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The Reynolds transport theorem: Application to ecological compartment modeling and case study of ecosystem energetics

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ABSTRACT

The Reynolds transport theorem (RTT) from mathematics and engineering has a rich history of success in mass transport dynamics and traditional thermodynamics. This paper introduces RTT as a complementary approach to traditional compartmental methods used in ecological modeling and network analysis. A universal system equation for a generic flow quantity is developed into a generic open-system differential expression for conservation of energy. Nonadiabatic systems are defined and incorporated into control volume (CV) and control surface (CS) perspectives of RTT where reductive assumptions in empirical data are then formally introduced, reviewed, and appropriately implemented. Compartment models are abstract, time-dependent systems of simultaneous differential equations describing storage and flow of conservative quantities between interconnected entities (the compartments). As such, they represent a set of flexible and somewhat informal, assumptions, definitions, algebraic manipulations, and graphical depictions subject to influence and selectively parsed expression by the modeler. In comparison, RTT compartment models are more rigorous and formal integro-differential equations and graphics initiated by the RTT universal system equation, forcing an ordered identification of simplifying assumptions, ending with clearly identified depictions of the transfer and transport of conservative substances in physical space and time. They are less abstract in the rigor of their equation development leaving less ambiguity to modeler discretion. They achieve greater consistency with other RTT compartment style models while possibly generating greater conformity with physical reality. Characteristics of the RTT approach are compared with those of a traditional compartment model of energy flow in an intertidal oyster-reef community.

1. Introduction

Originating in the mathematical development of physiological tracer theory, linear differential equation systems with constant coefficients are integral throughout the historical development of ecological network theory. In particular, the origin of compartment modeling can be attributed to the need for descriptive and pictorial representation of these mathematical models and the ecosystems they represented (e.g., Teorell, 1937; Sheppard and Householder, 1951; Patten, 1964; Brylinsky, 1972). *Compartment models* (Matis et al., 1979; O'Neill, 1979) and their associated mathematics are widely used to represent ecological networks of *stocks* x_i ($i = 1, 2, \ldots, n$) and *flows* f_{ij} ($i, j = 1, 2, \ldots, n$) of conservative substances (energy or matter). Inter-compartmental flows are generated by boundary *inputs* z_j terminating in boundary *outputs* y_i. Compartments as stocks, that is, transient *storages* of conserved substances, have little inherent formalism beyond a mathematical description of their rates of change by ordinary differential or difference equations. Ultimately, the combined pictorial, descriptive, and mathematical relations (e.g., assumptions, boundaries) remain abstractions heavily influenced by the modeler. Yet clear and consistent equation development, understanding, and interpretation are fundamental to the advancement and interpretation of widely disparate ecological network analyses (e.g., Hannon, 1979; Fath and Patten, 1999b; Gattie et al., 2006a,b; Schramski et al., 2006, 2007). To increase the rigor and consistency of compartment modeling, we introduce a formalism cultivated in engineering to describe and quantify mass transport and thermodynamic processes. The *Reynolds transport theorem* (Reynolds, 1903), through its development of an Eulerian control volume (CV) perspective, is a mature approach that formalizes flow and storage regimes and their corresponding equation development, explicitly ties pictorial representations to the mathematical representations, and ultimately opens ecological compartment modeling to the wider field of transport

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analysis. Although the terms and concepts of *compartment model* and *Reynolds transport theorem* can include non-linear and variable-coefficient methods, the present introduction restricts its focus to linear, constant-coefficient models.

A short review of Reynolds transport theorem (RTT) specifically articulating the CV and control surface (CS) concept is followed by development of the RTT energy conservation equation. Where RTT's widely generated conservation equations serve in a first-principle capacity to the study of transport dynamics, the condensed development below is a hybrid of several textbook methods (e.g., White, 2006; Munson et al., 2009), with most of the presentation emanating from Janna's (1993) derivation. The latter focuses on the essential physics of the flows and is particularly easy to understand. While subsequently engaging in an ecosystem energetics discussion specifically facilitated using the RTT energy conservation equation, clarifying and simplifying assumptions for ecological compartmental analysis and subsequent ecological network analysis (ENA) are identified. The entire RTT–CV methodology is then illustrated by reformulating a compartment model of energy flow and storage of an intertidal oyster-reef community in South Carolina (Dame and Patten, 1981) from the CV perspective.

2. Reynolds transport theorem control volume—review

Lagrangian and Eulerian perspectives in model development are both applicable to the study of mass or energy transfer. Lagrangian methodology, impractical for most reasonable ecological analyses and their attainable supporting data (although see Tollner and Kazanci, 2007; Kazanci et al., 2008; Matamba et al., 2009 this issue, for a recent development), addresses each individual particle's relevant characteristic as a function of time. Contrastingly, an Eulerian or CV method is applicable to the study of entire regions (fields of particles) of transactional flows. A CV analysis of a specific region can be established through the RTT conversion relating the time derivative of a material volume (often called the *system* in RTT analysis but we refer to it as the environment) to the rate of change of a material quantity within a specified region known as the control volume. Theoretically, a material volume is a closed system where energy but not mass crosses its boundary. An open-system CV (mass and energy can cross its boundary), judiciously chosen to represent the respective region or network of study, is usually bounded by an artificial but mathematically meaningful CS separating the region of study from the surrounding material volume environment. In RTT computations, the CS's orientation and location, particularly in transport analysis (conservation of mass), is critical and mathematically relevant. Although this orientation characteristic may not be immediately useful for the flows associated with ecological compartment modeling or ecological network analysis (ENA), the consistency in the use and treatment of the CS with established conservation mathematics in other disciplines will complement ENAs clarity, understanding, and future usefulness. Pictorially similar to compartmental analysis, a fixed CS is usually shown as a dashed line surrounding the CV as demonstrated in Fig. 1. The objective is

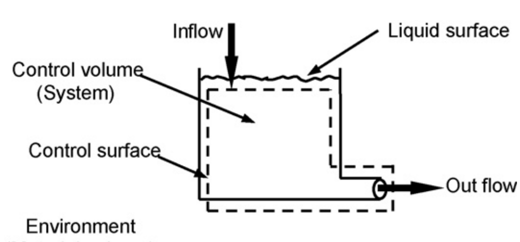

Fig. 1. Fixed control volume showing its corresponding control surface of liquid flowing through a holding tank.

