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Statistical-thermodynamics modelling of the built environment in relation to urban ecology

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Abstract

Various aspects of the built environment have important effects on ecology. Providing suitable metrics for the built forms so as to quantify and model their internal relations and external ecological footprints, however, remains a challenge. Here we provide such metrics focusing on the spatial distribution of 11,418 buildings within the city of Geneva, Switzerland. The size distributions of areas, perimeters, and volumes of the buildings follow approximately power laws, whereas the heights of the buildings follow a bimodal (two-peak) distributions. Using the Gibbs-Shannon entropy formula, we calculated area, perimeter, volume, and height entropies for 16 neighbourhoods (zones) in Geneva and show that they have positive correlations (R^2 = 0.43-0.84) with the average values of these parameters. Furthermore, the entropies of area, perimeter, and volume themselves are all positively correlated (R^2 = 0.87-0.91). Deriving entropy from Helmholtz free energy, we interpret entropy as a measure of spreading or expansion and provide an analogy between the entropy increase during the expansion of a solid and the entropy increase with the expansion of the built-up area in Geneva. Compactness of cities is widely thought to affect their ecology. Here we use the density of buildings and transport infrastructure as a measure of compactness. The results show negative correlation (R^2 = 0.39-0.54) between building density and the entropies of building area, perimeter, and volume. The calculated length-size distributions of the street network shows a negative correlations (R^2 = 0.70-0.76) with the number of streets per unit area as well as with the total street length per unit area. The number of buildings as well as populations (number of people) show sub-linear relations with both the annual heat demand (MJ) and CO_2 emissions (kg) for the 16 neighbourhoods. These relations imply that the heat demand and CO_2 emissions grow at a slower rate than either the number of buildings or the population. More specifically, the relations can be interpreted so that 1% increase in the number of buildings or the population is associated with some 0.8-0.9% increase in heat demand and CO_2 emissions. Thus, in terms of number of buildings and populations, large neighborhoods have proportionally less ecological footprints than smaller neighborhoods.

Keywords: Urban ecology, Built environment, Thermodynamics, Scaling, Spatial distribution, Helmholtz free energy

1. Introduction

Cities can be regarded as thermodynamic systems. They are sources of water vapour, trace gases and aerosol, and modify the surface roughness (thereby affecting the magnitude and direction of wind) and the moisture content of the soil (e.g., Costanza et al., 1997; Wallace and Hobbs, 2006). In addition, urban areas impact on land use, biogeochemical cycles, and hydrosystems (Grimm et al., 2008). Perhaps the best-known climatic effect of cities is the urban 'heat island', whereby dense cities have higher temperatures, particularly minimum temperatures, than the surrounding rural areas (Grimm et al., 2008). The heat islands impact on air quality and water resources. These and many other aspects of cities influence local and global climate and contribute to pollution (Chen et al., 2014), all of which affect the general ecosystem. In particular, urban areas are marked by biodiversity decrease (e.g., Grimm et al., 2008; Sanford et al., 2008; MacDougall et al., 2013). Biodiversity loss is widely thought to increase the vulnerability of the ecosystem (e.g., Odum and Barrett, 2004; MacDougall et al., 2013). While the relation between reduced biodiversity and vulnerability may not be as clear-cut as once thought (e.g., Jorgensen and Svirezhev, 2004), there is no doubt that urbanisation results in decreased biodiversity, and this effect is certainly of general importance.

There exist many methods of quantification and modelling in ecology as well as in urban systems (e.g., Maynard-Smith, 1978; Wilson, 2006; May and McLean, 2007; Alberti, 2008; Zang, 2009). In particular, classical and statistical thermodynamics have been used extensively over many years for modelling complex systems in general (Prigogine, 1967; Kondepudi and Prigogine, 1998), complex urban systems (Allen and Sanglier, 1978; Portugali, 1997; Batty, 2005), as well as ecological systems (Svirezhev, 2000; Jørgensen and Fath, 2004; Jørgensen and Svirezhev, 2004; Filchakova et al., 2007; Dewar and Porte, 2008; Giudice et al., 2009; Jørgensen et al., 1995 and 2007). For example, exergy (i.e. the maximum amount of useful work that a thermodynamic system can perform) analysis can be used for system optimisation in many engineering fields (Sciubba and Ulgiati, 2005). Similar methods of quantification and modelling, particularly using both classical thermodynamics and statistical thermodynamics, have been developed in urban systems. Examples include several works using thermodynamics and emergy concepts in urban systems (e.g., Odum, 1996; Huang, 1998; Brown et al., 2004; Huang and Chen, 2005; Bristow et al., 2013), gravity and maximum entropy models in transportation (Wilson, 1981; 2006; 2009; Simini et al., 2012), as well as information entropy (Zhang et al., 2006). While both emergy and exergy analysis quantitatively assess the resource consumption of physical systems using space and time integrated energy input/output models (Brown and Herendeen, 1997; Meillaud et al, 2004), recent comparisons suggest they are, as regards framework and approach, different (Sciubba and Ulgiati, 2005; Sciubba, 2010).

Despite all these studies, there has been little attempt to quantify the spatial distributions of the built environment and urban infrastructure using methods from statistical thermodynamics and information theory (Gudmundsson and Mohajeri, 2013; Mohajeri and Gudmundsson, 2014). In particular, there are hardly any studies on the size distributions of buildings within cities and between cities and how these size distributions relate to the ecological footprints of cities. The built-form parameters and their variation, under different ecological conditions, are thought to have strong impacts on the environment (Jabareen, 2006; Tratalos et al., 2007). It is also widely thought that compact urban forms are ecologically more sustainable than spread or dispersed forms (Alberti, 2007). This is because urban form, as reflected in the size distributions of buildings and transport infrastructures, affects energy use and energy efficiency of the built environment and thus the local climate, including the generation of heat islands. It is commonly argued that compact and mixed urban land use is more energy efficient and produces less pollution through reducing the average vehicle distances travelled (Alberti, 2007; Ewing and Cervero, 2010; Makido et al., 2012; Fragkias et al., 2013). In addition, the size distributions of buildings affect factors such as surface roughness, emission of greenhouse gases, and potential habitats for animals, particularly birds. All these factors, in turn, may affect biodiversity and vulnerability of the ecosystem (Alberti, 2007; Alberti and Marzluff, 2004.).

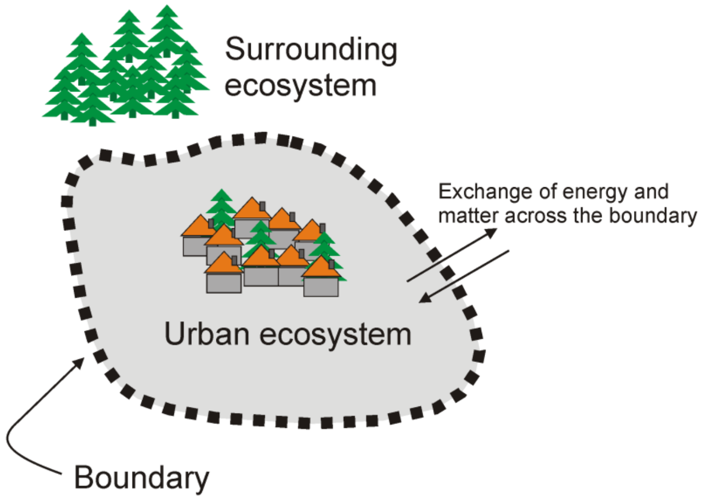

Fig. 1. City, as a thermodynamic system, is separated from its surroundings by a boundary (thick broken line) that allows the exchange energy and/or matter with the surroundings. A city is therefore an open thermodynamic system.

One difficulty in making an objective assessment of how much the built environment impacts on various ecological processes is that quantitative methods and general models that embrace both urban and ecological systems are not well developed. One aim of this study is to show that the Helmholtz free energy can be related to the statistical distributions as an indication of the useful energy and derive the general entropy formula from the Helmholtz free energy. The results are then applied to new data on the building configurations of the city of Geneva in Switzerland. The second aim is to use concepts from general statistical physics/information theory as a framework for quantifying the complexities of built environment in relation to ecology. In particular, we propose metrics for the size distributions of buildings and populations and their relation to urban compactness/dispersal, heat demand, and CO_2 emissions. We also discuss the general ecological implications of the results.

2. Statistical thermodynamics framework

Here we present the basic theory of statistical mechanics and, subsequently, information theory as related to the quantification of complex built environment systems. Statistical mechanics offers a microscopic basis for thermodynamics and a probabilistic treatment of all forms of matter so as to explain their bulk behaviour. In turn, information theory is presently widely regarded as offering a deeper foundation of statistical mechanics (e.g., Brillouin, 1956; Jaynes, 1957a,b: Ben-Naim, 2008; Volkenstein, 2009). All these three fields use the concept of entropy, originally measured as the input of heat at a given temperature to a system, and thus with the unit JK^{-1}. Subsequently, when the concept was given a probabilistic interpretation by Boltzmann and Gibbs the original unit was maintained simply by multiplying the logarithm of probability by the Boltzmann constant k_B. The entropy introduced by Shannon in relation to information theory does not have any specific physical unit; the unit used depends on the base of the logarithm used. There are currently many entropy measures - commonly with arbitrary units - but these can generally be related to the original thermodynamics/statistical mechanics entropy concepts and units after suitable manipulation.

A thermodynamic system is that part of the universe that is of the main interest in a particular thermodynamic study. The surroundings of the system are, strictly speaking, the rest of the universe. For practical purposes, however, the system is commonly that portion of the universe where the thermodynamic measurements are made. An urban ecosystem is an open thermodynamic system since it exchanges energy and matter with its surroundings (Fig. 1). For an urban ecosystem, matter is primarily transported across its boundary, that is, in and out of the system, by human activities, whereas the system exchanges energy partly through natural processes (e.g., radiation) and partly thorough human activities. For a particular urban ecosystem such as the city of Geneva then, for practical purposes, the surrounding ecosystem could be the adjacent rural areas. Alternatively, the surrounding system could be the country (Switzerland) within which the city is located, or Europe, or the entire surface of Earth.

The first law of thermodynamics refers to the conservation of energy and is given by:

$$dU = dQ + dW \qquad (1)$$

where dU is an infinitesimal change in the internal energy of the system when heat dQ is added to the system and work dW is done on the system. While dU is a proper state function (independent of the path taken) and thus an exact (or proper) differential, dQ and dW are both inexact (or imperfect) differentials. Here the path dependence of heat and work is assumed known (cf. Sommerfeld, 1964), so no special symbols for these are used for dQ and dW. The second law of thermodynamics states that during any natural process the total entropy of the universe (or the system and its surroundings) must be greater than or equal to zero. Entropy is commonly interpreted as a measure of disorder in a system. While this is helpful in some ways, it gives a better idea of entropy in many applications, particularly studies such as here for the built environment, to think of entropy in terms of spreading or dispersal.

