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Technical Note: A comparison of model and empirical measures of catchment scale effective energy and mass transfer

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Abstract

Recent work suggests that a coupled energy and mass transfer term (EEMT), that includes the energy associated with effective precipitation and primary production, may serve as a robust prediction parameter of critical zone structure and function. However, the models used to estimate EEMT have been solely based on long term climatological data with little validation using point to catchment scale empirical data. Here we compare catchment scale EEMT estimates generated using two distinct approaches: (1) EEMT modelled using the established methodology based on estimates of monthly effective precipitation and net primary production derived from climatological data, and (2) empirical catchment scale EEMT estimated using data from 86 catchments of the Model Parameterization Experiment (MOPEX) and MOD17A3 annual net primary production (NPP) product derived from Moderate Resolution Imaging Spectroradiometer (MODIS). Results indicated positive and significant linear correspondence between model and empirical measures but with modelled EEMT values consistently greater than empirical measures of EEMT. Empirical catchment estimates of the energy associated with effective precipitation (E_{PPT}) were calculated using a mass balance approach and base flow that accounts for water losses to quick surface runoff not accounted for in the climatologically modelled E_{PPT} . Similarly, local controls on primary production such as solar radiation and nutrient limitation were not explicitly included in the climatologically based estimates of energy associated with primary production (E_{BIO}) whereas these were captured in the remotely sensed MODIS NPP data. There was significant positive correlation between catchment aridity and the fraction of total energy partitioned into E_{BIO} , where the E_{BIO} increases as the average percentage catchment woody plant cover decreases. In summary, the data indicated strong correspondence between model and empirical measures of EEMT that agree well with catchment energy and water partitioning and plant cover.

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1 Introduction

A major challenge to the Earth sciences is to understand how energy, water, carbon, and sediment cycles and fluxes interact to control critical zone process, function and evolution (NRC, 2001). Recent studies indicate strong correlation of critical zone properties to a term referred to as effective energy and mass transfer (EEMT). This term represents the energy and mass transferred to the critical zone in the form of water in excess of evapotranspiration and biological production; therefore EEMT provides a measure of the energy available to perform work on the subsurface. Previous work demonstrated strong correlation of EEMT to measures of critical zone structure and function (Pelletier and Rasmussen, 2009; Rasmussen et al., 2005, 2011; Rasmussen and Tabor, 2007) and currently forms the basis for interdisciplinary research examining the coupling of water, carbon and sediment transport across a range of critical zone systems (Chorover et al., 2011). However, to date, the application and derivation of EEMT has been purely driven with long term average climate data, with no comparison of model estimates to empirical measures of EEMT to confirm model accuracy.

The objectives of this work were to (1) compare modelled to empirically derived values of EEMT at the catchment scale; and (2) elucidate how the relative partitioning of energy and mass transfer components among evaporation, base flow and biological production vary in response to climate. Building on the analyses of Troch et al. (2009), Brooks et al. (2011) and Rasmussen (2012), we use the Model Parameterization Experiment (MOPEX) catchment data and remotely sensed net primary productivity (NPP) data to empirically quantify climate, vegetation and catchment water balance interactions across a broad spatial and climate space.

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2 Materials and methods

2.1 Effective energy and mass transfer

The critical zone energy balance may be represented as the summation of energy and mass flux associated with energy, water, and carbon, tectonically forced gravity driven sediment transport, and the geochemical alteration of primary and secondary mineral phases. Following on previous work (Phillips, 2009; Volobuyev, 1974), the total critical zone energy (E_{Total}) balance can be stated as (Rasmussen et al., 2011):

$$E_{\text{Total}} = E_{\text{ET}} + E_{\text{PPT}} + E_{\text{BIO}} + E_{\text{ELEV}} + E_{\text{GEO}} + \sum E_i, \quad (\text{Jm}^{-2}\text{s}^{-1}) \quad (1)$$