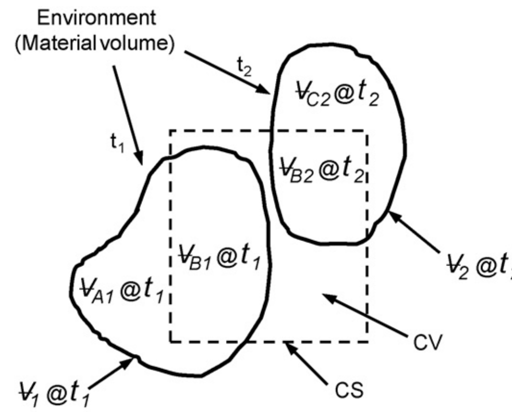

Fig. 2. The material volume, $\forall$, of an extensive property, S, at two sequential times, t_1 and t_2. The control volume of interest, $\forall_B$, is bounded by the control surface represented by a dashed line.

to relate the region outside the CS (environment) to that within the CV (system) and, by accounting for all of the mass or energy within the CV or crossing the CS, generate the conservation equations. The desired conversion derivation differs according to whether the control volume is fixed, deformable, or moving. For practicality within ENA and for the ease of presentation, we only articulate a fixed control volume derivation and application. The fixed CV procedure starts with the following universal integral equation as a closed environment of particles:

$$S_{\text{env}} = \iiint s\rho \, \mathrm{d}\forall. \tag{1}$$

Here, S_{env} is an extensive (mass dependent) conservative flow quantity (e.g., mass, energy, momentum, etc.) which we desire to monitor within a closed material volume environment, s is the corresponding intensive quantity (per unit mass–mass independent), ρ is the concentration or density (mass per unit volume), and $\forall$ is the environmental volume of interest. In Fig. 2, letting t be time, let the environmental volume at t_1, $\forall_1$, be represented by $\forall_{A1}$ plus $\forall_{B1}$, and later the volume at t_2, $\forall_2$, by $\forall_{B2}$ plus $\forall_{C2}$. The CV is bounded by the CS, represented by the dashed line. Change in the extensive property during the time interval t_1–t_2 can be written as,

$$\Delta S_{\text{env}} = (S_{B2} + S_{C2}) - (S_{A1} + S_{B1}). \tag{2}$$

Rearranging the terms to organize the extensive property inside and outside the prescribed CV, and dividing by the time interval, $\Delta t = t_2 - t_1$, the change in S per unit time is:

$$\left.\frac{\Delta S}{\Delta t}\right|_{\text{env}} = \frac{S_{B2} - S_{B1}}{\Delta t} + \frac{S_{C2} - S_{A1}}{\Delta t}. \tag{3}$$

The instantaneous rate of change is given in the limit:

$$\lim_{\Delta t \to 0} \left.\frac{\Delta S}{\Delta t}\right|_{\text{env}} = \lim_{\Delta t \to 0} \frac{S_{B2} - S_{B1}}{\Delta t} + \lim_{\Delta t \to 0} \frac{S_{C2} - S_{A1}}{\Delta t}, \tag{4}$$

where

$$\lim_{\Delta t \to 0} \left.\frac{\Delta S}{\Delta t}\right|_{\text{env}} = \left.\frac{\mathrm{d}S}{\mathrm{d}t}\right|_{\text{env}}. \tag{5}$$

The first right-hand-side term of (4) can be rewritten as the partial time rate of change of S within the control volume:

$$\lim_{\Delta t \to 0} \frac{S_{B2} - S_{B1}}{\Delta t} = \left.\frac{\partial S}{\partial t}\right|_{\text{CV}}. \tag{6}$$

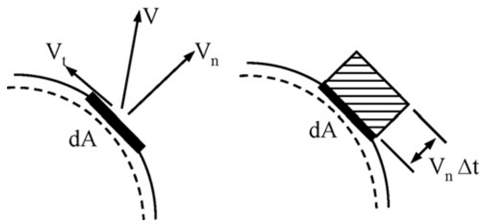

Fig. 3. Flow through a differential area dA of a control surface surrounding a control volume. V is the velocity of some entity through the differential area dA and is together comprised of its tangential V_t and normal V_n velocity components.

The second right-hand-side term in (4) represents the net rate of flow of S out of the control volume:

$$\lim_{\Delta t \to 0} \frac{S_{C2} - S_{A1}}{\Delta t} = \lim_{\Delta t \to 0} \frac{\delta S}{\Delta t}, \tag{7}$$

(where δ signifies the net rate out, a.k.a., out minus in). To obtain the specific limiting expression, this term requires additional manipulation using the Gauss–Green divergence theorem which converts the net flow out of the control volume to the specific flow of s along the portion of the perpendicular velocity vector V_n to the differential area element dA on the CS bounding the CV.