If a reversible process (a process that allows the system to return to its initial state) takes place (in a closed system) at a specific absolute temperature *T*, then the differential or infinitesimal change in entropy *dS* during the process is:

$$dS = \frac{dQ^{rev}}{T} \tag{2}$$

where dQ^{rev} is the infinitesimal amount of heat received by the system. Eq. (2) is one definition of entropy and implies that entropy increase due to heat transfer to a system from its surroundings is directly proportional to the received heat and inversely proportional to the absolute temperature at which the heat is received. In case the process is irreversible, then Eq. (2) becomes the Clausius inequality:

$$\oint \frac{dQ}{T} \leq 0 \tag{3}$$

More generally, the change in entropy can be given as:

$$dS = \frac{dQ^{rev}}{T} \geq \frac{dQ}{T} \tag{4}$$

for which equality applies if the process represented by the term on the right-hand side of the equality sign is reversible. *dS* is an exact differential (path independent) because *dQ* is changed into an exact differential when multiplied by T^{-1}.

For a reversible process, from Eq. (4):

$$dQ^{rev} = TdS \tag{5}$$

For gas of initial volume *V* subject to pressure *p*, the infinitesimal work *dW* in compressing the gas is:

$$dW = -pdV \tag{6}$$

Combining Eq. (6) with Eqs. (1) and (5) we get the fundamental equation in thermodynamics for a closed system, namely:

$$dU = TdS - pdV \tag{7}$$

This equation combines the first and second laws for a closed system; for an open one, a term allowing material exchange between the system and its surroundings must be added. All the quantities in Eq. (7) are state functions, namely the internal energy *U*, the temperature *T*, the entropy *S*, the pressure *p*, and the volume *V*, so that the equation applies also to irreversible processes and is valid for any process in a closed system. *V* and *S* are both extensive variables, that is, they depend on the size or extent of the thermodynamic system or, in other words, change with the quantity of material present in the system. By contrast, *p* and *T* are intensive variables, that is, they do not depend on the size of the system or the quantity of material that the system contains. *S* and *V* are also referred to as natural variables of the thermodynamic potential *U*.

A thermodynamic potential is a measure of the energy stored in a system and how that energy changes, subject to given constraints, when the system evolves towards equilibrium. Thus, the potentials determine the direction in which a natural process in a system is likely to go. Apart from entropy and internal energy, the main thermodynamic potentials are Helmholtz free energy *F*, Gibbs free energy *G*, and enthalpy *H*. The focus here is on Helmholtz free energy.

2.1. Helmholtz free energy

Free energy is the energy that is free or available to do work rather than being dissipated out of the system as heat. Helmholtz free energy can be interpreted as the energy available to do useful work in a system that has constant (fixed) temperature and volume. The variables that are held constant (fixed), such as temperature and volume for Helmholtz free energy, are referred to as the natural variables of that potential. The potential allows the thermodynamic calculations to focus on the system, rather than the system and its surroundings, and contains the same information about the thermodynamic system as the fundamental equation (Eq. 7).

The Helmholtz free energy *F* is defined as:

$$F = U - TS \tag{8}$$

where *U* is internal energy, *T* is temperature, and *S* is entropy. Differentiating Eq. (8) we obtain for an infinitesimal change:

$$dF = dU - TdS - SdT \tag{9}$$

Substituting Eq. (7) for *dU* in Eq. (9), we obtain:

$$dF = -SdT - pdV \tag{10}$$

For constant temperature then $dT = 0$, and:

$$dF = -pdV \tag{11}$$

Positive change in *F* means reversible work done on the system (by the surroundings), whereas negative change means reversible work done by the system on the surroundings. For constant temperature (no added heat), the infinitesimal change in work is, from Eq. (6), $dW = - pdV$, so that, from Eq. (11), we have:

$$dF = dW \tag{12}$$

which means that a positive change in the Helmholtz free energy of a thermodynamic system is equal to the reversible work done on that system by the surroundings When, in addition, the volume is constant (fixed grip in solid mechanics), then $dV = 0$ and:

$$dF = 0 \tag{13}$$

Thus, F has an extreme value at constant temperature and volume. It can be shown that the second derivative is positive, so that the extreme value is a minimum. In a process that results in an absolute temperature which is equal to that of the surroundings, the maximum work that can be obtained is equal to the decrease in the Helmholtz free energy.

2.2. The Boltzmann distribution, Helmholtz free energy, and entropy

The frequency distribution with which individual microstates occur in a system depends on temperature. When there are no constraints on the system, the maximum-entropy principle predicts a flat or uniform frequency distribution. By contrast, when the constraints are that the energy and number of objects (particles/atoms in statistical mechanics) in the system are constant (fixed), then the distribution becomes negative exponential. If the energy associated with a state of a thermodynamic system is denoted by ε then the probability of occurrence of that state $P(\varepsilon)$ is given by the Boltzmann distribution law (Widom, 2002):

$$P(\varepsilon) \propto e^{-\varepsilon / k_B T} \tag{14}$$

where k_B is the Boltzmann constant, T is the absolute temperature, and the term:

$$e^{-\varepsilon / k_B T} \tag{15}$$

is the Boltzmann factor. For a macroscopic thermodynamic system in equilibrium at temperature T, the probability P_i of finding the system in the given (micro) state i is, from Eq. (15):

$$P_i = \frac{e^{-E_i / k_B T}}{\sum_i e^{-E_i / k_B T}} \tag{16}$$

where E_i is the total mechanical energy. The denominator in Eq. (16), representing the sum over all the states i, assures that the sum of all the probabilities equals one, that is:

$$\sum_i P_i = 1 \tag{17}$$

and is referred to as the partition function, normally denoted by Z and given by:

$$Z = \sum_i e^{-\frac{E_i}{k_B T}} \tag{18}$$

Using Eq. (18), Eq. (16) can be written as:

$$P_i = Z^{-1} e^{-E_i / k_B T} \tag{19}$$

It follows from Eqs. (19) that the probability of a particle (atom, molecule, etc) occupying a given energy level is directly proportional to the exponential of the negative of its energy divided by the product of the Boltzmann constant and the absolute temperature. The Boltzmann distribution thus provides information on the frequency with which the microstates of the thermodynamic system occur for a given temperature.

Using the results in the Appendix (whose equations are denoted by A), from Eqs. (19) and (A14) it follows that Eq. (A15) can be rewritten in the following form:

$$S = -k_B \sum_i p_i \ln p_i \tag{20}$$

where we now use lower-case p for probability so as to fit with the practice in statistical mechanics and information theory. Equation (20) is the Gibbs-Shannon entropy formula; it is completely general and applies to any probability distribution. In case the probability distribution is uniform, which for discrete binned distributions implies that all the bins have equal heights, then we obtain the Boltzmann entropy formula. More specifically, if W is the number of microstates (or, here, bins), so that $p_i = 1/W$, then from Eq. (20) we get for a uniform distribution:

$$S = -k_B \sum_{i=1}^{W} \frac{1}{W} \ln \frac{1}{W} = k_B \ln W \tag{21}$$

which is the Boltzmann entropy formula and applicable to systems in thermodynamic equilibrium. Eq. (21) shows perhaps more clearly than Eq. (20) that entropy is basically the logarithm of probability multiplied by the Boltzmann constant. The Gibbs-Shannon entropy formula (Eq. 20) is also valid for thermodynamic systems that are not in equilibrium, such as systems that are not with constant energy (U), volume (V), or number of particles (N). Furthermore, the Gibbs-Shannon entropy formula is identical in form to the entropy formula in information theory, thereby linking statistical mechanics and information theory.

2.3. Relation with information theory

Shannon (1948) proposed the bit (*bi*nary digi*t*) as the fundamental unit of information, whereby the information contained in a message is found by translating the message into binary code and counting the digits of the resulting string of zeros and ones. Messages that are unusual, that is, indicate something unlikely, carry more information than those that are considered likely before they are received because unusual messages represent unlikely events and are thus difficult to forecast. When the unusual messages are received, however, they therefore provide more information that those that are highly likely or usual. More specifically, when a message has probability p_i, the information I obtained on receiving that message is given by (Luenberger, 2006, Desurvire, 2009):

$$I = \log \frac{1}{p_i} = -\log p_i \tag{22}$$

The logarithm (log) used here can have any base, the most common being natural, common, and base-2 logarithms. Different bases give different units for the calculated information. When the base is 10, the unit is Hartley, when the base is e, the unit is nat, and when the base is 2, the unit is bit. Here we use the base e and the unit is thus nat. Shannon (1948; cf. Shannon and Weaver, 1949) provided the following equation as a measure of information, which has exactly the same form as Eq. (20), namely:

$$H = -k \sum_{i}^{n} p_i \log p_i \tag{23}$$

where k (Shannon used capital K) is a positive constant. The value of k depends on the unit used. Eq. (23) implies as follows (cf. Jones and Jones, 2000; Yanofsky and Mannucci, 2008; Desurviere, 2009). The quantity expressed by Eq. (23) is a measure of information, choice and uncertainty. The entropy H = 0 if and only if all the probabilities but one are zero, in which case the received message or outcome is certain. For all other cases, the entropy H is positive and reaches a maximum when all the probabilities p_i in the probability distribution of Eq. (23) are equal, a uniform distribution. Then we know the least about the likely outcome before the message is received. Generally, the more equal the probabilities the higher the entropy. Maximum source entropy implies maximum uncertainty, but also maximum information from the received message.

The unit of the constant k in Eq. (23) is not physical but rather depends on the base of the logarithm used. The constant is commonly regarded as arbitrary with a unit value, so that the information entropy becomes dimensionless. When the second law of thermodynamics is derived from pure probability considerations, the result is the natural logarithm of probability. To fit the results with the entropy unit J K^{-1}, the log-probability results (in nat) are simply multiplied with $k_B = 1.38 \times 10^{-23}$ J K^{-1}. Similarly, multiplying the entropies for built environment data discussed here by the value of k_B yields the units of physical entropy. The calculated entropies of the building populations in the paper, however, are dimensionless and given in the unit of nat. This presentation corresponds to the Boltzmann's constant k_B being normalised to a factor 1. The entropies have a physical connection to development of the built environment because the construction of buildings requires energy and produces entropy.

3. Data and methods

3.1. Datasets

The sample of building configurations is restricted to a single city, Geneva in Switzerland (Fig. 2).

