\mathbf{r}}{\int_{\Omega_\iota} \rho_\iota \omega_{k\iota} \, \mathrm{d}\mathbf{r}} \\ &= \frac{1}{\rho^{\iota}\omega^{k\bar{\iota}}\mathscr{L}^{\iota}} \int_{\Omega_\iota} \rho_\iota \omega_{k\iota} \mathbf{v}_{k\iota} \, \mathrm{d}\mathbf{r} = \mathbf{v}^{\overline{k\iota}}.\end{aligned} \tag{6}$$

Of notational significance is the extension of the overline over the superscripts in various terms. The notation employed indicates that $\omega^{k\bar{\iota}}$ is the macroscale intrinsic mass average of the mass fraction of species $k$ obtained from

$$\omega^{k\bar{\iota}} = \langle \omega_{k\iota} \rangle_{\Omega_\iota,\Omega_\iota,\rho_\iota} = \frac{\int_{\Omega_\iota} \rho_\iota \omega_{k\iota} \, \mathrm{d}\mathbf{r}}{\int_{\Omega_\iota} \rho_\iota \, \mathrm{d}\mathbf{r}} = \frac{1}{\rho^{\iota}\mathscr{L}^{\iota}} \int_{\Omega_\iota} \rho_\iota \omega_{k\iota} \, \mathrm{d}\mathbf{r}. \tag{7}$$

In the notation for the macroscale velocity of species $k$ in entity $\iota$, the overline extends over both the species qualifier, $k$, and the entity qualifier, $\iota$, indicating that the weighting function is the mass density of species $k$ in entity $\iota$.

Since the macroscale properties are independent of microscale coordinates, they are unchanged when averaged over microscale coordinates. Operationally, this means they can be moved in and out of an averaging integral without error. For example, if $f^{\iota}$ is an intrinsic average of some microscale quantity $f_\iota$, then

$$\langle f^{\iota} \rangle_{\Omega_j,\Omega_k,w} = f^{\iota} \langle 1 \rangle_{\Omega_j,\Omega_k,w}. \tag{8}$$

Some macroscale properties are not obtained directly as averages of a single microscale quantity but are actually averages of combinations of microscale and other macroscale quantities. One example of this type of macroscale quantity is the macroscale stress tensor for an entity that is sometimes defined in terms of the average of the microscale stress tensor in combination with the microscale density and deviations of the microscale velocity from a macroscale value. The reason for this combination will become apparent in subsequent papers, but for now it is adequate to simply assert that we can define such a macroscale quantity. Introduction of special abbreviated notation for each special case of Eq. (1) would be impractical. Therefore, we will use a single special abbreviated notation, a double overbar in the superscript of the macroscale quantity, to designate a specially defined average. The precise meaning of the double-barred notation will vary depending on the macroscale quantity considered. Thus, the double-bar can be considered to be an alert that indicates the macroscale variable is not just a direct average of its microscale counterpart. As an example of the use of this notation, one form of the macroscale stress tensor may be designated as $\mathbf{t}^{\bar{\bar{\iota}}}$ and defined as

$$\mathbf{t}^{\bar{\bar{\iota}}} = \langle \mathbf{t}_\iota - \rho_\iota(\mathbf{v}_\iota - \mathbf{v}^{\bar{\iota}})(\mathbf{v}_\iota - \mathbf{v}^{\bar{\iota}}) \rangle_{\Omega_\iota,\Omega_\iota}. \tag{9}$$

Let us emphasize that if the double-bar notation is encountered in an equation, it means that the macroscale quantity under consideration is an average other than an intrinsic average or an intrinsic mass average. The actual definition of that double-bar average will be supplied in the notation section for each quantity. However, for purposes of continuing with the derivations of equations of interest, the precise definition of the macroscale quantity in terms of its microscale roots is less important than the fact that it represents a macroscale variable. For instance, once the transformation of microscale conservation equations to the macroscale has been carefully completed, it is more important in subsequent mathematical manipulations to recognize $\mathbf{t}^{\bar{\bar{\iota}}}$ as the macroscale stress tensor for entity $\iota$ than to recall its precise definition as given in Eq. (9). We emphasize, nonetheless, that precise knowledge of the definition of a macroscale quantity in terms of microscale precursors and other macroscale properties is essential for devising meaningful connections between microscale and macroscale theoretical formulations and for utilization of data measured at one scale in conjunction with the system description at another scale.

## 4. Averaging theorems

### 4.1. Overview

The development of macroscale conservation equations and macroscale thermodynamic expressions that are both consistent with the microscale and cast in terms of precisely defined variables can be facilitated by a set of theorems that support change of scale operations. The fundamental function of such theorems is straightforward: to transform the integrals of space and time derivatives to derivatives of integral quantities. Since macroscale variables developed using Definition 14 are composed of integrals of microscale quantities, or more generally combinations of microscale and macroscale quantities, derived macroscale equations should be expressed in terms of these averaged quantities and their derivatives. Averages of microscale temporal and spatial derivatives arise when the microscale conservation equations are averaged to the macroscale. These average derivatives are generally not readily accessible quantities. Averaging theorems provide a means to formulate rigorous models in which the derivatives have been converted to accessible quantities.

Some of the averaging theorems needed to facilitate the development of TCAT-based multiphase models are available, either existing through classical work in vector calculus or fluid mechanics (e.g. [27]), or through relatively recent focused work on the development of a large set of such theorems for a variety of entities [18]. For example, a collection of useful theorems for the transformation of surface and curve integral terms has been derived using generalized functions and tabulated. The most often used of these theorems are briefly summarized below and put into context of this work.

Recent work to extend microscale thermodynamics consistently to the macroscale [19] leads to new classes of integral expressions for which transformations to more common macroscale averaged forms is desirable. However, theorems to guide such transformations have not been published to the best of our knowledge. The lack of such theorems is an impediment to the development of rigorous closed macroscale models of multiphase transport phenomena based upon averaged microscale thermodynamics and thus is an impediment to the derivation of TCAT-based models. We summarize several types of expressions arising in such applications, and list and prove theorems to accomplish a useful set of transformations. Of course, the theorems developed may have utility beyond the immediate motivating set of applications.

### 4.2. Available theorems

Common textbooks dealing with vector calculus, fluid mechanics, and transport phenomena include Gauss' theorem, also commonly known as the divergence theorem, and various forms of the transport theorem (e.g. [8,27]). These common theorems are introduced and will be used as a point of departure for the discussion central to this work:

**Theorem 1** (Gauss' divergence theorem). *For a smooth continuous and differential vector function* $\mathbf{f}$ *defined over a domain* $\Omega \subset \mathbb{R}^3$ *that may deform with time* $t$ *due to boundary velocity* $\mathbf{w}$ *with closed boundary* $\Gamma$ *and outward normal from the boundary* $\mathbf{n}$

$$\int_{\Omega(t)} \nabla \cdot \mathbf{f}\, \mathrm{d}\mathfrak{r} = \int_{\Gamma(t)} \mathbf{n} \cdot \mathbf{f}\, \mathrm{d}\mathfrak{r}. \tag{10}$$

**Theorem 2** (Transport theorem). *For a smooth continuous and differential scalar function* $f$ *defined over a domain* $\Omega \subset \mathbb{R}^3$ *that may deform with time* $t$ *due to boundary velocity* $\mathbf{w}$ *with closed boundary* $\Gamma$ *and outward normal* $\mathbf{n}$

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega(t)} f\, \mathrm{d}\mathfrak{r} = \int_{\Omega(t)} \frac{\partial f}{\partial t} \mathrm{d}\mathfrak{r} + \int_{\Gamma(t)} f \mathbf{w} \cdot \mathbf{n}\, \mathrm{d}\mathfrak{r} \tag{11}$$

Theorems 1 and 2 are used classically in fluid mechanics and transport phenomena to transform integral statements of conservation principles into local conservation equations expressed in terms of differential operators. A similar but more comprehensive set of theorems is needed for the two-scale multiphase systems of interest in TCAT-based models. Specifically, the following classes of desirable transformations of integrals over a domain (phase volume, interface, or common curve) arise routinely in TCAT-based models:

- transformations of gradients, divergences, curls, and temporal derivatives of microscale functions to similar differential macroscale operators applied to integrals of functions over the domain and internal boundary terms;
- transformations of gradients, divergences, curls, and temporal derivatives of microscale functions to similar differential microscale operators applied at internal and external boundaries of the domain; and
- transformations of various derivatives of a deviation of a microscale scalar, vector, or tensor function from its macroscale counterpart to forms involving differentials of integrals of microscale functions, macroscale quantities, and boundary terms.

The first two classes of these transformations are well defined with each class having a total of 12 members (four derivative types for each of three entities) for a total of 24 transformations. All of these transformations have been developed and published as theorems and proved using generalized functions [18]. The generalized function approach has also been used to generate a variety of other theorems, including theorems involving three-scale averaging (microscale, macroscale, and megascale). Proofs of some subset of these theorems have appeared in the literature as well [18]. The existence of this large set of theorems is important because: (1) the development of TCAT-based models routinely requires the application of such transformations, and (2) theorems for the third class of transformations can be built upon these extant theorems. Examples of these first two classes of theorems and the details of how these existing theorems can be used to help prove certain important members of the third class of transformation are given in Section 4.3.

The third class of transformations has neither been precisely defined nor developed into a set of proven theorems. Because these transformations involve the evaluation of integrals of differential operators of the deviation between microscale and macroscale quantities, we collectively refer to this set of expressions as multiscale deviation transformations. To the best of our knowledge, this is the first work to catalog formally this important class of transformations that are essential tools in the development of rigorous models of transport phenomena in porous medium systems. The need to deal with deviation terms can arise, for example, when models based upon microscale thermodynamics are, in turn, averaged up to the macroscale and used to formulate an entropy inequality. This averaging of thermodynamics is a critical component of the TCAT approach [19].

### 4.3. Multiscale deviation theorems

In multiscale porous medium analysis, terms involving integrals of differential operators applied to properties of entity $\iota$, which may be a phase volume, interface, or common curve, of the form $f_\iota - f^\iota$ and $f_\iota - f^{\bar{\iota}}$ arise. The subscript denotes that $f_\iota$ is a microscale property of entity $\iota$ and the superscript $\iota$ or $\bar{\iota}$ is used to indicate a macroscale average as defined in the last section. Differences between microscale values and their macroscale counterparts arise for scalars, vectors, and tensors, as well as for a variety of different functional forms involving differential operators of multiscale deviations. Combinatorial considerations result in a large set of potential transformations. Since the need for such transformations will arise in TCAT model formulation, theorems are needed to facilitate the transformations of derivatives between scales. In this section, we focus on a subset of this class of transformations that arise frequently in TCAT-based model formulations.

Specifically, we focus on three types of transformations: products of microscale quantities with material derivatives of multiscale deviations of microscale and macroscale quantities for phase volumes, interfaces, and common curves. As mentioned in the previous section, the ability to refer to an existing set of multiscale theorems [18] will streamline the derivation of transformations from the microscale to the macroscale. We consider three specific theorems and a set of corollaries for each of these theorems.

#### 4.3.1. Multiscale deviations for a phase volume

The following theorems will be of subsequent use with multiscale deviations involving phase volume entities:

**Theorem 3.** (G[3,(3,0),0])

$$\int_{\Omega_\alpha} \nabla f_\alpha \,\mathrm{d}r = \nabla \int_{\Omega_\alpha} f_\alpha \,\mathrm{d}r + \sum_{\beta\neq\alpha} \int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha f_\alpha \,\mathrm{d}r. \tag{12}$$

**Theorem 4.** (T[3,(3,0),0])

$$\int_{\Omega_\alpha} \frac{\partial f_\alpha}{\partial t} \,\mathrm{d}r = \frac{\partial}{\partial t} \int_{\Omega_\alpha} f_\alpha \,\mathrm{d}r - \sum_{\beta\neq\alpha} \int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha \cdot \mathbf{v}_{\alpha\beta} f_\alpha \,\mathrm{d}r. \tag{13}$$

Where integration is performed over all the $\alpha$ phase volume within macroscale volume $\Omega$, $\mathbf{n}_\alpha$ is the outward normal vector from phase $\alpha$, and $\mathbf{n}_\alpha \cdot \mathbf{v}_{\alpha\beta}$ is both the normal component of the velocity of the $\alpha\beta$ interface and the normal component of the velocity of the material in the $\alpha\beta$ interface. The summation in these equations indicates that the surface integrations are performed over all interfaces between the $\alpha$ phase and other phases.

These two theorems are most commonly known as the spatial averaging theorem and the temporal averaging theorem, respectively [2,17,26]. The seemingly cryptic notation for naming these theorems used here corresponds to the carefully defined labels introduced when they were presented in the context of a collection of integration and averaging theorems for various entities [18]. These labels refer to the type of differential operator and dimensions considered at the microscale, the macroscale, and the megascale. A complete explanation of this labeling convention is available in the original work.

We extend this original notation to include the new class of multiscale deviation theorems considered in this work, which we will denote by a leading **M** in the naming convention for a multiscale deviation. We note that the **M** theorems are different from their predecessors in that they involve two functions, a material derivative based on a macroscale velocity, and both microscale and macroscale functions within the integrand.

