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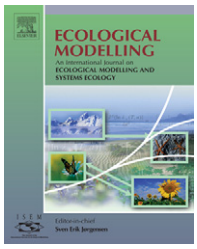

Defining an ecological thermodynamics using discrete simulation approaches

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ABSTRACT

New insights into interdisciplinary engineering endeavors, from classical modeling to nano–macroscale extrapolation and critical evaluation, weigh heavily on the pervasive nature of thermodynamics in the physical world. Just as statistical thermodynamic approaches provide a beneficial complement to a process-based macroscale thermodynamic approaches with physical systems, a Lagrangian approach to energetics in biological systems can, we believe, provide a beneficial complement to popular Eulerian approaches. Statistical thermodynamics is used as a springboard for some analogies that are similarly used to leap into the ecological scale. The Lagrangian simulation, a discrete simulation, is implemented with a spreadsheet approach, a discrete simulation approach, and a new stochastic differential equation solution approach. The Lagrangian approach complements the more widely used continuous (or Eulerian) simulation approaches such as STELLA or Environ theory approaches. The Lagrangian approach decomposes energy into small packets or ecological quanta. An ecological entropy is computed based on nodal contacts in the network, with the notion that nodal contact is analogous to molecular speed. In the cases shown, the results of ecological entropy appear generally consistent with thermodynamic entropy. A newly available simulation package (ECONET) enabled an easy Lagrangian approach to analyzing the Cone Springs and Oyster ecological models. An analogy between nodal contact numbers and molecular speed was developed to enable computation of an ecological entropy. There is a similarity between classical and ecological entropy based on similarity in shape of the Maxwell–Boltzmann distributions to the packet-nodal contact numbers. An ecological temperature can be defined based on this similarity. Selected ratios of ecological entropy versus classical macroscopic entropy appeared to have some degree of robustness. Other aspects of ecological thermodynamics remain to be developed. It is felt that the ecological thermodynamics approach presented offers an improved way to combine biochemical and ecological entropy. A sound combination of entropies at multiple scales will help bring together measurements at disparate scales.

1. Introduction

An ecological thermodynamics course should review the laws of thermodynamics in the classical sense. The course properly investigates some models showing how these laws describe solids and gases at the microscopic level in the context of isolated, closed and open systems. One must also realize that thermodynamic theory we have today was developed along a circuitous path (see Truesdell, 1980 for a historical overview of classical thermodynamics history).

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The inquiry herein pursued the following broad objectives:

- Evaluate the use of selected discrete simulation approaches for modeling movements of small entities within compartmental systems.
- Using discrete simulation approaches, initiate the development of an ecological thermodynamics that respects classical statistical thermodynamics and defines compatible concepts on ecological scales.

To build a rigorous basis for physically based design, ecological or otherwise, one must begin with energetics. The system must be clearly defined, thermodynamic coordinates must be identified, and an effective equation of state must be developed. Thermodynamic coordinates may include temperature, energy, constituents, and possibly ecological orientors. One may then analyze many systems to determine the relative robustness of the coordinate set. As trends begin to emerge, ecological engineering will be on its way to taking its place with other engineering disciplines.

An underlying sense pervaded that basing our definition of thermodynamic principles on molecular and atomic behavior was insufficient to describe ecological problems. Additional approaches were required to enable scaling from the molecular to the ecological temporal and spatial levels. The fundamental definition of entropy is based on a statistical distribution of molecular and atomic states. Once the distributions become multimodal, scale-up becomes problematic without some additional tools. The purpose of this presentation is to introduce an inquiry that may lead to new approaches for analyzing thermodynamics of ecosystems. The approach begins with considerations of systems and is oriented around network environ analyses (Patten, 1978; Gattie et al., 2005) and will be augmented by an alternative analyses based on a Lagrangian approach, described below.

2. Fundamental laws and approaches of general and statistical thermodynamics

2.1. *Zeroth law*

Two systems in thermal equilibrium with a third system are in thermal equilibrium with each other. The discussion of temperature underlies this discussion. Note that some authors refer to the zeroth law as the third law. Jorgensen (2001) analyses the numbers of observations needed to characterize an ecological system from an individual particle consideration and concludes that the task is nearly impossible.

It is interesting to speculate on what the zeroth law means in the ecological context, where the association to temperature with motion may become harder to describe.

2.2. *First law*

The first law is formulated to represent three ideas:

(1) the existence of an internal energy function, where internal energy may be due to temperature induced molecular movement, latent energy expressed in phase changes, or latent chemical energy expressed in chemical reactions;
(2) the principle of conservation of energy (and mass); and,
(3) the definition of heat as energy in transit by virtue of a temperature gradient.

2.3. *Closed system*

When a closed system whose surroundings are at a different temperature and on which mechanical work may be done undergoes a process, and then the energy transferred by non-mechanical means, equal to the difference between the change of internal energy and the mechanical work is called heat. Latent (phase change) and chemical energy are treated as components of the internal energy. A closed system analyses is inherently Eulerian, meaning that one focuses on flows at the boundary and assumes uniform conditions within the confined space.

2.4. *Open system*

The first law as applied to the open system says that the net energy change relative to the system boundaries is equal to the change of energy per unit time within the system. If the net change within the system is zero, the system is said to be in steady state if the inputs and outputs are also not changing with time. One usually analyses the open system using rate units. Cengel and Bowles (2002) provide some excellent examples of Eulerian first law analyses. One may also perform Lagrangian or discrete analyses on these systems, as will be demonstrated. There seems to be broad consensus that the first law is generally applicable to ecological systems of all scales. The ease of defining energy across a broad ranges of spatial and distance scales make this possible.

2.5. *Isolated system*

A system wherein no mass or energy is exchanged across the system boundary. Lagrangian analyses can potentially reveal dynamics of energy within an isolated system, whereas the Eulerian analyses provide little additional information.

2.6. *Second law*

The second law states that the net entropy generated in a process is equal or greater than zero. Zemansky and Dittman (1997) discuss the Clausius (impossible to construct a refrigerator requiring less work than that associated with the heat being transferred from a cold to a hot thermal energy reservoir) and Kelvin–Plank (impossible for a heat engine to do more work than the equivalent heat transferred from a hot to a cold thermal energy reservoir) variations of the second law. Both these variations essentially state that the perpetual motion machine is impossible. The reversible process generates zero entropy. Cengel and Bowles (2002) provide excellent examples of second law analyses with and without chemical reaction in nonliving systems. They consider isolated, closed and open systems. Entropy and second law analyses dictate the direction of a process. These concepts are also important in the notion of goal functions, further discussed below. Entropy is

related to the probability that a state will occur. Disorder is more likely to occur than an ordered system. Transition to a higher probability, more disordered state involves an increase in entropy. Whalley (1992) is one of many references that summarize our knowledge of classical entropy, macroscopically and microscopically.