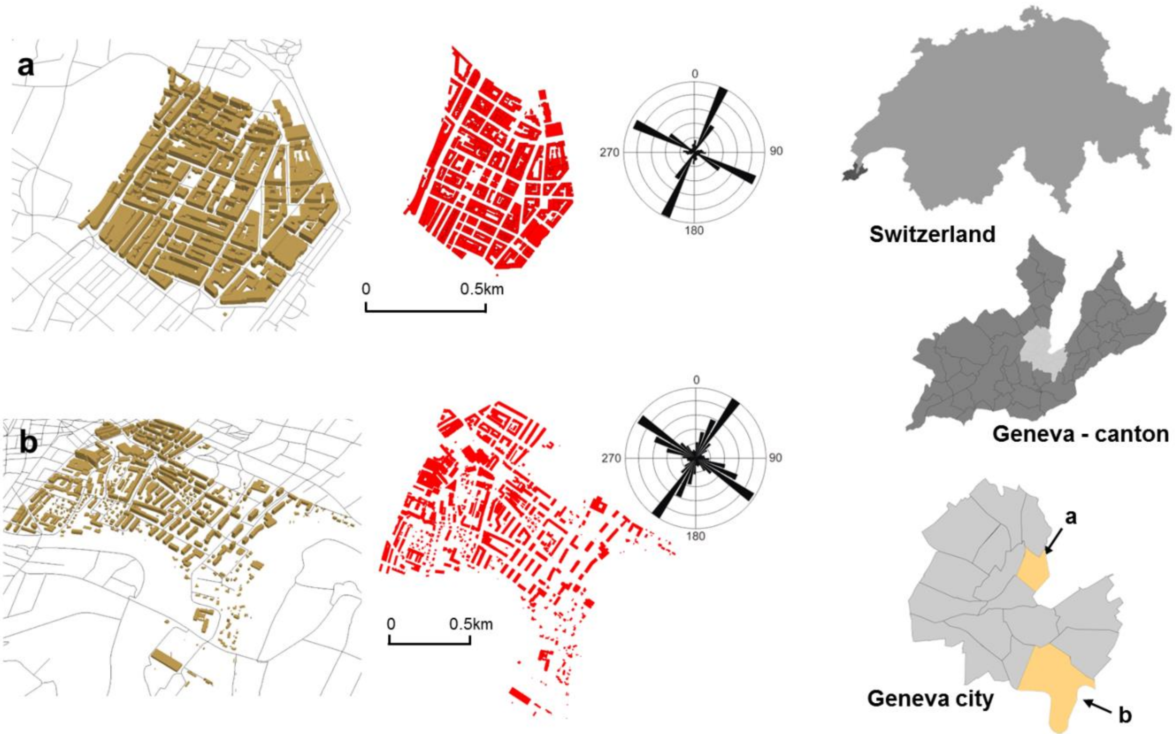

Fig. 2. Location of the city of Geneva in Switzerland and the 16 studied neighborhoods/zones of Geneva. A 3D view, a 2D (plan or map) view of the buildings, and the rose diagrams of the building orientations in (a) one of the old neighbourhoods/zones of Geneva (Paquis), (b) one of the more recent neighbourhoods/zones (Champel).

The 16 neighbourhoods or zones, however, have a large range in (1) building numbers, from 181 to 1193, (2) geographical environment (e.g., surrounding topography and location), and (3) population - from about 2 thousand to 23 thousand. All the 16 zones are defined by administrative boundaries as determined by Swiss Federal Statistical Office, which also provides the population data for 2013 (www.bfs.admin.ch). Building datasets are obtained from the Swisstopo (www.swisstopo.admin.ch) imported into ArcGIS for subsequent analyses. GIS tools are used to calculate the area, perimeter, volume of the buildings and their azimuths (orientations). Heat demand (integrated space heating and domestic hot water) and CO_2 emission datasets are based on measured and monitored data, but are available only for buildings with at least 5 users (inhabitants). The data is provided by SITG open access data (Système d'information géographique du territoire genevois; http://ge.ch/energie/suivi-energetique-des-batiments). Population data for buildings in which the heat demand and CO_2 emissions were measured (50% of the total number of buildings) are also provided by Office fédéral de la statistique OFS, Registre fédéral des bâtiments et des lodgements.

3.2. Heavy – tailed distributions

A bi-logarithmic plots yield straight lines for the heavy-tailed size distributions in Figs. (3, 4, 5) which can be approximated by power laws.

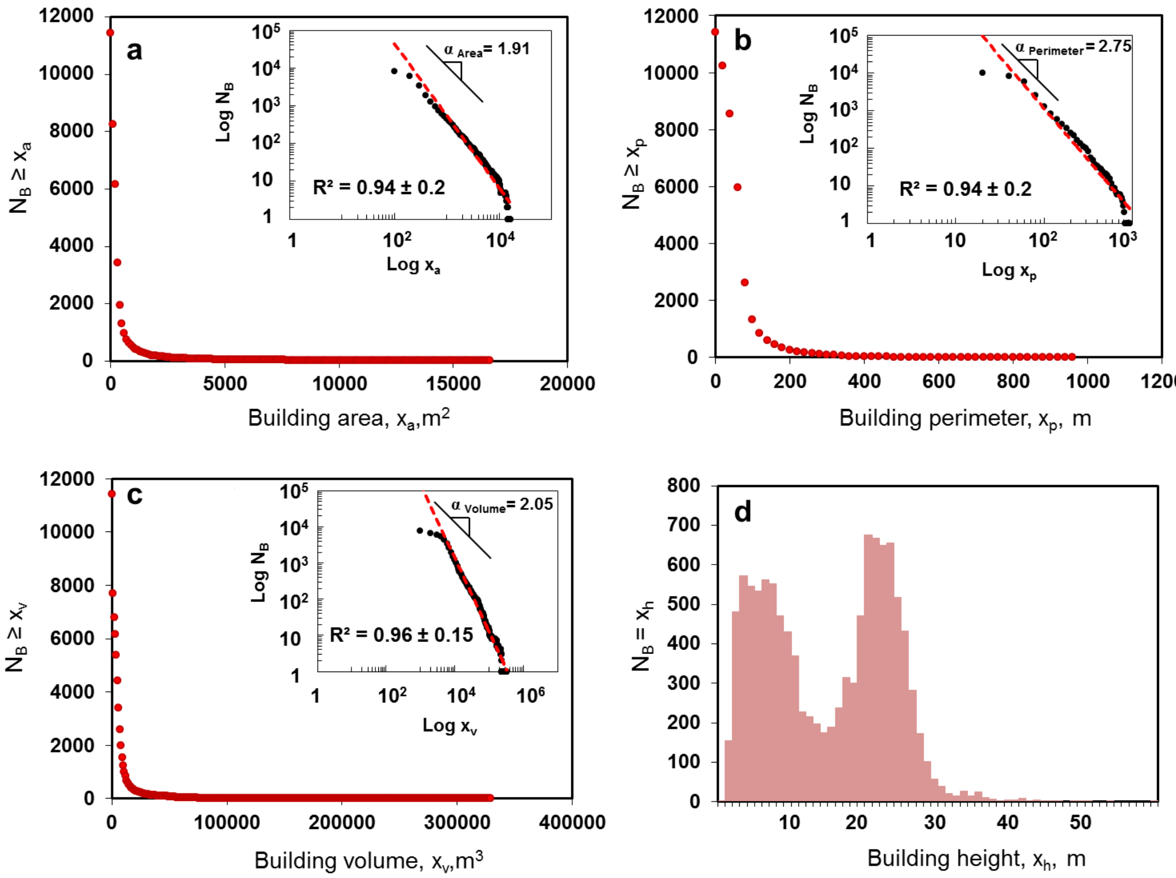

Fig. 3. Power-law size distributions of (a) building areas, x_a (b) building perimeters, x_p and (c) building volumes, x_v (11419 buildings) from the whole city of Geneva using an ordinary scale and, then, a log-log scale (insets).(d) Bimodal height distribution, x_h, of the same building data.

A power law may be expressed as a frequency (probability) distribution in the form:

$$p(x) = Cx^{-\alpha} \quad (24)$$

where *p(x)* is the frequency (probability) of buildings having area (or perimeter or volume) equal to *x*, *C* is a normalisation constant, and *α* is the scaling exponent. To obtain the bi-logarithmic (log-log) plots (Figs. 3-5), the logarithms of both sides of Eq. (24) are taken so as to obtain the linear equation:

$$\log p(x) = \log(C) - \alpha \log(x) \qquad (25)$$

Then standard regression methods are used to find a best-fit straight line describing the dataset. If the straight line of Eq. (25) fits the dataset well, the distribution is commonly regarded as a power law (Pisarenko and Rodkin 2010). However, more accurate tests such as likelihood-ratio tests (cf. Clauset et al., 2009) can be used for comparing the power-law fit with the one provided by other functions or alternative models (e.g., log-normal, exponential, and stretched exponential).

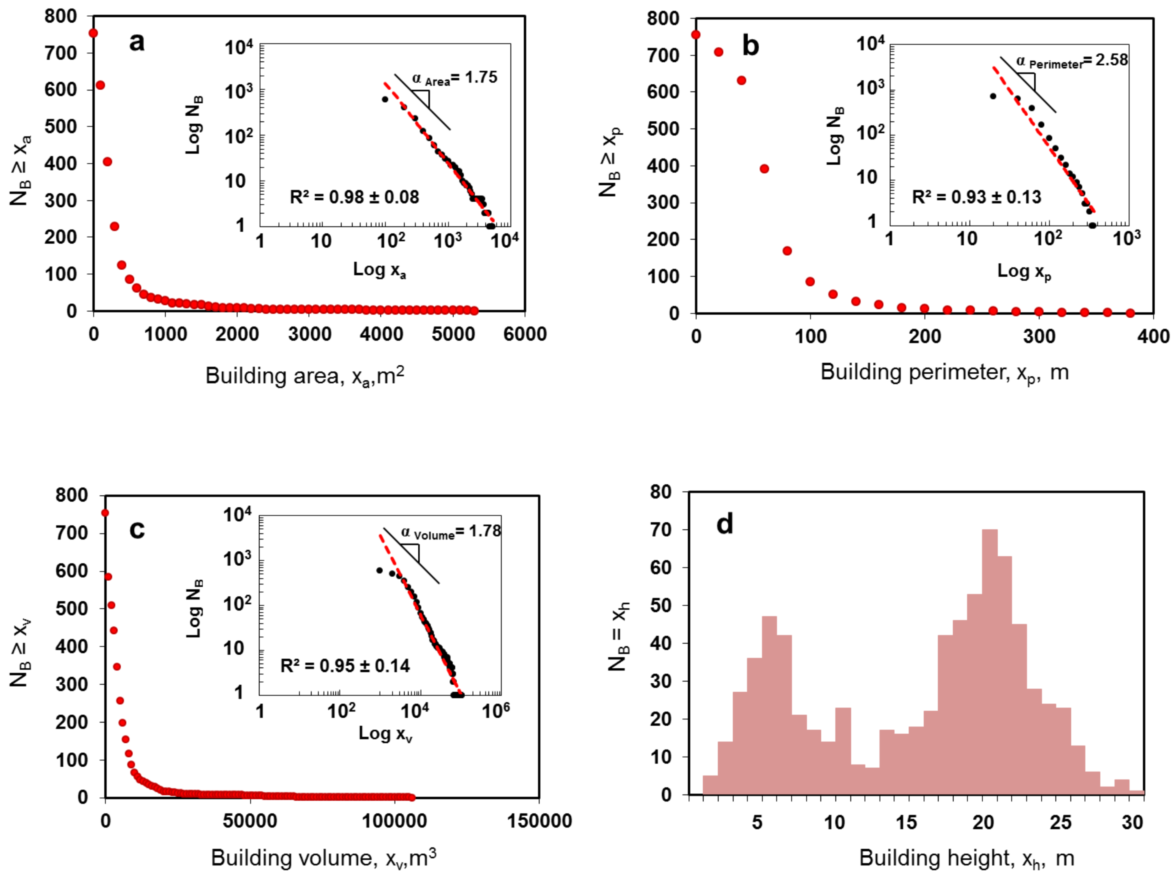

Fig. 4. Power-law size distribution of (a) building areas, (b) building perimeters, and (c) building volumes (754 buildings) from the old zone of Geneva (Paquis) in an ordinary scale and, then, a log-log scale (insets).(d) Bimodal height distribution of the same data.

