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Supplement of

Sensitivity analysis of an updated bidirectional air–surface exchange model for elemental mercury vapor

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1. Use of factorial design of experiments

Design of experiments is a series of tests in which purposeful changes are made to the input variables of a process systematically and the effects on response variables are measured. It is widely applied in the experiments involving many influencing factors, when it is necessary to study the combined effect of these factors. For a two-level design involving a high-level and a low-level value for each factor, the number of all possible combinations is 2^k (for example, for two factors the combinations is low-low, low-high, high-low and high-high), which also represent the number of experiments. This exponential relationship rapidly increases the number of experiments when the number of studied factors is increased. To reduce the experimental effort without losing the analytical power of the experiments, the number of experiment can be decreased strategically by choosing the experiments that investigate the main effects (i.e., the effect of single factor) and interaction effects of lower order. This is called fractional design and the number of experiment can be reduced by 2^p times (i.e., the number of experiment becomes 2^{k-p}). The term “Resolution” is used by statisticians to indicate how the experiments are chosen. For IV resolution design, all the main effects are completely isolated from confounding with all other experimental runs and the second-order (two-factor) interactions are maintained without confounding with higher order interactions. Based on the factorial experiment results, statistical test can be performed to understand the significance of each factor using P value.

An excellent online presentation on factorial design of experiments is also available at http://www.jhuapl.edu/techdigest/td/td2703/telford.pdf.

2. Initial parameter screening for bare lands

Normal plot of the standardized effects of 2^{11-6} (Figure s1) suggests significant effect from fraction of organic carbon, friction velocity, soil Hg content at 95% confidence level. The P-value of main effects from air temperature at 2 meters and scaling factor for reactivity of mercury on ozone (β_{Hg^0}) were close to 0.05 (0.069 and 0.073, respectively). For the second order interactions, air temperature and β_{Hg^0} are important. Therefore fraction of organic carbon, friction velocity, soil Hg concentration, air temperature, β_{Hg^0}, were chosen for the final 2^5 full factorial design.

3. Initial parameter screening for canopy system

The alias structure of the 2^{15-9} fractional design is complex (Figure s2). To ensure that the most significant factors are selected for the final full factorial design, all parameters confounded in alias system were chosen to run 2^{11-6} experiment except for air Hg^0 concentration because its weak significance ($P = 0.437$). From the results of the 2^{11-6} fractional design (Figure s3) result, the fraction of organic carbon, friction velocity, soil Hg concentration, β_{Hg^0}, soil moisture condition are significant. The P-value of main effects from Hg previously deposited to leaf stomata and air temperature were close to 0.05 (0.069 and 0.136, respectively). Therefore, fraction of organic carbon, friction velocity, soil Hg concentration, β_{Hg^0}, soil under moisture condition, Hg previously deposited to leaf stomata and air temperature were chosen to for another 2^{7-1} fractional experiments. Based on the results (Figure s7), the main effects from fraction of organic carbon, friction velocity, soil Hg concentration are significant. To get the full design, Hg previously deposited to leaf stomata and β_{Hg^0} were eliminated because of the relatively weaker significance.