**Theorem 5.** (M[3, (3, 0), 0]) *The volume average of a product of a microscale quantity $g_\alpha$ with a material derivative referenced to the macroscale mass average velocity of an entity $\iota$ of the difference between a microscale quantity $f_\alpha$ and its macroscale weighted average $f^{\bar{\bar{\alpha}}}$ can be expressed as a function of relative velocities at interfacial boundaries and macroscale quantities of the form*

$$\begin{aligned}\frac{1}{V}\int_{\Omega_\alpha} g_\alpha \frac{\mathrm{D}^{\bar{\iota}}\left(f_\alpha - f^{\bar{\bar{\alpha}}}\right)}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} &= \frac{\mathrm{D}^{\bar{\iota}}\left\{\epsilon^\alpha\left[(g_\alpha f_\alpha)^\alpha - g^\alpha f^{\bar{\bar{\alpha}}}\right]\right\}}{\mathrm{D}t} + \frac{\mathrm{D}^{\bar{\iota}}(\epsilon^\alpha g^\alpha)}{\mathrm{D}t} f^{\bar{\bar{\alpha}}} \\ &\quad - \frac{1}{V}\int_{\Omega_\alpha} \frac{\mathrm{D}^{\bar{\iota}} g_\alpha}{\mathrm{D}t} f_\alpha\,\mathrm{d}\mathbf{r} + \sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\cdot\left(\mathbf{v}^{\bar{\iota}} - \mathbf{v}_{\alpha\beta}\right) g_\alpha f_\alpha\,\mathrm{d}\mathbf{r},\end{aligned} \tag{14}$$

*where $\mathbf{v}^{\bar{\iota}}$ is the macroscale mass averaged velocity of entity $\iota$, $\mathbf{n}_\alpha$ is the microscale normal vector pointing outward from the $\alpha$ phase, $\mathbf{n}_\alpha\cdot\mathbf{v}_{\alpha\beta}$ is the component of the microscale velocity of the $\alpha\beta$ interface normal to the interface, $V$ is independent of time and position and is the measure of the averaging domain $\Omega$, $\Omega_\alpha \subset \Omega$ is the phase volume of phase $\alpha$, $\Omega_{\alpha\beta}$ is the interface between the $\alpha$ and $\beta$ phases, and the material derivative is defined as*

$$\frac{\mathrm{D}^{\bar{\iota}}}{\mathrm{D}t} = \frac{\partial}{\partial t} + \mathbf{v}^{\bar{\iota}}\cdot\nabla. \tag{15}$$

Although Theorem 5 and the material derivative are written explicitly in terms of the mass average velocity for entity $\iota$, $\mathbf{v}^{\bar{\iota}}$, in fact, any macroscale velocity may be employed, such as the intrinsic phase average, $\mathbf{v}^{\iota}$, or the mass average velocity of chemical species $i$ in entity $\iota$, $\mathbf{v}^{\overline{i\iota}}$. In actuality, the macroscale quantity denoted as $f^{\bar{\bar{\alpha}}}$ may be selected to be any useful macroscale function. For the context of porous medium modeling, it is typically some weighted average of the microscale quantity $f_\alpha$.

**Proof.** Note that

$$\frac{1}{V}\int_{\Omega_\alpha} g_\alpha \frac{\mathrm{D}^{\bar{\iota}}\left(f_\alpha - f^{\bar{\bar{\alpha}}}\right)}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} = \frac{1}{V}\int_{\Omega_\alpha} g_\alpha \frac{\mathrm{D}^{\bar{\iota}} f_\alpha}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} - \frac{1}{V}\int_{\Omega_\alpha} g_\alpha \frac{\mathrm{D}^{\bar{\iota}} f^{\bar{\bar{\alpha}}}}{\mathrm{D}t}\,\mathrm{d}\mathbf{r}. \tag{16}$$

The product rule may be employed to rearrange Eq. (16) to

$$\begin{aligned}\frac{1}{V}\int_{\Omega_\alpha} g_\alpha \frac{\mathrm{D}^{\bar{\iota}}\left(f_\alpha - f^{\bar{\bar{\alpha}}}\right)}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} &= \frac{1}{V}\int_{\Omega_\alpha} \frac{\mathrm{D}^{\bar{\iota}}(g_\alpha f_\alpha)}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} - \frac{1}{V}\int_{\Omega_\alpha} \frac{\mathrm{D}^{\bar{\iota}}\left(g_\alpha f^{\bar{\bar{\alpha}}}\right)}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} \\ &\quad - \frac{1}{V}\int_{\Omega_\alpha} \frac{\mathrm{D}^{\bar{\iota}} g_\alpha}{\mathrm{D}t} f_\alpha\,\mathrm{d}\mathbf{r} + \frac{1}{V}\int_{\Omega_\alpha} \frac{\mathrm{D}^{\bar{\iota}} g_\alpha}{\mathrm{D}t} f^{\bar{\bar{\alpha}}}\,\mathrm{d}\mathbf{r}\end{aligned} \tag{17}$$

Consider terms from the RHS of Eq. (17) in turn and simplify. The first term can be written as

$$\frac{1}{V}\int_{\Omega_\alpha} \frac{\mathrm{D}^{\bar{\iota}}(g_\alpha f_\alpha)}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} = \frac{1}{V}\int_{\Omega_\alpha} \frac{\partial(g_\alpha f_\alpha)}{\partial t}\,\mathrm{d}\mathbf{r} + \frac{1}{V}\int_{\Omega_\alpha} \mathbf{v}^{\bar{\iota}}\cdot\nabla(g_\alpha f_\alpha)\,\mathrm{d}\mathbf{r}. \tag{18}$$

Application of Theorem 4 to the first term on the RHS of Eq. (18) gives

$$\frac{1}{V}\int_{\Omega_\alpha} \frac{\partial(g_\alpha f_\alpha)}{\partial t}\,\mathrm{d}\mathbf{r} = \frac{\partial}{\partial t}\left(\frac{1}{V}\int_{\Omega_\alpha} g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}\right) - \sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\cdot\mathbf{v}_{\alpha\beta} g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}. \tag{19}$$

Now employ Theorem 3 to rearrange the second term on the RHS of Eq. (18) to

$$\frac{1}{V}\int_{\Omega_\alpha} \mathbf{v}^{\bar{\iota}}\cdot\nabla(g_\alpha f_\alpha)\,\mathrm{d}\mathbf{r} = \mathbf{v}^{\bar{\iota}}\cdot\nabla\left(\frac{1}{V}\int_{\Omega_\alpha} g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}\right) + \sum_{\beta\neq\alpha}\mathbf{v}^{\bar{\iota}}\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}\right). \tag{20}$$

Combining Eqs. (19) and (20) allows Eq. (18) to be written as

$$\begin{aligned}\frac{1}{V}\int_{\Omega_\alpha} \frac{\mathrm{D}^{\bar{\iota}}(g_\alpha f_\alpha)}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} &= \frac{\partial}{\partial t}\left(\frac{1}{V}\int_{\Omega_\alpha} g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}\right) + \mathbf{v}^{\bar{\iota}}\cdot\nabla\left(\frac{1}{V}\int_{\Omega_\alpha} g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}\right) \\ &\quad + \sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\cdot\left(\mathbf{v}^{\bar{\iota}} - \mathbf{v}_{\alpha\beta}\right) g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}.\end{aligned} \tag{21}$$

Next consider the second term on the RHS of Eq. (17), which can be expanded to

$$\frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\imath}}\left(g_\alpha f^{\bar{\bar{\alpha}}}\right)}{\mathrm{D}t}\mathrm{d}\mathbf{r}=\frac{1}{V}\int_{\Omega_\alpha}\frac{\partial\left(g_\alpha f^{\bar{\bar{\alpha}}}\right)}{\partial t}\mathrm{d}\mathbf{r}+\frac{1}{V}\int_{\Omega_\alpha}\mathbf{v}^{\bar{\imath}}\cdot\nabla\left(g_\alpha f^{\bar{\bar{\alpha}}}\right)\mathrm{d}\mathbf{r}. \tag{22}$$

Applying Theorems 3 and 4 to the RHS of Eq. (22) and rearranging gives

$$\frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\imath}}\left(g_\alpha f^{\bar{\bar{\alpha}}}\right)}{\mathrm{D}t}\mathrm{d}\mathbf{r}=\frac{\partial}{\partial t}\left(\frac{1}{V}\int_{\Omega_\alpha}g_\alpha f^{\bar{\bar{\alpha}}}\mathrm{d}\mathbf{r}\right)+\mathbf{v}^{\bar{\imath}}\cdot\nabla\left(\frac{1}{V}\int_{\Omega_\alpha}g_\alpha f^{\bar{\bar{\alpha}}}\mathrm{d}\mathbf{r}\right)+\sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot\left(\mathbf{v}^{\bar{\imath}}-\mathbf{v}_{\alpha\beta}\right)g_\alpha f^{\bar{\bar{\alpha}}}\mathrm{d}\mathbf{r} \tag{23}$$

or

$$\frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\imath}}\left(g_\alpha f^{\bar{\bar{\alpha}}}\right)}{\mathrm{D}t}\mathrm{d}\mathbf{r}=\frac{\mathrm{D}^{\bar{\imath}}\left(\epsilon^\alpha g^\alpha f^{\bar{\bar{\alpha}}}\right)}{\mathrm{D}t}+\sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot\left(\mathbf{v}^{\bar{\imath}}-\mathbf{v}_{\alpha\beta}\right)g_\alpha f^{\bar{\bar{\alpha}}}\mathrm{d}\mathbf{r}. \tag{24}$$

The third term on the RHS of Eq. (17) is the product of a microscale quantity and the material derivative of a microscale quantity, which cannot be simplified in any obvious manner.

Finally, consider the fourth term on the RHS of Eq. (17), which can be written as

$$\frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\imath}}g_\alpha}{\mathrm{D}t}f^{\bar{\bar{\alpha}}}\mathrm{d}\mathbf{r}=\frac{1}{V}\int_{\Omega_\alpha}\frac{\partial g_\alpha}{\partial t}f^{\bar{\bar{\alpha}}}\mathrm{d}\mathbf{r}+\frac{1}{V}\int_{\Omega_\alpha}\mathbf{v}^{\bar{\imath}}\cdot\nabla g_\alpha f^{\bar{\bar{\alpha}}}\mathrm{d}\mathbf{r}. \tag{25}$$

Application of Theorems 3 and 4 to the RHS of Eq. (25) gives

$$\frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\imath}}g_\alpha}{\mathrm{D}t}f^{\bar{\bar{\alpha}}}\mathrm{d}\mathbf{r}=\frac{\partial}{\partial t}\left(\frac{1}{V}\int_{\Omega_\alpha}g_\alpha\,\mathrm{d}\mathbf{r}\right)f^{\bar{\bar{\alpha}}}+\mathbf{v}^{\bar{\imath}}\cdot\nabla\left(\frac{1}{V}\int_{\Omega_\alpha}g_\alpha\,\mathrm{d}\mathbf{r}\right)f^{\bar{\bar{\alpha}}}+\sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot(\mathbf{v}^{\bar{\imath}}-\mathbf{v}_{\alpha\beta})g_\alpha f^{\bar{\bar{\alpha}}}\mathrm{d}\mathbf{r} \tag{26}$$

or

$$\frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\imath}}g_\alpha}{\mathrm{D}t}f^{\bar{\bar{\alpha}}}\mathrm{d}\mathbf{r}=\frac{\mathrm{D}^{\bar{\imath}}(\epsilon^\alpha g^\alpha)}{\mathrm{D}t}f^{\bar{\bar{\alpha}}}+\sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot(\mathbf{v}^{\bar{\imath}}-\mathbf{v}_{\alpha\beta})g_\alpha f^{\bar{\bar{\alpha}}}\mathrm{d}\mathbf{r}. \tag{27}$$

Substituting Eqs. (21), (24), and (27) into Eq. (17) yields

$$\frac{1}{V}\int_{\Omega_\alpha}g_\alpha\frac{\mathrm{D}^{\bar{\imath}}(f_\alpha-f^{\bar{\bar{\alpha}}})}{\mathrm{D}t}\mathrm{d}\mathbf{r}=\frac{\partial}{\partial t}\left(\frac{1}{V}\int_{\Omega_\alpha}g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}\right)+\mathbf{v}^{\bar{\imath}}\cdot\nabla\left(\frac{1}{V}\int_{\Omega_\alpha}g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}\right)+\sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot(\mathbf{v}^{\bar{\imath}}-\mathbf{v}_{\alpha\beta})g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}-\frac{\mathrm{D}^{\bar{\imath}}(\epsilon^\alpha g^\alpha f^{\bar{\bar{\alpha}}})}{\mathrm{D}t}-\frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\imath}}g_\alpha}{\mathrm{D}t}f_\alpha\,\mathrm{d}\mathbf{r}+\frac{\mathrm{D}^{\bar{\imath}}(\epsilon^\alpha g^\alpha)}{\mathrm{D}t}f^{\bar{\bar{\alpha}}}. \tag{28}$$

The fact that

$$\frac{\partial}{\partial t}\left(\frac{1}{V}\int_{\Omega_\alpha}g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}\right)+\mathbf{v}^{\bar{\imath}}\cdot\nabla\left(\frac{1}{V}\int_{\Omega_\alpha}g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}\right)=\frac{\mathrm{D}^{\bar{\imath}}[\epsilon^\alpha(g_\alpha f_\alpha)^\alpha]}{\mathrm{D}t}, \tag{29}$$

allows for rearrangement of Eq. (28) to

$$\frac{1}{V}\int_{\Omega_\alpha}g_\alpha\frac{\mathrm{D}^{\bar{\imath}}(f_\alpha-f^{\bar{\bar{\alpha}}})}{\mathrm{D}t}\mathrm{d}\mathbf{r}=\frac{\mathrm{D}^{\bar{\imath}}\left\{\epsilon^\alpha\left[(g_\alpha f_\alpha)^\alpha-g^\alpha f^{\bar{\bar{\alpha}}}\right]\right\}}{\mathrm{D}t}+\frac{\mathrm{D}^{\bar{\imath}}(\epsilon^\alpha g^\alpha)}{\mathrm{D}t}f^{\bar{\bar{\alpha}}}-\frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\imath}}g_\alpha}{\mathrm{D}t}f_\alpha\,\mathrm{d}\mathbf{r}+\sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot(\mathbf{v}^{\bar{\imath}}-\mathbf{v}_{\alpha\beta})g_\alpha f_\alpha\,\mathrm{d}\mathbf{r} \tag{30}$$

which is the identity given in Theorem 5. □

Several corollaries to Theorem 5 can be proven. A subset of these will be used routinely in deriving TCAT-based models.

