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Short communication

Application of a statistical emulator to fire emission modeling

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A B S T R A C T

We have demonstrated the use of an advanced Gaussian-Process (GP) emulator to estimate wildland fire emissions over a wide range of fuel and atmospheric conditions. The Fire Emission Production Simulator, or FEPS, is used to produce an initial set of emissions data that correspond to some selected values in the domain of the input fuel and atmospheric parameters for the purpose of training the emulator. The emulated emissions are found to be within ±5% of the FEPS simulated emissions, providing confidence in the potential use of the GP-emulator for this and other similar applications. Cluster analysis for 1000 emulator-produced posterior samples spanning a wide-range of fuel and environmental conditions suggest that the emulator not only produces valid results but also preserves the physical relationships between the fire emission and the fuel and environmental conditions. Results show that the GP-emulator could be used as an alternative to the simulations from the FEPS modeling system when four or more input parameters related to fuel type, fuel moisture, and weather condition are allowed to vary. This work also provides a conceptual basis for constructing a nation-wide emissions inventory based on a trained GP-emulator representing the complex geographic distribution of fuel types and environmental conditions.

1. Introduction

A Gaussian-Process (GP) emulator is a Bayesian-based statistical tool that treats a set of input and output parameters as indices to stochastic Gaussian functions with a set of mean and covariance values emerging from the input/output parameters. Examples of other algorithms that approach the problem of interpolation or prediction in a non-Bayesian framework could be linear/non-linear regression models where a significant assumption of the relationship between the input/output is made, or data-demanding artificial neural network algorithms. Rasmussen (1996) compared up to 7 different methods with large input/output datasets and concluded that the Bayesian approach coupled with a Gaussian process outperforms other traditional methods. For a complete description of how a GP-emulator could be constructed, refer to Chiles and Delfiner (1999), Cressie (1993), Rasmussen and Williams (2006). Several recent studies have applied GP-emulator to complex geophysical processes. Tokmakian and Challenor (2014) and Tokmakian et al. (2012) have shown how GP-emulators could be used to gain specific understanding of complex geophysical systems and interactions within these systems. They also demonstrated how emulators, when trained with data from atmospheric general circulation models (AGCM) and observations, become a powerful tool to assess uncertainties related to the non-linearity in ocean–atmosphere interactions. Holden et al. (2013) demonstrated how an emulator could be used to give spatially and temporally downscaled climate projections, while Gómez et al. (2012), for an extra-terrestrial application, showed how the emulation of historic galactic formation could help with the analyses of the current observations of Milky Way-like galaxies. The advantages of fast statistical models lie in the ability of producing large data sets emulating the simulator while performing at a fraction of the computational cost. An example of an application we have chosen here is for fire emissions modeling.

Wildland fires, whether natural or human-ignited, have one

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thing in common, and that is the release of oxocarbons, hydrocarbons, and particulate matter. Fire smoke can have profound environmental impacts that range from degradation of visibility (Shelby and Speaker, 1990; Toman et al., 2004), production of regional haze and smog (van der Werf et al., 2010; Phuleria et al., 2005) and alteration of ecosystem respiration and production (Amiro et al., 2010). Smoke from large fires can affect local, regional, and global climate by modifying the earth's radiative balance and altering cloud and precipitation patterns (Oris et al., 2013; Liu et al., 2014). In addition to its impact on natural environments, fire smoke also poses a direct risk to human health (Dennekamp and Abramson, 2011; Johnston et al., 2012). The uncertainty in fire emissions comes not only from the misrepresentation of fuel and environmental conditions, but also from the different methods and assumptions used in fire emission models. Various tools or models have been developed to aid in estimating fire emissions. These models vary in their parameterizations and assumptions and the scale at which they are applied (French et al., 2011). These fire emission models are used to estimate emissions from wildfires and prescribed burns for use in air-quality assessment as well as in atmospheric dispersion models. One of the major uncertainties arising from air pollution dispersion tools is the accuracy of the emission sources at the ground level. The other uncertainty comes from humidity and temperature that play a major role in determining the dispersive characteristics of smoke (Hoadley et al., 2003). Fire emissions are usually specified in numerical and analytical models as a function of the size of the area being burned, fuel characteristics including the amount and type of biomass and its moisture content, a combustion efficiency, an emission factor that relates the burned and emitted mass to the biomass burned (Seiler and Crutzen, 1980) and weather conditions such as near surface wind speed and atmospheric stability. Uncertainties in each one of these factors contribute unequally to the overall uncertainty of the estimated emissions. French et al. (2011) compared 5 different widely used models and concluded that despite the 25% range agreement amongst these models, the largest uncertainty of carbon and particulate emissions comes from the difficulty in quantifying the emissions during the smoldering process, the spatial variability of fuel loading (amount of fuel per unit area) and weather conditions that determine the fuel condition.