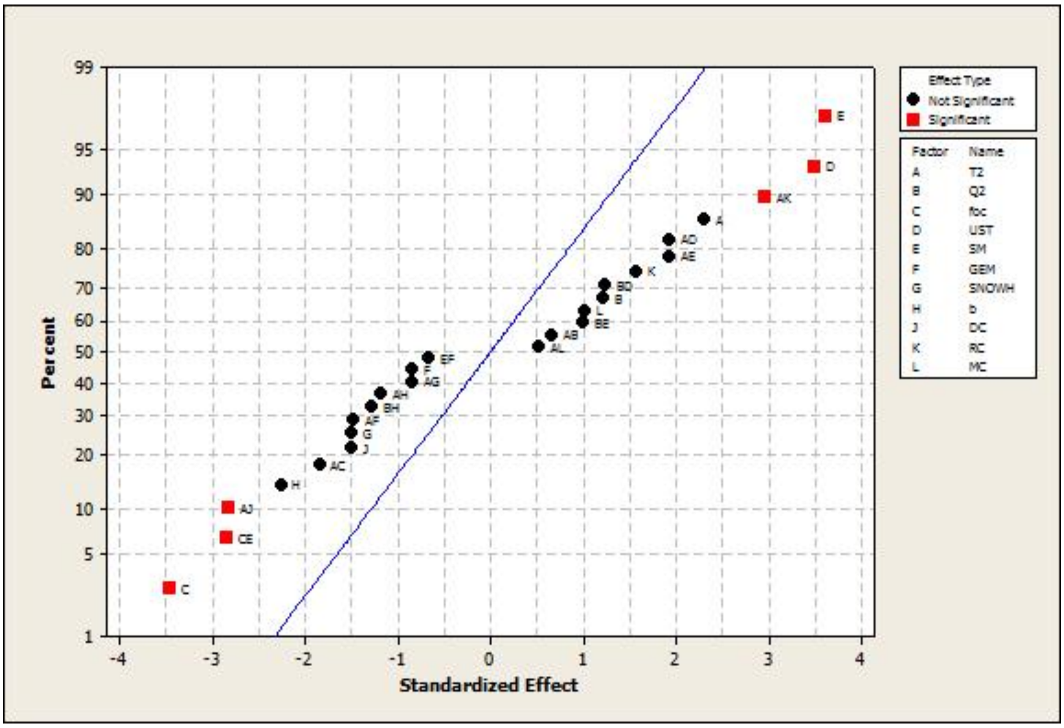

Figure s1: Results of 2^{11-6} fractional design for bare lands. Significance at $P<0.05$. T denotes air temperature at 2 meters, Q2 denotes water vapor mixing ratio, foc denotes fraction of organic carbon in surface soil, UST denotes friction velocity, SM denotes soil total Hg concentration, GEM denotes air Hg(0) concentration, SNOWH denotes snow depth, b denotes scaling factor of reactivity Hg, DC denotes dew condition, RC denotes rain condition, MC denotes moist soil condition. Alias information for significant terms: T*DC + Q2*SNOWH + foc*UST + SM*b, T*RC + Q2*MC+ foc*b + UST*SM, foc*SM + UST*b + SNOWH*MC + DC*RC.