The introduction of living entities in a system complicates the estimation of entropy from a microscopic sense. The macroscopic balance is still regarded as valid, with the entropy generation term being the impacted parameter. Aoki (2001) gives an excellent summary of efforts to compute macroscopic entropy balances in ecological systems. The above statements imply that organisms are on a trajectory leading to death.

Zemansky and Dittman (1997) provide a concise overview of statistical thermodynamics for gases and solids. They argue that number of energy states possible for a set of particles far exceed the number of particles in a gas. The thermodynamic number (Ω) of a particular macro state is given by

$$\Omega = \frac{g_1^{N_1}}{N_1!}\frac{g_2^{N_2}}{N_2!}\cdots \quad (1)$$

where g_i represents the number of quantum states yielding energy e_i and N_i represents the number of particles at that energy. The thermodynamic number is identical to the number of ways a sample of N_i particles can be drawn (with replacement) from a population when particles N_i are indistinguishable. Eq. (1) states that the total thermodynamic number is the product of the numbers of the respective N_i.

The Maxwell–Boltzmann theory enables statements concerning temperature as shown in Fig. 1. In our case, we are in effect looking at contact numbers in lieu of molecular speed, so the temperature indicator would be a contact number indicator. The Maxwell–Boltzmann distribution is the probability density of molecule numbers at a given speed as shown in Eq. (2).

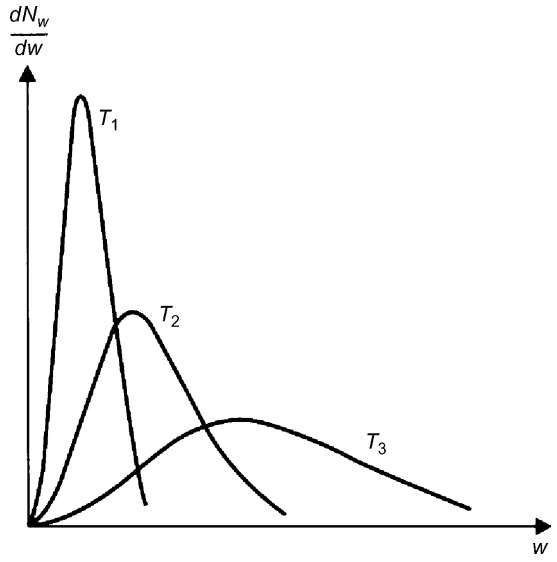

Fig. 1 – Hypothetical Maxwell–Boltzmann distributions showing the effect of temperature ($T_1 < T_2 < T_3$) on the distribution of molecular speeds w (from Zemansky and Dittman, 1997).

$$\frac{dN}{dw} = \frac{2N}{\sqrt{2\pi}}\left(\frac{m}{kT}\right) w^2 e^{-0.5mw^2/kT} \quad (2)$$

where N is the number of molecules at speed w, w the molecular speed (L/T), k the Boltzmann constant, T is the absolute temperature (K)

Eq. (2) is the culmination of a rather lengthy derivation given by Zemansky and Dittman (1997). The right hand side of Eq. (2) defines the Maxwell–Boltzmann velocity distribution. Note the effect of temperature on the distribution shape as highlighted in Fig. 1.

Zemansky and Dittman (1997) give the following formulation for entropy as derived from statistical mechanics.

$$S = -k\sum_{i=1}^{\infty} N_i \ln\frac{N_i}{g_i} + kN \rightarrow S_{\text{specific}} \approx k\sum_{i=1}^{\infty} \ln\frac{1}{p_i} \quad (3)$$

In our case, contact number is analogous to molecular speed, the mass of the packet (unity here) is analogous to the molecular mass, m; the number of possible quantum energy states that the packet may be distributed over (g) is analogous to the number of contacts possible in the nodal network; the number of molecules at speed w is analogous to the number of packets N_i contacting a specified 'i' number of network nodes; the equivalent of the Boltzmann constant k is not specifically defined. The probability p_i is the ratio of the number of states over the number of possible contacts. It is noted that other formulations for the thermodynamic probability exist and lead to modified forms of the Maxwell–Boltzmann distribution.

3. A Lagrangian view of Eulerian systems

Before defining the Lagrangian systems approach, we review the classical Eulerian approach. The classical Eulerian system is one that identifies a conserved currency (e.g., mass or energy) and quantifies various network properties of systems. A Eulerian approach common in the ecological community is the use of simulation packages such as STELLA for solving systems of first order differential equations (ODEs) for dynamic analyses of nodal states within systems. Network environ analyses (NEA), developed by Patten (1978) is typical of a steady state Eulerian approach wherein an input–output approach is taken to describe flows within nodal networks. Another Eulerian approach with many similarities to NEA includes Ascendancy analyses (Ulanowicz, 2000). An ascendancy analysis is similar to NEA in initial setup. The major difference in the approach is in the network properties computed.

The Lagrangian approach begins with typical continuous flow systems and discretizes them into finite sized entities that may be directed along various paths based on probabilities. Thus, the Lagrangian approach is a special case of discrete simulation and may be analyzed with discrete simulation techniques. Discrete simulation is sporadically used in ecological research (see Atkinson and Shorrocks, 1981). Techniques involving Markov analyses could be viewed as discrete and are somewhat common (see Puterman, 1994) but little used compared to continuous simulation approaches such as

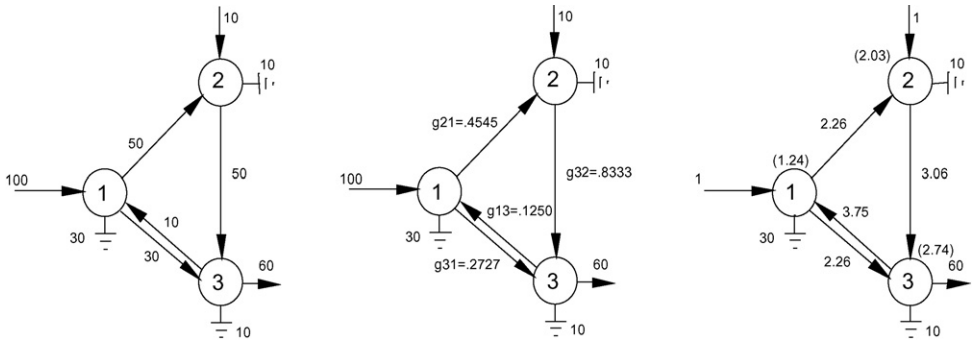

Fig. 2 – Archetypical network environ showing energy flow through a simple three-node system with two inputs, a recycle loop, dissipation and an output.

STELLA. Accounts of the Lagrangian variant of discrete simulation are sparse.