Consider Fig. 3 showing a differential area dA on the CS. The tangential velocity V_t carries no matter out of the CV by crossing the CS. All matter leaving dA can be assumed in the normal direction represented by the normal component of the velocity V_n. During Δt, the mass crossing dA is then:

$$\mathrm{d}m = \rho\, \mathrm{d}\forall \tag{8}$$

where, the differential volume is the three dimensional product of the cross-sectional area and height:

$$\mathrm{d}\forall = (V_n \Delta t)\, \mathrm{d}A. \tag{9}$$

Assuming the amount of S moving through the area dA is

$$\delta S = s\, \mathrm{d}m, \tag{10}$$

substitute (8) and (9) into (10) and divide through by Δt to obtain:

$$\frac{\delta S}{\Delta t} = s \rho V_n\, \mathrm{d}A. \tag{11}$$

In the limit as Δt approaches zero:

$$\lim_{\Delta t \to 0} \frac{\delta S}{\Delta t} = \iint_{CS} s \rho V_n\, \mathrm{d}A. \tag{12}$$

The main premise with the surface integral of (12) is that the CS and its location and orientation are relevant and critical to the mathematics describing the conservation equations in transport analysis. Although the choice of CS location and orientation remains with the modeler, the variation in its location is often used to a modeler's advantage. Substituting (5), (6), and (12) into (4) generates the general RTT conservation equation for an open control volume system:

$$\left.\frac{\mathrm{d}S}{\mathrm{d}t}\right|_{env} = \left.\frac{\partial S}{\partial t}\right|_{CV} + \iint_{CS} s \rho V_n\, \mathrm{d}A \tag{13}$$

In practical terms Eq. (13) states:

|instantaneous time rate of change of S in an environment of particles| = |instantaneous time rate of accumulation of *nonumber* S within the control volume| + |amount of S leaving the control volume minus the amount of S entering|

The difference between the time rate of change of S in the environment and the time rate of change of S in the CV is the net amount of S leaving the CV. The RTT–CV equation framework, extending and augmenting ecological compartmental analysis, allows for a consistent and clarifying elaboration of transport energetics, as shown next.

3. Reynolds transport theorem control volume—conservation of energy

Assumptions necessary to express the conservation equation for energy in a form compatible with ecological field data will serve to contrast the complexity of ecosystem energetics and existing modeling capabilities. Energy conservation in an adiabatic, closed system is given by:

$$\mathrm{d}W = (E_2 - E_1) = \mathrm{d}E. \tag{14}$$

The net work performed on the system, dW, is defined as the change in energy ($E_2 - E_1$) of the system, where E_1 and E_2 indicate initial and final states. Work, W, quantifies the interaction of a system with its surroundings (in effect, work crossing the system boundary) and includes, for example: shaft, electric and magnetic, viscous shear, or flow work. Numerous energy forms can constitute the total energy, E, of a macroscopic system including, for example: internal, kinetic, gravitational potential, electrostatic, chemical, nuclear, magnetic, or strain energy.

For a nonadiabatic, diathermic, closed system, energy conservation is defined as,

$$Q \equiv (E_2 - E_1) - W, \tag{15}$$

where the difference between the change of energy of the system and the work done on the system is the heat of interaction of the process (Q and W are positive for heat added to or work performed on the system). Rearranging (15), and writing in a differential form:

$$\mathrm{d}E = \mathrm{d}Q + \mathrm{d}W, \tag{16}$$

where dQ reflects the net energy transfer driven by the temperature difference between two systems. Actions commonly represented by dQ are radiation, convection, and conduction. The energy in a system (control volume, CV) changes by an amount equal to that which crosses the system boundary (control surface, CS) where energy can cross a boundary in the form of heat transfer (Q) or work (W) for the closed system of (16). To account for the mass flow of an open system, using (13) let $S = E$ and $s = E/m = e$ where the RTT open-system conservation of energy equation becomes,

$$\left.\frac{\mathrm{d}E}{\mathrm{d}t}\right|_{env} = \left.\frac{\partial E}{\partial t}\right|_{CV} + \iint_{CS} e \rho V_n\, \mathrm{d}A \tag{17}$$

Considering (16), for the control volume system coincident with the environment at an instant of time,

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \left[\frac{\mathrm{d}Q}{\mathrm{d}t} + \frac{\mathrm{d}W}{\mathrm{d}t}\right]_{env} = \left[\frac{\mathrm{d}Q}{\mathrm{d}t} + \frac{\mathrm{d}W}{\mathrm{d}t}\right]_{CV}, \tag{18}$$

Substituting (18) into (17) yields,

$$\left[\frac{\mathrm{d}Q}{\mathrm{d}t} + \frac{\mathrm{d}W}{\mathrm{d}t}\right]_{CV} = \left.\frac{\partial E}{\partial t}\right|_{CV} + \iint_{CS} e \rho V_n\, \mathrm{d}A, \tag{19}$$

where the heat transfer rate to the CV, dQ/dt, plus the rate of work performed on the CV, dW/dt, equals (for a non-steady-state system) the energy accumulation rate in the CV, $\partial E/\partial t|_{CV}$, plus the energy associated with mass entering or leaving the system across the CS, $\iint_{CS} e \rho V_n\, \mathrm{d}A$ (e.g., kinetic, potential, chemical, nuclear, etc.). Eq. (19) represents the first law of thermodynamics (law of conservation) for an open system. Thermodynamic analysis of a given open system involves independently evaluating the rates of heat transfer and work done on the system, the rate of energy accumulation, and changes in specific forms of energy associated with mass flows across the system's boundaries.