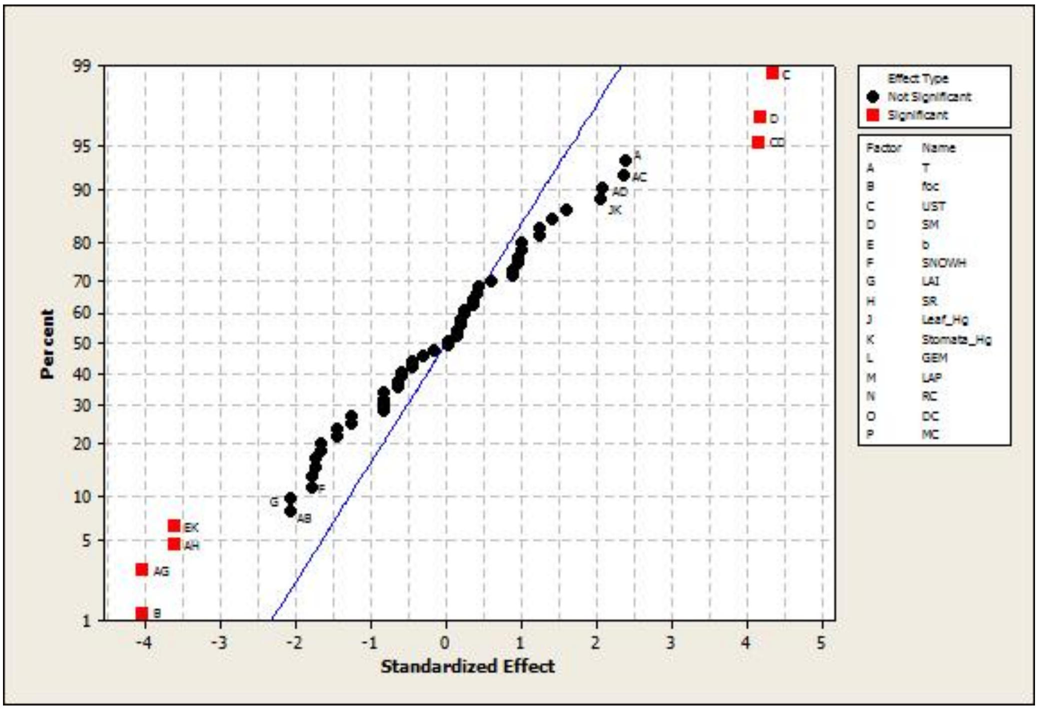

Figure s2: Results of 2^{15-9} fractional design for canopy system. Significance at $P<0.05$. T denotes air temperature at 2 meters, foc denotes fraction of organic carbon in surface soil, UST denotes friction velocity, SM denotes soil total Hg concentration, b denotes scaling factor of reactivity Hg, SNOWH denotes snow depth, LAI denotes Leaf area index , SR denotes solar irradiation, Leaf_Hg denotes Hg concentration in leaf rinse, Stomata_Hg denotes Hg previously deposited to leaf stomata, GEM denotes air Hg(0) concentration, LAP denotes leaf-air partitioning coefficient, DC denotes dew condition, RC denotes rain condition, MC denotes moist soil condition. Alias information for significant terms: T*LAI + foc*UST, T*SR + foc*SM, UST*SM + LAI*SR + GEM*LAP, b*Stomata_Hg + RC*MC.