Given the large number of factors involved in specifying emissions, a full understanding of the contributions from each factor to the uncertainties of estimated emissions is difficult because it requires a large number of tests and model runs. Similarly, a complete understanding of the sensitivity of the total emissions to individual factors and interactions of multiple factors also poses a significant challenge. This challenge can be met by the use of statistical tools. In this study, we demonstrate the potential use of a GP-emulator constructed for the Models and Data Analysis Initiative (MADAI: www.madai-public.cs.unc.edu) (O'Hagan, 2006; Oakley and O'Hagan, 2004) as an alternative to a large number of simulations using a simulator, which in this case is the fire emission model.

What we will show in this short contribution is a new area of applications of a statistical emulator: the area of fire emissions modeling. Fire emission models usually involve a large number of input parameters and it is difficult to fully understand how the interactions among the input parameters affect the emissions output. We will show that the emulator, after being trained by output data of simulated emissions and their corresponding input parameters, can be used to easily expand the emissions database to cover a wide variety of the fuel and atmospheric conditions, thus enabling a better understanding of the dependency of fire emissions to variations of the input parameters and their interactions. In addition to improving the current understanding, the outcome of this study will provide an alternative way of specifying the emissions during a fire event without having to actually run an emissions model, because the emulator itself has been “trained” by the emissions model. The proven success of the GP-emulator to emulate the FEPS model could also suggest a conceptual framework that would allow for constructing a geographic information system or GIS-based nation-wide emission inventory where fuel models (defined here by the fuel type and environmental conditions) are very complex in their geographic distribution and type.

2. Methodology

In this study, we aim to achieve a successful emulation of wildland fire emissions. We will use a specific fire emissions dynamic simulator to produce a small dataset of input parameters and emissions output values that will be used to train an emulator to produce the desired emission products. The results from the emulator will then be validated with a new set of simulated results based on the emulator's posterior, or newly produced, samples.

2.1. The simulator

The numerical simulator used in this study for dynamically relating fire emissions to the control input parameters is the Fire Emission Production Simulator (FEPS) (Anderson et al., 2004), which is used by many fire and forest managers in the U.S. to estimate fuel consumption and fire emissions and has been successfully integrated into smoke modeling frameworks such as the BlueSky framework (Larkin et al., 2009). Through a graphically driven user interface, FEPS allows users to customize all input variables (such as fuel loading, fuel moisture, consumption, fire growth, hourly meteorological data, etc) for their specific needs and locations in order to calculate emissions for a wide range of fuel and environmental conditions. For fuel loading, the user has the flexibility to choose from 5 natural fuel loading profiles (canopy, shrub, grass, woody, litter), 2 slash fuels (broadcast and piles) and a duff layer as an additional fuel profile, or choose from 24 predefined National Fire Danger Rating System (NFDRS) fuel models (Bradshaw et al., 1984). FEPS also allows the user to enter a time varying meteorological field from surface weather stations or numerical weather forecasts, including wind speed at transport height, wind speed at the flame level, and an atmospheric stability class of the ambient atmosphere. For fuel moisture, the user can assign one of six moisture profiles for every fuel type. The output of FEPS includes an emission rate report that contains carbon monoxide (CO), carbon dioxide (CO_2), methane (CH_4), and 2.5-micron particulate matter ($PM_{2.5}$). A complete description of FEPS, including its algorithms and equations, can be found in Anderson et al. (2004).

For this study, FEPS is first used to produce emissions of CO, CH_4 and $PM_{2.5}$ with three input parameters, namely fuel loading (mass or percent of fuel burned per unit area, pB), fuel moisture content (FM), and wind speed (WS), for a fixed fuel type. The same FEPS simulations are repeated for another fuel type, thus, increasing the number of input parameters from three to four (the additional parameter being pB of the new fuel type). By increasing the number of input parameters (hence increasing the training parameter dimensions of the emulator), we aim to investigate whether this process could improve the emulator results. For simplicity, the FEPS simulations assume a fire that lasts for 1 h and burns 1 acre. The burn areas are additive, i.e., the amount of emissions would double if the areas burned double.