A prototype ecology represented by the figure below was analyzed using network environ theory and a "particle" simulation approach. The network environ theory, based on state space and input–output modeling approaches represents a classical Eulerian approach to solving the problem and can be easily applied to problems of many scales. The particle simulation approach represents a Lagrangian ride through the system and is inherently more difficult to apply because every detail must be specified in theory. It appears at first glance to be dynamic in that pulses or packets of energy or mass are sent through the system in a discrete fashion from some known starting state. The starting state is an arbitrary zero mass or energy state that is admitably meaningless. The transition probabilities from one node to the next are indeed similar to those in the transport matrix from network environ analyses and are derived assuming steady state. One possible connection with a dynamic analyses is that one may see an output response with zero inputs; however further investigations are needed.

Nodes in the Lagrangian model receive inputs from other indicated nodes based on probabilities of total mass or energy at that node. For example, node 1 receives 110 energy units in Fig. 2. In the steady state condition, 50 of those units go to node 2, for a probability of 0.4525 as shown in Fig. 2. One must compute the transport probabilities for each node as shown in Fig. 2. An excel spreadsheet provides a suitable platform for a very simple implementation of the Lagrangian concept. It should be noted that the scheme for managing the energy balance in the Lagrangian approach implies that energy in equals energy out, a direct application of the first law.

The basic challenge and potential of the Lagrangian analyses is to track the route traveled by each packet of mass or energy. One must also provide timing information for the movement of the packets through the systems, usually from a statistical distribution. Energy packets in Fig. 2 represent 0.1 energy units. A group of 1000 packets were introduced into the network at node 1 and 100 were introduced into the network at node 2 for each pulse event. The direction of the packets to a given node depends on the probability of flow in a given direction. The probability is figured by dividing the flow in a given direction by the total outgoing flow from the respective nodes.

Energy packets enter the system at an arbitrarily defined state of "1". Passage through a node causes an incremental change of the state by 1. Therefore, packets entering at node 1 have a state of "2" as they go to node 2 or node 3. Packets traveling the longest path would have a value of "4" as they returned to node 1. Due to the recycle between node 3 and node 1, multiple system snapshots are required to determine the distribution of states contained in the nodes. Each snapshot was made after passage of packets around the longest route back to node 1. After four snapshots, packets can have accumulated as many as 13 different state increments, with state number (e.g., history) becoming exponentially more complicated with each pulse event. The analysis was limited to four snapshots due to logistic considerations in using the Excel platform. The probability of energy persisting in the network with a high state becomes very low. Knowledge of energy state persisting in the network may provide insights into network behavior, thus we desire to track energy state distributions. Results shown in Figs. 3–5 were obtained by considering 1000 realizations with uniform random numbers providing the basis of probability calculations for each realization.

Some packets of energy at a given node may represent very low quality energy while some represent reasonably high quality energy. The assumption is that travel through the network degrades the quality of the energy. The low quality energy history represents past history. A working hypothesis of this inquiry is that interesting possibilities may exist when one places very low quality energy along side of high quality energy. In a true steady state analyses, packets can accumu-

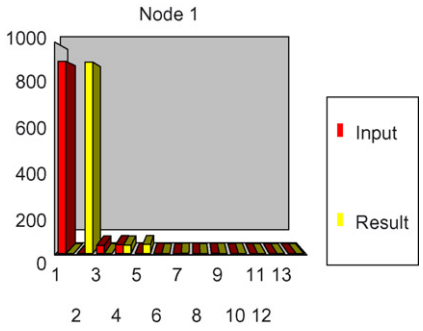

Fig. 3 – Histogram showing hypothetical states of energy packets residing in node 1 after four pulses, based on an average over 10 runs.

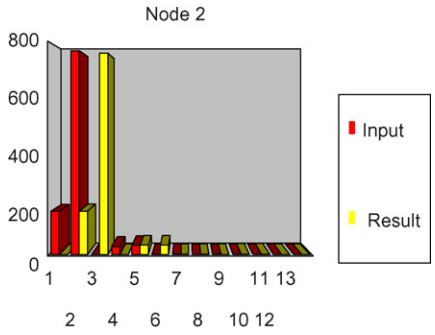

Fig. 4 – Histogram showing hypothetical states of energy packets residing in node 2 after four pulses, based on an average over 10 runs.

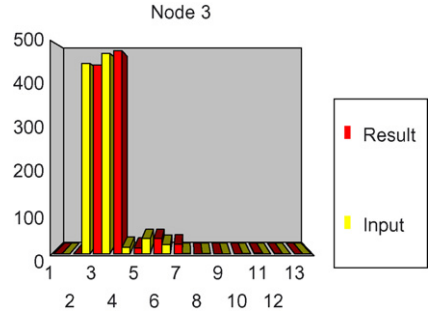

Fig. 5 – Histogram showing hypothetical states of energy packets residing in node 3 after four pulses, based on an average over 10 runs.

late very low energy levels, albeit the probability of observing these packets becomes extremely small as will be seen below.

Energy qualities of the nodes of Fig. 2 are shown in Figs. 3–5, respectively assuming four pulse events. The fact that some packets at node 1 are not 1000 is due to the recycle from node 3. Similar explanations exist for the other nodes. The fact that the distributions each could be viewed as similar to the Maxwell–Boltzmann distributions from classical statistical thermodynamics is of interest.

Details of history at node 1 are shown in Fig. 6. The Shannon information entropy is shown along with the Boltzmann entropy (where the Boltzmann constant is arbitrarily assigned as 1). The mixing of packets with different energy states and resulting effects of 'far from equilibrium' conditions (De Groot and Mazur, 1984) occur is of interest from a thermodynamic viewpoint. Each network will have different properties due to its inputs, outputs, elements, and element connections.

Another aspect of the Lagrangian analyses is to consider what the number of nodal contacts that the energy packets in a given node have completed. Each packet of energy by definition contacts a packet one time in the process of entering and leaving a node. This simple approach does not introduce the storage concept, which may result in multiple contacts between entrance and exit. Results are summarized in Table 1. The input contact average at node 1 is notably higher than 1 due to the recycle with node 3. As one proceeds to node 2, the contact is nearly two because the impact of recycle with node 3 is greatly diminished. Node 3 is complicated by the input from 1 and 2. The most interesting note that the effective change of each node is slightly higher that a simple contact.