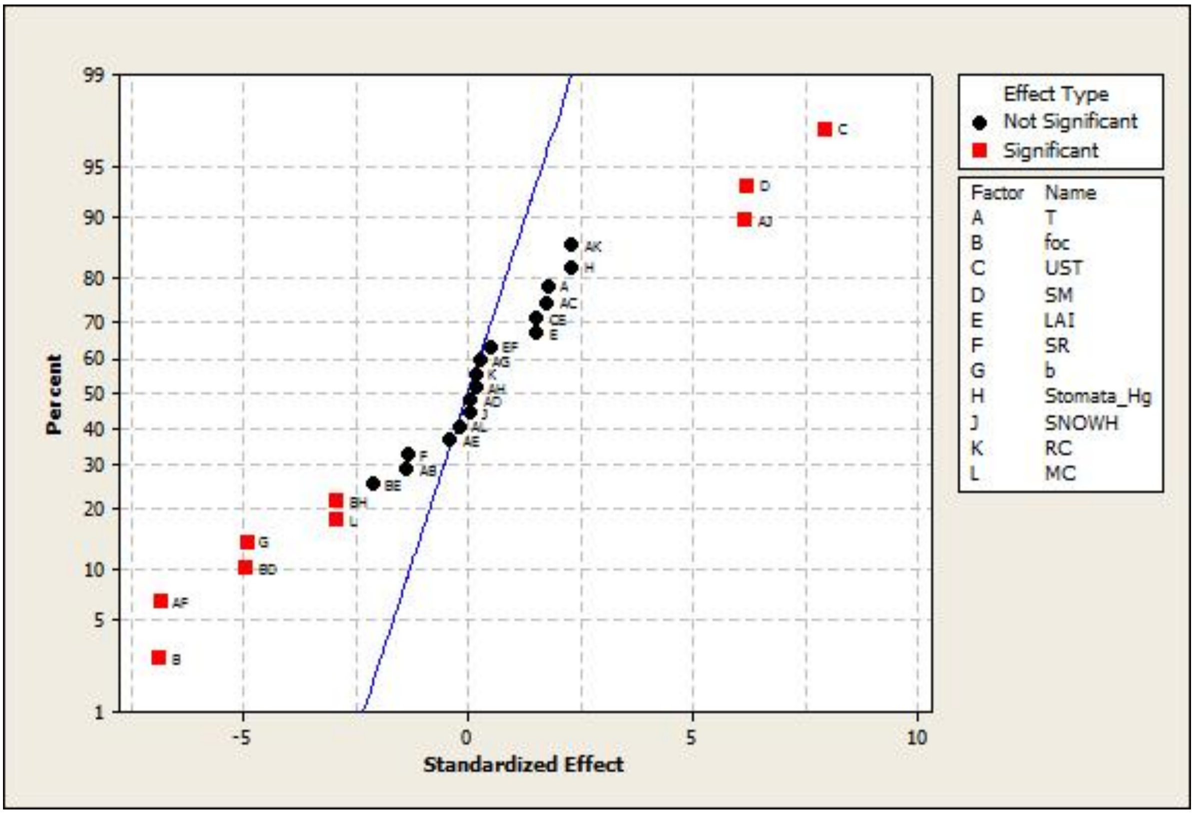

Figure s3: Results of 2^{11-6} fractional design for canopy system. Significance at P<0.05. T denotes air temperature at 2 meters, foc denotes fraction of organic carbon in surface soil, UST denotes friction velocity, SM denotes soil total Hg concentration, LAI denotes leaf area index, SR denotes solar irradiation, b denotes scaling factor of reactivity Hg, Stomata_Hg denotes Hg previously deposited to leaf stomata, SNOWH denotes snow depth, RC denotes rain condition, MC denotes moist soil condition. Alias information for significant terms: T*SR + foc*UST + SM*b + Stomata_Hg*MC, T*SNOWH + foc*b + UST*SM + LAI*Stomata_Hg, foc*LAI + SM*MC + b*Stomata_Hg, foc*Stomata_Hg + UST*MC + LAI*b + SR*RC.

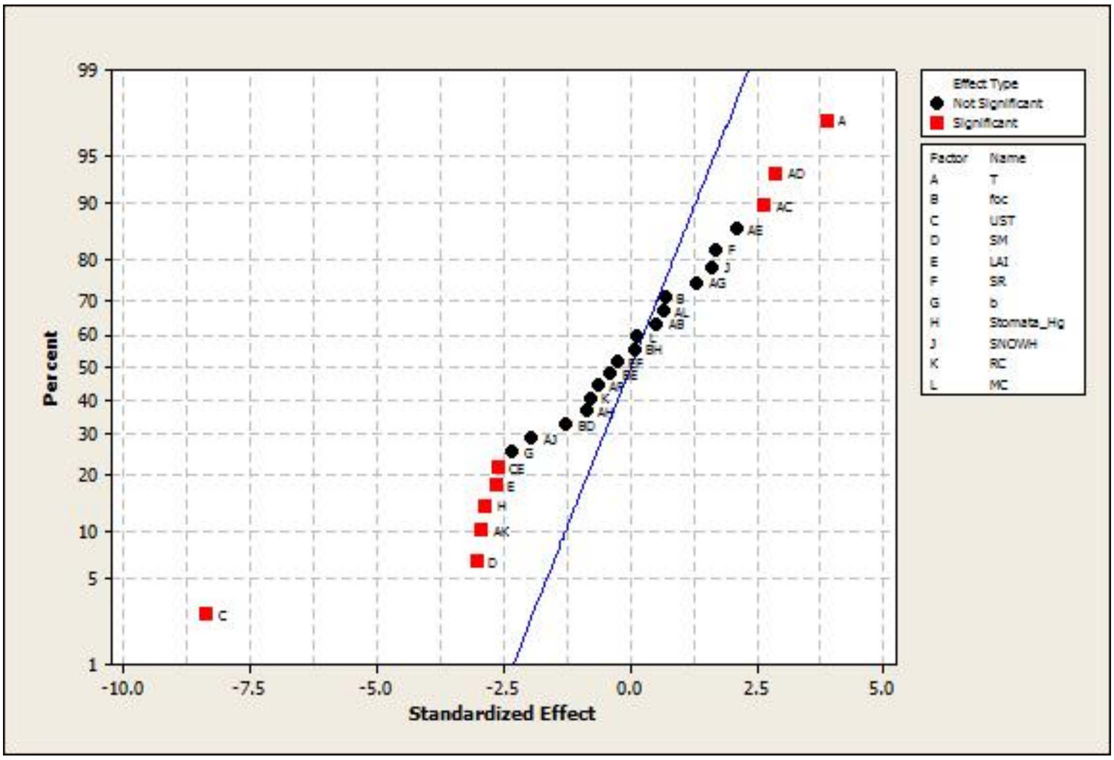

Figure s4: Results of 2^{11-6} fractional design for foliage. Significance at $P<0.05$. T denotes air temperature at 2 meters, foc denotes fraction of organic carbon in surface soil, UST denotes friction velocity, SM denotes soil total Hg concentration, LAI denotes leaf area index, SR denotes solar irradiation, b denotes scaling factor of reactivity Hg, Stomata_Hg denotes Hg previously deposited to leaf stomata, SNOWH denotes snow depth, RC denotes rain condition, MC denotes moist soil condition. Alias information for significant terms: T*SR + foc*UST + SM*b + Stomata_Hg*MC, T*SNOWH + foc*b + UST*SM + LAI*Stomata_Hg, foc*LAI + SM*MC + b*Stomata_Hg, foc*Stomata_Hg + UST*MC + LAI*b + SR*RC.