Table 1
Summary of the input/output parameters and values used in preparing the emulator training set from FEPS. Blue and green colors correspond to experiment 1 (three-input parameter) and 2 (four-input parameter) respectively. pBf1 and pBf2 correspond to percent burn of fuel type 1 (broadcast) and fuel type 2 (shrub); FM and WS correspond to fuel moisture and wind speed, respectively.

	FM	WS (ms^{-1})	pBf1 (%)	pBf2 (%)
Number of input parameter combinations to FEPS: 240 for exp1 432 for exp2	1 (very dry) 3 (moderate) 6 (very wet)	1, 5, 10, 20	5, 20, 40, 60, 80, 100 or 5 (step 5) to 100	5, 20, 40, 60, 80, 100
Output from FEPS	$PM_{2.5}$ (gs^{-1})	CO (gs^{-1})	CH_4 (gs^{-1})	
Max. (exp1, exp2) Mean (exp1, exp2) Std. deviation (exp1, exp2)	154, 203 50, 77 37, 44	1905, 2506 609, 936 455, 539	90, 118 29, 44 21, 25	

A summary of the simulated FEPS input/output is given in Table 1. The parameters in Table 1 are then used to train the GP-emulator. These parameters were prepared by running FEPS driven by FM, WS, pBf1 and pBf2 as inputs and producing the particulate and gaseous emissions as output. The sensitivity of the emissions of the three output species, CO, CH_4, and $PM_{2.5}$, to the changes in the input parameters is investigated using the large posterior samples generated by the trained emulator.

2.2. The emulator

We used a GP-emulator trained by simulated inputs/outputs from FEPS. The GP-emulator used in this study is part of the open source statistical packages developed by the Models and Data Initiative program (MADAI: www.madai-public.cs.unc.edu). The statistical package tools and thorough documentation can be downloaded from here (https://madai-public.cs.unc.edu/statistical-tools/distribution-sampling-library). The trained GP-emulator can then be used as a surrogate to FEPS simulations and generate posterior samples of which selected samples can be validated against equivalent FEPS simulations.

The emulator is first trained by the FEPS output for selected input parameter values described in Table 1. Once trained, the GP-emulator is then used to produce 100 posterior samples (input and output parameters). For validation purposes, FEPS is run again with those 100 input parameters to produce a set of output parameters representing 'true' emissions. The outputs in the 100 posterior samples representing the emulated emissions are compared against the 'true' emissions. Fig. 1 summarizes the necessary steps involved in the emulation of the FEPS modeling system.

A total of 4 sensitivity experiments to GP-emulator tuning parameters are carried out to reach the best combination of control setting parameters that produce the least relative bias between the simulated and the emulated results. We have also advanced systematically from the emulation of one, two, three and four input parameters to check for consistency or errors in the application.