4. Conservation of energy—ecosystem energetics

Representing an ecosystem with a practical formulation of (19) is the next logical, but difficult, step. Ecosystem types vary widely and, correspondingly, are continuous tradeoffs between the rates of heat transfer dQ/dt, work dW/dt, energy stored $\partial E/\partial t|_{CV}$, and the energy associated with mass flow across CS boundaries, $\iint_{CS} e\rho V_n \, dA$. For example, consider solar radiation is converted to gravitational potential energy through the heating of water, subsequent evaporation, and ultimate precipitation. Atmospheric winds are the kinetic energy produced from the solar heating of the biosphere. Primary producers use solar radiation to convert raw materials of lower chemical energy (H_2O, CO_2) to higher energy compounds (e.g., carbohydrates). Secondary consumers use photosynthetic products to increase their biomass and produce useful work. Additional complexities exist in the widely variable inefficiencies in these processes lost to the greater environment as heat eventually radiated back to space. Although detailed energy balances of specific ecosystems or their components exist, for example, green leaves (Aber and Melillo, 2001) and bodies of water (the psychometric chart in all elementary thermodynamics texts), as of yet, data acquisition for network analyses of energy flow has been pragmatically limited to food-web style contact graphs (Odum, 1956, 1957; Tilly, 1968; Williams and Crouthamel, 1972; Dame and Patten, 1981; Martinez, 1995; Pimm, 2002).

The energetics of ecological network models are very limited or simplified. Most elements of heat transfer, work, and internal energy change are loosely combined into respiration. Except for primary producers, which convert electromagnetic energy to chemical energy, all flows crossing boundaries between other compartments are in the form of chemical energy (e.g., carbohydrates). Output flows, leaving the system boundary (no consumer available within the defined system), include energies associated with or grouped into component metabolism (basal and non-basal respiration), net component growth (e.g., Hannon, 1973), and exported biomass (e.g., mortality, food ingested but not assimilated, etc.). Variations exist on the groupings of these system-level output energy flows (e.g., Odum, 1957; Hannon, 1979, 1985; Dame and Patten, 1981), yet these groupings reveal little about the work, heat transfer, or energy of mass transfer associated with ecological processes.

5. Conservation of energy—ecological network analysis

The RTT–CV formulation of energy conservation is uniquely effective and accurate acknowledging the different types, and therefore to some extent the qualities, of energy potential, thus improving model presentation and communication. Compartment modeling in the general sense has not accomplished this, or at best, achieves this type of insight with difficulty (see later, oyster model example). However, reducing RTT's Eq. (19) with appropriate assumptions, into a typical ENA conservation equation capable of receiving the usual field data, compliments compartment modeling by providing insight into the gap between the expansive understanding of ecosystem energetics and the current methodologies used to model this activity. The rate of work dW/dt performed by or on an organism physically moving materials, or an abiotic compartment moving vertically closer to earth, is usually combined into the rate of heat transfer term dQ/dt representing incoming or outgoing energy not specifically associated with mass flow across a boundary (loosely qualified as respiration or solar radiation). Subsequently for compartment-modeling analysis, Eq. (19) consolidates to the following form for one-dimensional flow,

$$\left.\frac{dQ}{dt}\right|_{CV} = \left.\frac{\partial E}{\partial t}\right|_{CV} + \sum_{\substack{\text{out}\\ \text{CS}}} (\dot{m}e)_{\text{out}} - \sum_{\substack{\text{in}\\ \text{CS}}} (\dot{m}e)_{\text{in}} \tag{20}$$

Here, intensive or mass-specific energy, e (e.g., kJ/kg), and associated mass flow, $\dot{m}$ (e.g., kg/s), are combined in the concept of biomass, representing stored chemical energy. At steady-state, with no net accumulation of energy in the CV, $\partial E/\partial t|_{CV} = 0$, Eq. (20) is often simplified to,

$$\left.\frac{dQ}{dt}\right|_{CV} = \sum_{\substack{\text{out}\\ \text{CS}}} (\dot{m}e)_{\text{out}} - \sum_{\substack{\text{in}\\ \text{CS}}} (\dot{m}e)_{\text{in}} \tag{21}$$

where the rate of heat transfer from and to the system, $\pm dQ/dt|_{CV}$, could be confused with the missing rate of accumulation term, $\partial E/\partial t|_{CV}$. If the system is assumed adiabatic, $dQ/dt|_{CV}$, Eq. (20) becomes,

$$\left.\frac{\partial E}{\partial t}\right|_{CV} = \sum_{\substack{\text{in}\\ \text{CS}}} (\dot{m}e)_{\text{in}} - \sum_{\substack{\text{out}\\ \text{CS}}} (\dot{m}e)_{\text{out}}, \tag{22}$$

which is subtly but distinctly different than Eq. (21). Considering Eqs. (20)–(22), various forms of energy on the left-hand sides—e.g., inputs, $+dQ/dt$, as radiation, outputs, $-dQ/dt$, as respiration, and storage accumulations, $\pm\partial E/\partial t|_{CV}$, as biomass are often written interchangeably with the incoming and outgoing mass flow terms on the right-hand sides. To begin clarifying such issues of energy commensurability that go untreated in compartment modeling, each of the n scalar equations of an n-compartment energy model can be written as a corresponding conservation equation for an n-CV model using Eq. (19) as the universal starting point. As this discussion illustrates, first principles, definitions, assumptions, and algebraic manipulations are clearly different aspects of model development where RTT can compliment compartment modeling and help introduce an orderly progression of steps into the modeling process and final model representation.