where E_{ET} is energy and mass flux associated with evapotranspiration, E_{PPT} is heat energy associated with effective precipitation, E_{BIO} is net primary productivity energy and mass transfer, E_{ELEV} is potential energy associated with gravity driven transport of sediment, E_{GEO} is geochemical potential of chemical weathering, and E_i is any other external energy and mass input such as dust or anthropogenic inputs. The E_{ELEV} and E_{GEO} terms encompass the physical and chemical transfers of energy and mass associated with denudation and mineral transformation and may be orders of magnitude less than the water, radiant, and carbon flux terms (Phillips, 2009). In contrast, E_{ET} represents the largest component of E_{Total} and is typically several orders of magnitude greater than the sum of the remaining energy and mass flux terms (Minasny et al., 2008). However, E_{ET} represents the transfer of water and radiant energy back to the atmosphere and thus has limited potential for performing chemical or physical work on the subsurface. Therefore, here we focus on the components of E_{Total} that can perform chemical and physical work on the subsurface, the sum of which Rasmussen et al. (2011) refer to as “effective energy and mass transfer” (EEMT) and define as follows:

$$\text{EEMT} = E_{\text{PPT}} + E_{\text{BIO}}, \quad (\text{Jm}^{-2}\text{s}^{-1}) \quad (2)$$

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where EEMT represents the summation of energy transferred to the subsurface critical zone as the heat transfer associated with effective precipitation, that water in excess of evapotranspiration (E_{PPT}), and chemical energy associated with reduced carbon compounds derived from primary production (E_{BIO}).

In brief, the components of modelled EEMT estimates (Eq. 2) have units of $\text{J m}^{-2} \text{s}^{-1}$, or W m^{-2} and are calculated using traditional monthly water balance techniques (e.g. Arkley, 1963) and net primary production estimates (Lieth, 1975) as follows:

$$E_{\text{PPT}} = F \cdot c_w \cdot \Delta T \quad (\text{J m}^{-2} \text{s}^{-1}) \quad (3)$$

where F is mass flux of base flow [$\text{kg m}^{-2} \text{s}^{-1}$], c_w is specific heat of water [$\text{J kg}^{-1} \text{K}^{-1}$], and $\Delta T = T_{\text{ambient}} - T_{\text{ref}}$ [K] with T_{ambient} the ambient temperature at time of water flux and T_{ref} set at 273.15 K; and

$$E_{\text{BIO}} = \text{NPP} \cdot h_{\text{BIO}} \quad (\text{J m}^{-2} \text{s}^{-1}) \quad (4)$$

where NPP is mass flux of carbon as net primary production [$\text{kg m}^{-2} \text{s}^{-1}$], and h_{BIO} the specific biomass enthalpy [J kg^{-1}] fixed at a value of $22 \times 10^6 \text{ J kg}^{-1}$.

2.2 Modelled effective energy and mass transfer

Previous applications of the EEMT framework (Chorover et al., 2011; Pelletier and Rasmussen, 2009; Rasmussen, 2012; Rasmussen et al., 2005, 2011; Rasmussen and Tabor, 2007; Sheldon and Tabor, 2009) have largely focused on using relatively easy to obtain annual and monthly precipitation and temperature data to calculate local water and energy balance to derive the components needed for E_{PPT} and E_{BIO} . Specifically, for E_{PPT} the F term is approximated using effective precipitation: $P_{\text{eff}} = \text{PPT} - \text{PET}$ [$\text{kg m}^{-2} \text{s}^{-1}$], where PET is potential evapotranspiration calculated following Thornthwaite and Mather (1957). The net primary production (NPP) term is calculated using a modified form of the sigmoid equation of Lieth (1975) relating NPP

to mean annual temperature: $NPP = 3000 \left[1 + e^{(1.315 - 0.1197)} \right]^{-1} [\text{g m}^{-2} \text{yr}^{-1}]$. Using this equation, NPP is calculated at monthly time steps for all months of $PPT > PET$, and scaled to a monthly time step based on each months percentage of one year (i.e. $\text{days}_{\text{month}}/\text{days}_{\text{year}}$). Here the energy model components (E_{PPT} and E_{BIO}) calculated using this approach will be termed $E_{PPT\text{-}MODEL}$ and $E_{BIO\text{-}MODEL}$, and their sum referred to as $EEMT_{MODEL}$.