Is all energy equal in the potential work it can accomplish? It is assumed herein that each time an energy bundle passes through a node, it accumulates states (e.g., history) related to the number of nodes it has passed while within the system. The total energy within a system may therefore contain a diverse history. The heart of the Lagrangian analysis is to develop that history for each node in the system. Having this history enables one to compute a measure of homogeneity of the energy known as the Shannon information entropy in a classical sense. It was interesting to compute the Shannon information entropy analogue along with the Boltzmann entropy analogue for the inputs and outputs of each node based on distributions of the respective conditions similar to those shown in Fig. 6. To keep from confusing these 'entropies' with accepted thermodynamic counterparts, we use SE instead of *S* for ecological entropy. The Shannon information entropy (SE_{Inform}) and specific Boltzmann ecological entropy ($SE_{Sp\ Boltz}$) are respectively computed using the following equations:

$$SE_{Inform} = -k_B \sum_{State=1}^{No.\ States} p_i \log_2 p_i, \quad \text{where } p_i = \frac{node_i}{\sum_{State=1}^{No.States} node_i};$$

$$SE_{Sp\ Boltz} = \sum_{State=1}^{No.\ States} k_B \operatorname{Ln}\left(\frac{1}{p_i}\right) \tag{4}$$

Note that $\log_2 p_i$ and $\operatorname{Ln} 1/p_i$ were forced to zero if $p_i = 0$.

Shannon and Boltzmann entropy values at the entrance and exit of each bin are shown in Table 1. Details of the entropy calculations for node 1 are also shown in Fig. 6. Nodes

Input to Node 1					Output from Node 1			
State	Mean	SD	Shannon Entropy	Bolt. Entropy.	Mean	SD	Shannon Entropy	Bolt. Entropy.
1	912.6	9.08	-0.1204	0.0915	0	0.00	0.0000	0.0000
2	0	0.00	0.0000	0.0000	908.1	8.79	-0.1263	0.0964
3	39	7.53	-0.1825	3.2442	0	0.00	0.0000	0.0000
4	41.6	4.77	-0.1908	3.1797	40.4	3.89	-0.1870	3.2089
5	1.1	1.10	-0.0108	6.8124	43.3	8.84	-0.1961	3.1396
6	2	1.56	-0.0179	6.2146	1	1.25	-0.0100	6.9078
7	0.1	0.32	-0.0013	9.2103	2.8	1.48	-0.0237	5.8781
8	1.2	1.23	-0.0116	6.7254	0.2	0.42	-0.0025	8.5172
9	2.4	1.71	-0.0209	6.0323	2	1.70	-0.0179	6.2146
10	0	0.00	0.0000	0.0000	2	1.56	-0.0179	6.2146
11	0	0.00	0.0000	0.0000	0.2	0.42	-0.0025	8.5172
12	0	0.00	0.0000	0.0000	0	0.00	0.0000	0.0000
13	0		0.0000	0.0000	0	0.00	0.0000	0.0000
	1000		0.5564	41.5104	1000		0.5839	48.6944

Fig. 6 – Example histograms showing details of contacts of packets entering and leaving node 1 after four pulses.

Table 1 – Summary of Nodal Inputs and Actions for the hypothetical model of Fig. 2

Node	Input contact average	Output result average	Effective change	SE_{inform}	SE_{Boltz} [a]	Entropy trends[b]		
						SE_{inform}	SE_{Boltz}	S_{Macro}
1	1.25	2.26	1.01	0.556 0.585	41.51 48.69	+	+	0.1024
2	2.03	3.06	1.03	1.093 1.143	44.81 43.28	+	–	0.0341
3	3.75	2.74	1.01	1.467 1.455	58.38 64.70	–	+	0.0341
Combined	–	–	–	3.116 3.183	144.7 156.7	+	+	0.1707

[a] An arbitrary value of 1.0 is assigned to the Boltzmann constant. Energy units here are arbitrary.
[b] A positive sign connotes an increase in entropy due to the nodal action.

1 and 2 showed an increase in information entropy and a decrease in Boltzmann entropy. Node 3 exhibited the opposite behavior, due to the recycle with node 1. Node 3 was moving in a different direction relative to equilibrium than were nodes 1 and 2. Jorgensen and Svirezhev (2004) seem to rely on the Shannon entropy more so than the Boltzmann entropy. The macroscopic entropy is positive for all nodes and consequently the entire system. The dissipative effects coupled with the accumulation of capacity to do work is consistent with Prigogine's assertion (see Prigogine and Stengers, 1984) that thermodynamic systems, while dissipating much energy, may have small zones moving further from equilibrium. A more exhaustive analysis of this system and additional systems may provide additional insights as to which definition of entropy is the best for ecological systems. The ecology entropy calculation here is not process based as is the case with macroscopic entropy; ecological entropy looks at state changes independent of process.

In our simplified network, node 2 has the highest output result average (Table 1). It would be interesting to know the point on the *x*-axis where the free energy ceases decreasing and begins to increase. Some tagged experimentation may help resolve this question in a variety of network configurations.

One may estimate the macroscopic entropy of each of the nodes. Entropy may be written as follows:

$$\Delta\dot{S} = \Delta\dot{S}_{exch} + \Delta\dot{S}_{gen} \quad (5)$$

where $\Delta\dot{S}$ is the change in entropy production rate in the system ($E/K - T$), $\Delta\dot{S}_{exch}$ the entropy exchange rate ($E/K - T$), and $\Delta\dot{S}_{gen}$ is the entropy generation rate ($E/K - T$)

In the above formulations, units are energy (E) per degree K per time unit. At steady state, $\Delta\dot{S}$ due to thermal effects is zero. The exchange entropy is a function of dissipated heat, $-Q/T$ where T is taken at 293 K. The macroscopic entropy of each node may be expressed as:

$$\Delta\dot{S} = 0 = \Delta\dot{S}_{exch} + \Delta\dot{S}_{gen} \rightarrow \Delta\dot{S}_{gen} = \Delta\dot{S}_{Macro} = \frac{\dot{Q}_{diss}}{293\,K} \quad (6)$$

Results are shown in Table 1. Following Michaelian (2005), we combine the results of the nodes represent theresults for the system. It is interesting to note that both the statistical and macroscopic approaches suggest net entropy for the entire system. The work of relating these findings to other outputs of network environ analyses remains to be completed.

It is interesting to explore some parallels between the classical statistical thermodynamics definition of thermodynamic probability as shown in Eq. (1) and the ecological thermodynamic probability leading to the distributions in Figs. 3–5. In classical thermodynamics, g_i represents the number of possible quantum state combinations leading to a given energy level e_i. One possible ecological parallel to g_i is the number of possible contact combinations leading to a given energy level e_i. In classical thermodynamics, N_i represents the number of atoms/molecules having energy level e_i. The ecological parallel is the number of energy packets having energy level e_i. The energy packet thus becomes the basic quanta of energy in this analysis.

It is also interesting to consider the distributions of contact in the context of available free energy. As the number of contacts increases, the net free energy would generally decrease. The enzyme suits necessary to metabolize further compounds would presumably increase in complexity. However, life processes, create local niches wherein free energy increases as biological organizational processes. We believe that the likelihood of complexity increase occurring with a given ecological quanta is directly related to persistence in the network.