Note, for comparison, that a linear, scalar, energy-balance formulation for one of $i = 1, \ldots, n$ compartments, plus environment, $i = 0$, of a corresponding compartmental system, $E = (E_i)_{n\times 1}$, is often written by inspection and tradition as:

$$\begin{aligned}\frac{dE_i}{dt} &= \text{inflow} - \text{outflow} = [c_{i0}E_0 + c_{i1}E_1 + c_{i2}E_2 + \ldots \\ &\quad + c_{ii}^{\text{in}}E_i + \ldots + c_{in}E_n] - [c_{0i}E_i + c_{1i}E_i + c_{2i}E_i + \ldots \\ &\quad + c_{ii}^{\text{out}}E_i + \ldots + c_{ni}E_i].\end{aligned} \tag{23}$$

Here, each coefficient, c_{ij} ($i, j = 0, \ldots, n$), denotes the fraction of substance storage E_j in compartment j that flows via a direct link, $f_{ij} = c_{ij}E_j$, to the stock E_i in compartment i. The first bracketed terms represent the total substance flow into compartment i (incoming throughflow, T_i^{in}) and those on the right denote total flows out (outgoing throughflow, T_i^{out}). The terms $c_{i0}E_0$ and $c_{0i}E_i$ denote boundary inputs, z_i, and outputs, y_i, respectively, to and from the system. The system boundary is in effect delimited by these particular transfers, and may be real or virtual; it corresponds to the CS of the RTT formulation. The latter is concrete, however, and occurs in physical space-time, while the former is abstract in the context of the space-free compartmental formulation. The $c_{ii}^{\text{in}}E_i$ and $c_{ii}^{\text{out}}E_i$ terms in (23) signify the compartment's contributions and deductions to and from itself. The self contributions are positive, zero, or negative in accordance with the three possibilities $c_{ii}^{\text{in}}E_i > c_{ii}^{\text{out}}E_i$, $c_{ii}^{\text{in}}E_i = c_{ii}^{\text{out}}E_i$,

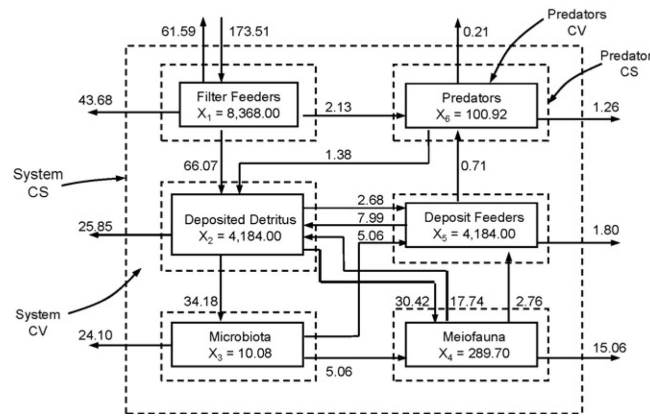

Fig. 4. Energy flows ($\text{kJ m}^{-2}\,\text{d}^{-1}$) and standing crops ($\text{kJ m}^{-2}$) in an intertidal oyster reef (Dame and Patten, 1981). Figure includes the system control volume (CV) and the system control surface (CS) and an example (Predators) of a typical sub-group's CV and CS. Defining the appropriate CV's and CS's is required per the Reynolds transport theorem. Figure shows the inter-CV flows f_{ij}, input boundary flows z_i, and output boundary flows y_j. No self-loops, $f_{ii} = 0$, exist in this model. For energy modeling, often the environment and CS boundaries are considered coincident at an instant of time to aid algebra.

and $c_{ii}^{\text{in}} E_i < c_{ii}^{\text{out}} E_i$. These net self-flows accordingly reflect (positively, neutrally, or negatively) the compartment's contribution to the rate of change of its own accumulation or standing stock, $\text{d}E_i/\text{d}t$ as initiated by Eq. (23). The ambiguity of these self-flows as flows or quasi-storages in their relation to the other flows, the system boundary, and the resultant, $\text{d}E_i/\text{d}t$, is one of the conceptual difficulties with compartment models that the RTT mathematical formulation resolves, or at least avoids, as later discussed.

6. Conservation of energy—energy flow in an intertidal oyster reef

Dame and Patten's (1981) steady-state compartment model of an intertidal oyster-reef community in coastal South Carolina, USA is depicted in Fig. 4. Feeding type and size determine the grouping CV's of this system, which correspond to the compartments as originally given. Filter Feeders, Deposit Feeders, and Predators are macroscopic organisms, while Meiofauna and Microbiota are progressively smaller living forms. A single input of phytoplankton and suspended detrital particles, acquired through filter feeding, serves as the trophic base of the community driving the system. Boundary output processes include resuspension, mortality, and respiration. The remaining inter-compartmental, inter-CV flows are due either to feeding, or egestion to the deposited detrital compartment.