2.3 Empirical effective energy and mass transfer

To meet this work's objective of comparing $EEMT_{MODEL}$ to empirical EEMT estimates ($EEMT_{MODIS\text{-}MOPEX}$) we used a subset of eighty-six catchments from the MOPEX database (data available at <http://www.nws.noaa.gov/oh/mopex>) spanning the time period from 2000–2009 following on the analyses of Troch et al. (2009) and Brooks et al. (2011) to estimate E_{PPT} ($E_{PPT\text{-}MOPEX}$) and used MODIS data for the same 86 catchments to estimate E_{BIO} ($E_{BIO\text{-}MODIS}$). The selected catchments span a broad climate space with substantial variation in water availability and vegetation cover (Duan et al., 2006). The catchments average 3477 km^2 in size, ranging from 134 to $10\,329 \text{ km}^2$; annual precipitation ranges from ~ 650 to 1800 mm yr^{-1} , and mean annual temperature spans 10 to 22°C . Additionally, the catchments exhibit minimal snow storage to avoid issues of winter-to-spring water carryover or snow water loss to sublimation (Brooks et al., 2011).

Empirical E_{PPT} was estimated from monthly MOPEX precipitation, temperature and discharge data using a catchment balance approach (L'vovich, 1979):

$$W = PPT - SR = ET + F + BIO \quad (\text{kg m}^{-2} \text{s}^{-1}) \quad (5)$$

where W is subsurface or catchment wetting, PPT is precipitation, SR is quick runoff, or the immediate increase in surface discharge due to rainfall and represents water that is not available to do work on the system, ET is mass of water returned to the atmosphere by evapotranspiration, F is base flow and equivalent to the fraction of

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precipitation available to flux through the soil and participate in weathering processes and solute transport, and BIO is the mass of water incorporated into biomass via primary production. Discharge (Q) was partitioned to SR and F based on the analysis of Brooks et al. (2011). The E_{PPT} term was then calculated using catchment base flow and air temperature as: $E_{PPT-MOPEX} = F \cdot c_w \cdot \Delta T$. Values of E_{PPT} were calculated on a monthly basis and summed to provide an annual measure of E_{PPT} , here termed $E_{PPT-MOPEX}$.

The energy associated with evapotranspiration was derived from catchment estimates of actual evapotranspiration (AET) calculated as:

$$AET = PPT - Q \quad (\text{kgm}^{-2}\text{s}^{-1}). \quad (6)$$

This was converted to an energy term as:

$$E_{ET-MOPEX} = AET \cdot h_v \quad (\text{Jm}^{-2}\text{s}^{-1}) \quad (7)$$

where h_v is the latent heat of evaporation [Jkg^{-1}].

Annual net primary production for each MOPEX catchment was taken from the MODIS data product MOD17A3 for the period 2000–2009 (Zhao and Running, 2010) (data available in GeoTiff format from the Numerical Terradynamic Simulation Group at: ftp://ftp.ntsg.umd.edu/pub/MODIS/Mirror/MOD17_Science_2010/MOD17A3/Geotiff). The MOD17 data product provides annual estimates of NPP [$\text{gCm}^{-2}\text{yr}^{-1}$] at 1 km pixel resolution. The algorithm for NPP includes parameters for short-wave downward solar radiation, the fraction of photosynthetically active radiation adsorbed by plants, vapor pressure deficit, temperature, light use efficiency, and maintenance respiration (Running et al., 2004). After download, the MODIS NPP data were subset to exclude any areas of no data including surface water bodies and any urban/developed areas within the MOPEX catchments. Annual $E_{BIO-MODIS}$ was calculated as in Eq. (4):

$$E_{BIO-MODIS} = NPP \cdot h_{BIO}.$$

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The empirical energy balance estimates calculated using the MOPEX and MODIS data were summed to provide a “measured EEMT” where:

$$EEMT_{MOPEX-MODIS} = E_{PPT-MOPEX} + E_{BIO-MODIS} \quad (Jm^{-2}s^{-1}). \quad (8)$$