A fundamental premise of network environ analyses is that the system is at steady state. Considering the Lagrangian analyses, the subtle difference between 'steady state' and 'dynamic equilibrium' becomes interesting. (We view 'static equilibrium' or equilibrium unqualified as connoting no motion.) A system can have equal inputs and outputs from the Eulerian viewpoint and be at a macroscopic 'steady state' or 'dynamic equilibrium' but still be changing its configuration on the microscale. This we feel a specification of 'steady state' and/or 'dynamic equilibrium' require a scale qualifier.

According to Reynolds (1968), the Shannon information entropy is equivalent to the Gibbs definition of entropy (where we have taken the Boltzmann constant equal to unity). The Boltzmann distribution assumes that quantum states are equally possible in the universe of Ω numbers of quantum states. The Gibbs (or Shannon information) formulation does

not impose this restriction. It is felt that the Shannon formulation may be more appropriate at this juncture. Resolving the apparent discrepancy between the Shannon and Boltzmann entropy trends would be aided by a similar analyses of additional models.

ARENA (see Kelton et al., 2004), a discrete simulation framework, enables one to track attributes of individual packets was used to reproduce the spreadsheet results presented above. The ARENA model adds a contemporary graphical user interface to the classic SIMON discrete system (see Pegden et al., 1995) and has some capability for continuous simulation. The student version of ARENA is limited in the availability of custom interfaces and limited in the number of entities that may be moving within a system during a simulation run. The student version (which may be freely copied) has a complete implementation of SIMON (hereafter referred to as SIMON/ARENA) and the limit of 150 entities has not had an adverse impact on problems addressed to date. Working at the SIMON level is recommended initially in order to acquire the feel of discrete simulation methodology.

SIMON/ARENA enables one to control timing of the packets through the system via the use of common statistical distributions. The discrete simulation package treats each node as a queue (with user selectable ordering), a seizure operation, where the node 'takes possession' of the packet and executes an operation. Operational counts and process time tallies are possible. A user programmable time delay is used to simulate the residence time. Decision branching using probabilities from network environ analyses is easily implemented. A portion of the model for one node is shown in Fig. 7.

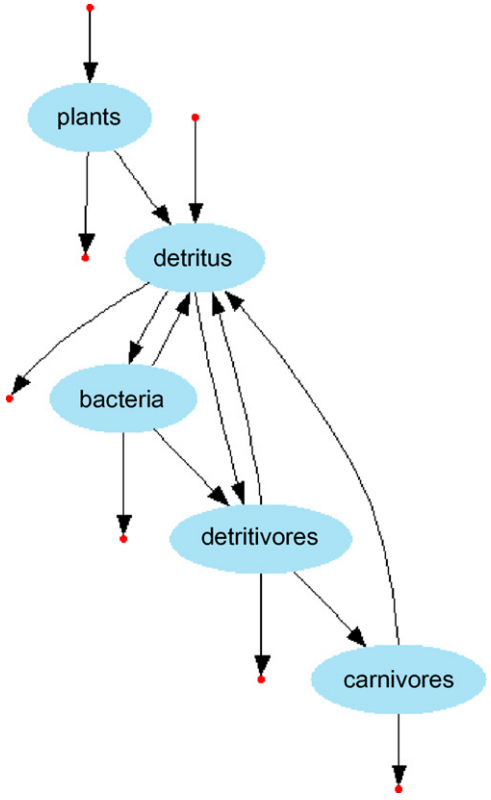

Fig. 7 – Schematic of the Cone Springs model as rendered by ECONET.

The SIMON/ARENA framework provides additional flexibility for stamping each packet with a unique identifier associated with passage through each network node. This package can also be used to model ecological problems of greater complexity. This package also enables non-steady state analyses. The storage features of network environ analyses can also be incorporated in a straightforward away. The SIMON/ARENA discrete modeling package also enables one to move beyond the limit of three or four passes. An analysis of the simple model shown in Fig. 2 yielded results similar to those presented above. Using SIMON/ARENA enables one to exercise minute control of a packet through a particular node. The control is so detailed that minute manipulation may not be practical because the data to justify specifics would be difficult to obtain.

3.1. *Lagrangian analyses of two ecological systems*

Programming SIMON/ARENA to track individual elements is a relatively cumbersome task because of the minute control requirements. An advanced modeling and differential equation solution package known as 'ECONET' (see Kazanci, in press) has been configured to solve systems of deterministic or stochastic differential equations with particle tracking (Tollner and Kazanci, 2007). ECONET is similar to STELLA in that it provides solutions to a series of first order continuous ODEs arising from typical control volume analyses. Rather than the detailed process programming required by SIMON/ARENA, ECONET uses a chemical mass action approach for managing the movement of energy or mass packets (or quanta) from one node to the next.

The important ECONET enhancement now available is the capability of solving stochastic ODEs based on Gillespie's stochastic algorithm (Gillespie, 1977). A particle-tracking feature now under development enables Lagrangian-type particle tracking. We are applying the ECONET Lagrangian particle tracking approach to an ecological thermodynamic analyses of two well publicized data sets: Cone Springs (Ulanowicz, 2000) and Oyster reef (Dame and Patten, 1981).

The Cone Springs model is shown schematically in Fig. 7. The ECONET model was run two different times with two different packet sizes. An indication that a robust steady state values of stocks was reached was that the total number of packets in the system was about 6900 in both runs with similar distributions among the nodes. The nodes in the analyses included plants, bacteria, detritivors, carnivors and detritus. Results for one run are shown in Figs. 7–10. Fig. 8 shows the path from a starting condition to steady state. Steady state was reached in approximately 0.5 time units. The number of iterations over two time units was about 137,000. Particles passing through the system numbered about 34,000. Histograms of packet numbers versus nodal contacts are shown in Fig. 9. A composite histogram of packet numbers vs. nodal contacts is shown in semilog form in Fig. 10. The results for individual nodes take on the shape of the Maxwell–Boltzmann distribution and the linear tail in Fig. 10 follows from the log transform. The detritus node was dominating in this model.