Control surfaces circumscribe the CVs of each compartment and the system as a whole. The scalar version of the universal scale-free formula (1) for the ith control volume, CV_i, is:

$$[S_{\text{env}} = \iiint s\rho\, \text{d}\forall]_i . \tag{1a}$$

This expression corresponds to the general scalar equation for compartments, Eq. (23), in the compartment-modeling paradigm. The subsequently derived RTT conservation Eq. (17a) generates the law of conservation open system energy balance (19a) for each modeled compartment CV_i, $i = 1, \ldots, 6$ and the total system CV_i, $i = 7$:

$$\left[\left.\frac{\text{d}E}{\text{d}t}\right|_{\text{env}} = \left.\frac{\partial E}{\partial t}\right|_{\text{CV}} + \iint_{\text{CS}} e\rho V_n\, \text{d}A\right]_i , \tag{17a}$$

$$\left[\left[\frac{\text{d}Q}{\text{d}t} + \frac{\text{d}W}{\text{d}t}\right]_{\text{CV}} = \left.\frac{\partial E}{\partial t}\right|_{\text{CV}} + \iint_{\text{CS}} e\rho V_n\, \text{d}A\right]_i \tag{19a}$$

Assuming either that no net work, $\text{d}W_i/\text{d}t$, is performed on each CV_i or that an unknown amount of work is reasonably represented within the net heat flow rate, $\text{d}Q_i/\text{d}t$, and the flows associated with the surface integral term on the right-hand-side are spatially one-dimensional (represented as difference of simple summations), an open system energy-balance expression is written:

$$\left[\left.\frac{\text{d}Q}{\text{d}t}\right|_{\text{CV}} = \left.\frac{\partial E}{\partial t}\right|_{\text{CV}} + \sum_{\substack{\text{out}\\ \text{CS}}} (\dot{m}e)_{\text{out}} - \sum_{\substack{\text{in}\\ \text{CS}}} (\dot{m}e)_{\text{in}}\right]_i \tag{20a}$$

or at steady-state with $\partial E/\partial t|_{\text{CV}} = 0$,

$$\left[\left.\frac{\text{d}Q}{\text{d}t}\right|_{\text{CV}} = \sum_{\substack{\text{out}\\ \text{CS}}} (\dot{m}e)_{\text{out}} - \sum_{\substack{\text{in}\\ \text{CS}}} (\dot{m}e)_{\text{in}}\right]_i \tag{21a}$$

Accounting for the energy flows across each control volume's CS_i, the energy balance for the Filter Feeders (CV_1) is written,

$$-q_{01} = (\dot{m}e_{01} + \dot{m}e_{61} + \dot{m}e_{21})_{\text{out}} - (\dot{m}e_{01})_{\text{in}}. \tag{21b}$$

Here, e represents intensive energy flow per unit mass (kJ/kg) and q, where for ease of presentation $q = \text{d}Q/\text{d}t$, is mass-free energy flow (e.g., respiratory heat, in kJ/d). Mass flows, $\dot{m}$, carry units of kg/d, such that the extensive energy flows, $\dot{m}e_{ij}$, are expressed in kJ/d. The entire equation is divided by m^2 to accommodate the oyster reef empirical data. Each term (in $\text{kJ m}^{-2}\,\text{d}^{-1}$) then represents a power density, i.e., the rate of energy flow per unit of oyster-reef area. The left-hand side, q_{01} (61.69 $\text{kJ m}^{-2}\,\text{d}^{-1}$), is respiration waste heat. The right-hand-side outbound, $\dot{m}e_{01}$, $\dot{m}e_{61}$, and $\dot{m}e_{21}$ (43.68, 2.13, and 66.07 $\text{kJ m}^{-2}\,\text{d}^{-1}$, respectively) and inbound, $\dot{m}e_{10}$ (173.51 $\text{kJ m}^{-2}\,\text{d}^{-1}$) flows are due to predation, egestion, and feeding which are mass flow energy transfers. Assuming similar CV_i's and CS_i's for the rest of the system, including the total system (21h), the energy balances are,

$$0 = (\dot{m}e_{02} + \dot{m}e_{32} + \dot{m}e_{42} + \dot{m}e_{52})_{\text{out}} - (\dot{m}e_{24} + \dot{m}e_{25} + \dot{m}e_{26} + \dot{m}e_{21})_{\text{in}}, \tag{21c}$$

$$-q_{03} = (\dot{m}e_{43} + \dot{m}e_{53})_{\text{out}} - (\dot{m}e_{32})_{\text{in}}, \tag{21d}$$

$$-q_{04} = (\dot{m}e_{24} + \dot{m}e_{54})_{\text{out}} - (\dot{m}e_{24} + \dot{m}e_{34})_{\text{in}}, \tag{21e}$$

$$-q_{05} = (\dot{m}e_{25} + \dot{m}e_{65})_{\text{out}} - (\dot{m}e_{52} + \dot{m}e_{54} + \dot{m}e_{53})_{\text{in}}, \tag{21f}$$

$$-q_{06} = (\dot{m}e_{06} + \dot{m}e_{26})_{\text{out}} - (\dot{m}e_{65} + \dot{m}e_{61})_{\text{in}}, \tag{21g}$$

$$-q_{01} - q_{03} - q_{04} - q_{05} - q_{06} = (\dot{m}e_{01} + \dot{m}e_{02} + \dot{m}e_{06})_{\text{out}} - (\dot{m}e_{10})_{\text{in}}, \tag{21h}$$

where the flow out of Deposited Detritus (2) across the system CS, $\dot{m}e_{02}$, is due to resuspension, not respiration (q_{02}).

Eqs. (21b)–(21h) can be further simplified notationally, for example employing the input–interflow–output notations introduced in the text following Eq. (23). Then, Eqs. (20b)–(20h) become:

$$y_1 + f_{61} + f_{21} = z_1, \tag{21i}$$

$$y_2 + f_{32} + f_{42} + f_{52} = f_{24} + f_{25} + f_{26} + f_{21}, \tag{21j}$$

$$y_3 + f_{43} + f_{53} = f_{32}, \tag{21k}$$

$$y_4 + f_{24} + f_{54} = f_{24} + f_{34}, \tag{21m}$$

$$y_5 + f_{25} + f_{65} = f_{52} + f_{54} + f_{53}, \tag{21p}$$

$$y_6 + f_{26} = f_{65} + f_{61}, \tag{21q}$$

$$y_1 + y_2 + y_3 + y_4 + y_5 + y_6 = z_1 \tag{21r}$$

With this, compartmental and RTT-based modeling become joined, notationally as well as conceptually.