2.4 Catchment energy partitioning

5 The values of $EEMT_{MODEL}$, $E_{PPT-MODEL}$ and $E_{BIO-MODEL}$ were compared to $EEMT_{MOPEX-MODIS}$, $E_{PPT-MOPEX}$ and $E_{BIO-MODIS}$ to check the validity of the model approach and values. In addition, the relative partitioning of total critical zone energy (E_{TOTAL}) to $E_{ET-MOPEX}$, $E_{PPT-MOPEX}$ and $E_{BIO-MODIS}$ were calculated for each catchment as a fraction of E_{TOTAL} , so that:

$$10 \quad \frac{E_{ET-MOPEX}}{E_{TOTAL}} + \frac{E_{PPT-MOPEX}}{E_{TOTAL}} + \frac{E_{BIO-MODIS}}{E_{TOTAL}} = \frac{E_{ET-MOPEX}}{E_{TOTAL}} + \frac{EEMT_{MOPEX-MODIS}}{E_{TOTAL}} = 1. \quad (9)$$

For simplicity E_{GEO} and E_{ELEV} have not been included. The relative partitioning of E_{TOTAL} was compared to the aridity index, or the ratio of potential evapotranspiration to precipitation ($\frac{PET_{MOPEX}}{PPT_{MOPEX}}$) as a more traditional measure of water availability (Budyko, 1974).

15 Further, we compared the fraction of catchment woody plant cover to $\frac{EEMT_{MOPEX-MODIS}}{E_{TOTAL}}$ and to the fraction of EEMT partitioned to E_{BIO} where: $F_{BIO} = E_{BIO}/EEMT = \frac{E_{BIO-MODIS}}{EEMT_{MOPEX-MODIS}}$. The percentage catchment woody cover was derived from the 2001 National Land Cover Database (NLCD, Homer et al., 2007) available for download from the Multi-Resolution Land Characterization (MRLC) Consortium (http://www.mrlc.gov/nlcd01_data.php). Greater detail and data summary is included in Brooks et al. (2011).

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3 Results and discussion

3.1 Model and empirical data comparison

Modelled values of EEMT, E_{PPT} and E_{BIO} were all linearly and significantly ($p < 0.0001$) correlated with their respective empirical values derived from the MOPEX and MODIS datasets (Fig. 1). The liner regressions indicate that $\text{EEMT}_{\text{MOPEX-MODIS}}$, $E_{\text{PPT-MOPEX}}$ and $E_{\text{BIO-MODIS}}$ were, on average, 0.57 to 0.48 to 0.67 times less than $\text{EEMT}_{\text{MODEL}}$, $E_{\text{PPT-MODEL}}$ and $E_{\text{BIO-MODEL}}$, respectively. The strong linear correlations between model and empirical data indicate that while the magnitude of $\text{EEMT}_{\text{MODEL}}$ in previous work relating EEMT to critical zone properties and process may be overestimated (Chorover et al., 2011; Pelletier and Rasmussen, 2009; Rasmussen, 2012; Rasmussen et al., 2005, 2011; Rasmussen and Tabor, 2007; Sheldon and Tabor, 2009), the overall trends relative to EEMT remain valid.

The over prediction of $E_{\text{PPT-MODEL}}$ relative to $E_{\text{PPT-MOPEX}}$ is a function of the catchment water balance approach applied to the MOPEX data that accounts for losses of precipitation to quick runoff, water that would otherwise be partitioned to base flow and E_{PPT} . In the selected MOPEX catchments, quick runoff increases linearly and significantly with increasing precipitation, with an average of 10 % of precipitation partitioned to quick runoff and a range of ~ 0.5 to 30 %. Analysis of the residuals of $\text{EEMT}_{\text{MODEL}}$ and $E_{\text{PPT-MODEL}}$ relative to an ideal 1 : 1 fit indicates that quick runoff accounts for ~ 35 % ($p < 0.0001$) of the variance in both $\text{EEMT}_{\text{MODEL}}$ and $E_{\text{PPT-MODEL}}$ residuals, and data indicate significant decrease in the model residuals with greater quick runoff (Fig. 2). The monthly water balance used for $\text{EEMT}_{\text{MODEL}}$ does not account for quick runoff, or that the fraction of rainfall that leaves the catchment too quickly to perform work, and thus over predicts the water available for base flow and E_{PPT} . Additionally, the catchment water balance employed here assumes that the change in storage may be neglected over annual time scales; however, it is possible there is unaccounted storage of water within the catchments that would lead to an underestimation of $E_{\text{PPT-MOPEX}}$.