For power laws derived from histograms the scaling exponent α (Eq. 24) depends on the chosen bin width. To overcome (partly) this dependency on bin width, we use cumulative frequency distributions rather than histograms. Then we plot the probability *P(x)* that *x* has a value greater than or equal to *x*, namely:

$$P(x) = \int_x^\infty p(x')dx' \tag{26}$$

If the frequency size distribution follows a power law, $p(x) = Cx^{-\alpha}$, then:

$$P(x) = C\int_x^\infty x'^{-\alpha} dx' = \frac{C}{\alpha - 1} x^{-(\alpha-1)} \tag{27}$$

A log-log plot of *P(x)* (Eq. 25) again yields a straight line, but its slope is shallower; that is, its scaling exponent is smaller than that of *p(x)* in Eq. (24). One benefit is that the cumulative frequency distribution tends to smooth out the irregularities (noise) in a dataset (cf. Newman 2005; Clauset et al. 2009).

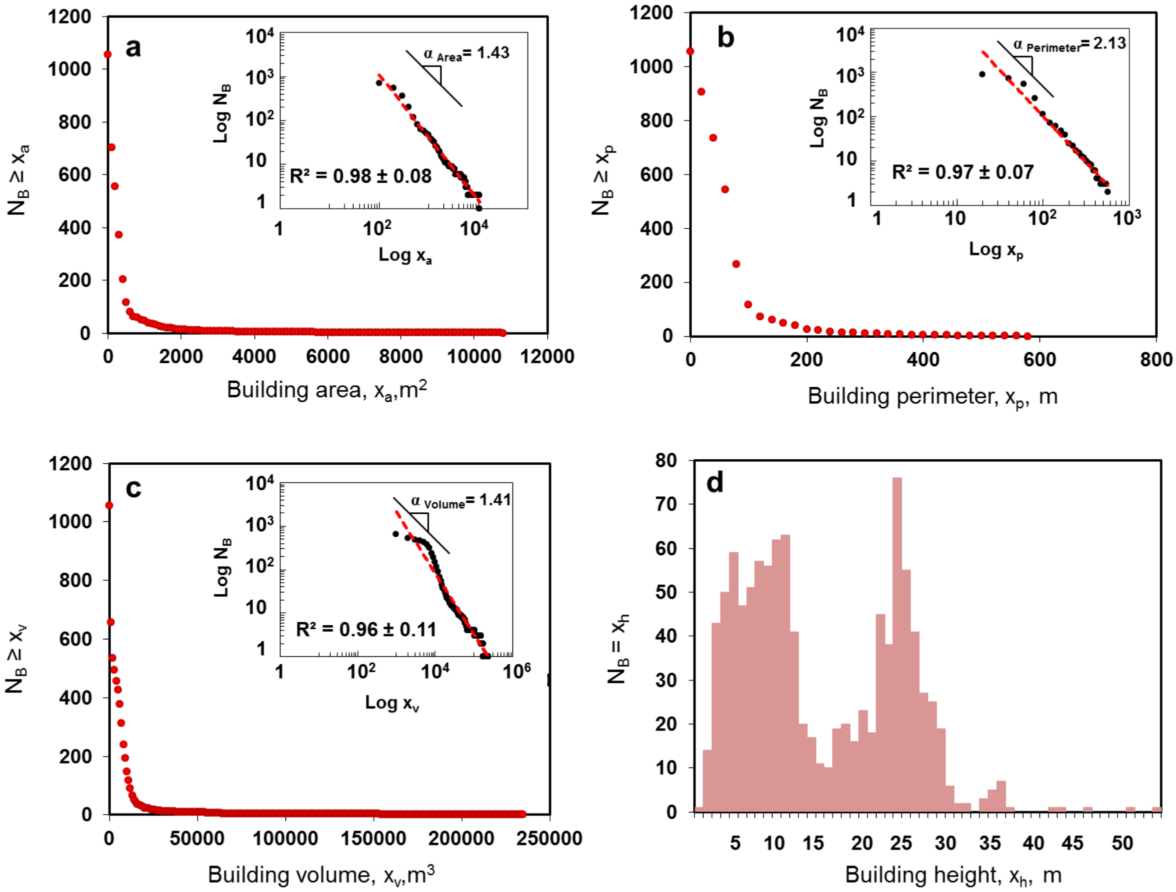

Fig. 5. Power-law size distribution of (a) building areas, (b) building perimeters, and (c) building volumes (1055 buildings) from the more recent zone of Geneva (Champel) in an ordinary scale and, then, a log-log scale (insets).(d) Bimodal height distribution of the same data.

3.3. Entropy

For a general probability distribution, such as the size-frequency distribution of buildings, the entropy, H or S, is given by the Gibbs-Shannon equation, Eqs. (20, 23) (Brillouin 1956; Laurendeau 2005; Volkenstein 2009). In Eq. (23) k is a positive constant (Boltzmann constant k_B), n is the number of classes or bins with nonzero probabilities of buildings (bins containing building counts), and p_i is the probability of buildings falling in the i-th bin (the probability of the i-th bin). The minus sign for k ensures a positive value for the entropy. Eq. (23) shows a general relation between entropy H or S and probability p_i; it is equally valid for equilibrium and non-equilibrium systems (e.g., Panagiotopolus 2012). By definition, the sum of the probabilities for all the bins equals one. The probabilities are a measure of the chances of randomly selected buildings from a population falling into a particular bin; only those bins that contain at least one building are included. For a uniform distribution, all the bins have the same frequency, whereby the entropy would reach its maximum value (Eq. 21).

Equations (5) and (7) imply that the greater the bin number and the smaller the bin width, the greater is the entropy for a given data set (cf. Singh 1997; Mays et al. 2002). However, the number of bins cannot exceed a certain limit, for example, the number of analysed buildings. To minimise the effect of bin size on entropy calculations, all the bin widths used here for the specific parameters are equal: 100 m^2 for area distributions, 20 m for perimeter distributions, 1000 m^3 for volume distributions, and 1 m for the height distributions.

4. Results

The main equations derived and discussed above can be used as quantitative metrics for the built environment. The following parameters were measured: areas, perimeters, volumes, and heights of the buildings in 16 neighbourhoods in Geneva (Tables 1 and 2). We divided the main analysis into three parts: the whole city (Fig. 3), a selected inner and older part (name: Paquis) of the city (Fig. 4), and a selected outer and more recent part (name: Champel) of the city (Fig. 5). The dataset on the entire city contains 11,418 buildings (Fig. 3). On plotting the building-area size distribution (Figs. 3 - 5), we see that the areas, perimeters, and volumes follow power-law size distributions, but not the building heights. All the height-size distributions are bimodal (double peak) distributions (Figs. 3d, 4d, and 5d). This means that there is one set showing a roughly normal distribution with a small mean height, and another set showing a roughly normal distribution about a much greater mean height.

It is perhaps surprising that the volume-size distributions of the buildings are power laws given that the heights follow bimodal distributions. Clearly, the height enters the volume, so that we might expect the bimodal shape of the height distributions to be reflected in the shape of the volume distributions. However, the area size distributions all follow power laws (Figs. 3-5). Because the areas enter the volume through two dimensions whereas the height enters through one dimension, it follows that the areas dominate in the volume-size distributions, which therefore become not bimodal but rather power law distributions.

4.1. Entropies of the size distributions

We used Eqs. (20) and (23) to calculate the entropies of the various building size distributions. The results (Table 2) show that the entropy varies considerably between the selected inner and outer zones of the city of Geneva and in general within the 16 zones of the city (Fig. 6). Consider first the area size distribution (Figs. 3a, 4a, and 5a). Focusing first on the inner and outer zone in comparison with the city as a whole (Table 2), the entropy of the outer zone (Champel) is the largest (2.66), followed by that of the city as a whole (2.590), that of the inner zone (Paquis) being the smallest (2.29). Thus, the entropy of the area-size distribution for the whole city is in-between those of the inner and outer neighbourhoods (Table 2). The same results are obtained for the entropies of the other power-law size distributions, namely of perimeter and volume: the outer neighbourhood (Champel) has the largest entropies, followed by those of the city as a whole, whereas the inner neighbourhood (Paquis) has the smallest entropies (Table 2).