7. Discussion

Ecology can be defined as the biological science of environment, but in its history it has often lost sight of what is system and what is environment given that it is an amorphous field of niches, populations, communities, etc. with corresponding amorphous boundaries. The classical homogeneous differential equations of population ecology, devoid as they are of explicit nonhomogeneous connection to environment, are a prime example of this lapse. Compartment models reconnect ecology to its object of interest because they always describe open, dissipative systems that always require environmental inputs and outputs to function. The boundaries of compartmental models are explicit or implicit, but always present, and their further rendering as control surfaces in the Reynolds transport sense tends to make them more concrete and physical than is typically demonstrated in the time-dependant compartmental modeling. Conceptually, compartments and control volumes are equivalent entities, both fully under the control of the modeler to define. The rigidity of form provided by the Reynolds transport CV, however, helps establish a more rigorous implementation of the compartment concept—a connection helpful for the broader ENA because inter-CV flows and CV storages maintain consistent definitions at model conception and subsequent analytical interpretations. The inside/outside distinction is maintained in the RTT approach and, because engineers deal with more concrete systems than systems ecologists, CV's are inherently more physical (the triple-integral defined physical volume, for example) than their abstract compartmental counterparts designed to be flexible with large, complex, multifaceted, and diffuse ecological systems.

Both the compartmental and RTT approaches are internally consistent. In the latter, consistency starts with the universal system Eq. (1) which mathematically represents each CV at all scales of hierarchical organization relevant to the system in question. In compartment models, consistency is reflected in the conservation principles for energy and matter (Patten et al., 1997), the (2nd-law-based) dissipation principle for energy (Straskraba et al., 1999), and openness which follows from the latter (Jørgensen et al., 1999). Mass and energy balance equations reflect this triad of bedrock solid physical principles. The universal system Eq. (1) of RTT is equally valid for each hierarchal sub-grouping, as demonstrated in Eqs. (21b)–(21g), and also the entire system as shown in Eq. (21h). The equation is fundamentally more capable, temporally and spatially, than space-free compartment models, of incorporating further inclusions, elaborations, and improvements at all hierarchical levels. In applications to energetics, the simultaneously simple but comprehensive treatment of system-wide energy in its diverse forms made possible by RTT provides a universal starting point for comparative analyses that enhances compartmental modeling. Fluid dynamics' Navier–Stokes equations, chemistry's oxidation–reduction balances, and physics' conservation of electric charge are all examples of conservation-based sciences with similar, and somewhat elegant, mathematical foundations. Providing a physically consistent mathematical extension of compartmental analysis joins this field to the greater disciplines of conservation science, opening it and its extensions to ecological network analysis (e.g., Christian and Thomas, 2000, 2003; Fath and Patten, 1999a,b; Gattie et al., 2006a,b; Schramski et al., 2006, 2007; and others) to wider participation.

Subsequent assumptions, definitions, algebraic development, and descriptions starting from Eq. (1) establish a compartment-modeling consistency. Disparate equation development methods are normal in compartment modeling where a comprehensive list of simplifying assumptions is rarely articulated. Definitions, their substitutions, and algebraic manipulations are often combined with minimal descriptions. The lack of consistency serves as minor time-consuming nuisances to those familiar with the field and as genuine impedances to those potential representatives from disparate fields of conservation science needed to embrace and further augment compartmental modeling. The universal system Eq. (1) forces a reasonably ordered presentation of assumptions and definitions to develop a suitable working equation [e.g., Eq. (21)] relevant to the question or data available. Further implementation of (21) demonstrates the RTT consistency with the compartmental approach. Most notably, assumptions (spatial and temporal interpretations, simplifications, combinations, etc.) and definitions (substitutions) generally precede, as they should, final algebraic manipulations.

The RTT–CV model is sufficiently definitive to begin laying a formal foundation to previously abstract concepts. Consider that absent a formal definition, a compartment self-flow out and back to itself over one path length has been articulated as both a flow and a quasi-storage related entity (Odum, 1957; Fath and Patten, 1999a; Patten, 1981, 1982). In the vast majority of models in the literature to date, the observed field-acquired data corresponding to the self-flow terms have been zero or inconsequential and therefore, assumed zero. However, although rare, empirically observed self-loops do exist in the literature (e.g., Odum, 1957; Hannon, 1979). Absent a formal framework in compartmental analysis, the self-flow idea is difficult to discuss and defend from at least the two perspectives of ecological field interpretations (data collection) and the subsequent model development (mathematical representations). Ambiguity has persisted.

Formally derived from the RTT integral calculus operations (Gauss–Green divergence theorem), however, a mass-specific flow is only recognized in the conservation equation as a flow if it crosses the CS. If it does cross the CS (and then eventually returns back across the CS into the CV), a self-flow becomes one flow of many on the right-hand-side of the conservation equation contributing to a CV storage's accumulation. As such, a self-flow included in this manner does not inherit, over the other flows, any special mathematical recognition or, in particular, quasi-storage status. If a flow does not cross the defined CS of the control volume, then by definition, the flow does not exist in the right-hand-side terms of the conservation equation. When a flow remains within the predetermined CV, the RTT conservation equation has no capacity to include or review the flow's essence or activity and by this model definition is not a flow. Admittedly, although the analytical description is definitive, the ecological significance of a self-flow, particularly as it pertains to data collection from the field, still remains unclear and requires more work in both compartment and ecological network analysis. However, the current RTT initiated equation development allows us to articulate this discussion. The ecological significance of a self-flow can be temporarily sidestepped since the self-flow algebraic terms (with zero values generally substituted later) can be clearly defined and remain with no disruption to subsequent equation development.