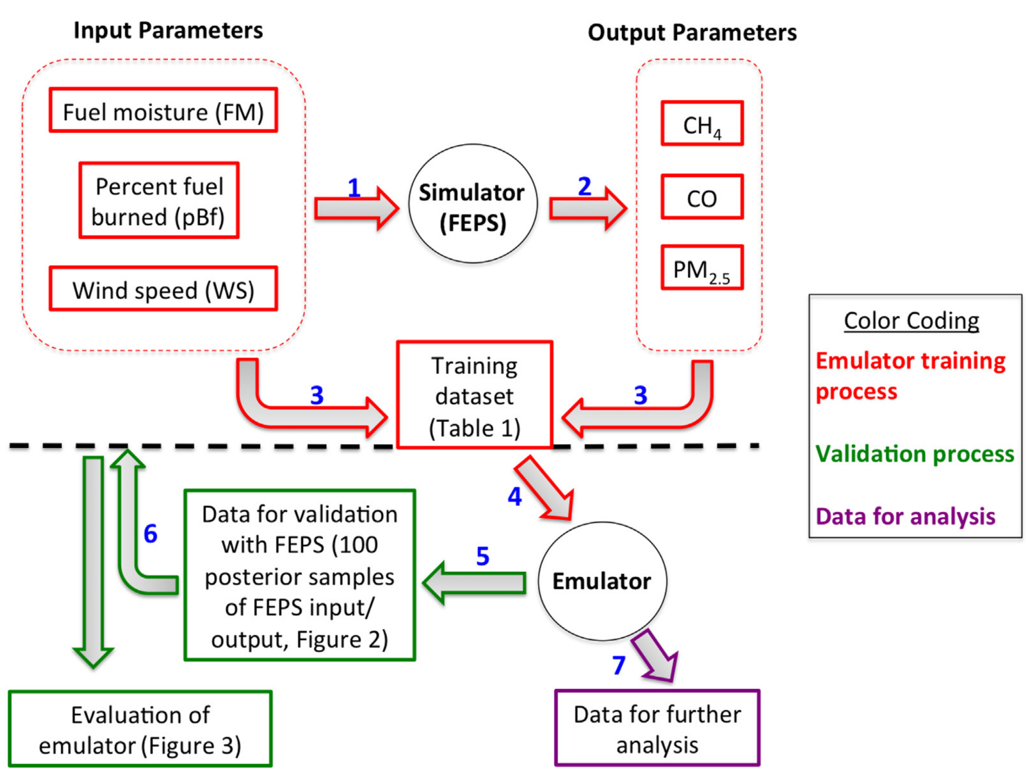

Fig. 1. Flow chart showing the necessary steps needed for the emulation process. The color coding key shows the three major stages required prior to using data from the emulations for analysis. The blue numbers indicate the process sequence; using the simulator to produce a training dataset and train the emulator (numbers 1, 2, 3, and 4); the validation process (number 5) of comparing a subset of posterior samples produced by the emulator with the output from the simulator at the same sampling points (numbers 5 and 6); and finally the usage of the emulator to produce data ready for further analysis (number 7). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

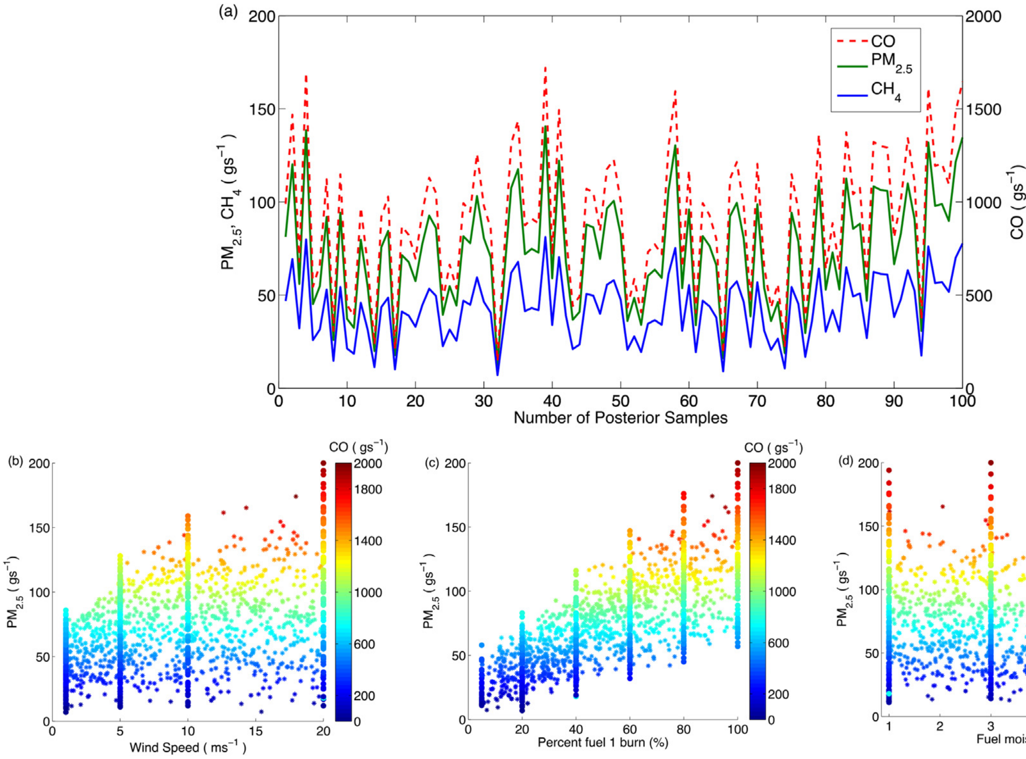

Fig. 2. (a) The co-variation of the emulated 100 posterior outputs, (b to d) the filled parameter space (star symbol, total of 1000 samples) produced by the trained GP-emulator with 432 training points (vertical straight-line points). The emissions from CH_4 showed similar results and are not presented in this figure.