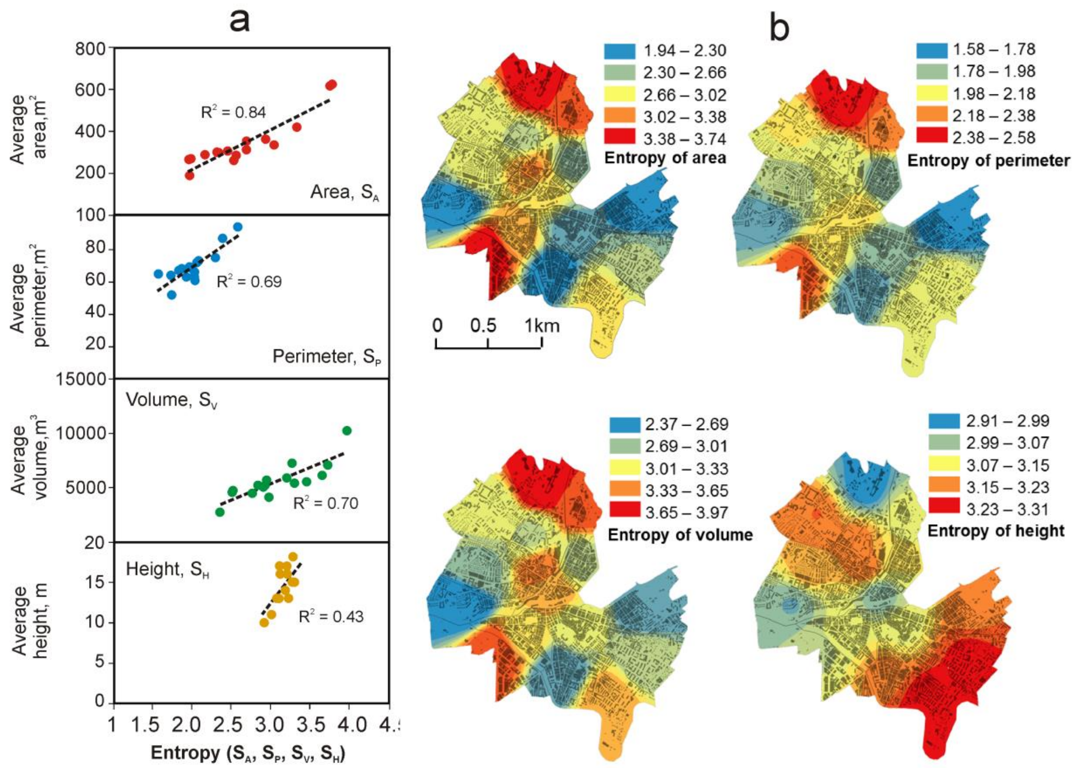

Fig. 6. Average area, perimeter, volume, and height versus associated entropies. The maps show the distributions of area, perimeter, volume, and height entropies for 16 zones in Geneva.

Entropy is commonly interpreted as a measure of 'disorder' in a system, but may also be regarded as a measure of spreading or dispersal. When the 'constraints' on a thermodynamic system are relaxed, such as by making more space available for its particles or objects, the entropy tends to increase. Here we see that the greater the arithmetic averages of the area, perimeter, and volume, the greater is the corresponding entropy (Tables 1, 2). To test if such a correlation between entropy and average values of these parameters exists, we analysed all the 16 zones of the city of Geneva (Fig. 2). The results (Fig. 6a) show high linear correlations (the coefficient of determination, R^2, ranging from 0.69 to 0.84) between the entropies and the average values of these three parameters, thereby further supporting our conclusions from the more limited data. There is also a correlation between average building height and entropy, but less significant (R^2 = 0.43) excluding an outlier for the St-Gervais zone.

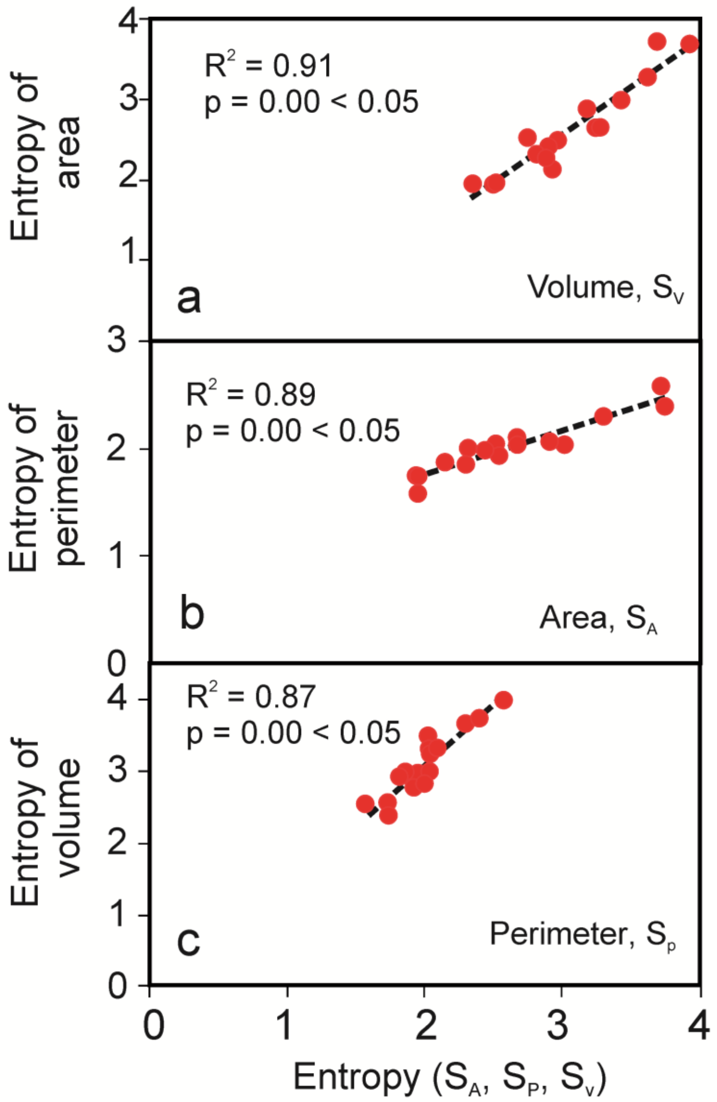

Fig. 7. The relation between entropies of the size distributions of area, perimeter, and volume. The coefficient of determination (R^2) and the associated significance p-values) are given for each linear correlation.

The distributions of the entropies of all the four parameters are perhaps better visualised in map view (Fig. 6b). The results show that entropy distributions of the three parameters area, perimeter, and volume, are broadly similar. In particular, the lowest entropies of these three parameters are in the inner and older zones of the city, whereas the highest entropies are in the outermost zones, far away from the old centre of the city. By contrast, the entropy distributions of building heights are quite different. While the entropy in the old central zones is still low, the extreme entropy values occur at the north and south ends of the city.

Thus, the highest height entropy is in the southernmost part of the city while the lowest entropy is in the northernmost part. The height distribution is bimodal and thus widely different from the power-law size distributions of the area, perimeter, and volume distributions.

Further analysis shows that the entropies of the size distributions of these three parameters, namely area, perimeter, and volume, are strongly correlated (Fig. 7). We tested the correlations for all the 16 zones of Geneva and found that the coefficient of determination, R^2, of these entropies varies from 0.87 to 0.91. While these parameters are not clearly independent, these strong linear correlations suggest that the entropy results for one parameter, for example building area, can be used to forecast the entropies of the other parameters, here the perimeters and volumes of the buildings.

4.2. Expansion of urban and ecological systems: a thermodynamic analogy

Urban areas and ecological systems are not isolated but rather open thermodynamic systems (Fig. 1) due to the fact that they receive energy and matter and interact with their surroundings. Thermodynamic potentials such Helmholtz free energy (Eqs. 8 and A9) can be used to model the expansion of both urban and ecological systems. Here the focus is on the urban systems. An urban neighbourhood or zone that has, on average, higher number of buildings or higher total street length than some other zones may be regarded as having expanded. This applies particularly within individual cities. For example, some studies with a focus on transport infrastructure have shown increasing average street length in the networks with increasing distance from the dense city centre (e.g. Gudmundsson and Mohajeri, 2013).

The expansion of an urban area may be regarded as analogous to stretching or expansion of an elastic body. We consider here a one-dimensional version of such an expansion, but the results are easily generalised to two or three dimensions. If the initial length of the elastic rod is L_i and the final length is L_f, then during the application of the tensile force f the length increases by $dL = L_f - L_i$. It then follows that the work done by the force is fdL. Substituting fdL for $-pdV$ in Eq. (10) we get the change in Helmholtz free energy as:

$$dF = -SdT + fdL \tag{28}$$

By analogy with Eq. (A6) then for constant length of the rod, the entropy S is related to the change in Helmholtz free energy, from Eq. (28), as follows:

$$S = -\left(\frac{\partial F}{\partial T}\right)_L \tag{29}$$

Similarly, from Eq. (28) and for constant temperature the tensile or extension force f is related to the change in Helmholtz free energy through the equation:

$$f = \left(\frac{\partial F}{\partial T} \right)_T \quad (30)$$

Applying the mathematical property of exact differentials (Ragone, 1995) to Eq. (28), and denoting the infinitesimal tension by df, we obtain:

$$\left(\frac{\partial S}{\partial L} \right)_T = -\left(\frac{\partial f}{\partial T} \right)_L \quad (31)$$

which is a Maxwell relation. For linear elastic solids the one-dimensional Hooke's law may be stated as the ratio of normal stress σ to normal strain ε, thus:

$$\sigma = E\varepsilon \quad (32)$$

where *E* is Young's modulus, a measure of stiffness or springiness of the solid. By definition, normal stress is force per unit area and normal strain is change in length divided by the original length. Thus, we have:

$$\sigma = \frac{df}{A} \quad (33)$$

where *A* is the area, and

$$\varepsilon = \frac{dL}{L} \quad (34)$$

Combining Eqs. (32-34), we obtain for Young's modulus the relation:

$$E = \frac{L}{A} \left(\frac{\partial f}{\partial L} \right)_T \quad (35)$$

Solids normally expand on being heated. One measure of this expansion is the linear expansivity α, which is here the fractional change in dimension of the body (here in length of the rod) per degree change in temperature. In the present notation, the linear expansivity may be presented as:

$$\alpha = \frac{1}{L}\left(\frac{\partial L}{\partial T}\right)_f \tag{36}$$

the subscript f meaning that the tensile or extension force is constant. Using Eqs. (35) and (36), we can find a new expression for the right-hand side of Eq. (31) thus:

$$\left(\frac{\partial f}{\partial T}\right)_L = -\left(\frac{\partial f}{\partial L}\right)_T \left(\frac{\partial L}{\partial T}\right)_f = -EA\alpha \tag{37}$$

It therefore follows that the change in entropy with change in length or expansion of the rod, from Eqs. (31) and (36), becomes:

$$\left(\frac{\partial S}{\partial L}\right)_T = EA\alpha \tag{38}$$

which shows that so long as α is positive (normally the case except for rubber), the entropy increases with expansion of the solid. Although the result is here derived for solids, it applies as well to fluids; when gas expands, so that the volume occupied by the gas increases, its entropy increases. And, more generally, allowing matter to expand, for example by moving certain constraints, tends to increase the entropy. By analogy, entropy of the built environment, as reflected in increasing average area, average perimeter, or average volume of buildings, increases the configuration urban entropy (Fig. 6).

4.3. Ecological implications

Urban form is widely regarded as an important factor that affects ecological systems (e.g., Burton et al., 1996; 2000; Jabareen, 2006). In particular, compact urban form is thought to be ecologically favourable in the sense of using less energy per capita – both in terms of energy use in the built environment and energy (fuel) consumption for transportation (e.g., Jabareen, 2006). In addition, compact urban form uses less land and, on the assumption of using less energy per capita, is thought to produce less pollution.