**Corollary 1.** (MC[3,(3,0),0]) *The volume average of a material derivative referenced to the macroscale mass average velocity of an entity $\imath$ of the difference between a microscale quantity $f_\alpha$ and its intrinsic volume average $f^\alpha$ can be expressed as a function of relative velocities at interfacial boundaries and macroscale quantities of the form*

$$\frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\imath}}(f_\alpha-f^\alpha)}{\mathrm{D}t}\mathrm{d}\mathbf{r}=\sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot(\mathbf{v}^{\bar{\imath}}-\mathbf{v}_{\alpha\beta})(f_\alpha-f^\alpha)\,\mathrm{d}\mathbf{r}=\sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot(\mathbf{v}^{\bar{\imath}}-\mathbf{v}_{\alpha\beta})f_\alpha\,\mathrm{d}\mathbf{r}+f^\alpha\frac{\mathrm{D}^{\bar{\imath}}\epsilon^\alpha}{\mathrm{D}t}, \tag{31}$$

*where $\mathbf{v}^{\bar{\imath}}$ is the macroscale mass averaged velocity of entity $\imath$, $\mathbf{n}_\alpha$ is the microscale normal vector pointing outward from the $\alpha$ phase, $\mathbf{n}_\alpha\cdot\mathbf{v}_{\alpha\beta}$ is the component of the microscale velocity of the $\alpha\beta$ interface normal to the interface, $V$ is independent of time and position and is the measure of the averaging domain $\Omega$, $\Omega_\alpha\subset\Omega$ is the phase volume of* *phase* $\alpha$, *and* $\Omega_{\alpha\beta}$ *is the interface between the* $\alpha$ *and* $\beta$ *phases.*

**Proof.** Theorem 5 is

$$\frac{1}{V}\int_{\Omega_\alpha} g_\alpha \frac{\mathrm{D}^{\bar{\iota}}(f_\alpha - f^{\bar{\bar{\alpha}}})}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} = \frac{\mathrm{D}^{\bar{\iota}}\left\{\epsilon^\alpha\left[(g_\alpha f_\alpha)^\alpha - g^\alpha f^{\bar{\bar{\alpha}}}\right]\right\}}{\mathrm{D}t} + \frac{\mathrm{D}^{\bar{\iota}}(\epsilon^\alpha g^\alpha)}{\mathrm{D}t} f^{\bar{\bar{\alpha}}} - \frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\iota}} g_\alpha}{\mathrm{D}t} f_\alpha\,\mathrm{d}\mathbf{r} + \sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot(\mathbf{v}^{\bar{\iota}} - \mathbf{v}_{\alpha\beta}) g_\alpha f_\alpha\,\mathrm{d}\mathbf{r}, \tag{32}$$

If $g_\alpha$ is a constant then $g_\alpha = g^\alpha = g$, and its derivative will be zero. Eq. (32) may then be divided by $g$ to eliminate it and obtain

$$\frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\iota}}(f_\alpha - f^{\bar{\bar{\alpha}}})}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} = \frac{\mathrm{D}^{\bar{\iota}}\left[\epsilon^\alpha\left(f^\alpha - f^{\bar{\bar{\alpha}}}\right)\right]}{\mathrm{D}t} + \frac{\mathrm{D}^{\bar{\iota}}\epsilon^\alpha}{\mathrm{D}t} f^{\bar{\bar{\alpha}}} + \sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot(\mathbf{v}^{\bar{\iota}} - \mathbf{v}_{\alpha\beta}) f_\alpha\,\mathrm{d}\mathbf{r}, \tag{33}$$

where use has been made of the fact that $(f_\alpha)^\alpha$ is the intrinsic volume average $f^\alpha$. Now consider the case where the macroscale quantity $f^{\bar{\bar{\alpha}}}$ is the intrinsic volume average $f^\alpha$ and rearrange the order of the terms so that Eq. (33) simplifies to

$$\frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\iota}}(f_\alpha - f^\alpha)}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} = \sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot(\mathbf{v}^{\bar{\iota}} - \mathbf{v}_{\alpha\beta}) f_\alpha\,\mathrm{d}\mathbf{r} + f^\alpha\frac{\mathrm{D}^{\bar{\iota}}\epsilon^\alpha}{\mathrm{D}t} \tag{34}$$

which is the second identity in Corollary 1.

The last term on the RHS of Eq. (34) can be written as

$$f^\alpha\frac{\mathrm{D}^{\bar{\iota}}\epsilon^\alpha}{\mathrm{D}t} = f^\alpha\left(\frac{\partial\epsilon^\alpha}{\partial t} + \mathbf{v}^{\bar{\iota}}\cdot\nabla\epsilon^\alpha\right). \tag{35}$$

From Theorems 3 and 4 note that

$$f^\alpha\mathbf{v}^{\bar{\iota}}\cdot\nabla\epsilon^\alpha = f^\alpha\mathbf{v}^{\bar{\iota}}\cdot\nabla\left(\frac{1}{V}\int_{\Omega_\alpha}\mathrm{d}\mathbf{r}\right) = -f^\alpha\mathbf{v}^{\bar{\iota}}\cdot\left(\sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\,\mathrm{d}\mathbf{r}\right) \tag{36}$$

and

$$f^\alpha\frac{\partial\epsilon^\alpha}{\partial t} = f^\alpha\frac{\partial}{\partial t}\left(\frac{1}{V}\int_{\Omega_\alpha}\mathrm{d}\mathbf{r}\right) = f^\alpha\left(\sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot\mathbf{v}_{\alpha\beta}\,\mathrm{d}\mathbf{r}\right). \tag{37}$$

Combining Eqs. (34)–(37) gives

$$\frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\iota}}(f_\alpha - f^\alpha)}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} = \sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot(\mathbf{v}^{\bar{\iota}} - \mathbf{v}_{\alpha\beta})(f_\alpha - f^\alpha)\,\mathrm{d}\mathbf{r} \tag{38}$$

which is the first identity in Corollary 1, and this completes the proof. □

**Corollary 2.** (MV[3,(3,0),0]) *The volume average of a vector product of a microscale vector quantity* $\mathbf{g}_\alpha$ *with a material derivative referenced to the macroscale mass average velocity of an entity* $\iota$ *of the difference between a microscale vector quantity* $\mathbf{f}_\alpha$ *and a macroscale vector quantity* $\mathbf{f}^{\bar{\bar{\alpha}}}$ *can be expressed as a function of relative velocities at interfacial boundaries and macroscale quantities of the form*

$$\frac{1}{V}\int_{\Omega_\alpha}\mathbf{g}_\alpha\cdot\frac{\mathrm{D}^{\bar{\iota}}(\mathbf{f}_\alpha - \mathbf{f}^{\bar{\bar{\alpha}}})}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} = \frac{\mathrm{D}^{\bar{\iota}}\left\{\epsilon^\alpha\left[(\mathbf{g}_\alpha\cdot\mathbf{f}_\alpha)^\alpha - \mathbf{g}^\alpha\cdot\mathbf{f}^{\bar{\bar{\alpha}}}\right]\right\}}{\mathrm{D}t} + \frac{\mathrm{D}^{\bar{\iota}}(\epsilon^\alpha\mathbf{g}^\alpha)}{\mathrm{D}t}\cdot\mathbf{f}^{\bar{\bar{\alpha}}} - \frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\iota}}\mathbf{g}_\alpha}{\mathrm{D}t}\cdot\mathbf{f}_\alpha\,\mathrm{d}\mathbf{r} + \sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot(\mathbf{v}^{\bar{\iota}} - \mathbf{v}_{\alpha\beta})\mathbf{g}_\alpha\cdot\mathbf{f}_\alpha\,\mathrm{d}\mathbf{r} \tag{39}$$

*where* $\mathbf{v}^{\bar{\iota}}$ *is the macroscale mass averaged velocity of entity* $\iota$, $\mathbf{n}_\alpha$ *is the microscale normal vector pointing outward from the* $\alpha$ *phase,* $\mathbf{n}_\alpha\cdot\mathbf{v}_{\alpha\beta}$ *is the component of the microscale velocity of the* $\alpha\beta$ *interface normal to the interface,* $V$ *is independent of time and position and is the measure of the averaging domain* $\Omega$, $\Omega_\alpha\subset\Omega$ *is the phase volume of phase* $\alpha$, *and* $\Omega_{\alpha\beta}$ *is the interface between the* $\alpha$ *and* $\beta$ *phases.*

**Proof.** Proof of this corollary follows directly from the proof of Theorem 5 by extension to vector quantities. □

**Corollary 3.** (MT[3,(3,0),0]) *The volume average of a tensor product of a second-rank microscale tensor quantity* $\mathbf{g}_\alpha$ *with a material derivative referenced to the macroscale mass average velocity of an entity* $\iota$ *of the difference between a second-rank microscale tensor quantity* $\mathbf{f}_\alpha$ *and a second-rank macroscale tensor quantity* $\mathbf{f}^{\bar{\bar{\alpha}}}$ *can be expressed as a function of relative velocities at interfacial boundaries and macroscale quantities of the form*

$$\frac{1}{V}\int_{\Omega_\alpha}\mathbf{g}_\alpha : \frac{\mathrm{D}^{\bar{\iota}}(\mathbf{f}_\alpha - \mathbf{f}^{\bar{\bar{\alpha}}})}{\mathrm{D}t}\,\mathrm{d}\mathbf{r} = \frac{\mathrm{D}^{\bar{\iota}}\left\{\epsilon^\alpha[(\mathbf{g}_\alpha : \mathbf{f}_\alpha)^\alpha - \mathbf{g}^\alpha : \mathbf{f}^{\bar{\bar{\alpha}}}]\right\}}{\mathrm{D}t} + \frac{\mathrm{D}^{\bar{\iota}}(\epsilon^\alpha\mathbf{g}^\alpha)}{\mathrm{D}t} : \mathbf{f}^{\bar{\bar{\alpha}}} - \frac{1}{V}\int_{\Omega_\alpha}\frac{\mathrm{D}^{\bar{\iota}}\mathbf{g}_\alpha}{\mathrm{D}t} : \mathbf{f}_\alpha\,\mathrm{d}\mathbf{r} + \sum_{\beta\neq\alpha}\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\cdot(\mathbf{v}^{\bar{\iota}} - \mathbf{v}_{\alpha\beta})\mathbf{g}_\alpha : \mathbf{f}_\alpha\,\mathrm{d}\mathbf{r} \tag{40}$$

*where* $\mathbf{v}^{\bar{\iota}}$ *is the macroscale mass averaged velocity of entity* $\iota$, $\mathbf{n}_\alpha$ *is the microscale normal vector pointing outward from the* $\alpha$ *phase*, $\mathbf{n}_\alpha \cdot \mathbf{v}_{\alpha\beta}$ *is the component of the microscale velocity of the* $\alpha\beta$ *interface normal to the interface*, $V$ *is independent of time and position and is the measure of the averaging domain* $\Omega$, $\Omega_\alpha \subset \Omega$ *is the phase volume of phase* $\alpha$, *and* $\Omega_{\alpha\beta}$ *is the interface between the* $\alpha$ *and* $\beta$ *phases.*

**Proof.** Proof of this corollary follows directly from the proof of Theorem 5 by extension to tensor quantities. □

### 4.3.2. Multiscale deviations for an interface

Next we consider transformations of multiscale deviations for interface quantities. To aid the development of the theorem and corollaries of interest, the following previously derived theorems are of use [18]:

**Theorem 6.** (G[2,(3,0),0])

$$\int_{\Omega_{\alpha\beta}} \nabla' f_{\alpha\beta}\,\mathrm{d}\mathfrak{r} = \nabla \int_{\Omega_{\alpha\beta}} f_{\alpha\beta}\,\mathrm{d}\mathfrak{r} - \nabla\cdot\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha f_{\alpha\beta}\,\mathrm{d}\mathfrak{r} + \int_{\Omega_{\alpha\beta}} (\nabla'\cdot\mathbf{n}_\alpha)\mathbf{n}_\alpha f_{\alpha\beta}\,\mathrm{d}\mathfrak{r} + \sum_{\gamma\neq\alpha,\beta}\int_{\Omega_{\alpha\beta\gamma}} \mathbf{m}_{\alpha\beta} f_{\alpha\beta}\,\mathrm{d}\mathfrak{r}, \tag{41}$$

*where*

$$\nabla' = \nabla - \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot\nabla. \tag{42}$$