The Oyster model is shown schematically in Fig. 11. The ECONET model was run two different times with two different packet sizes. An indication that a robust steady state

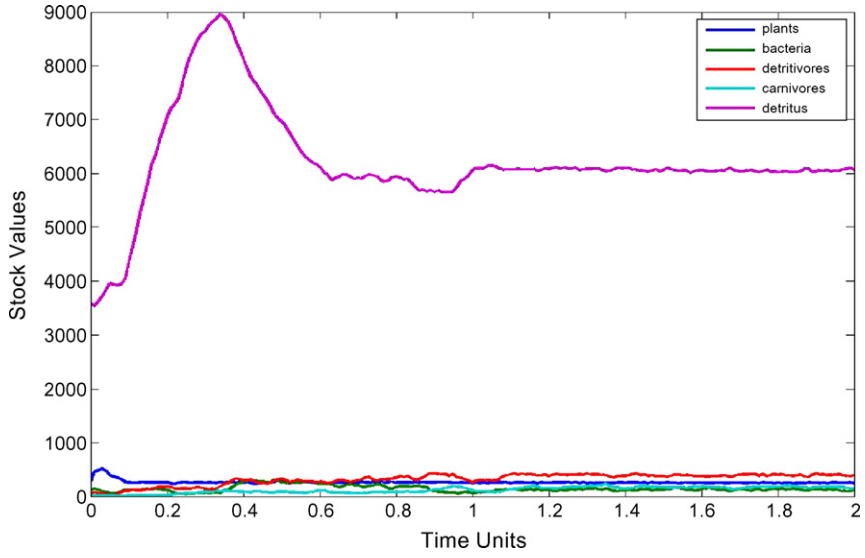

Fig. 8 – Stock values vs. time units in a Cone Springs ECONET model run.

values of stocks was reached was that the total number of packets in the system was about 40,000 in both runs with similar distributions among the nodes. The nodes in the analyses included filter feeders, deep detritus, microbiota, meofauna, deep feeders and predators. Results for one run are shown in Figs. 12–14. Fig. 12 shows the path from a starting condition to steady state. Steady state was reached in approximately 1000 time units. The number of iterations over two time units was about 3.2 million. Particles passing through the system numbered just over 1 million. Histograms of packet numbers vs. nodal contacts are shown in Fig. 13. A composite histogram of packet numbers vs. nodal contacts is shown in semilog form in Fig. 14. The results for individual nodes take on the shape of the Maxwell–Boltzmann distribution and the linear tail in Fig. 14 follows from the log transform. The filter feeders node followed by the deep detritus node was dominating in this model.

The Maxwell–Boltzmann distribution shape is discernable in the Cone Springs and Oyster models. Each model tends to be dominated by one or two nodes. It is tempting to simply add the entropy from the respective nodes; however, the more correct way appears be to accumulate the packets numbers contacting the respective node numbers and recomputed the entropy, since the logarithm is not a linear function. These

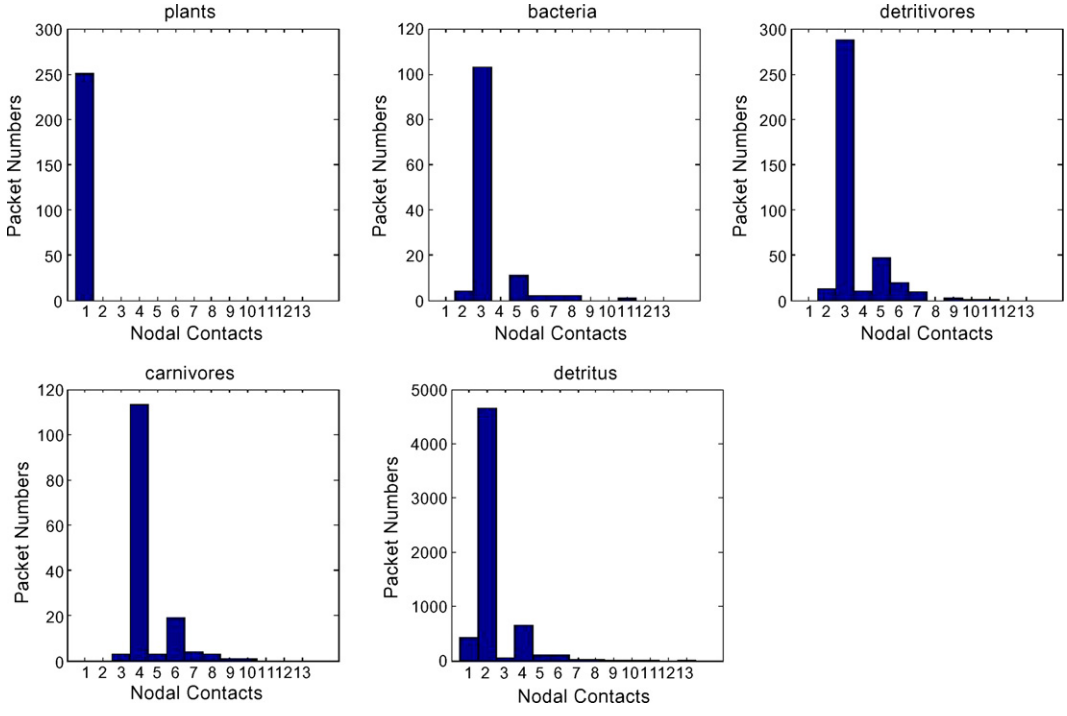

Fig. 9 – Final plot matrix of packet numbers vs. nodal contacts by node for the Cone Springs model run shown in Fig. 8.

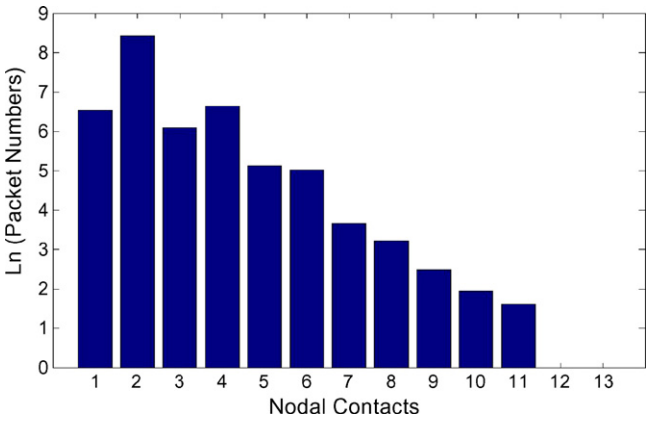

Fig. 10 – Cumulative plot of the natural logarithm of packet numbers versus nodal contacts for the Cone Spring model run of Fig. 8.