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The model E_{BIO} is based on the temperature of those months where $\text{PPT} > \text{PET}$. This model does not account for local scale variation in photosynthetically active radiation, water redistribution, and nutrient limitation, all factors that limit primary production under natural conditions (Melillo et al., 1993; Newman et al., 2006). The algorithm for calculating $\text{NPP}_{\text{MODIS}}$ considers many of these limitations either directly or indirectly (Running et al., 2004) and thus the over prediction of $E_{\text{BIO-MODEL}}$ relative to $E_{\text{BIO-MODIS}}$ is likely a function of the lack of parameterization and mechanism in the $E_{\text{BIO-MODEL}}$ framework.

The monthly water balance based $\text{EEMT}_{\text{MODEL}}$ used in previous work thus presents a potential transfer or upper bound of available energy and mass to the critical zone. The strong linear correlation between $\text{EEMT}_{\text{MODEL}}$ and $\text{EEMT}_{\text{MOPEX-MODIS}}$ however, reinforces the validity of previous correlations of EEMT to critical zone structure and function, i.e. the relationships should express the same functional relationship to EEMT, albeit at somewhat lower EEMT values.

3.2 Energy and mass partitioning

The relative partitioning of E_{TOTAL} to $E_{\text{BIO-MODIS}}$, $E_{\text{PPT-MOPEX}}$, and $E_{\text{ET-MOPEX}}$ exhibited clear and non-linear relationships with the aridity index (Fig. 3). Values of $\frac{E_{\text{ET-MOPEX}}}{E_{\text{TOTAL}}}$ ranged from 0.97 to 0.995 (Fig. 3a), indicating that evapotranspiration accounts for as much as 99.5 % of the total energy balance, a finding supported by numerous studies documenting Earth surface energy and mass balances (e.g. Minasny et al., 2008; Phillips, 2009; Rasmussen et al., 2011; Wilcox et al., 2003). Correspondingly, $\text{EEMT}_{\text{MOPEX-MODIS}}$ accounts for only 0.5 to 3.0 % of E_{TOTAL} (Fig. 3b). However, despite the relatively small fraction of energy and mass transfer partitioned to $\text{EEMT}_{\text{MOPEX-MODIS}}$, $\text{EEMT}_{\text{MOPEX-MODIS}}$ represents the work available to perform work on the subsurface and thus drive subsurface critical zone process and function.

The ratios of $\frac{E_{\text{PPT-MOPEX}}}{E_{\text{TOTAL}}}$ and $\frac{E_{\text{ET-MOPEX}}}{E_{\text{TOTAL}}}$ exhibited significant nonlinear decrease and increase, respectively, with increasing aridity index (Fig. 3a and c). These data indicate