**Theorem 7.** (T[2,(3,0),0])

$$\int_{\Omega_{\alpha\beta}} \frac{\partial' f_{\alpha\beta}}{\partial t}\,\mathrm{d}\mathfrak{r} = \frac{\partial}{\partial t}\int_{\Omega_{\alpha\beta}} f_{\alpha\beta}\,\mathrm{d}\mathfrak{r} + \nabla\cdot\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot\mathbf{v}_{\alpha\beta} f_{\alpha\beta}\,\mathrm{d}\mathfrak{r} - \int_{\Omega_{\alpha\beta}} (\nabla'\cdot\mathbf{n}_\alpha)\mathbf{n}_\alpha\cdot\mathbf{v}_{\alpha\beta} f_{\alpha\beta}\,\mathrm{d}\mathfrak{r} - \sum_{\gamma\neq\alpha,\beta}\int_{\Omega_{\alpha\beta\gamma}} \mathbf{m}_{\alpha\beta}\cdot\mathbf{v}_{\alpha\beta\gamma} f_{\alpha\beta}\,\mathrm{d}\mathfrak{r}, \tag{43}$$

*where*

$$\frac{\partial'}{\partial t} = \frac{\partial}{\partial t} + \mathbf{v}_{\alpha\beta}\cdot\mathbf{n}_\alpha\mathbf{n}_\alpha\cdot\nabla. \tag{44}$$

Where integration is performed over all the $\alpha\beta$ interface within macroscale volume $\Omega$, $\mathbf{n}_\alpha$ is the outward normal vector from the $\alpha$ phase on the $\alpha\beta$ interface, $\mathbf{m}_{\alpha\beta}$ is orthogonal to $\mathbf{n}_\alpha$ and is the outward normal vector from the $\alpha\beta$ interface along its edge, $\nabla'$ is the microscale surficial del operator on the $\alpha\beta$ interface, $\mathbf{f}'_{\alpha\beta} = \mathbf{f}_{\alpha\beta} - \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot\mathbf{f}_{\alpha\beta}$ is a microscale vector that is tangent to the $\alpha\beta$ interface, the operator $\partial'/\partial t$ denotes the partial derivative with respect to time for a point fixed to a moving interface, and $\mathbf{m}_{\alpha\beta}\cdot\mathbf{v}_{\alpha\beta\gamma}$ is both the component of the velocity of the $\alpha\beta\gamma$ common curve bounding the $\alpha\beta$ interface in the direction tangent to the interface but normal to its edge and the component of the velocity of the material in the $\alpha\beta\gamma$ common curve in the same direction. The summation in these equations indicates that the common curve integrations are performed over all curves forming the boundary of the $\alpha\beta$ interface.

**Theorem 8.** (M[2,(3,0),0]) *The volume average of a product of a microscale quantity* $g_{\alpha\beta}$ *with a material derivative, referenced to the macroscale mass average velocity of an entity* $\iota$, *restricted to a position on a potentially moving interface* $\alpha\beta$ *of the difference between a microscale quantity* $f_{\alpha\beta}$ *and a macroscale quantity* $f^{\overline{\overline{\alpha\beta}}}$ *can be expressed as a function of relative velocities and macroscale quantities of the form*

$$\begin{aligned}
\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}'^{\bar{\iota}}(f_{\alpha\beta} - f^{\overline{\overline{\alpha\beta}}})}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}
&= \frac{\mathrm{D}^{\bar{\iota}}\left\{\epsilon^{\alpha\beta}\left[(g_{\alpha\beta}f_{\alpha\beta})^{\alpha\beta} - g^{\alpha\beta}f^{\overline{\overline{\alpha\beta}}}\right]\right\}}{\mathrm{D}t} + \frac{\mathrm{D}^{\bar{\iota}}(\epsilon^{\alpha\beta}g^{\alpha\beta})}{\mathrm{D}t}f^{\overline{\overline{\alpha\beta}}} \\
&\quad + \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta} - \mathbf{v}^{\bar{\iota}})g_{\alpha\beta}(f_{\alpha\beta} - f^{\overline{\overline{\alpha\beta}}})\,\mathrm{d}\mathfrak{r}\right) \\
&\quad + \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot\left(\mathbf{v}_{\alpha\beta} - \mathbf{v}^{\bar{\iota}}\right)g_{\alpha\beta}\,\mathrm{d}\mathfrak{r}\right)f^{\overline{\overline{\alpha\beta}}} \\
&\quad - \frac{1}{V}\int_{\Omega_{\alpha\beta}} (\nabla'\cdot\mathbf{n}_\alpha)\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta} - \mathbf{v}^{\bar{\iota}})g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}\mathfrak{r} \\
&\quad + \left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}f_{\alpha\beta}\mathbf{n}_\alpha\mathbf{n}_\alpha\,\mathrm{d}\mathfrak{r}\right) : \mathbf{d}^{\bar{\iota}} \\
&\quad - \sum_{\gamma\neq\alpha,\beta}\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} \mathbf{m}_{\alpha\beta}\cdot(\mathbf{v}_{\alpha\beta\gamma} - \mathbf{v}^{\bar{\iota}})g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}\mathfrak{r} \\
&\quad - \frac{1}{V}\int_{\Omega_{\alpha\beta}} \frac{\mathrm{D}'^{\bar{\iota}}g_{\alpha\beta}}{\mathrm{D}t}f_{\alpha\beta}\,\mathrm{d}\mathfrak{r},
\end{aligned} \tag{45}$$

*where* $\mathbf{v}^{\bar{\iota}}$ *is the macroscale mass averaged velocity of entity* $\iota$, $\epsilon^{\alpha\beta}$ *is the specific interfacial area of the* $\alpha\beta$ *interface*, $\mathbf{n}_\alpha$ *is the microscale unit vector normal to the* $\alpha\beta$ *interface pointing outward from the* $\alpha$ *phase*, $\mathbf{n}_\alpha\cdot\mathbf{v}_{\alpha\beta}$ *is the component of the microscale velocity of the* $\alpha\beta$ *interface normal to the interface*, $\mathbf{d}^{\bar{\iota}}$ *is the macroscale rate of strain tensor of entity* $\iota$, $\mathbf{m}_{\alpha\beta}$ *is a unit vector normal to the common curve edge of* $\alpha\beta$ *and tangent to* $\alpha\beta$, $V$ *is independent of time and position and is the measure of the averaging domain* $\Omega$, $\Omega_{\alpha\beta}$ *is the* $\alpha\beta$ *interface within* $\Omega$, $\Omega_{\alpha\beta\gamma}$ *for all* $\gamma$ *is the common curve that bounds* $\Omega_{\alpha\beta}$ *within* $\Omega$, *and* $\mathrm{D}'^{\bar{\iota}}/\mathrm{D}t$ *is a material derivative referenced to* $\mathbf{v}^{\bar{\iota}}$ *and restricted to the interface* $\alpha\beta$ *defined as*

$$\frac{\mathrm{D}'^{\bar{\iota}}}{\mathrm{D}t} = \frac{\partial'}{\partial t} + \mathbf{v}^{\bar{\iota}}\cdot\nabla' \tag{46}$$

**Proof.** Note that

$$\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}'^{\bar{\iota}}(f_{\alpha\beta}-f^{\overline{\overline{\alpha\beta}}})}{\mathrm{D}t}\,\mathrm{d}r = \frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}'^{\bar{\iota}}f_{\alpha\beta}}{\mathrm{D}t}\,\mathrm{d}r - \frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}'^{\bar{\iota}}f^{\overline{\overline{\alpha\beta}}}}{\mathrm{D}t}\,\mathrm{d}r, \tag{47}$$

where, based on definitions (42), (44) and (46),

$$\frac{\mathrm{D}'^{\bar{\iota}}}{\mathrm{D}t} = \frac{\partial}{\partial t} + (\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})\cdot\mathbf{n}_\alpha\mathbf{n}_\alpha\cdot\nabla + \mathbf{v}^{\bar{\iota}}\cdot\nabla = \frac{\mathrm{D}^{\bar{\iota}}}{\mathrm{D}t} + (\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})\cdot\mathbf{n}_\alpha\mathbf{n}_\alpha\cdot\nabla. \tag{48}$$

The first term on the RHS of Eq. (47) will be addressed first. Application of the product rule gives

$$\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}'^{\bar{\iota}}f_{\alpha\beta}}{\mathrm{D}t}\,\mathrm{d}r = \frac{1}{V}\int_{\Omega_{\alpha\beta}} \frac{\mathrm{D}'^{\bar{\iota}}(g_{\alpha\beta}f_{\alpha\beta})}{\mathrm{D}t}\,\mathrm{d}r - \frac{1}{V}\int_{\Omega_{\alpha\beta}} \frac{\mathrm{D}'^{\bar{\iota}}g_{\alpha\beta}}{\mathrm{D}t}f_{\alpha\beta}\,\mathrm{d}r. \tag{49}$$

Expand the derivative in the first term on the RHS making use of Eq. (46). Also, since $\mathbf{v}^{\bar{\iota}}$ is a macroscale quantity, it may be moved outside the integral such that Eq. (49) becomes

$$\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}'^{\bar{\iota}}f_{\alpha\beta}}{\mathrm{D}t}\,\mathrm{d}r = \frac{1}{V}\int_{\Omega_{\alpha\beta}} \frac{\partial'(g_{\alpha\beta}f_{\alpha\beta})}{\partial t}\,\mathrm{d}r + \mathbf{v}^{\bar{\iota}}\cdot\frac{1}{V}\int_{\Omega_{\alpha\beta}}\nabla'(g_{\alpha\beta}f_{\alpha\beta})\,\mathrm{d}r - \frac{1}{V}\int_{\Omega_{\alpha\beta}} \frac{\mathrm{D}'^{\bar{\iota}}g_{\alpha\beta}}{\mathrm{D}t}f_{\alpha\beta}\,\mathrm{d}r. \tag{50}$$

Applying Theorem 7 to the first integral and Theorem 6 to the second integral on the RHS of Eq. (50) yields

$$\begin{aligned}
\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}'^{\bar{\iota}}f_{\alpha\beta}}{\mathrm{D}t}\,\mathrm{d}r
&= \frac{\partial}{\partial t}\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r\right) + \nabla\cdot\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\mathbf{n}_\alpha\cdot\mathbf{v}_{\alpha\beta}g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r \\
&\quad - \frac{1}{V}\int_{\Omega_{\alpha\beta}}(\nabla'\cdot\mathbf{n}_\alpha)\mathbf{n}_\alpha\cdot\mathbf{v}_{\alpha\beta}g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r \\
&\quad - \sum_{\gamma\neq\alpha,\beta}\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\mathbf{m}_{\alpha\beta}\cdot\mathbf{v}_{\alpha\beta\gamma}g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r \\
&\quad + \mathbf{v}^{\bar{\iota}}\cdot\nabla\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r \\
&\quad - \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\mathbf{n}_\alpha g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r\right)\cdot\mathbf{v}^{\bar{\iota}} \\
&\quad + \frac{1}{V}\int_{\Omega_{\alpha\beta}}(\nabla'\cdot\mathbf{n}_\alpha)\mathbf{n}_\alpha\cdot\mathbf{v}^{\bar{\iota}}g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r \\
&\quad + \sum_{\gamma\neq\alpha,\beta}\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\mathbf{m}_{\alpha\beta}\cdot\mathbf{v}^{\bar{\iota}}g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r - \frac{1}{V}\int_{\Omega_{\alpha\beta}}\frac{\mathrm{D}'^{\bar{\iota}}g_{\alpha\beta}}{\mathrm{D}t}f_{\alpha\beta}\,\mathrm{d}r.
\end{aligned} \tag{51}$$

Apply the product rule to the third from the last term in Eq. (51) and make use of the fact that the macroscale velocity $\mathbf{v}^{\bar{\iota}}$ may be moved inside the integral such that

$$\begin{aligned}
\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\mathbf{n}_\alpha g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r\right)\cdot\mathbf{v}^{\bar{\iota}}
&= \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\mathbf{n}_\alpha\cdot\mathbf{v}^{\bar{\iota}}g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r\right) \\
&\quad - \left(\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\mathbf{n}_\alpha g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r\right):\mathbf{d}^{\bar{\iota}},
\end{aligned} \tag{52}$$

where $\mathbf{d}^{\bar{\iota}}$ is the rate of strain tensor defined as

$$\mathbf{d}^{\bar{\iota}} = \frac{1}{2}\left[\nabla\mathbf{v}^{\bar{\iota}} + (\nabla\mathbf{v}^{\bar{\iota}})^{\mathrm{T}}\right]. \tag{53}$$

Substitution of Eq. (52) into Eq. (51) and collection of terms provides

$$\begin{aligned}
\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}'^{\bar{\iota}}f_{\alpha\beta}}{\mathrm{D}t}\,\mathrm{d}r
&= \frac{\mathrm{D}'^{\bar{\iota}}\left[\epsilon^{\alpha\beta}\left(g_{\alpha\beta}f_{\alpha\beta}\right)^{\alpha\beta}\right]}{\mathrm{D}t} \\
&\quad + \nabla\cdot\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r \\
&\quad - \frac{1}{V}\int_{\Omega_{\alpha\beta}}(\nabla'\cdot\mathbf{n}_\alpha)\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r \\
&\quad - \sum_{\gamma\neq\alpha,\beta}\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\mathbf{m}_{\alpha\beta}\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\iota}})g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r \\
&\quad - \frac{1}{V}\int_{\Omega_{\alpha\beta}}\frac{\mathrm{D}'^{\bar{\iota}}g_{\alpha\beta}}{\mathrm{D}t}f_{\alpha\beta}\,\mathrm{d}r + \left(\frac{1}{V}\int_{\Omega_{\alpha\beta}}\mathbf{n}_\alpha\mathbf{n}_\alpha g_{\alpha\beta}f_{\alpha\beta}\,\mathrm{d}r\right):\mathbf{d}^{\bar{\iota}}.
\end{aligned} \tag{54}$$