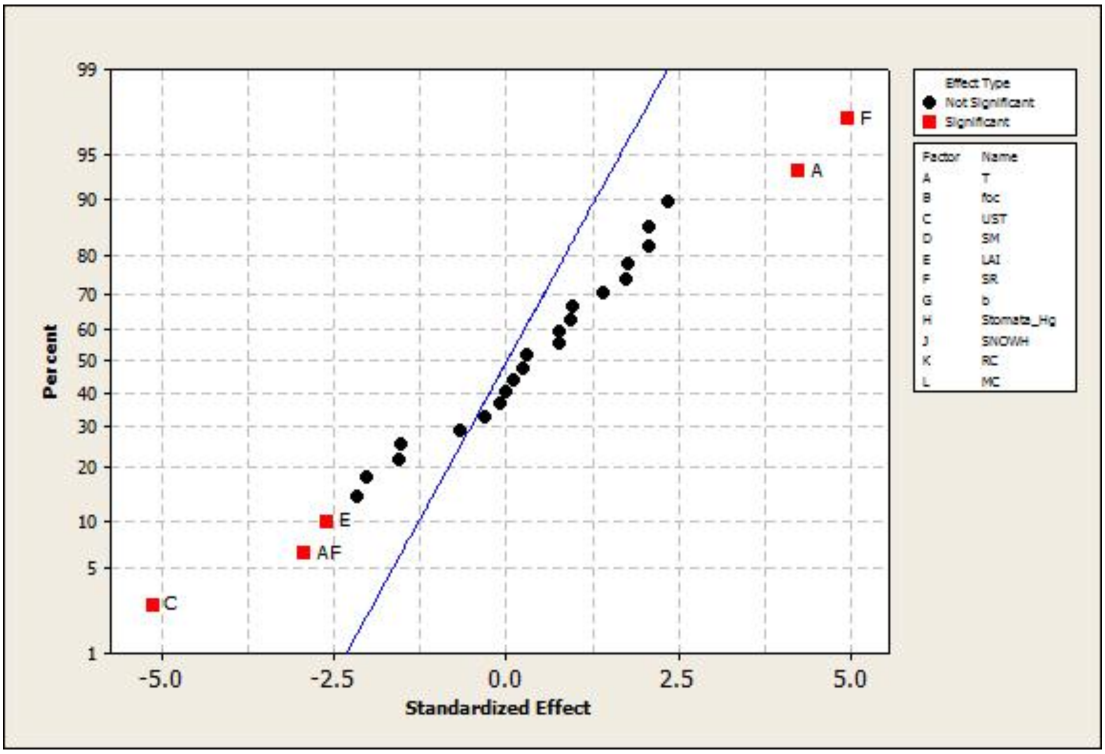

Figure s5: Results of 2^{11-6} fractional design for cuticle. Significance at $P<0.05$. T denotes air temperature at 2 meters, foc denotes fraction of organic carbon in surface soil, UST denotes friction velocity, SM denotes soil total Hg concentration, LAI denotes leaf area index, SR denotes solar irradiation, b denotes scaling factor of reactivity Hg, Stomata_Hg denotes Hg previously deposited to leaf stomata, SNOWH denotes snow depth, RC denotes rain condition, MC denotes moist soil condition. Alias information for significant terms: T*SR + foc*UST + SM*b + Stomata_Hg*MC, T*SNOWH + foc*b + UST*SM + LAI*Stomata_Hg, foc*LAI + SM*MC + b*Stomata_Hg, foc*Stomata_Hg + UST*MC + LAI*b + SR*RC.