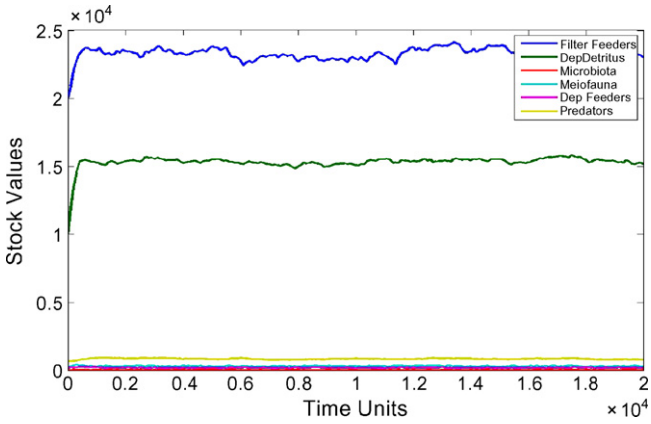

Fig. 12 – Stock values vs. time units in an Oyster reef model ECONET run.

results are shown in Tables 2 and 3 along with the macroscopic entropy for each node. It is interesting to note that the analysis thus far treats every node as equal in terms of effect on the energy packet. It is conceivable that one could bring to bear an appropriate Maxwell–Boltzmann type of biochemical entropy to packets leaving each node in an additional post-processing step. This may enable an addition of biochemical entropy to ecological entropy in a way that goes beyond a simple addition of the type used by Jorgensen and Svirezhev (2004) when they added biochemical and information entropy.

A summary of selected entropy ratios for all three models evaluated is shown in Table 4. The Boltzmann entropy computed using total nodal contacts in the system versus the Boltzmann entropy summed for each node (B.lumped/B.nodal) was fairly consistent over all models. The related ratios involving Shannon entropy (Shan. lumped/Shan. Nodal) was not as consistent. The essential nonlinearity of the entropy definition is obvious in that these ratios are far from unity as one would expect from a linear process. This raises a doubt that the sum of the entropy in a system is simply the sum of nodal entropies.

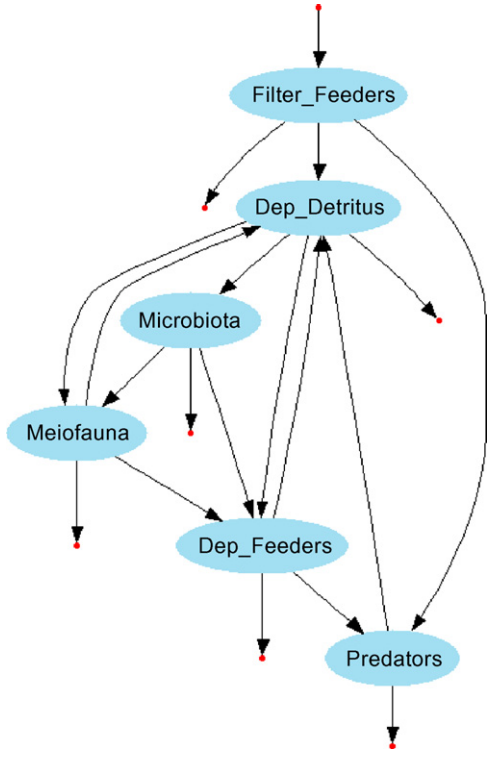

Fig. 11 – Schematic of the Oyster reef model as rendered by ECONET.

Table 2 – Summary of Nodal Inputs and Actions for the Cone Springs model run of Fig. 8

Node	SE_{inform}	SE_{Boltz}	S_{Macro}
Bacteria	1.04	23.30	11.18
Carnivores	1.26	27.57	0.69
Detritivors	1.42	33.45	6.19
Detritus	1.27	59.10	10.61
Plants	0.00	0.00	6.84
Total system	1.68	55.39	
Nodal sum	4.99	143.42	35.51

Note: The energy units are kcal/m^2 year. An arbitrary value of 1.0 is assigned to the Boltzmann constant.

Table 3 – Summary of Nodal Inputs and Actions for the Oyster model run of Fig. 12

Node	Shannon entropy	Boltzmann entropy	Macroscopic entropy
Filter feeder	0.00	0.00	31.34
Dep. Detritus	1.15	80.00	7.69
Microbiota	1.36	11.58	7.18
Meofauna	1.57	27.16	4.46
Dep. feeders	1.94	29.15	0.54
Preditors	1.31	39.70	0.49
Total system	1.53	91.05	
Nodal sum	7.34	187.60	51.7

Note: The energy units are converted from kcal/m^2 day to kcal/m^2 year. An arbitrary value of 1.0 is assigned to the Boltzmann constant.

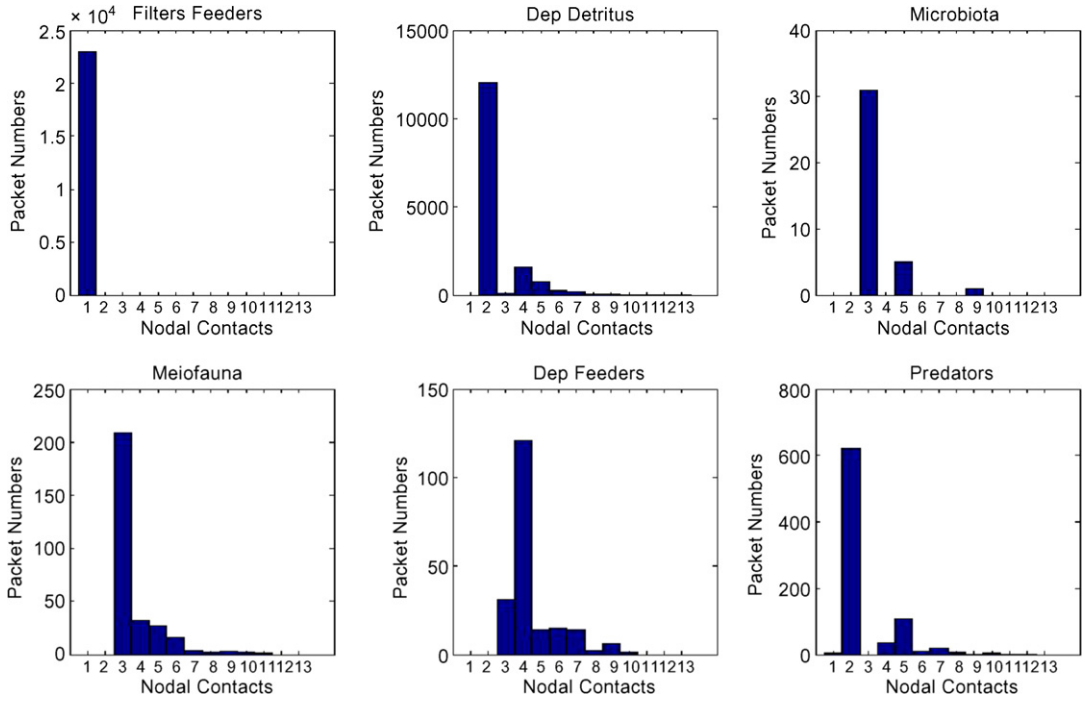

Fig. 13 – Final plot matrix of packet numbers vs. nodal contacts by node for the Oyster model run in Fig. 12.