While urban areas are generally thought to be marked by biodiversity decrease (e.g., Grimm et al., 2008; Sanford et al., 2008; MacDougall et al., 2013), some authors suggest the opposite. For example, in a study of biodiversity in cities in Switzerland, Home et al. (2010) suggest that cities are the sites of high biodiversity, partly because of heat-island effects, and partly because cities provide the sites for a variety of imported exotic plants and animals that can thrive in the urban ecosystem but could not exist in its rural surroundings. This applies particularly to various thermophilous plants and animals that prefer urban systems. Based on these different views, it is clear that quantitative studies are needed so as to explore not only the exact ecological impacts of different urban forms and densities (urban compactness) but also how the impact may change from one place to another.

One principal point widely regarded as being in favour of the compact city is that compact cities use urban land more efficiently and reduce the urban sprawl, which has considerable ecological benefits (e.g., Jabareen, 2006; Tratalos et al., 2007). One difficulty, however, is to decide on the criteria for assessing the compactness of a city, since the compactness normally varies through time. During the growth of many cities, there are periods when expansion dominates alternating with periods when densification (increasing compactness) dominates (e.g., Strano et al., 2012; Mohajeri and Gudmundsson, 2014). The expansion of cities generally increases the land coverage and thus changes the land-use and drives other types of environmental change. By analogy with the expansion of solids (Section 4.2), and the relation between city growth and entropy, entropy is likely to increase during city expansion and decreases during densification and increased compactness. This suggestion is supported by results on the relationships between entropy and street-network expansion/densification for many cities (Mohajeri and Gudmundsson, 2014). In addition, entropy of transport networks tends to increase with increasing distance from the central dense parts of the cities (e.g. Gudmundsson and Mohajeri, 2013).

For Geneva it is clear that the inner zone (Paquis) is much more compact than the outer zone (Champel). This difference is reflected in land (site) coverage by buildings, which is about 45% in the inner zone compared with about 18% in the outer zone, but also in the ratio between the total built volume and the associated land area – that is, the volume/area ratio (Table 3). For the inner zone the volume/area ratio is about 7.7 but about 3.2 for the outer zone. The compactness is also reflected in the population density, which is about 22,000 people per km^2 in the inner zone compared with about 10,000 people per km^2 in the outer zone. Overall, the parameters reflecting compactness are generally similar for the outer zone as for the city as a whole, whereas those for the inner zone are generally much higher than either of these (Table 3).

For the 16 zones in Geneva, plots of the building density (number of buildings per km^2) against the entropies of building volume, perimeter, and area show negative linear correlations (Fig. 8a-c). The correlations between building density and entropy of perimeters ($R^2 = 0.54$) and area ($R^2 = 0.52$) are reasonably strong, but less so between building density and entropy of volume ($R^2 = 0.39$). The calculated p-values suggest that all these correlations are statistically significant (Fig. 8). The results also show a clear negative linear correlation between the street density and the street-length entropy. We use two definitions of street density namely, the number of streets per unit area (Fig 8d) and the total (cumulative) street length per unit area (Fig. 8e). The relation between street densities and length entropies is strong ($R^2 = 0.76$ and 0.70) which is also indicated in the calculated p-values (Figs. 8d and e).

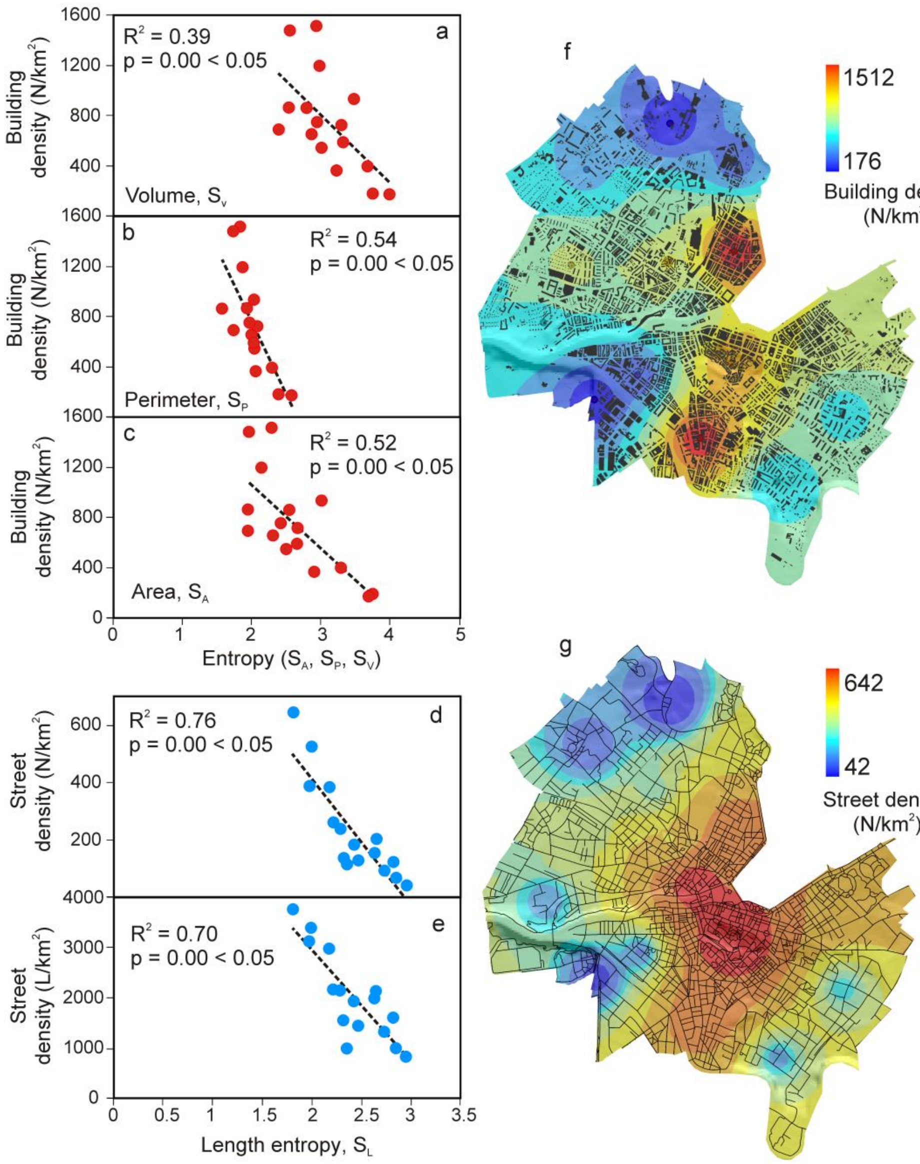

Fig. 8. Entropy of size distributions against density for the buildings and street networks of 16 zones in Geneva. (a) Entropies of building volumes, entropies of building perimeters (b), and entropies of building areas (c) versus building density (number of buildings N per km^2). (d) Length-entropy against street density (number of streets N per km^2), (e) Length-entropy versus street density (total street-length per km^2). p-values show the significance of R^2 for each linear correlation. The maps show the gradients of building density (f) and the infrastructure density namely, street density (g) from the city centre to the outer parts of the city for the 16 zones in Geneva.

Entropy is a measure of spreading (Gudmundsson and Mohajeri, 2013; Mohajeri and Gudmunsson, 2014) and thus one measure of the building and transport-network configurations. As the average built form parameters (area, perimeter, volume, and height) increase in size, the spreading measured by entropy increases (Fig. 6a; Tables 1 and 2). Conversely, as the building density increases and the average built-form parameters decrease, the spreading becomes less and so does the entropy (Fig. 8a). Similarly, as the average distance between streets decreases (the city becomes more compact), their average length decreases and the spreading as measured by entropy decreases (Fig. 8d and e; Gudmundsson and Mohajeri, 2013). Thus, the more compact the built-up areas and the more confined the street network, the lower are their entropies. The result is in agreement with well-known thermodynamic effects of constraints; increasing the constraints (reducing the available volume or area) normally decreases the entropy (Reiss, 1996). We also show maps of the gradients of building density (Fig. 8f) and street density (Fig. 8g) for the 16 zones in Geneva.

Another measure of the ecological impact of cities is the heat demand and associated CO_2 emissions by the built-up areas. The heat demand in the neighbourhoods of Geneva is not only related to the parameters of the built form but also to other factors (e.g. household size, income). The latter include the construction period, that is, the age of the buildings, insulation and local microclimate as well as complex socio-economic factors, such as income and number of people living in a particular household. All these parameters can change from one building to another and from one zone to another zone within the Geneva city. Whether the energy use (heat demand) and carbon emissions relate primarily to the built form as such, or to insulation, construction periods, or socio-economic factors remains to be explored.

There have been comparatively few empirical studies as to whether the environmental impacts of urban areas becomes proportionally less or greater with increasing population (Zucchetto, 1983; Oliveira et al., 2014; Mohajeri et al., 2015). To explore this impact, we compare the number of people living in the 16 studies zones of Geneva and the number of buildings in each zone with the associated heat demand and CO_2 emissions (Figs. 9, 10, 11). As mentioned in Section 3, the measurement data for heat demand and CO_2 emissions within each neighbourhood in Geneva cover only about half the buildings in each zone. We therefore consider only those buildings and associated populations for which the heat demand and CO_2 emissions data are available.

The correlation between the number of buildings and the average annual heat demand (MJ) and annual CO_2 emissions (kg) is sub-linear, meaning that the scaling exponent α in the relation is less than 1 (Fig. 9). The exponent and the 95% confidence intervals (*CI*) are as follows: $\alpha = 0.89$, *CI* = [0.79-0.99] for Fig. 9a; $\alpha = 0.90$, *CI* = [0.79-1.01] for Fig. 9b. The sub-linear relations show that for all the 16 zones, the heat demand and CO_2 emissions grow at slower rates than the number of buildings. The relations can also be interpreted so that 1% increase in number of buildings is associated with about 0.9% increase in heat demand and CO_2 emissions. This implies that as the number of buildings increases, proportionally less heat is consumed and less CO_2 emitted and thus less ecological footprints.
Similarly, comparisons between the populations on one hand and the annual heat demand (MJ) and CO_2 emissions (kg) on the other hand show sub-linear relationships (Fig. 10). The scaling exponent at the 95% confidence intervals (*CI*) is $\alpha = 0.81$, *CI* = [0.62-0.99] for Fig.

10a; α = 0.82, *CI* = [0.64-1.00] for Fig. 10b. These relations imply that as the population increases proportionally less fuel for heating per capita is consumed and less CO_2 per capita is emitted (cf. Fig. 11). These relations can also be interpreted so that 1% increase in the population is associated with about 0.81% increase in fuel consumption and 0.82% increase in CO_2 emissions, thereby proportionally decreasing ecological footprints. It follows that in terms of population, larger zones are more energy efficient and environmentally friendly than smaller ones.