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greater energy and mass partitioned to evapotranspiration with increasing water limitation, with nearly 100 % of E_{TOTAL} partitioned to ET at $\text{PET}_{\text{MOPEX}}/\text{PPT}_{\text{MOPEX}}$ values greater than 1.0. In contrast, the ratio $\frac{E_{\text{BIO-MODIS}}}{E_{\text{TOTAL}}}$ exhibited a threshold type relationship with aridity index (Fig. 3d). This ratio exhibited substantial variation, from 0.6 to 1.0 % of E_{TOTAL} in energy-limited systems where $\text{PET}_{\text{MOPEX}}/\text{PPT}_{\text{MOPEX}} < 1$. The relatively large variance likely reflects local variation and control of biological production in these systems. In the water-limited systems, where $\text{PET}_{\text{MOPEX}}/\text{PPT}_{\text{MOPEX}} > 1$, $E_{\text{BIO-MODIS}}/E_{\text{TOTAL}}$ decreased substantially and exhibited little variation with average values of 0.5 % of E_{TOTAL} . The relative lack of variation in these systems is likely a function of strong water limitation on biological production and optimization of biological water use efficiency (e.g. Huxman et al., 2004; Troch et al., 2009). Previous work indicates that in water-limited systems EEMT is dominated by E_{BIO} indicating any available water is tied up in primary production and coupled water-carbon cycles, with limited water resources available for base flow, subsurface leaching, or soil development.

The relative partitioning of E_{TOTAL} to $\text{EEMT}_{\text{MOPEX-MODIS}}$ demonstrates a moderate and significant positive correlation ($R^2 = 0.39$; $p < 0.0001$) with increasing woody plant cover across the MOPEX catchments (Fig. 4a). Similarly, the fraction of $\text{EEMT}_{\text{MOPEX-MODIS}}$ derived from $E_{\text{BIO-MODIS}}$ significantly decreased with increasing woody plant cover ($R^2 = 0.31$; $p < 0.0001$, Fig. 4b). These data confer previous results that “low” EEMT systems are typically water limited and dominated by primary production as the principle component of EEMT (e.g. Rasmussen, 2012). The “high” EEMT systems, while exhibiting the greatest woody plant cover, are principally dominated by energy associated with E_{PPT} despite relatively greater rates of primary production. In the water-limited systems, any water available in excess of evapotranspiration is partitioned to primary production, with minimal water remaining for base flow and E_{PPT} . Thus the systems express low EEMT values dominated by E_{BIO} . In contrast, the wet, energy-limited systems have substantial water in excess of evapotranspiration, facilitating greater base flow and E_{PPT} , relatively high EEMT, and greater subsurface development.

4 Summary

The comparison of simple monthly water balance based estimates of EEMT to direct empirical measures of EEMT at the catchment scale indicates strong positive, linear correlation between model and measured values. The empirical measures thus confirm previously published trends in EEMT and the relationship of EEMT to various measures of critical zone structure and function. The monthly water balance model consistently over predicted both the water and biological components of EEMT due to a lack of accounting for precipitation losses to quick runoff in the water component and the simplicity of modelled net primary production that does not account for local water redistribution, terrain controlled variation in radiation and nutrient limitations. The relative partitioning of the critical zone energy balance to evapotranspiration, water and biological energy and mass transfers varied consistently with aridity index and woody plant cover.

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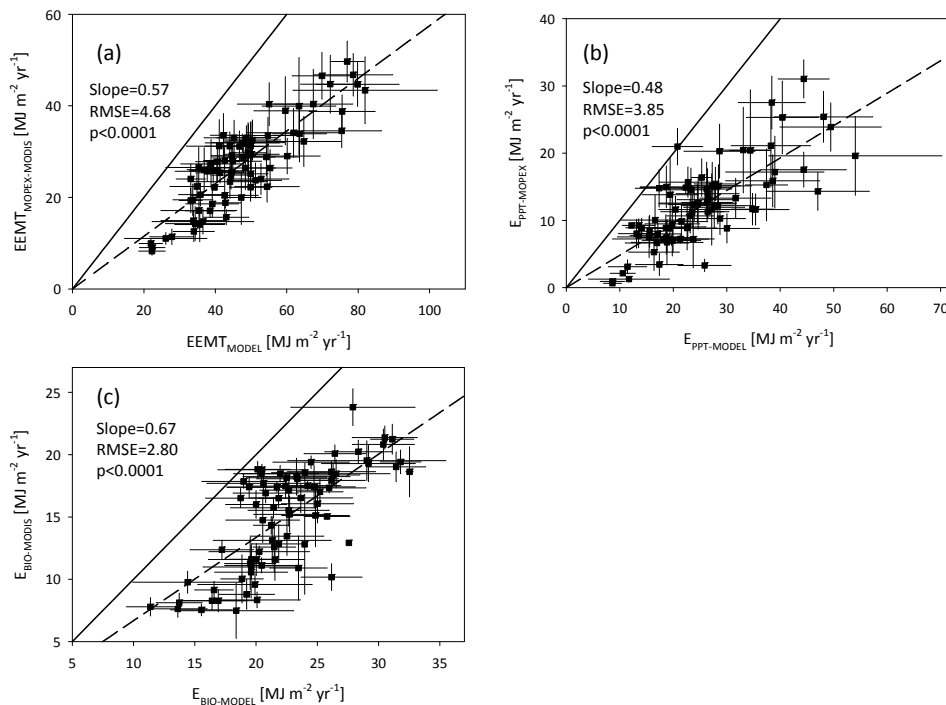