Eq. (13)'s explicit representation of the control surface promotes wider consideration and integration of the pictorial and mathematical portions of the compartmental modeling process. Although not immediately useful in ecological compartment analysis, the CS as a line of demarcation can witness and mathematically articulate a variety of transitions and transformations. In fluid dynamics the CS is capable of serving as a highly accurate monitoring-modeling point wherein fluids cross at various directions and velocities. The geometric location of the CS, the geometric direction, and the physical quality (velocity, pressure, height, etc.) of the respective fluid flows as they cross are usually essential concerns where flows are assessed and quantified through various forms of Eq. (13) to assure that all mass or energy is accounted for in the conservation sense. In compartment modeling, the definition or description of a *flow* across the respective CS can also vary considerably. For example, flows represent nitrification as ammonium in one CV transforming to a nitrate in a subsequent CV or ingestion as particulate nitrogen in a phytoplankton CV are consumed to become particulate nitrogen in a heterotroph CV (Christian and Thomas, 2000, 2003). Energy stocks in compartment models are typically represented by the energy content associated with a particular biomass grouping. The energy flows are then the respective biomass exchanges of biotic and abiotic CVs through ingestion, egestion, mortality, respiration, etc. or flow not associated with mass transport such as insolation. Whether abstract or explicit flows, the RTT–CV mathematical model tied to its pictorial representation is capable of providing judiciously vague to very explicit spatial definition to the physical occurrence modeled.

The abbreviated development of the energy conservation Eqs. (19)–(22) begins to identify the abundance of assumptions necessary to arrive at a suitable energy-analysis equation for ecological purposes. Energy within ecosystems has a variety of manifestations only coarsely represented by the quantity of terms in a comprehensive energy conservation equation. Furthermore, energy continuously transforms itself through a variety of forms and thereby cycles (Patten, 1985) through a combinatorial vast array of microscopic fluxes as it degrades ultimately to the predictable diurnally cycled heat radiating back to space. These assumptions and the corresponding lumping of terms are rarely discussed in depth beyond the pertinent energy-flow description leading directly to the simplified Eqs. (21i)–(21r). For example, the output flow respiration term r_i, in Hannon's (1973) summary of Odum's (1957) Silver Springs model combines three energy terms: (1) heat flow out due to respiration, (2) net component growth of energy content, and (3) energy content of exported biomass. These three terms involve three distinctly different energy manifestations (and energy qualities) in the conservation equation, respectively: (1) the heat flow out due to respiration is $\mathrm{d}Q/\mathrm{d}t$, (2) the net component growth of energy content represents the non-steady-state accumulation term $\partial E/\partial t|_{CV}$, and (3) the energy content of the exported biomass is an energy flow associated with mass flow which is one of the terms in the mass-specific energy summation $\sum_{\substack{\text{out}\\ \text{CS}}} (\dot{m}e)_{\text{out}}$. For the most part, this differentiation of the forms of energy adds nothing to the current compartment-modeling methodology. However, as the quality of energy or total energy investment garners heightened awareness in ecological studies (Odum, 1996; Brown and Ulgiati, 2001; Sciubba, 2004, 2005; Jørgensen, 2005), identifying appropriate simplifying assumptions is becoming necessary to elicit and foster a wider understanding of ecosystem energetics and corresponding network analyses. As of yet, these assumptions have not been consistently articulated with regard to compartmental modeling development. The Reynolds transport equations (13) and (17) provide a foundational framework to adequately describe all assumptions leading to the final conservation equations. These assumptions, like all assumptions should, can now be used and then subsequently evaluated for their impact on the final results. They can also be isolated and independently explored in later studies.

Table 1
Summary of a Reynolds transport theorem control volume model's complimentary aspects to ecological network analysis's compartmental modeling pertaining to the modeling of energy storage and flow in ecological networks.

Compartmental model	Reynolds transport theorem control volume model
Order of differential equation development less formal and generally more modeler dependent	Order of differential equation development more formal and generally more RTT process dependent (first principles, assumptions, definitions, algebra, interpretation)
Time dependent equations where mathematical model is loosely tied to pictorial model	Time and space dependent equations where mathematical model can be explicitly tied to pictorial model
Energy types are identified by the modeler	Energy types are mathematically explicit through established RTT development methodology

8. Conclusions

Table 1 consolidates RTT's substantive and therefore potential complimentary improvements to compartmental analysis. Where compartment modeling, although abstract, can ultimately be successful at accounting for all conserved quantities, RTT's formal CV developmental process provides structure and order to the introduction of first principles, assumptions, definitions, algebraic manipulations, and graphical presentations. This ordered progression, among other attributes, uniquely illuminates different types (and therefore different qualities) of energy transfers. In short, existing compartment analysis of ecosystems is a successful but implicit process of equation and graphical construction with the order and content of development heavily influenced by the modeler. The RTT–CV is a consistent model development methodology that informs compartmental analysis and ultimately ecological network analysis, helps to communicate across disparate disciplines, and most importantly, will help in the classroom as this material makes its transition from journals to textbooks where uniform and consistent methods are essential.

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