Next consider the second term on the RHS of Eq. (47). Since the derivative is of a macroscale quantity, it may be expanded using the second equality in Eq. (48) giving

$$\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}'^{\bar{\iota}}f^{\overline{\overline{\alpha\beta}}}}{\mathrm{D}t}\,\mathrm{d}r = \frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}^{\bar{\iota}}f^{\overline{\overline{\alpha\beta}}}}{\mathrm{D}t}\,\mathrm{d}r + \frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})\cdot\mathbf{n}_\alpha\mathbf{n}_\alpha\cdot\nabla f^{\overline{\overline{\alpha\beta}}}\,\mathrm{d}r. \tag{55}$$

The material derivative in the first integral on the RHS and the gradient in the second integral are macroscopic expressions. Therefore, they may be moved outside the integrals. The remaining part of the first integral defines a surficial average such that the equation becomes

$$\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}'^{\bar{\iota}}f^{\overline{\overline{\alpha\beta}}}}{\mathrm{D}t}\,\mathrm{d}r = \epsilon^{\alpha\beta}g^{\alpha\beta}\frac{\mathrm{D}^{\bar{\iota}}f^{\overline{\overline{\alpha\beta}}}}{\mathrm{D}t} + \left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})\cdot\mathbf{n}_\alpha\mathbf{n}_\alpha\,\mathrm{d}r\right)\cdot\nabla f^{\overline{\overline{\alpha\beta}}}. \tag{56}$$

Then the product rule may be applied to both terms to obtain

$$\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}'^{\bar{\iota}} f^{\overline{\overline{\alpha\beta}}}}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}$$
$$= \frac{\mathrm{D}^{\bar{\iota}}\left[\epsilon^{\alpha\beta}(g^{\alpha\beta} f^{\overline{\overline{\alpha\beta}}})\right]}{\mathrm{D}t} - f^{\overline{\overline{\alpha\beta}}}\frac{\mathrm{D}^{\bar{\iota}}(\epsilon^{\alpha\beta} g^{\alpha\beta})}{\mathrm{D}t}$$
$$+ \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})g_{\alpha\beta} f^{\overline{\overline{\alpha\beta}}}\,\mathrm{d}\mathfrak{r}\right)$$
$$- \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})g_{\alpha\beta}\,\mathrm{d}\mathfrak{r}\right) f^{\overline{\overline{\alpha\beta}}}, \tag{57}$$

where $f^{\overline{\overline{\alpha\beta}}}$ has been moved inside the integral in the third term on the RHS.

Subtraction of Eq. (57) from Eq. (54) and collecting terms yields

$$\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta}\frac{\mathrm{D}'^{\bar{\iota}}(f_{\alpha\beta} - f^{\overline{\overline{\alpha\beta}}})}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}$$
$$= \frac{\mathrm{D}^{\bar{\iota}}\left\{\epsilon^{\alpha\beta}\left[(g_{\alpha\beta} f_{\alpha\beta})^{\alpha\beta} - g^{\alpha\beta} f^{\overline{\overline{\alpha\beta}}}\right]\right\}}{\mathrm{D}t} + \frac{\mathrm{D}^{\bar{\iota}}(\epsilon^{\alpha\beta} g^{\alpha\beta})}{\mathrm{D}t} f^{\overline{\overline{\alpha\beta}}}$$
$$+ \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})g_{\alpha\beta}(f_{\alpha\beta} - f^{\overline{\overline{\alpha\beta}}})\,\mathrm{d}\mathfrak{r}\right)$$
$$+ \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})g_{\alpha\beta}\,\mathrm{d}\mathfrak{r}\right) f^{\overline{\overline{\alpha\beta}}}$$
$$- \frac{1}{V}\int_{\Omega_{\alpha\beta}} (\nabla'\cdot\mathbf{n}_\alpha)\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})g_{\alpha\beta} f_{\alpha\beta}\,\mathrm{d}\mathfrak{r}$$
$$+ \left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} g_{\alpha\beta} f_{\alpha\beta}\mathbf{n}_\alpha\mathbf{n}_\alpha\,\mathrm{d}\mathfrak{r}\right) : \mathbf{d}^{\bar{\iota}}$$
$$- \sum_{\gamma\neq\alpha,\beta}\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} \mathbf{m}_{\alpha\beta}\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\iota}})g_{\alpha\beta} f_{\alpha\beta}\,\mathrm{d}\mathfrak{r}$$
$$- \frac{1}{V}\int_{\Omega_{\alpha\beta}} \frac{\mathrm{D}'^{\bar{\iota}} g_{\alpha\beta}}{\mathrm{D}t} f_{\alpha\beta}\,\mathrm{d}\mathfrak{r} \tag{58}$$

which completes the proof. □

**Corollary 4.** (MC[2, (3, 0), 0]) *The surface average of a material derivative referenced to a macroscale mass averaged velocity for entity* $\iota$ *and restricted to a position on a potentially moving interface* $\alpha\beta$ *of the difference between a microscale quantity* $f_{\alpha\beta}$ *and its intrinsic average* $f^{\alpha\beta}$ *can be expressed as a function of relative velocities at interfacial boundaries and macroscale quantities of the form*

$$\frac{1}{V}\int_{\Omega_{\alpha\beta}} \frac{\mathrm{D}'^{\bar{\iota}}(f_{\alpha\beta} - f^{\alpha\beta})}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}$$
$$= \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})(f_{\alpha\beta} - f^{\alpha\beta})\,\mathrm{d}\mathfrak{r}\right)$$
$$- \frac{1}{V}\int_{\Omega_{\alpha\beta}} (\nabla'\cdot\mathbf{n}_\alpha)\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})(f_{\alpha\beta} - f^{\alpha\beta})\,\mathrm{d}\mathfrak{r}$$
$$+ \left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} (f_{\alpha\beta} - f^{\alpha\beta})\mathbf{n}_\alpha\mathbf{n}_\alpha\,\mathrm{d}\mathfrak{r}\right) : \mathbf{d}^{\bar{\iota}}$$
$$- \sum_{\gamma\neq\alpha,\beta}\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} \mathbf{m}_{\alpha\beta}\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\iota}})(f_{\alpha\beta} - f^{\alpha\beta})\,\mathrm{d}\mathfrak{r}, \tag{59}$$

*where* $\mathbf{v}^{\bar{\iota}}$ *is the macroscale mass averaged velocity of entity* $\iota$, $\epsilon^{\alpha\beta}$ *is the specific interfacial area of the* $\alpha\beta$ *interface,* $\mathbf{n}_\alpha$ *is the microscale unit vector normal to the* $\alpha\beta$ *interface pointing outward from the* $\alpha$ *phase,* $\mathbf{n}_\alpha\cdot\mathbf{v}_{\alpha\beta}$ *is the component of the microscale velocity of the* $\alpha\beta$ *interface normal to the interface,* $\mathbf{d}^{\bar{\iota}}$ *is the macroscale rate of strain tensor of entity* $\iota$, $\mathbf{m}_{\alpha\beta}$ *is a unit vector normal to the common curve edge of* $\alpha\beta$ *and tangent to* $\alpha\beta$, $V$ *is independent of time and position and is the measure of the averaging domain* $\Omega$, $\Omega_{\alpha\beta}$ *is the* $\alpha\beta$ *interface within* $\Omega$, $\Omega_{\alpha\beta\gamma}$ *for all* $\gamma$ *is the common curve that bounds* $\Omega_{\alpha\beta}$ *within* $\Omega$, *and* $\mathrm{D}'^{\bar{\iota}}/\mathrm{D}t$ *is a material derivative referenced to* $\mathbf{v}^{\bar{\iota}}$ *and restricted to the interface* $\alpha\beta$.

**Proof.** Proof of this corollary follows directly from the proof of Theorem 8 with $g_{\alpha\beta} = 1$. Use is also made of Theorems 6 and 7 with $f_{\alpha\beta} = 1$. □

**Corollary 5.** (MV[2, (3, 0), 0]) *The volume average of a product of a microscale vector quantity* $\mathbf{g}_{\alpha\beta}$ *with a material derivative, referenced to the macroscale mass average velocity of an entity* $\iota$, *restricted to a position on a potentially moving interface* $\alpha\beta$ *of the difference between a microscale vector quantity* $\mathbf{f}_{\alpha\beta}$ *and a macroscale vector quantity* $\mathbf{f}^{\overline{\overline{\alpha\beta}}}$ *can be expressed as a function of relative velocities and macroscale quantities of the form*

$$\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{g}_{\alpha\beta}\cdot\frac{\mathrm{D}'^{\bar{\iota}}(\mathbf{f}_{\alpha\beta} - \mathbf{f}^{\overline{\overline{\alpha\beta}}})}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}$$
$$= \frac{\mathrm{D}^{\bar{\iota}}\left\{\epsilon^{\alpha\beta}\left[(\mathbf{g}_{\alpha\beta}\cdot\mathbf{f}_{\alpha\beta})^{\alpha\beta} - \mathbf{g}^{\alpha\beta}\cdot\mathbf{f}^{\overline{\overline{\alpha\beta}}}\right]\right\}}{\mathrm{D}t} + \frac{\mathrm{D}^{\bar{\iota}}(\epsilon^{\alpha\beta}\mathbf{g}^{\alpha\beta})}{\mathrm{D}t}\cdot\mathbf{f}^{\overline{\overline{\alpha\beta}}}$$
$$+ \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta}\cdot(\mathbf{f}_{\alpha\beta} - \mathbf{f}^{\overline{\overline{\alpha\beta}}})\,\mathrm{d}\mathfrak{r}\right)$$
$$+ \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta}\,\mathrm{d}\mathfrak{r}\right)\cdot\mathbf{f}^{\overline{\overline{\alpha\beta}}}$$
$$- \frac{1}{V}\int_{\Omega_{\alpha\beta}} (\nabla'\cdot\mathbf{n}_\alpha)\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta}\cdot\mathbf{f}_{\alpha\beta}\,\mathrm{d}\mathfrak{r}$$
$$+ \left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{g}_{\alpha\beta}\cdot\mathbf{f}_{\alpha\beta}\mathbf{n}_\alpha\mathbf{n}_\alpha\,\mathrm{d}\mathfrak{r}\right) : \mathbf{d}^{\bar{\iota}}$$
$$- \sum_{\gamma\neq\alpha,\beta}\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} \mathbf{m}_{\alpha\beta}\cdot(\mathbf{v}_{\alpha\beta}-\mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta}\cdot\mathbf{f}_{\alpha\beta}\,\mathrm{d}\mathfrak{r}$$
$$- \frac{1}{V}\int_{\Omega_{\alpha\beta}} \frac{\mathrm{D}^{\bar{\iota}}\mathbf{g}_{\alpha\beta}}{\mathrm{D}t}\cdot\mathbf{f}_{\alpha\beta}\,\mathrm{d}\mathfrak{r}, \tag{60}$$

*where $\mathbf{v}^{\bar{\iota}}$ is the macroscale mass averaged velocity of entity $\iota$, $\epsilon^{\alpha\beta}$ is the specific interfacial area of the $\alpha\beta$ interface, $\mathbf{n}_\alpha$ is the microscale unit vector normal to the $\alpha\beta$ interface pointing outward from the $\alpha$ phase, $\mathbf{n}_\alpha \cdot \mathbf{v}_{\alpha\beta}$ is the component of the microscale velocity of the $\alpha\beta$ interface normal to the interface, $\mathbf{d}^{\bar{\iota}}$ is the macroscale rate of strain tensor of entity $\iota$, $\mathbf{m}_{\alpha\beta}$ is a unit vector normal to the common curve edge of $\alpha\beta$ and tangent to $\alpha\beta$, $V$ is independent of time and position and is the measure of the averaging domain $\Omega$, $\Omega_{\alpha\beta}$ is the $\alpha\beta$ interface within $\Omega$, $\Omega_{\alpha\beta\gamma}$ for all $\gamma$ is the common curve that bounds $\Omega_{\alpha\beta}$ within $\Omega$, and $\mathrm{D}^{\prime\bar{\iota}}/\mathrm{D}t$ is a material derivative referenced to $\mathbf{v}^{\bar{\iota}}$ and restricted to the interface $\alpha\beta$.*