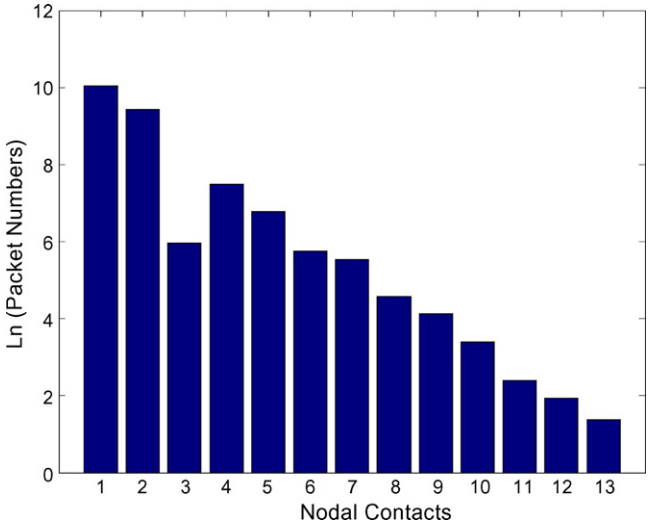

Fig. 14 – Cumulative plot of the natural logarithm of packet numbers versus nodal contacts for the Oyster reef model run of Fig. 12.

The respective comparisons of lumped/macro entropies provided consistent results in the ecological models. The Cone Springs and Oyster models had some similarity in that they were dominated by one or two nodes. There is no compelling reason to choose the Shannon information entropy over the Boltzmann entropy based on the lumped entropy/macroscopic entropy ratios. The same may be said for the nodal sum to macroscopic entropy ratios with the ecological systems. The arbitrary system shown in Fig. 2 varied greatly, which is not surprising given the arbitrary energy units. Another contributing factor to the difference may also have been that the arbitrary system was not dominated by a single node, as were the other ecological models.

4. Potential benefits of the Lagrangian analyses

The Lagrangian analysis approach offers the capability to view a conventional Eulerian model from additional viewpoints. The statistical thermodynamics approach has been of immense value to physicists and engineers for understanding materials properties. Likewise, we believe that a statistical approach (be it the one we propose or one that others may

Table 4 – Comparison of Shannon, Boltzmann and macroscopic entropy ratios on the indicated models

Model	Shan. lumped/Shan. Nodal	B.lumped/B. Nodal	Shan. lumped/ macro	B.lumped/ macro	Shan. Nodal/macro	B. Nodal/ macro
Fig. 2	0.60	0.43	10.99	356.47	18.32	834.87
Cone Springs	0.34	0.39	0.05	1.56	0.14	4.04
Oyster	0.21	0.49	0.03	1.76	0.14	3.63

propose) can further enlighten us on some key interactions observed at the macroscopic level of ecological modeling. For example, our models tend to show that there are always some 'packets' of energy (or mass) that circulate in the network for long periods of time. Network configurations that result in this circulation may impart some proclivity for emerging properties. Our approach at least provides an inroad for quantification of these properties that could be put to field test.

The second potential utility of the Lagrangian approach for modeling relates to the understanding of scaling from the bench to the field and on to the ecological unit. For example, if a point or line source disturbance is placed on a boundary, can we identify some scaling relationships that give insight to how the effect impacts a space? We believe so and are now commencing some analyses towards this end.

5. Summary

The ecological thermodynamics approach presented here respects the isolated, closed and open systems as defined by classical thermodynamics. The first law of thermodynamics is contained herein as well in that energy is still conserved. The nature of the energy (e.g., internal, other) needs further definition. The second law is respected in that the entropy is similar and a scheme is available for what we believe will be a more appropriate combination of classical and ecological entropy.

Much work remains. Many aspects of ecological thermodynamics remain to be developed. The molecular speed–nodal contact analogy leads to an association between thermodynamic temperature and an ecological temperature via the Maxwell–Boltzmann distribution. We have yet to define other thermodynamic properties such as internal energy, pressure and other properties.

Nodal processes as handled by the Spreadsheet, SIMON/ARENA (Pegden et al., 1995) and ECONET approaches must be further explored. They should be further compared and contrasted with STELLA ODE-based approaches and input–output approaches such as Environ analyses (Patten, 1978). The spreadsheet approached used was based on the probabilities of going to the next node (or being dissipated) that were generated with the Patten (1978) environ theory. Similarly, the SIMON/ARENA approach also used these probabilities. SIMON/ARENA provides flexibility in terms of nodal size, storage and probability choices. ECONET on the other hand uses mass action approaches common in reaction kinetics. None of the approaches base transport from one node to the next on respective gradients and conductance coefficients.

The Maxwell–Boltzmann distribution is not necessarily the only distribution from classical thermodynamics that may be applicable. Maxwell–Boltzmann represents molecular gas velocity. One may describe solids using a related distribution known as the Bose–Einstein distribution, which describes molecular vibration speed. Statistical thermodynamics for liquids is not well developed (Zemansky and Dittman, 1997). We are focusing on the Maxwell–Boltzmann distribution as a type for approximation purposes only.

At what point does the free energy of the material represented by multiple nodal contacts represent or correlate with compounds with increasing free energy? Such an occurrence would be consistent with the notion of Prigogine and Stengers (1984) that enclaves of organization occur in regions where much dissipative activity occurs. The fact that this may be happening is a by-product of life.

A careful look at how cycling occurs in ecological systems and associating the cycling with the blending of mass and/or energy of varying states may offer insights into ecological behavior in the future. It is believed that systems offering highly diverse energy and mass will likely be much more robust than those with simplified more simplified dynamics. The ability to track 'extreme event' particles offers many exciting possibilities and in our view forms the potential connection to contemporary ecological thermodynamic theory by Jorgensen (2001) and Jorgensen and Svirezhev (2004) and co-workers and Patten (1978) and co-workers such as Fath et al. (2004). It is felt that the Lagrangian analyses presented herein will enable us to bridge measurement and observation scales in a more seamless manner than will other approaches currently available.

6. Conclusions

An analogy between nodal contact numbers and molecular speed was developed to enable computation of an ecological entropy. There is a similarity between classical and ecological entropy based on similarity in shape of the Maxwell–Boltzmann distributions to the packet-nodal contact numbers. An ecological temperature can be defined based on this similarity. The similarity leads to some promising concepts for entropy calculation. Other aspects of ecological thermodynamics remain to be developed.

The discrete or Lagrangian modeling approach can be implemented with spreadsheets (not recommended), with specialized packages such as SIMON/ARENA or with a new stochastic, particle tracking ODE solver that is newly available. Some questions remain regarding the details of exactly how the SIMON/ARENA, ECONET and input–output approaches move energy or mass from one node to another.

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