Fig. 1. The relationship between **(a)** effective energy and mass transfer (EEMT) quantified using MOPEX baseflow and MODIS net primary production data ($EEMT_{MOPEX-MODIS}$) relative to modeled EEMT ($EEMT_{MODEL}$), **(b)** water transferred heat energy input derived from MOPEX baseflow data ($E_{PPT-MOPEX}$) and modeled heat transfer ($E_{PPT-MODEL}$), and **(c)** biological chemical energy input derived from MODIS net primary production ($E_{BIO-MODIS}$) and modeled primary production ($E_{BIO-MODEL}$). The 1 : 1 relationship are noted as solid lines and the dashed lines represent best fit linear functions fit with an intercept of zero. Error bars are standard errors of the annual means over the period of record.

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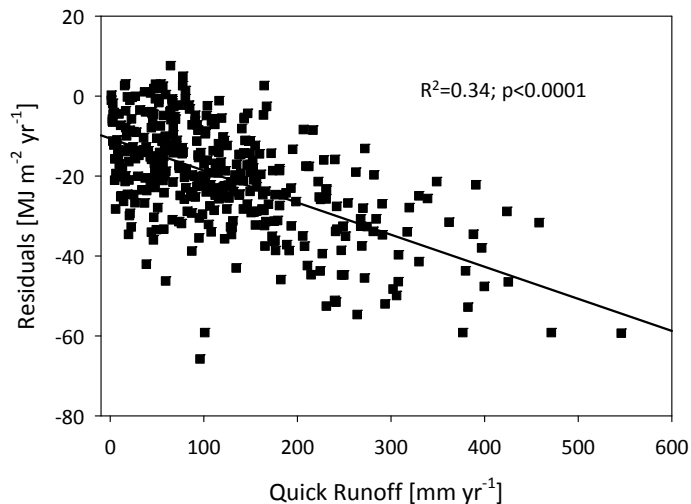


Fig. 2. The relationship between the residuals of the 1 : 1 fit between $EEMT_{MODEL}$ and $EEMT_{MOPEX-MODIS}$ relative to quick runoff. Data includes all observation years. The solid line is the best fit linear regression.