**Proof.** Proof of this corollary follows directly from the proof of Theorem 8 by extension to vector quantities. □

**Corollary 6.** (MT[2, (3, 0), 0]) *The volume average of a product of a second-rank microscale tensor quantity $\mathbf{g}_{\alpha\beta}$ with a material derivative, referenced to the macroscale mass average velocity of an entity $\iota$, restricted to a position on a potentially moving interface $\alpha\beta$ of the difference between a second-rank microscale tensor quantity $\mathbf{f}_{\alpha\beta}$ and a second-rank macroscale tensor quantity $\mathbf{f}^{\overline{\overline{\alpha\beta}}}$ can be expressed as a function of relative velocities and macroscale quantities of the form*

$$
\begin{aligned}
\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{g}_{\alpha\beta} : \frac{\mathrm{D}^{\prime\bar{\iota}}(\mathbf{f}_{\alpha\beta} - \mathbf{f}^{\overline{\overline{\alpha\beta}}})}{\mathrm{D}t}\,\mathrm{d}r
&= \frac{\mathrm{D}^{\bar{\iota}}\left\{\epsilon^{\alpha\beta}\left[(\mathbf{g}_{\alpha\beta} : \mathbf{f}_{\alpha\beta})^{\alpha\beta} - \mathbf{g}^{\alpha\beta} : \mathbf{f}^{\overline{\overline{\alpha\beta}}}\right]\right\}}{\mathrm{D}t} + \frac{\mathrm{D}^{\bar{\iota}}(\epsilon^{\alpha\beta}\mathbf{g}^{\alpha\beta})}{\mathrm{D}t} : \mathbf{f}^{\overline{\overline{\alpha\beta}}} \\
&\quad + \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta} - \mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta} : (\mathbf{f}_{\alpha\beta} - \mathbf{f}\overline{\overline{\alpha\beta}})\,\mathrm{d}r\right) \\
&\quad + \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{n}_\alpha\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta} - \mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta}\,\mathrm{d}r\right) : \mathbf{f}^{\overline{\overline{\alpha\beta}}} \\
&\quad - \frac{1}{V}\int_{\Omega_{\alpha\beta}} (\nabla'\cdot\mathbf{n}_\alpha)\mathbf{n}_\alpha\cdot(\mathbf{v}_{\alpha\beta} - \mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta} : \mathbf{f}_{\alpha\beta}\,\mathrm{d}r \\
&\quad + \left(\frac{1}{V}\int_{\Omega_{\alpha\beta}} \mathbf{g}_{\alpha\beta} : \mathbf{f}_{\alpha\beta}\mathbf{n}_\alpha\mathbf{n}_\alpha\,\mathrm{d}r\right) : \mathbf{d}^{\bar{\iota}} \\
&\quad - \sum_{\gamma\neq\alpha,\beta}\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} \mathbf{m}_{\alpha\beta}\cdot(\mathbf{v}_{\alpha\beta} - \mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta} : \mathbf{f}_{\alpha\beta}\,\mathrm{d}r \\
&\quad - \frac{1}{V}\int_{\Omega_{\alpha\beta}} \frac{\mathrm{D}^{\bar{\iota}}\mathbf{g}_{\alpha\beta}}{\mathrm{D}t} : \mathbf{f}_{\alpha\beta}\,\mathrm{d}r, \qquad (61)
\end{aligned}
$$

*where $\mathbf{v}^{\bar{\iota}}$ is the macroscale mass averaged velocity of entity $\iota$, $\epsilon^{\alpha\beta}$ is the specific interfacial area of the $\alpha\beta$ interface, $\mathbf{n}_\alpha$ is the microscale unit vector normal to the $\alpha\beta$ interface pointing outward from the $\alpha$ phase, $\mathbf{n}_\alpha \cdot \mathbf{v}_{\alpha\beta}$ is the component of the microscale velocity of the $\alpha\beta$ interface normal to the interface, $\mathbf{d}^{\bar{\iota}}$ is the macroscale rate of strain tensor of entity $\iota$, $\mathbf{m}_{\alpha\beta}$ is a unit vector normal to the common curve edge of $\alpha\beta$ and tangent to $\alpha\beta$, $V$ is independent of time and position and is the measure of the averaging domain $\Omega$, $\Omega_{\alpha\beta}$ is the $\alpha\beta$ interface within $\Omega$, $\Omega_{\alpha\beta\gamma}$ for all $\gamma$ is the common curve that bounds $\Omega_{\alpha\beta}$ within $\Omega$, and $\mathrm{D}^{\prime\bar{\iota}}/\mathrm{D}t$ is a material derivative referenced to $\mathbf{v}^{\bar{\iota}}$ and restricted to the interface $\alpha\beta$.*

**Proof.** Proof of this corollary follows directly from the proof of Theorem 8 by extension to tensor quantities. □

### *4.3.3. Multiscale deviations for a common curve*

Next we consider transformations of multiscale deviations for common curve quantities. To aid the development of the theorem and corollaries of interest, the following previously derived theorems are of use [18].

**Theorem 9.** (G[1, (3, 0), 0])

$$
\begin{aligned}
\int_{\Omega_{\alpha\beta\gamma}} \nabla'' f_{\alpha\beta\gamma}\,\mathrm{d}r &= \nabla\int_{\Omega_{\alpha\beta\gamma}} f_{\alpha\beta\gamma}\,\mathrm{d}r - \nabla\cdot\int_{\Omega_{\alpha\beta\gamma}} (\mathbf{I} - \mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma}) f_{\alpha\beta\gamma}\,\mathrm{d}r \\
&\quad - \int_{\Omega_{\alpha\beta\gamma}} \mathbf{l}_{\alpha\beta\gamma}\cdot\nabla''\mathbf{l}_{\alpha\beta\gamma} f_{\alpha\beta\gamma}\,\mathrm{d}r \\
&\quad + \sum_{\delta\neq\alpha,\beta,\gamma} (\mathbf{e}_{\alpha\beta\gamma} f_{\alpha\beta\gamma})|_{\alpha\beta\gamma\delta}, \qquad (62)
\end{aligned}
$$

*where*

$$\nabla'' = \mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma}\cdot\nabla. \qquad (63)$$

**Theorem 10.** (T[1, (3, 0), 0])

$$
\begin{aligned}
\int_{\Omega_{\alpha\beta\gamma}} \frac{\partial'' f_{\alpha\beta\gamma}}{\partial t}\,\mathrm{d}r
&= \frac{\partial}{\partial t}\int_{\Omega_{\alpha\beta\gamma}} f_{\alpha\beta\gamma}\,\mathrm{d}r + \nabla\cdot\int_{\Omega_{\alpha\beta\gamma}} (\mathbf{I} - \mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot\mathbf{v}_{\alpha\beta\gamma} f_{\alpha\beta\gamma}\,\mathrm{d}r \\
&\quad + \int_{\Omega_{\alpha\beta\gamma}} \mathbf{l}_{\alpha\beta\gamma}\cdot\nabla''\mathbf{l}_{\alpha\beta\gamma}\cdot\mathbf{v}_{\alpha\beta\gamma} f_{\alpha\beta\gamma}\,\mathrm{d}r \\
&\quad - \sum_{\delta\neq\alpha,\beta,\gamma} (\mathbf{e}_{\alpha\beta\gamma}\cdot\mathbf{v}_{\alpha\beta\gamma\delta} f_{\alpha\beta\gamma})|_{\alpha\beta\gamma\delta}, \qquad (64)
\end{aligned}
$$

*where*

$$\frac{\partial''}{\partial t} = \frac{\partial}{\partial t} + \mathbf{v}_{\alpha\beta\gamma}\cdot(\mathbf{I} - \mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot\nabla. \qquad (65)$$

Where integration is performed over all the $\alpha\beta\gamma$ common curve within macroscale volume $\Omega$, $\mathbf{l}_{\alpha\beta\gamma}$ is the unit vector tangent to the $\alpha\beta\gamma$ common curve, $\mathbf{e}_{\alpha\beta\gamma}$ is the unit vector tangent to the $\alpha\beta\gamma$ common curve oriented to be positive outward from the curve at its endpoints, $\nabla''$ is the microscale curvilinear del operator along the $\alpha\beta\gamma$ common curve, $\mathbf{f}''_{\alpha\beta\gamma} = \mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma}\cdot\mathbf{f}_{\alpha\beta\gamma}$ is the microscale vector component, tangent to the $\alpha\beta\gamma$ common curve, of a general microscale vector $\mathbf{f}_{\alpha\beta\gamma}$, $\mathbf{v}_{\alpha\beta\gamma\delta}$ is the microscale velocity of the $\alpha\beta\gamma\delta$ common point at the end of the common curve, the operator $\partial''/\partial t$ denotes the partial derivative with respect to time at a point fixed on the moving $\alpha\beta\gamma$ common curve, and $(\mathbf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot\mathbf{v}_{\alpha\beta\gamma}$ is both the velocity of the $\alpha\beta\gamma$ common curve normal to the curve, and the velocity of the material in the $\alpha\beta\gamma$ common curve normal to the curve. The summation in these equations indicates that the evaluations are performed at all the common points at the ends of common curves.

**Theorem 11.** (M[1, (3, 0), 0]) *The volume average of a product of a microscale quantity $g_{\alpha\beta\gamma}$ with a material derivative referenced to the macroscale mass average velocity of an entity $\imath$ restricted to a position on a potentially moving curve $\alpha\beta\gamma$ of the difference between a microscale quantity $f_{\alpha\beta\gamma}$ and a macroscale quantity $f^{\overline{\overline{\alpha\beta\gamma}}}$ can be expressed as a function of relative velocities and macroscale quantities of the form*

$$\begin{aligned}
&\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} g_{\alpha\beta\gamma}\frac{\mathrm{D}''^{\bar{\imath}}(f_{\alpha\beta\gamma}-f^{\overline{\overline{\alpha\beta\gamma}}})}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}\\
&\quad=\frac{\mathrm{D}^{\bar{\imath}}\left\{\epsilon^{\alpha\beta\gamma}\left[(g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})^{\alpha\beta\gamma}-g^{\alpha\beta\gamma}f^{\overline{\overline{\alpha\beta\gamma}}}\right]\right\}}{\mathrm{D}t}+\frac{\mathrm{D}^{\bar{\imath}}(\epsilon^{\alpha\beta\gamma}g^{\alpha\beta\gamma})}{\mathrm{D}t}f^{\overline{\overline{\alpha\beta\gamma}}}\\
&\qquad+\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\imath}})g_{\alpha\beta\gamma}(f_{\alpha\beta\gamma}-f^{\overline{\overline{\alpha\beta\gamma}}})\,\mathrm{d}\mathfrak{r}\right)\\
&\qquad+\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}_{\alpha\beta\gamma}\cdot\nabla''\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\imath}})g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\\
&\qquad+\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\imath}})g_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\right)f^{\overline{\overline{\alpha\beta\gamma}}}\\
&\qquad-\frac{1}{V}\sum_{\delta\neq\alpha,\beta,\gamma}[\mathbf{e}_{\alpha\beta\gamma}\cdot(\mathbf{v}_{\alpha\beta\gamma\delta}-\mathbf{v}^{\bar{\imath}})g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}]|_{\alpha\beta\gamma\delta}\\
&\qquad-\frac{1}{V}\int_{\Omega\alpha\beta\gamma}\frac{\mathrm{D}''^{\bar{\imath}}g_{\alpha\beta\gamma}}{\mathrm{D}t}f_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\\
&\qquad+\left(\frac{1}{V}\int_{\Omega\alpha\beta\gamma}(g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})(\mathbf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\,\mathrm{d}\mathfrak{r}\right):\mathbf{d}^{\bar{\bar{\imath}}},
\end{aligned}\tag{66}$$

*where $\mathbf{v}^{\bar{\imath}}$ is the macroscale mass averaged velocity of entity $\imath$, $\epsilon^{\alpha\beta\gamma}$ is the specific length of the $\alpha\beta\gamma$ common curve, $\mathbf{l}_{\alpha\beta\gamma}$ is the microscale unit vector tangent to the $\alpha\beta\gamma$ common curve, $(\mathbf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot\mathbf{v}_{\alpha\beta\gamma}$ is the component of the microscale velocity of the $\alpha\beta\gamma$ common curve normal to the curve, $\mathbf{d}^{\bar{\bar{\imath}}}$ is the macroscale rate of strain tensor of entity $\imath$, $\mathbf{e}_{\alpha\beta\gamma}$ is a unit vector tangent to common curve $\alpha\beta\gamma$ at its endpoints and positive outward from the curve, $V$ is independent of time and position and is the measure of the averaging domain $\Omega$, $\Omega_{\alpha\beta\gamma}$ is the $\alpha\beta\gamma$ common curve within $\Omega$, $\Omega_{\alpha\beta\gamma\delta}$ for all $\delta$ is the set of end points of the $\Omega_{\alpha\beta\gamma}$ common curve within $\Omega$, and $\mathrm{D}''^{\bar{\imath}}/\mathrm{D}t$ is a material derivative referenced to $\mathbf{v}^{\bar{\imath}}$ and restricted to the common curve $\alpha\beta\gamma$ defined as*

$$\frac{\mathrm{D}''^{\bar{\imath}}}{\mathrm{D}t}=\frac{\partial''}{\partial t}+\mathbf{v}^{\bar{\imath}}\cdot\nabla''.\tag{67}$$

**Proof.** Note that

$$\begin{aligned}
&\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} g_{\alpha\beta\gamma}\frac{\mathrm{D}''^{\bar{\imath}}(f_{\alpha\beta\gamma}-f^{\overline{\overline{\alpha\beta\gamma}}})}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}\\
&\quad=\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} g_{\alpha\beta\gamma}\frac{\mathrm{D}''^{\bar{\imath}}f_{\alpha\beta\gamma}}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}-\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} g_{\alpha\beta\gamma}\frac{\mathrm{D}''^{\bar{\imath}}f^{\overline{\overline{\alpha\beta\gamma}}}}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}.
\end{aligned}\tag{68}$$

Based on Eqs. (63), (65) and (67)

$$\begin{aligned}
\frac{\mathrm{D}''^{\bar{\imath}}}{\mathrm{D}t}&=\frac{\partial}{\partial t}+(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\imath}})\cdot(\mathbf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot\nabla+\mathbf{v}^{\bar{\imath}}\cdot\nabla\\
&=\frac{\mathrm{D}^{\bar{\imath}}}{\mathrm{D}t}+(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\imath}})\cdot(\mathbf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot\nabla.
\end{aligned}\tag{69}$$