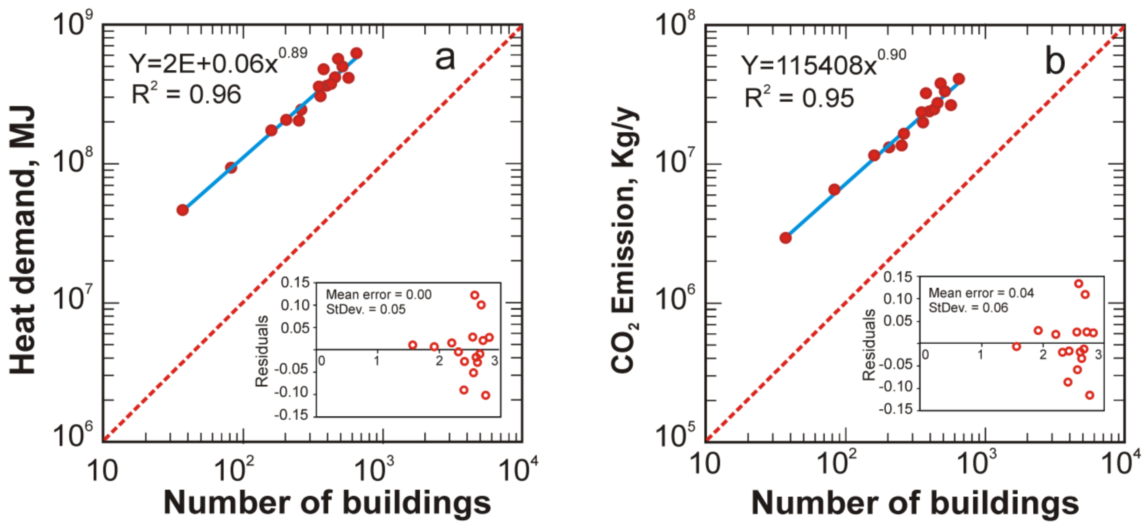

Fig. 9. Number of buildings against annual heat demand (MJ) and CO_2 emissions (kg) for the 16 zones in Geneva (broken straight line is for a slope of 1, in which case the power of x in the inset equations would be 1). (a) Sub-linear relation between number of buildings and heat demand with the scaling exponent α = 0.89 ± 0.05 (R^2 = 0.96 ± 0.06) and associated residuals for the single line fit in (a). (b) Sub-linear relation between number of buildings and CO_2 emissions with the scaling exponent α = 0.90 ± 0.05 (R^2 = 0.95 ± 0.06) and associated residuals for the single line fit in (b).

For a standard least-square linear regression, a measure of the goodness-of-fit between the calculated regression lines and the actual data can be obtained from the residuals of the curve-fitting procedure (Berendsen, 2011; Hughes and Hase, 2010; Motulsky, 2010). If the relation is statistically significant then the residuals should ideally be normally distributed about a zero mean and without any obvious structure. The residual plots for the population versus heat demand (MJ) and CO_2 emissions are shown on the insets in Fig. 10. For the population versus heat demand (Fig. 10a), the mean of the residuals is 0.00, indicating that there is no clear structure. The standard deviation is 0.11, and the range (the difference between the maximum and minimum residual) is -0.43. For the population versus CO_2 emissions (Fig. 10b), the mean of the residuals is again 0.00 (so no clear structure). The standard deviation is 0.11, and the range is -0.42. The residuals are roughly normally distributed around a zero mean and all the residuals range between -1 and 1.

We also mapped the annual heat demand (MJ) per capita and the CO_2 emissions (tonne) per capita in the city of Geneva (Fig. 11). Both maps show similar structure, indicating a decrease in heat demand per capita (Fig. 11a) and CO_2 emissions per capita (Fig. 11b) from the core (city centre) to the outer parts. One possible explanation of these gradients may relate to the rather poor insulation of the buildings in the city centre compared with the more recent parts. This is, however, only one of several possible explanations, which need to be explored further when new data for the heat demand and CO_2 emissions for all the buildings (Fig. 8f) become available.

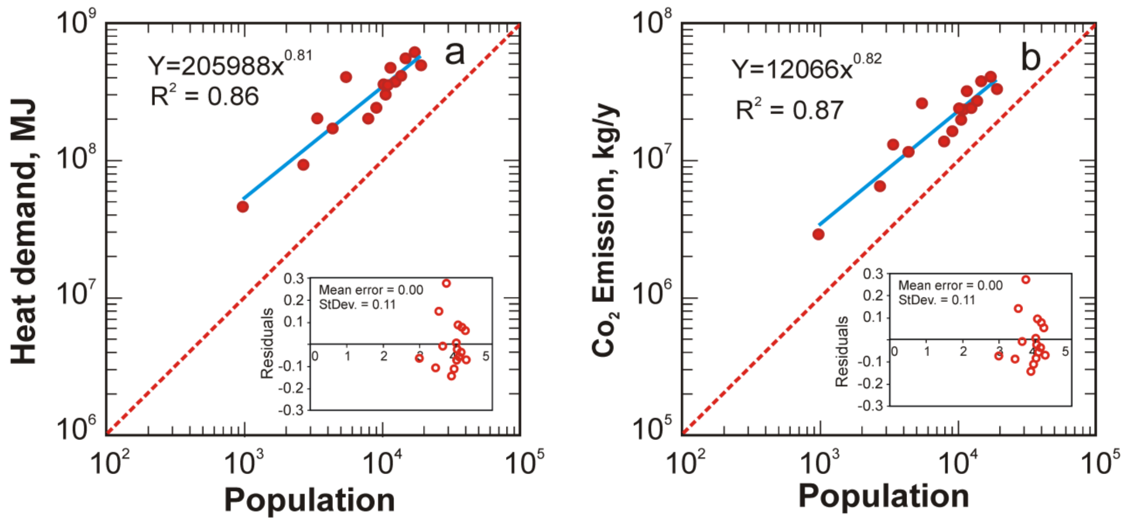

Fig. 10. Population against annual heat demand (MJ) and CO_2 emissions (kg) for the 16 zones in Geneva. (a) Sub-linear relation between population and heat demand with the scaling exponent $\alpha = 0.81 \pm 0.08$ ($R^2 = 0.86 \pm 0.11$) and associated residuals for the single line fit in (a). (b) Sub-linear relation between population and CO_2 emissions with the scaling exponent $\alpha = 0.82 \pm 0.08$ ($R^2 = 0.87 \pm 0.11$) and associated residuals for the single line fit in (b).

5. Discussion and conclusions

There has been considerable discussion as to what urban forms are ecologically most favourable. Many have suggested that compact cities are ecologically favourable, since they use less energy per capita, thereby producing less pollution, and also use less land (e.g., Jabareen, 2006; Alberti, 2007; Tratalos et al., 2007). There is, however, considerable debate as to exact ecological impact of compact urban forms, and many of the proposed relationships between urban form and ecological factors are not well developed. This is partly because comparatively little quantitative research has been made as to these relationships (e.g., Alberti, 2007; Tratalos et al., 2007; Tannier et al., 2012). Also, to develop models and metrics that can be used and generalised for quantifying both the built environment and ecological processes remains a challenge.

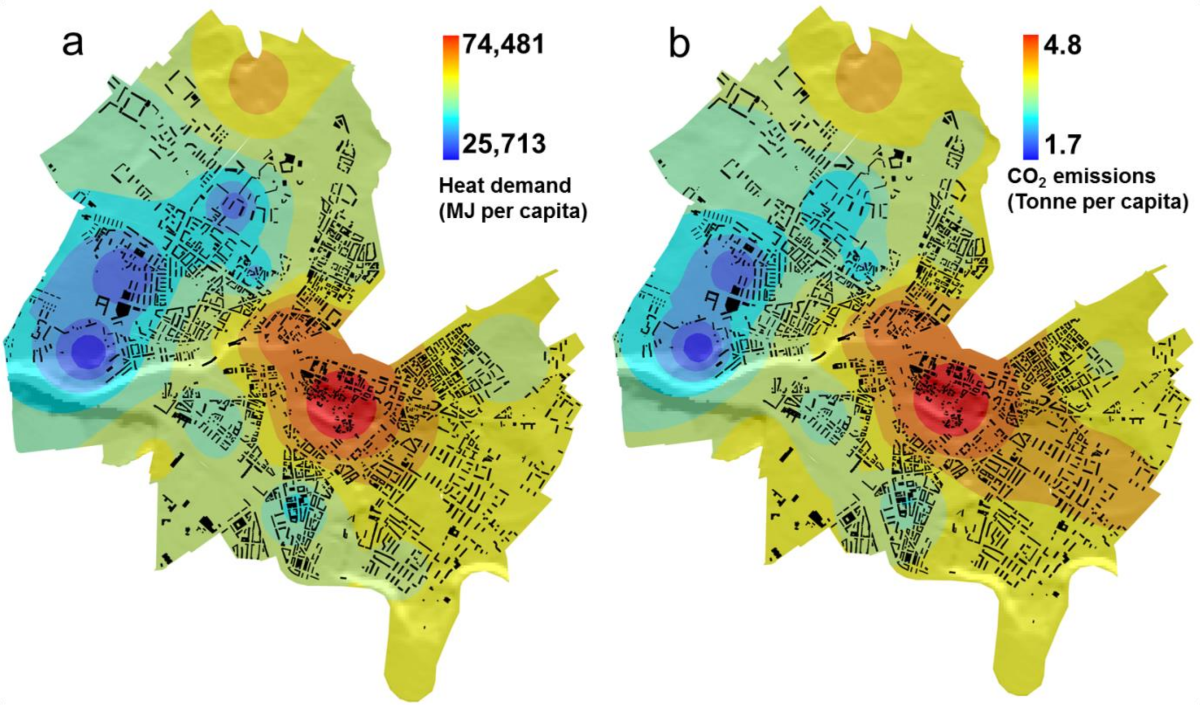

Fig. 11. Gradients of annual heat demand (MJ) per capita (a) and CO_2 emissions (t/yr) per capita (b) based on available data for the 16 zones in Geneva.

In this paper we provide methods for quantification of the spatial distributions and compactness of the built form. These methods provide results which can then be used for quantitative assessment of the impact of the built form on ecological systems. This quantification is partly through the Helmholtz free energy. The Helmholtz free energy can be related to the Gibbs-Shannon entropy, which provides a suitable metric of various built-form parameters. By analogy with the expansion of an elastic solid (here a rod, but easily generalised to two or three dimensions) subject to a tensile force, we show that the extension of the elastic body results in increase in entropy and interpret the expansion of the built area in Geneva, and the associated entropy increase, as in some ways an analogous process, resulting in increasing entropy with urban expansion or spreading.