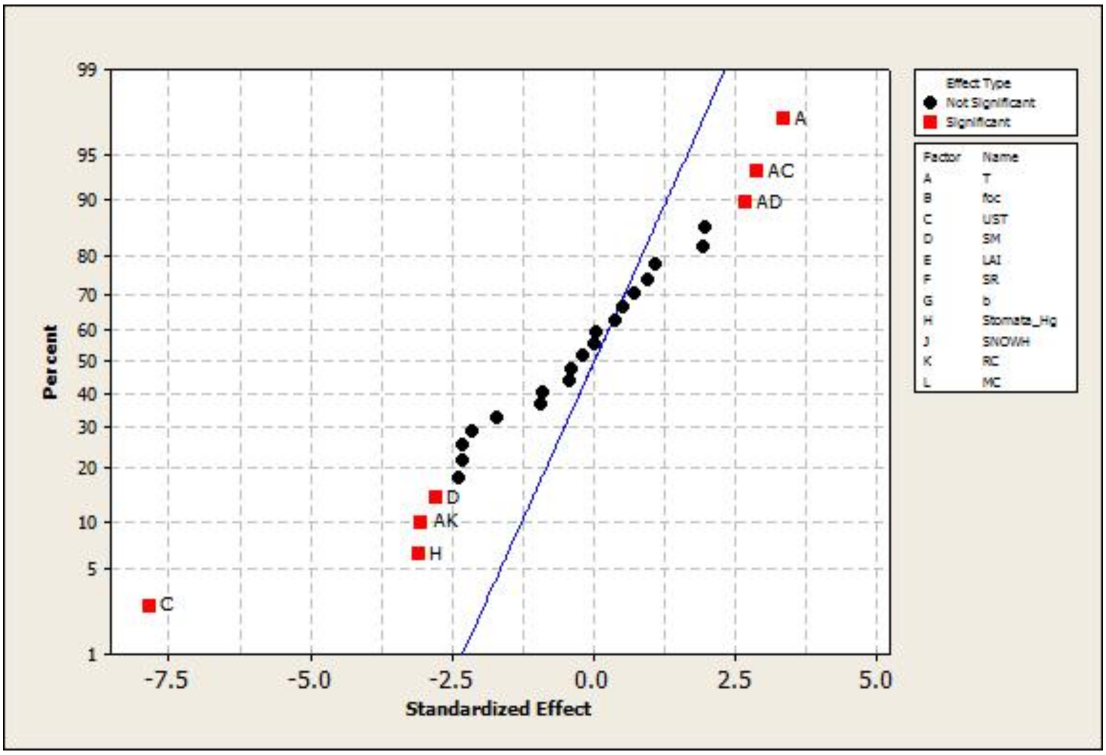

Figure s6: Results of 2^{11-6} fractional design for stamata. Significance at P<0.05. T denotes air temperature at 2 meters, foc denotes fraction of organic carbon in surface soil, UST denotes friction velocity, SM denotes soil total Hg concentration, LAI denotes leaf area index, SR denotes solar irradiation, b denotes scaling factor of reactivity Hg, Stomata_Hg denotes Hg previously deposited to leaf stomata, SNOWH denotes snow depth, RC denotes rain condition, MC denotes moist soil condition. Alias information for significant terms: T*SR + foc*UST + SM*b + Stomata_Hg*MC, T*SNOWH + foc*b + UST*SM + LAI*Stomata_Hg, foc*LAI + SM*MC + b*Stomata_Hg, foc*Stomata_Hg + UST*MC + LAI*b + SR*RC.