3. Results and discussion

Fig. 2a shows the emulated 100 sample emissions of the three species. The emissions for the three species vary consistently among the sampling points. Fig. 2b shows three examples of selected points used to train the GP-emulator (the vertical straight lines) and the 1000 posterior samples produced by the trained GP-emulator. The posterior samples fill in the space amongst the training points and are shown to have a matching magnitude distribution depicted by the color intensity of one of the output emissions (CO). These results reveal the basic function of the GP-emulator, and that is to correctly interpolate between the training points and provide a large number of new samples that could be used for further analysis.

The emulator was developed with variety of applications in mind and users are allowed to select parameters in order to optimize the performance of the emulator for their specific application. For this application, two emulator setup parameters related to the order of the regression model and the type of training algorithm are found to have most influence on the emulation results. For the experiment with three input parameters, the combination of a first order regression model and the exhaustive training algorithm appear to have yielded smaller bias compared to higher order regression and the basic training algorithm (dark blue line of stat4 case in Fig. 3a). Still, the bias is large at ±20% for almost 90% of the sampled data (Fig. 3b). However, a substantial reduction in the overall bias is achieved by the introduction of the fourth input parameter with at least 90% of the 100 validation points having a bias within ±5% (light blue line of stat4 in Fig. 3b). Fig. 3b shows the cumulative frequency of the bias where the mean bias of the four-input parameter experiments was −0.8% with the standard deviation of 4.4%. Increasing the input parameters from three to four by including a new fuel type (with the parameter pBf2) improved the emulation results substantially regardless of the regression models and training algorithms used.

To fully explore the sensitivity of the three emission outputs to the four input parameters (pBf1, pBf2, FM and WS), we have used 1000 emulator-produced posterior samples and clustered the output by the k-means algorithm. The algorithm sorts the samples into four different clusters as shown by different colors in Fig. 4. The $PM_{2.5}$ emissions are shown here, but the other two emission outputs produced similar results and only their means are presented in Fig. 4. Naturally, the clusters are ordered based on their average values that could be categorized as low, medium-low, medium—high, and high emission scenarios. The mean of each input parameter that corresponds to every cluster is calculated and shown in Fig. 4 (inside the color coded boxes). It is to be noted here that these clusters and the corresponding mean values for the four input parameters are a result of the GP-emulator output, not the actual FEPS model output. These results show that pBf1 (a part of slash fuel group in FEPS that produces more intense fires and emissions) is correlated with the increase in emissions and has the largest relative change between clusters compared to other input parameters. The other fuel type pBf2 (that comes from the natural fuels category in FEPS and produces less intense fires and emissions) has weak influence on changing the emissions from one cluster to the other. The results also show that the sensitivity of the emission to fuel moisture is weak as indicated by the very little change of mean FM values between the clusters. Wind speeds, on the other hand, are correlated with the increase in emissions, but the impact, judging by the relative change of the mean values between clusters, is not as strong as the input parameter pBf1. These results, which reveal the true physical dynamics relating the input parameters to the expected fire emissions, add more confidence in the potential use of GP-emulator posterior samples as surrogates to FEPS simulated emissions.