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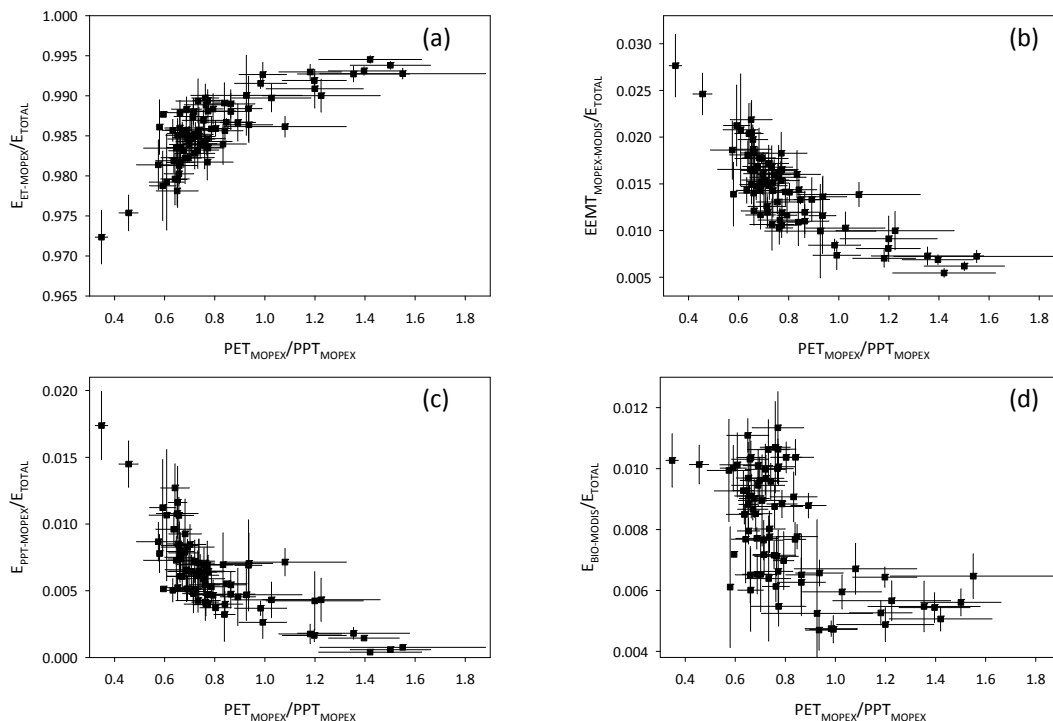


Fig. 3. The relationship between **(a)** energy partitioned to evapotranspiration (E_{ET}), **(b)** effective energy and mass transfer (EEMT) that is the sum of E_{BIO} and E_{PPT} , **(c)** water transferred heat energy from baseflow (E_{PPT}), and **(d)** biological chemical energy (E_{BIO}) normalized to the total energy consumed (E_{TOTAL}) that is the sum of E_{BIO} , E_{PPT} and E_{ET} relative to the ratio of potential evapotranspiration to precipitation (PET/PPT). Error bars are standard errors of the annual means over the period of record.

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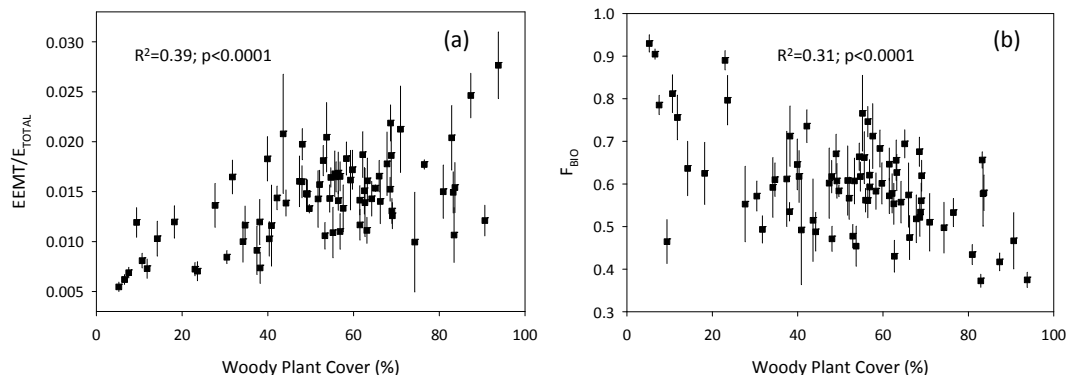


Fig. 4. The relationship between **(a)** effective energy and mass transfer (EEMT) normalized to the total energy consumed (E_{TOTAL}) relative to catchment percent woody plant cover and **(b)** the fraction of EEMT derived from biological energy input (F_{BIO}) relative to catchment percent woody plant cover. Error bars are standard errors of the annual means over the period of record for $EEMT/E_{TOTAL}$ and F_{BIO} . Woody plant cover was taken from the 2001 NLCD that does not represent annual variation in percent woody plant cover. As such, error bars were not included for percent woody plant cover.

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