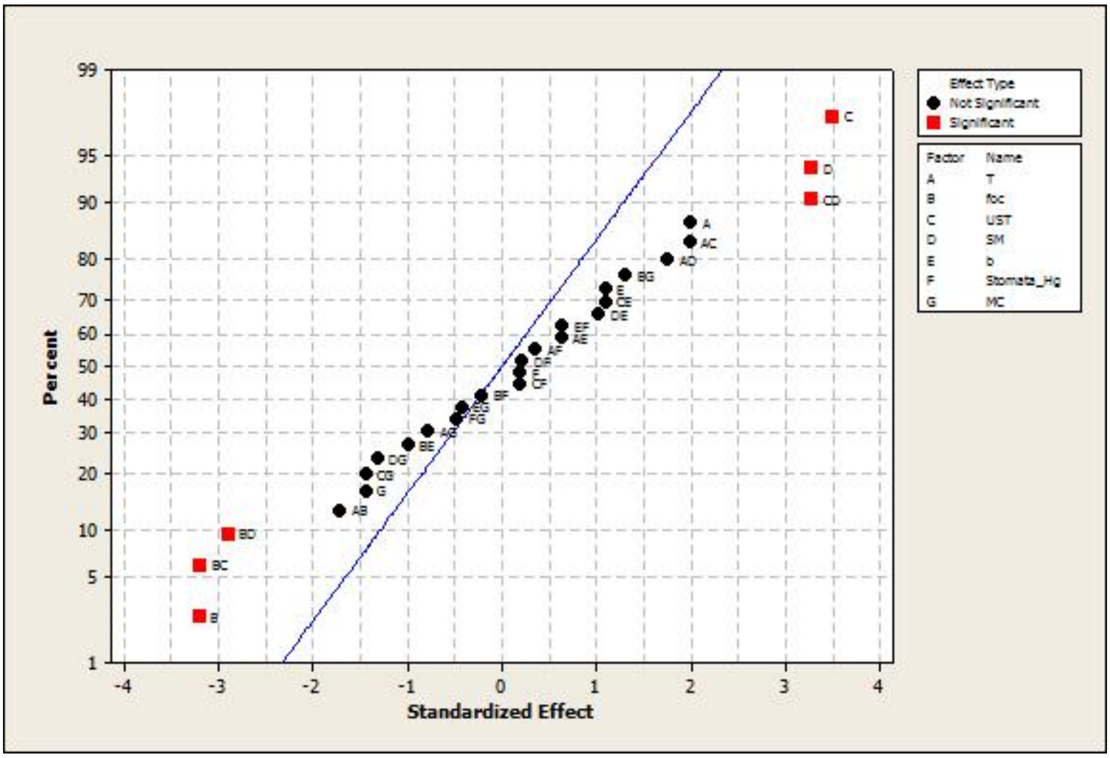

Figure s7: Results of 2^{7-1} fractional design for canopy system. Significance at $P<0.05$. T denotes air temperature at 2 meters, foc denotes fraction of organic carbon in surface soil, UST denotes friction velocity, SM denotes soil total Hg concentration, MC denotes moist soil condition. Alias information for significant terms: T*SR + foc*UST + SM*b + Stomata_Hg*MC, T*SNOWH + foc*b + UST*SM + LAI*Stomata_Hg, foc*LAI + SM*MC + b*Stomata_Hg, foc*Stomata_Hg + UST*MC + LAI*b + SR*RC.

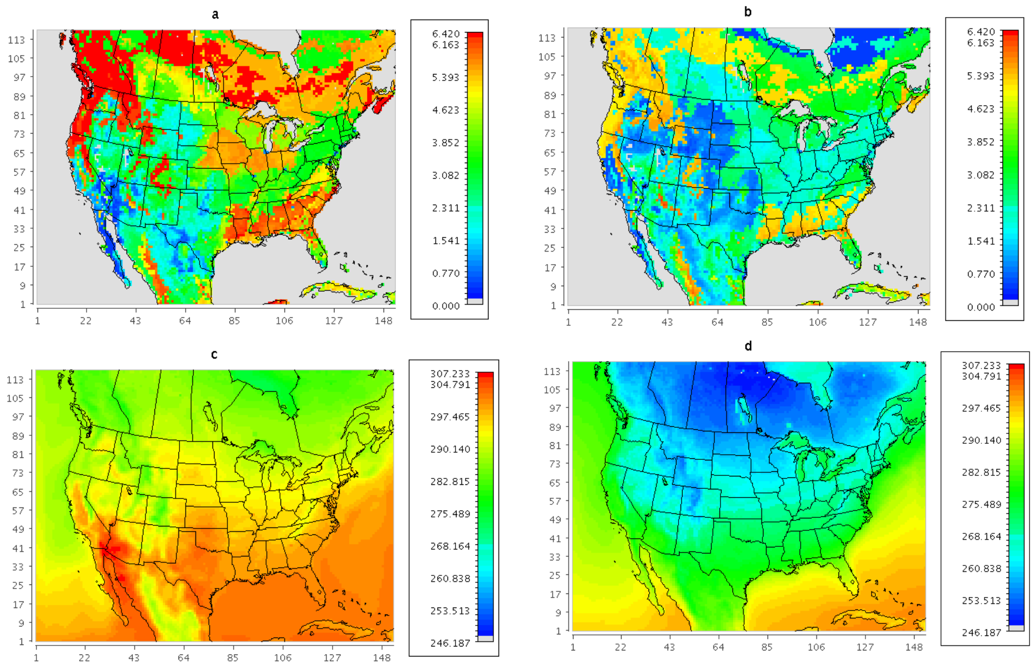

Figure s8: (a) the average spatial distribution of LAI (m^2 m^{-2}) in the summer month; (b) the average spatial distribution of LAI (m^2 m^{-2}) in the winter month; (c) the average spatial distribution of air temperature at 2 meters (K) in the summer month; (d) the average spatial distribution of air temperature at 2 meters (K) in the winter month