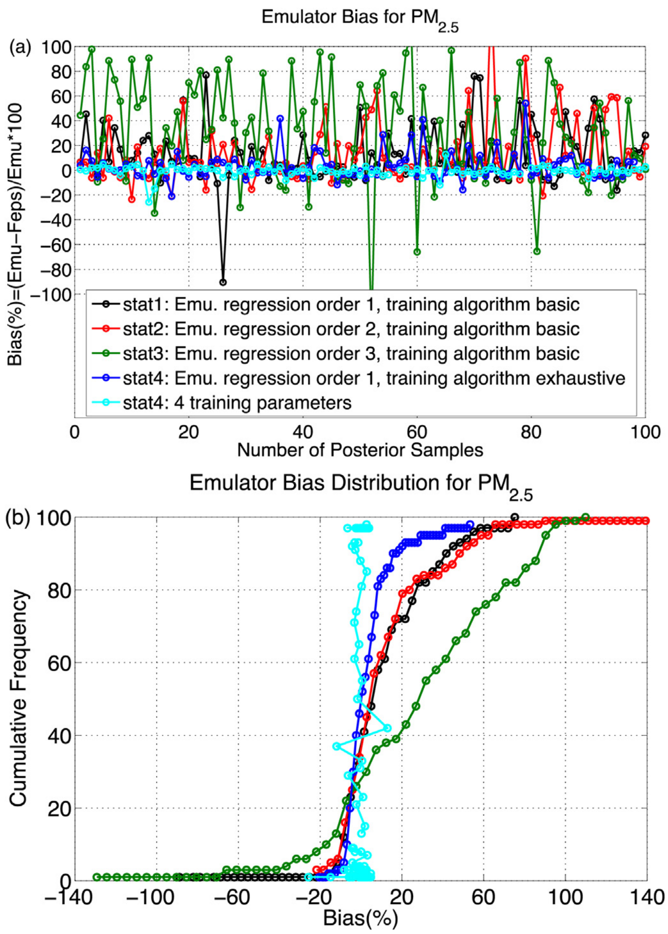

Fig. 3. (a) Relative bias (y-axis, (emulator-FEPS/emulator)*100) between the FEPS simulated results for $PM_{2.5}$ concentrations and the emulated results by the GP-emulator. Four different GP-emulator settings were used (stat1 to 4: see figure inset). (b) Cumulative frequency of the relative bias between the FEPS simulated and GP-emulator emulated results. Both figures have a common legend shown in (a).

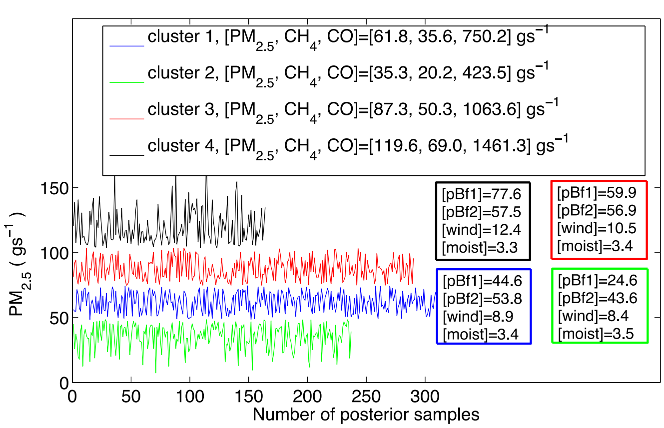

Fig. 4. A k-means cluster for 1000 posterior samples (four clusters) and the corresponding mean (in brackets) output emission parameters and the associated mean of the four input parameters of every cluster (inside the color coded boxes). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

4. Conclusion

We have investigated the performance of a GP-emulator driven by a Bayesian framework to emulate the complex physical interactions among several factors contributing to wildland fire emissions. The emulated emissions for three species, CO, CH_4 and $PM_{2.5}$, from wildland fire are within ±20% of the simulated emissions when three input parameters (fuel loading, fuel moisture and wind speed) are allowed to vary. The relative bias decreased to ±5% when an additional input parameter, fuel type, is included. Further analysis with 1000 emulator-produced posterior samples representing fire emission and input fuel and environmental properties suggest that the emulator not only produces valid results, but also a large dataset that preserves the relationship between the input and output parameters. An example was provided by relating the maximum emissions to the fuel type known to produce the highest emission rates.

This study represents a pilot-investigation and a proof of concept towards potential use of a GP-emulator to effectively produce fire emissions that span a wide range of fuel and atmospheric conditions. A trained emulator with fast statistical algorithms is capable of producing a very large dataset of valid emission results driven by a smaller set of simulated emissions and the corresponding input parameter values. Although the primary objective of this work is to conceptualize a framework that would allow for constructing a GIS-based nation-wide emission inventory where fuel models (defined here by the fuel type and environmental conditions) are very complex in their geographic distribution and type, one could also allude to various other possible objectives. This work also provides the preliminary results for constructing automated look-up tables relating fire emissions to fuel and environmental properties, which could then be coupled to operational smoke and atmospheric dispersion models driven by weather forecasts or observations. The emulator could also be used to construct an ensemble of fire emission outputs not only driven by one simulator (like FEPS) but with other emissions models. This approach would allow for an uncertainty reduction (due to the incorporation of a collection of fire emission model outputs) and ensemble-based predictions facilitated by a GP emulator.

Although the approach adopted in this study emphasizes the success of the proposed simple statistical methodology in tackling complex environmental physical processes, a continuous case-by-case validation process is necessary. We also recommend that the number and size of training parameters be as large as possible (limited by practicability). In theory, the more feedback processes included in a physical system, the more the need arises to include extra input/output training parameters. Unfortunately, there are no guidelines on the relationships of the number of training parameters required and the complexity of the physical process under investigation.

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