Application of the product rule to the first term on the RHS of Eq. (68) yields

$$\begin{aligned}
\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} g_{\alpha\beta\gamma}\frac{\mathrm{D}''^{\bar{\imath}}f_{\alpha\beta\gamma}}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}&=\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\frac{\mathrm{D}''^{\bar{\imath}}(g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}\\
&\quad-\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\frac{\mathrm{D}''^{\bar{\imath}}g_{\alpha\beta\gamma}}{\mathrm{D}t}f_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}.
\end{aligned}\tag{70}$$

Expand the derivative in the first term on the RHS making use of Eq. (67). Also, since $\mathbf{v}^{\bar{\imath}}$ is a macroscale quantity, it may be moved outside the integral, such that Eq. (70) becomes

$$\begin{aligned}
\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} g_{\alpha\beta\gamma}\frac{\mathrm{D}''^{\bar{\imath}}f_{\alpha\beta\gamma}}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}&=\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\frac{\partial''(g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})}{\partial t}\,\mathrm{d}\mathfrak{r}\\
&\quad+\mathbf{v}^{\bar{\imath}}\cdot\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\nabla''(g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})\mathrm{d}\mathfrak{r}\\
&\quad-\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\frac{\mathrm{D}''^{\bar{\imath}}g_{\alpha\beta\gamma}}{\mathrm{D}t}f_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}.
\end{aligned}\tag{71}$$

Apply Theorems 10 and 9 to the first and second integrals on the RHS of Eq. (71), respectively, to obtain

$$\begin{aligned}
&\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} g_{\alpha\beta\gamma}\frac{\mathrm{D}''^{\bar{\imath}}f_{\alpha\beta\gamma}}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}\\
&\quad=\frac{\partial}{\partial t}\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\right)\\
&\qquad+\nabla\cdot\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot\mathbf{v}_{\alpha\beta\gamma}g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\\
&\qquad+\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}_{\alpha\beta\gamma}\cdot\nabla''\mathbf{l}_{\alpha\beta\gamma})\cdot\mathbf{v}_{\alpha\beta\gamma}g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\\
&\qquad-\frac{1}{V}\sum_{\delta\neq\alpha,\beta,\gamma}(\mathbf{e}_{\alpha\beta\gamma}\cdot\mathbf{v}_{\alpha\beta\gamma\delta}g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})|_{\alpha\beta\gamma\delta}\\
&\qquad+\mathbf{v}^{\bar{\imath}}\cdot\nabla\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\right)
\end{aligned}$$

$$-\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}\,\mathrm{d}\mathbf{r}\right)\cdot\mathbf{v}^{\bar{\bar{\imath}}}$$
$$-\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}_{\alpha\beta\gamma}\cdot\nabla''\mathbf{l}_{\alpha\beta\gamma})g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}\,\mathrm{d}\mathbf{r}\right)\cdot\mathbf{v}^{\bar{\bar{\imath}}}$$
$$+\frac{1}{V}\sum_{\delta\neq\alpha,\beta,\gamma}(\mathbf{e}_{\alpha\beta\gamma}g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})|_{\alpha\beta\gamma\delta}\cdot\mathbf{v}^{\bar{\bar{\imath}}}-\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\frac{D'''^{\bar{\bar{\imath}}}g_{\alpha\beta\gamma}}{\mathrm{D}t}f_{\alpha\beta\gamma}\,\mathrm{d}\mathbf{r}. \tag{72}$$

Apply the product rule to the third from the last term in Eq. (72) and make use of the fact that the macroscale velocity $\mathbf{v}^{\bar{\bar{\imath}}}$ may be moved inside the integral, such that

$$\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})(g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})\,\mathrm{d}\mathbf{r}\right)\cdot\mathbf{v}^{\bar{\bar{\imath}}}$$
$$=\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot\mathbf{v}^{\bar{\bar{\imath}}}(g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})\,\mathrm{d}\mathbf{r}\right)$$
$$-\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})(g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})\,\mathrm{d}\mathbf{r}\right):\mathbf{d}^{\bar{\bar{\imath}}}, \tag{73}$$

where $\mathbf{d}^{\bar{\bar{\imath}}}$ is the rate of strain tensor defined as

$$\mathbf{d}^{\bar{\bar{\imath}}}=\frac{1}{2}\left[\nabla\mathbf{v}^{\bar{\bar{\imath}}}+(\nabla\mathbf{v}^{\bar{\bar{\imath}}})^{\mathrm{T}}\right]. \tag{74}$$

Substitution of Eq. (73) into Eq. (72) and collection of terms gives

$$\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}g_{\alpha\beta\gamma}\frac{\mathrm{D}'''^{\bar{\bar{\imath}}}f_{\alpha\beta\gamma}}{\mathrm{D}t}\,\mathrm{d}\mathbf{r}$$
$$=\frac{\mathrm{D}^{\bar{\bar{\imath}}}\left[\epsilon^{\alpha\beta\gamma}(g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})^{\alpha\beta\gamma}\right]}{\mathrm{D}t}$$
$$+\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\bar{\imath}}})g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}\,\mathrm{d}\mathbf{r}\right)$$
$$+\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}_{\alpha\beta\gamma}\cdot\nabla''\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\bar{\imath}}})g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}\,\mathrm{d}\mathbf{r}$$
$$-\frac{1}{V}\sum_{\delta\neq\alpha,\beta,\gamma}[\mathbf{e}_{\alpha\beta\gamma}\cdot(\mathbf{v}_{\alpha\beta\gamma\delta}-\mathbf{v}^{\bar{\bar{\imath}}})g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}]|_{\alpha\beta\gamma\delta}$$
$$-\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\frac{D'''^{\bar{\bar{\imath}}}g_{\alpha\beta\gamma}}{\mathrm{D}t}f_{\alpha\beta\gamma}\,\mathrm{d}\mathbf{r}$$
$$+\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})(g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})\,\mathrm{d}\mathbf{r}\right):\mathbf{d}^{\bar{\bar{\imath}}}. \tag{75}$$

Next consider the second term on the RHS of Eq. (68). Since the derivative is of a macroscale quantity, it may be expanded using the second equality provided in Eq. (69) to obtain

$$\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}g_{\alpha\beta\gamma}\frac{\mathrm{D}'''^{\bar{\bar{\imath}}}f^{\overline{\overline{\alpha\beta\gamma}}}}{\mathrm{D}t}\,\mathrm{d}\mathbf{r}$$
$$=\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}g_{\alpha\beta\gamma}\frac{\mathrm{D}^{\bar{\bar{\imath}}}f^{\overline{\overline{\alpha\beta\gamma}}}}{\mathrm{D}t}\,\mathrm{d}\mathbf{r}$$
$$+\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}g_{\alpha\beta\gamma}(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\bar{\imath}}})\cdot(\mathbf{l}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot\nabla f^{\overline{\overline{\alpha\beta\gamma}}}\,\mathrm{d}\mathbf{r}. \tag{76}$$

The material derivative in the first integral on the RHS of Eq. (76) and the gradient in the second integral are macroscopic expressions. Therefore, they may be moved outside the integral. The remaining part of the first integral defines an average over the common curve such that the equation becomes

$$\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}g_{\alpha\beta\gamma}\frac{\mathrm{D}'''^{\bar{\bar{\imath}}}f^{\overline{\overline{\alpha\beta\gamma}}}}{\mathrm{D}t}\,\mathrm{d}\mathbf{r}$$
$$=\epsilon^{\alpha\beta\gamma}g^{\alpha\beta\gamma}\frac{\mathrm{D}^{\bar{\bar{\imath}}}f^{\overline{\overline{\alpha\beta\gamma}}}}{\mathrm{D}t}$$
$$+\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}g_{\alpha\beta\gamma}(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\bar{\imath}}})\cdot(\mathbf{l}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\,\mathrm{d}\mathbf{r}\right)\cdot\nabla f^{\overline{\overline{\alpha\beta\gamma}}}. \tag{77}$$

Then the product rule may be applied to both terms on the RHS of Eq. (77) to obtain

$$\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}g_{\alpha\beta\gamma}\frac{\mathrm{D}'''^{\bar{\bar{\imath}}}f^{\overline{\overline{\alpha\beta\gamma}}}}{\mathrm{D}t}\,\mathrm{d}\mathbf{r}$$
$$=\frac{\mathrm{D}^{\bar{\bar{\imath}}}\left[\epsilon^{\alpha\beta\gamma}(g^{\alpha\beta\gamma}f^{\overline{\overline{\alpha\beta\gamma}}})\right]}{\mathrm{D}t}-f^{\overline{\overline{\alpha\beta\gamma}}}\frac{\mathrm{D}^{\bar{\bar{\imath}}}(\epsilon^{\alpha\beta\gamma}g^{\alpha\beta\gamma})}{\mathrm{D}t}$$
$$+\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\bar{\imath}}})g_{\alpha\beta\gamma}f^{\overline{\overline{\alpha\beta\gamma}}}\,\mathrm{d}\mathbf{r}\right)$$
$$-\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\bar{\imath}}})g_{\alpha\beta\gamma}\,\mathrm{d}\mathbf{r}\right)f^{\overline{\overline{\alpha\beta\gamma}}}, \tag{78}$$

where the macroscale quantity $f^{\overline{\overline{\alpha\beta\gamma}}}$ has been moved inside the integral in the third term on the RHS. Subtraction of Eq. (78) from Eq. (75) and collection of terms gives

$$\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}g_{\alpha\beta\gamma}\frac{\mathrm{D}'''^{\bar{\bar{\imath}}}(f_{\alpha\beta\gamma}-f^{\overline{\overline{\alpha\beta\gamma}}})}{\mathrm{D}t}\,\mathrm{d}\mathbf{r}$$
$$=\frac{\mathrm{D}^{\bar{\bar{\imath}}}\left\{\epsilon^{\alpha\beta\gamma}[(g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})^{\alpha\beta\gamma}-g^{\alpha\beta\gamma}f^{\overline{\overline{\alpha\beta\gamma}}}]\right\}}{\mathrm{D}t}+\frac{\mathrm{D}^{\bar{\bar{\imath}}}(\epsilon^{\alpha\beta\gamma}g^{\alpha\beta\gamma})}{\mathrm{D}t}f^{\overline{\overline{\alpha\beta\gamma}}}$$
$$+\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\bar{\imath}}})g_{\alpha\beta\gamma}(f_{\alpha\beta\gamma}-f^{\overline{\overline{\alpha\beta\gamma}}})\,\mathrm{d}\mathbf{r}\right)$$

$$
\begin{aligned}
&+\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}_{\alpha\beta\gamma}\cdot\nabla''\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\iota}})g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\\
&+\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathsf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\iota}})g_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\right)f^{\overline{\overline{\alpha\beta\gamma}}}\\
&-\frac{1}{V}\sum_{\delta\neq\alpha,\beta,\gamma}\left[\mathbf{e}_{\alpha\beta\gamma}\cdot(\mathbf{v}_{\alpha\beta\gamma\delta}-\mathbf{v}^{\bar{\iota}})g_{\alpha\beta\gamma}f_{\alpha\beta\gamma}\right]|_{\alpha\beta\gamma\delta}\\
&-\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\frac{\mathrm{D}''^{\bar{\iota}}g_{\alpha\beta\gamma}}{\mathrm{D}t}f_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\\
&+\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(g_{\alpha\beta\gamma}f_{\alpha\beta\gamma})(\mathsf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\,\mathrm{d}\mathfrak{r}\right):\mathbf{d}^{\bar{\bar{\iota}}},
\end{aligned}
\tag{79}
$$

which completes the proof. □

**Corollary 7.** (MC[1,(3,0),0]) *The volume average of a material derivative referenced to the macroscale mass average velocity of an entity $\iota$ of the difference between a microscale quantity $f_{\alpha\beta\gamma}$ and its intrinsic volume average $f^{\alpha\beta\gamma}$ can be expressed as a function of relative velocities and macroscale quantities of the form*

$$
\begin{aligned}
&\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\frac{\mathrm{D}''^{\bar{\iota}}(f_{\alpha\beta\gamma}-f^{\alpha\beta\gamma})}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}\\
&\quad=\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathsf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\iota}})(f_{\alpha\beta\gamma}-f^{\alpha\beta\gamma})\,\mathrm{d}\mathfrak{r}\right)\\
&\qquad+\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}_{\alpha\beta\gamma}\cdot\nabla''\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\iota}})(f_{\alpha\beta\gamma}-f^{\alpha\beta\gamma})\,\mathrm{d}\mathfrak{r}\\
&\qquad-\frac{1}{V}\sum_{\delta\neq\alpha,\beta,\gamma}[\mathbf{e}_{\alpha\beta\gamma}\cdot(\mathbf{v}_{\alpha\beta\gamma\delta}-\mathbf{v}^{\bar{\iota}})(f_{\alpha\beta\gamma}-f^{\alpha\beta\gamma})]|_{\alpha\beta\gamma\delta}\\
&\qquad+\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathsf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})(f_{\alpha\beta\gamma}-f^{\alpha\beta\gamma})\,\mathrm{d}\mathfrak{r}\right):\mathbf{d}^{\bar{\bar{\iota}}},
\end{aligned}
\tag{80}
$$