The calculations indicate that the higher the entropy of zones within Geneva city the greater the average areas, perimeters, and volumes of the buildings of the zone (Fig. 6). Entropy is commonly used as a measure of disorder, but in the present context may be regarded as a measure of spreading or dispersal of these three parameters, which characterise the geometric aspects of the buildings. In contrast to these three parameters, which follow power-law size distributions, the height distributions of buildings follow a bimodal distribution. The distribution of the entropies of these metrics of the built form in Geneva are perhaps best visualised in map view (Fig. 6). The results show that the entropies of building areas, perimeters, and volumes correlate well through the city, whereas the entropy of building heights has a very different distribution within the city.

The results for Geneva presented here indicate that the increase in entropy with increasing average values of the built-form parameters (area, perimeter, volume) can be formally related to spreading. Another indicator of city expansion or spreading is the number of buildings and population size. We find a sub-linear relation between population and number of buildings on one hand, and heat demand and CO_2 emissions on the other hand for the 16 studied zones of Geneva (Figs. 9-11). The sub-linearity indicates that less heat is consumed per capita and less CO_2 emitted per capita with increasing number of buildings or population sizes. The results indicate that the larger populations and number of buildings are more energy efficient and have less ecological footprints than smaller ones.

The statistical-physics models presented here provide new insights into the complex relationship between the built environment and ecology. The methods provide metrics that can be interpreted in terms of dispersal and compactness of the built form and their relations with entropy through the Helmholtz free energy. These measures are here used to relate some parameters of the built environment with general urban-ecology concepts, such as the ecological effects of compactness. While there are some indications showing that increasing city compactness correlates with declining ecosystem performance, the variability is great and the quantitative data is, as yet, comparatively limited (Tratalos et al., 2007). Further development of the methods and results presented here should include additional CO_2 emission and heat-demand data on that half the buildings for which measurements are still lacking. Also, the relations between different urban patterns (dense, disperse) and the heat demand and CO_2 emissions can be expanded so as to include many cities in Switzerland and elsewhere.

Clearly, much work remains to be done in developing models to optimise the built form under different ecological conditions so as to minimise negative urban ecological effects. In addition, general models and alternative metrics are needed to be able integrate better urban and ecological systems. The proposed metrics for handling spatial complexity in urban systems can be expanded and used for analysing and quantifying various parameters of ecological systems. Thus, the statistical thermodynamics approach used here may be generally useful for analysing and understanding better how urban and ecological systems interact and how changes in built-form parameters can affect the urban ecosystem.

Acknowledgments

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Appendix

We can use the Boltzmann distribution, the partition function, and the Helmholtz free energy to derive a general formula for entropy. Using the symbol β for the term $1/k_BT$, Eq. (18) becomes:

$$Z = \sum_i e^{-\beta E_i} \qquad \text{(A1)}$$

The mean energy of the microsystem is the expected energy value <E>, which is just the probabilities P_i times the energies E_i, or:

$$\langle E \rangle = \sum_i P_i E_i \qquad \text{(A2)}$$

Using Eqs. (19, A1), Eq. (A2) can be rewritten as:

$$\langle E \rangle = \frac{1}{Z}\sum_i E_i e^{-\beta E_i} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -\frac{\partial \ln Z}{\partial \beta} \qquad \text{(A3)}$$

or in terms of temperature, recalling that $\beta = 1/k_BT$, as:

$$\langle E \rangle = k_B T^2 \frac{\partial \ln Z}{\partial T} \qquad \text{(A4)}$$

The mean energy can now be related to the Helmholtz free energy by identifying the mean energy with the internal energy of the thermodynamic system so that $\langle E \rangle = U$. From Eq. (8), which assumes constant volume, we have:

$$\langle E \rangle = U = F + TS \qquad \text{(A5)}$$

Also, from Eq. (10):

$$S = -\left(\frac{\partial F}{\partial T}\right)_V \qquad \text{(A6)}$$

Using Eq. (A6) for the entropy S in Eq. (A5) we obtain:

$$U = F - T\frac{\partial F}{\partial T} = T^2\left(\frac{F}{T^2} - \frac{1}{T}\frac{\partial F}{\partial T}\right) \qquad \text{(A7)}$$

which can be rewritten as:

$$U = T^2 \frac{\partial}{\partial T}\left(\frac{-F}{T}\right) \qquad \text{(A8)}$$

From Eqs. (A4) and (A8), using the identity $\langle E \rangle = U$, it follows that Helmholtz free energy may be written in the well-known form:

$$F = -k_B T \ln Z \tag{A9}$$

Using $\beta = 1/k_B T$, Eq. (A9) can also be written in the form:

$$Z = e^{-\beta F} \tag{A10}$$

Equations (A9) and (A10) provide a link between the microscopic world, as specified through microstates, and the everyday macroscopic world which is described by the Helmholtz free energy. Eq. (A6) provides a relationship between Helmholtz free energy *F* and entropy *S*. Using this relationship, then on differentiating Eq. (A9) we get:

$$S = -\left(\frac{\partial F}{\partial T}\right) = \frac{\partial (k_B T \ln Z)}{\partial T} = k_B \left[\ln Z + T\left(\frac{\partial \ln Z}{\partial T}\right) \right] \tag{A11}$$

The volume *V* is here constant and, for systems with variable number of particles *N*, then their number is also assumed constant. Eq. (A11) establishes a clear relationship between entropy *S* and Helmholtz free energy *F* but can be written in a different and generally more useful form, namely the Gibbs-Shannon entropy formula, which can be derived as follows. We complete the differentiation of the logarithm of *Z* with respect to *T*, using Eq. (A1) for Z, to obtain:

$$\frac{\partial \ln Z}{\partial T} = \frac{1}{Z}\left(\sum_i e^{-E_i/k_B T} \times \frac{E_i}{k_B T^2}\right) \tag{A12}$$

and then combine Eqs. (A11) and (A12) to obtain the entropy *S* as:

$$S = k_B \ln Z + k_B \frac{1}{Z}\left(\sum_i e^{-E_i/k_B T} \times \frac{E_i}{k_B T}\right) \tag{A13}$$

From Eq. (19) we have:

$$\ln P_i = -\frac{E_i}{k_B T} - \ln Z \tag{A14}$$

Rearranging the terms in Eq. (A113) and using negative sign for k_B in order to make the entropy positive (the natural logarithm of the probability range between 0 and 1 is negative) we get:

$$S = -k_B \sum_i \frac{1}{Z} e^{-E_i / k_B T} \times \left(\frac{E_i}{k_B T} + \ln Z \right) \tag{A15}$$

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Table 1. Statistical Data for 16 neighbourhoods in the city of Geneva

Geneva neighborhoods	Building numbers, [-]	Population, [-]	Ave. area [m^2]	Ave. perimeter, [m]	Ave. volume, [m^3]	Ave. height, [m]
Bâtie – Acacias	420	4889	623	87	7082	13
Bouchet – Moillebeau	874	15052	260	61	4120	13
Champel	**1055**	**18237**	**311**	**66**	**5415**	**15**
Charmilles – Châtelaine	988	23128	284	63	4480	14
Cité – Centre	1193	7914	286	68	5694	17
Délices – Grottes – Montbrillant	638	13921	334	63	5552	16
Eaux-Vives – Lac	1174	20791	264	65	4566	16
Florissant – Malagnou	762	14462	297	68	5215	15
Grand-Pré – Vermont	464	10481	305	69	5161	16
Jonction	836	15806	361	72	5898	16
La Cluse	738	16298	267	64	4732	17
O.N.U.	181	2237	615	94	10263	10
Pâquis	**754**	**10878**	**299**	**67**	**5081**	**16**
Sécheron	272	6907	418	75	6141	13
St-Gervais – Chantepoulet	408	4550	351	73	7262	19
St-Jean – Aire	661	9606	188	52	2725	11

Table 2. Entropy calculations (area, perimeter, volume, height) and annual heat demand (MJ) and associated CO_2 (tonne) per capita, for 16 neighbourhoods/zones in the city of Geneva. Heat demand and CO_2 emissions (the last two columns) are calculated based on available data and not cover the whole existing buildings.

Geneva neighborhoods	Entropy area (nat)	Entropy perimeter (nat)	Entropy volume (nat)	Entropy height (nat)	Annual heat demand MJ per capita	CO_2 emissions, tonne per capita
Bâtie – Acacias	3.73	2.39	3.73	3.09	39534	2.65
Bouchet – Moillebeau	2.50	2.04	2.99	3.23	32593	2.16
Champel	**2.66**	**2.03**	**3.31**	**3.30**	**37918**	**2.59**
Charmilles – Châtelaine	2.53	1.93	2.78	3.19	26029	1.76
Cité – Centre	2.14	1.87	2.96	3.12	74481	4.84
Délices – Grottes – Montbrillant	3.00	2.03	3.47	3.22	28810	1.89
Eaux-Vives – Lac	1.94	1.58	2.53	3.22	36030	2.39
Florissant – Malagnou	2.31	2.00	2.85	3.28	41064	2.82
Grand-Pré – Vermont	2.42	1.97	2.93	3.21	26909	1.83
Jonction	2.90	2.06	3.21	3.13	29776	1.97
La Cluse	1.96	1.74	2.54	3.21	30396	2.02
O.N.U.	3.70	2.58	3.97	2.92	47438	2.99
Pâquis	**2.29**	**1.84**	**2.92**	**3.14**	**35317**	**2.35**
Sécheron	3.29	2.30	3.66	3.11	34610	2.41
St-Gervais – Chantepoulet	2.66	2.09	3.28	3.02	60751	3.90
St-Jean – Aire	1.95	1.75	2.37	3.02	25713	1.73

Table 3. Density calculations of the built environment and transport infrastructure for 16 neighbourhoods/zones in the city of Geneva

Geneva neighborhoods	Building density (n/km^2)	Street density (n/km^2)	Street density (total length ./km^2)	Population density (n/km^2)	Land coverage (%)	Volume/area ratio
Bâtie – Acacias	182	69	10096	2122	11	1.29
Bouchet – Moillebeau	546	94	13313	9401	14	2.25
Champel	**589**	**127**	**14586**	**10176**	**18**	**3.19**
Charmilles – Châtelaine	861	184	19402	20155	24	3.86
Cité – Centre	1195	642	37535	7929	34	6.81
Délices – Grottes – Montbrillant	934	239	21471	20387	31	5.19
Eaux-Vives – Lac	863	260	21742	15287	23	3.94
Florissant – Malagnou	654	137	15663	12406	19	3.41
Grand-Pré – Vermont	751	154	20035	16973	23	3.88
Jonction	363	114	10086	6861	13	2.14
La Cluse	1476	388	31306	32596	39	6.98
O.N.U.	176	42	8487	2172	11	1.8
Pâquis	**1512**	**385**	**29852**	**21808**	**45**	**7.68**
Sécheron	395	205	21415	10027	17	2.42
St-Gervais – Chantepoulet	722	526	33886	8056	25	5.25
St-Jean – Aire	691	123	16204	10043	13	1.88