*where $\mathbf{v}^{\bar{\iota}}$ is the macroscale mass averaged velocity of entity $\iota$, $\epsilon^{\alpha\beta\gamma}$ is the specific length of the $\alpha\beta\gamma$ common curve, $\mathbf{l}_{\alpha\beta\gamma}$ is the microscale unit vector tangent to the $\alpha\beta\gamma$ common curve, $(\mathsf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot\mathbf{v}_{\alpha\beta\gamma}$ is the component of the microscale velocity of the $\alpha\beta\gamma$ common curve normal to the curve, $\mathbf{d}^{\bar{\bar{\iota}}}$ is the macroscale rate of strain tensor of entity $\iota$, $\mathbf{e}_{\alpha\beta\gamma}$ is a unit vector tangent to common curve $\alpha\beta\gamma$ at its endpoints and positive outward from the curve, $V$ is independent of time and position and is the measure of the averaging domain $\Omega$, $\Omega_{\alpha\beta\gamma}$ is the $\alpha\beta\gamma$ common curve within $\Omega$, $\Omega_{\alpha\beta\gamma\delta}$ for all $\delta$ is the set of end points of the $\Omega_{\alpha\beta\gamma}$ common curve within $\Omega$, and $\mathrm{D}''^{\bar{\iota}}/\mathrm{D}t$ is a material derivative referenced to $\mathbf{v}^{\bar{\iota}}$ and restricted to the common curve $\alpha\beta\gamma$.*

**Proof.** This corollary follows directly from the proof of Theorem 11 with $g_{\alpha\beta\gamma}=1$. Use is also made of Theorems 9 and 10 with $f_{\alpha\beta}=1$. □

**Corollary 8.** (MV[1,(3,0),0]) *The volume average of a product of a microscale vector quantity $\mathbf{g}_{\alpha\beta\gamma}$ with a material derivative referenced to the macroscale mass average velocity of an entity $\iota$ restricted to a position on a potentially moving curve $\alpha\beta\gamma$ of the difference between a microscale vector quantity $\mathbf{f}_{\alpha\beta\gamma}$ and a macroscale vector quantity $\mathbf{f}^{\overline{\overline{\alpha\beta\gamma}}}$ can be expressed as a function of relative velocities and macroscale quantities of the form*

$$
\begin{aligned}
&\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\mathbf{g}_{\alpha\beta\gamma}\cdot\frac{\mathrm{D}''^{\bar{\iota}}(\mathbf{f}_{\alpha\beta\gamma}-f^{\overline{\overline{\alpha\beta\gamma}}})}{\mathrm{D}t}\,\mathrm{d}\mathfrak{r}\\
&\quad=\frac{\mathrm{D}^{\bar{\iota}}\left\{\epsilon^{\alpha\beta\gamma}\left[(\mathbf{g}_{\alpha\beta\gamma}\cdot\mathbf{f}_{\alpha\beta\gamma})^{\alpha\beta\gamma}-\mathbf{g}^{\alpha\beta\gamma}\cdot f^{\overline{\overline{\alpha\beta\gamma}}}\right]\right\}}{\mathrm{D}t}\\
&\qquad+\frac{\mathrm{D}^{\bar{\iota}}(\epsilon^{\alpha\beta\gamma}\mathbf{g}^{\alpha\beta\gamma})}{\mathrm{D}t}\cdot f^{\overline{\overline{\alpha\beta\gamma}}}\\
&\qquad+\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathsf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta\gamma}\cdot(\mathbf{f}_{\alpha\beta\gamma}-f^{\overline{\overline{\alpha\beta\gamma}}})\,\mathrm{d}\mathfrak{r}\right)\\
&\qquad+\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{l}_{\alpha\beta\gamma}\cdot\nabla''\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta\gamma}\cdot\mathbf{f}_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\\
&\qquad+\nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathsf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma}-\mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\right)\cdot\mathbf{f}^{\overline{\overline{\alpha\beta\gamma}}}\\
&\qquad-\frac{1}{V}\sum_{\delta\neq\alpha,\beta,\gamma}\left[\mathbf{e}_{\alpha\beta\gamma}\cdot(\mathbf{v}_{\alpha\beta\gamma\delta}-\mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta\gamma}\cdot\mathbf{f}_{\alpha\beta\gamma}\right]|_{\alpha\beta\gamma\delta}\\
&\qquad-\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}\frac{\mathrm{D}''^{\bar{\iota}}\mathbf{g}_{\alpha\beta\gamma}}{\mathrm{D}t}\cdot\mathbf{f}_{\alpha\beta\gamma}\,\mathrm{d}\mathfrak{r}\\
&\qquad+\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}}(\mathbf{g}_{\alpha\beta\gamma}\cdot\mathbf{f}_{\alpha\beta\gamma})(\mathsf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\,\mathrm{d}\mathfrak{r}\right):\mathbf{d}^{\bar{\bar{\iota}}},
\end{aligned}
\tag{81}
$$

*where $\mathbf{v}^{\bar{\iota}}$ is the macroscale mass averaged velocity of entity $\iota$, $\epsilon^{\alpha\beta\gamma}$ is the specific length of the $\alpha\beta\gamma$ common curve, $\mathbf{l}_{\alpha\beta\gamma}$ is the microscale unit vector tangent to the $\alpha\beta\gamma$ common curve, $(\mathsf{I}-\mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot\mathbf{v}_{\alpha\beta\gamma}$ is the component of the microscale velocity of the $\alpha\beta\gamma$ common curve normal to the curve, $\mathbf{d}^{\bar{\bar{\iota}}}$ is the macroscale rate of strain tensor of entity $\iota$, $\mathbf{e}_{\alpha\beta\gamma}$ is a unit vector tangent to common curve $\alpha\beta\gamma$ at its endpoints and positive outward from the curve, $V$ is independent of time and position and is the measure of the averaging domain $\Omega$, $\Omega_{\alpha\beta\gamma}$ is the $\alpha\beta\gamma$ common curve within $\Omega$, $\Omega_{\alpha\beta\gamma\delta}$ for all $\delta$ is the set of end points of the $\Omega_{\alpha\beta\gamma}$ common curve within $\Omega$, and $\mathrm{D}''^{\bar{\iota}}/\mathrm{D}t$ is a material derivative referenced to $\mathbf{v}^{\bar{\iota}}$ and restricted to the common curve $\alpha\beta\gamma$.*

**Proof.** Proof of this corollary follows directly from the proof of Theorem 11 by extension to vector quantities. □

**Corollary 9.** (MT[1,(3,0),0]) *The volume average of a product of a second-rank microscale tensor quantity $\mathbf{g}_{\alpha\beta\gamma}$ with a material derivative referenced to the macroscale mass average velocity of an entity $\iota$ restricted to a position on a potentially moving curve $\alpha\beta\gamma$ of the difference* *between a second-rank microscale tensor quantity $\mathbf{f}_{\alpha\beta\gamma}$ and a second-rank macroscale tensor quantity $\mathbf{f}^{\overline{\overline{\alpha\beta\gamma}}}$ can be expressed as a function of relative velocities and macroscale quantities of the form*

$$\begin{aligned}
&\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} \mathbf{g}_{\alpha\beta\gamma} : \frac{\mathrm{D}''^{\bar{\iota}}(\mathbf{f}_{\alpha\beta\gamma} - \mathbf{f}^{\overline{\overline{\alpha\beta\gamma}}})}{\mathrm{D}t}\mathrm{d}\mathbf{r} \\
&= \frac{\mathrm{D}^{\bar{\iota}}\left\{\epsilon^{\alpha\beta\gamma}\left[(\mathbf{g}_{\alpha\beta\gamma} : \mathbf{f}_{\alpha\beta\gamma})^{\alpha\beta\gamma} - \mathbf{g}^{\alpha\beta\gamma} : \mathbf{f}^{\overline{\overline{\alpha\beta\gamma}}}\right]\right\}}{\mathrm{D}t} \\
&\quad + \frac{\mathrm{D}^{\bar{\iota}}(\epsilon^{\alpha\beta\gamma}\mathbf{g}^{\alpha\beta\gamma})}{\mathrm{D}t} : \mathbf{f}^{\overline{\overline{\alpha\beta\gamma}}} \\
&\quad + \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} (\mathbf{I} - \mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma} - \mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta\gamma} : (\mathbf{f}_{\alpha\beta\gamma} - \mathbf{f}^{\overline{\overline{\alpha\beta\gamma}}})\,\mathrm{d}\mathbf{r}\right) \\
&\quad + \frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} (\mathbf{l}_{\alpha\beta\gamma}\cdot\nabla''\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma} - \mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta\gamma} : \mathbf{f}_{\alpha\beta\gamma}\,\mathrm{d}\mathbf{r} \\
&\quad + \nabla\cdot\left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} (\mathbf{I} - \mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot(\mathbf{v}_{\alpha\beta\gamma} - \mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta\gamma}\,\mathrm{d}\mathbf{r}\right) : \mathbf{f}^{\overline{\overline{\alpha\beta\gamma}}} \\
&\quad - \frac{1}{V}\sum_{\delta\neq\alpha,\beta,\gamma} \left[\mathbf{e}_{\alpha\beta\gamma}\cdot(\mathbf{v}_{\alpha\beta\gamma\delta} - \mathbf{v}^{\bar{\iota}})\mathbf{g}_{\alpha\beta\gamma} : \mathbf{f}_{\alpha\beta\gamma}\right]\big|_{\alpha\beta\gamma\delta} \\
&\quad - \frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} \frac{\mathrm{D}''^{\bar{\iota}}\mathbf{g}_{\alpha\beta\gamma}}{\mathrm{D}t} : \mathbf{f}_{\alpha\beta\gamma}\,\mathrm{d}\mathbf{r} \\
&\quad + \left(\frac{1}{V}\int_{\Omega_{\alpha\beta\gamma}} (\mathbf{g}_{\alpha\beta\gamma} : \mathbf{f}_{\alpha\beta\gamma})(\mathbf{I} - \mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\,\mathrm{d}\mathbf{r}\right) : \mathbf{d}^{\bar{\bar{\iota}}},
\end{aligned} \tag{82}$$

*where $\mathbf{v}^{\bar{\iota}}$ is the macroscale mass averaged velocity of entity $\iota$, $\epsilon^{\alpha\beta\gamma}$ is the specific length of the $\alpha\beta\gamma$ common curve, $\mathbf{l}_{\alpha\beta\gamma}$ is the microscale unit vector tangent to the $\alpha\beta\gamma$ common curve, $(\mathbf{I} - \mathbf{l}_{\alpha\beta\gamma}\mathbf{l}_{\alpha\beta\gamma})\cdot\mathbf{v}_{\alpha\beta\gamma}$ is the component of the microscale velocity of the $\alpha\beta\gamma$ common curve normal to the curve, $\mathbf{d}^{\bar{\bar{\iota}}}$ is the macroscale rate of strain tensor of entity $\iota$, $\mathbf{e}_{\alpha\beta\gamma}$ is a unit vector tangent to common curve $\alpha\beta\gamma$ at its endpoints and positive outward from the curve, $V$ is independent of time and position and is the measure of the averaging domain $\Omega$, $\Omega_{\alpha\beta\gamma}$ is the $\alpha\beta\gamma$ common curve within $\Omega$, $\Omega_{\alpha\beta\gamma\delta}$ for all $\delta$ is the set of end points of the $\Omega_{\alpha\beta\gamma}$ common curve within $\Omega$, and $\mathrm{D}''^{\bar{\iota}}/\mathrm{D}t$ is a material derivative referenced to $\mathbf{v}^{\bar{\iota}}$ and restricted to the common curve $\alpha\beta\gamma$.*

**Proof.** Proof of this corollary follows directly from the proof of Theorem 11 by extension to tensor quantities. □

## 5. Discussion

The description of scales, averaging operators, summary of existing theorems, and proof of a new set of deviation theorems and corollaries has laid the foundation for a consistent, first-principles-based formulation of closed models that describe multiphase flow and transport phenomena. Future work will refer to the results collected in this paper and in the preceding paper in this series [19] as new closed models are built. The detailed calculations presented here will not be repeated in future works; rather, we will simply rely upon the final results.

As the goal of this series is to formulate a novel set of closed models, it seems reasonable to take stock of the work needed to do so. The work performed to date, along with previous efforts to derive conservation equations, is a sufficient foundation for a rather detailed exploration of single- and two-fluid-phase models. However, the additional work required to complete the analysis is nontrivial. For example, the application of this work to single-phase flow will require significant detailed calculations regarding the conversion of microscale thermodynamics to an appropriate macroscale form and the closure of the resultant model. Our preliminary efforts along these lines have revealed the necessity of utilizing some mathematical manipulations that are codified in this paper as theorems and their corollaries. This preliminary work has also shown conditions under which traditional models provide reasonable descriptions of the physics, when the models will be inadequate, and how more complete models can be formulated. We will report the details of this work in the near future.

## 6. Summary and conclusions

This work focused on the development of fundamental notions and basic mathematical identities needed to advance the TCAT approach. Specific items accomplished include the following:

- the systems of concern were described as deterministic systems with two distinct scales, a microscale, or pore scale, and a macroscale, or porous medium continuum scale;
- the entities involved in these systems were described to include phase volumes, interfaces, common curves, and common points;
- basic definitions and systems properties were summarized;
- a compact notation was introduced to enable concise model development and closure and was related to traditional notation for clarity;
- key available averaging theorems needed to produce models were summarized;
- several new averaging theorems and corollaries that can be used to developed TCAT-based models were listed and proven; and
- the current status of this work was placed in the context of future steps needed to produce complete, consistent, well-posed models of porous medium systems.

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