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Testing hadronic-model predictions of depth of maximum of air-shower profiles and ground-particle signals using hybrid data of the Pierre Auger Observatory

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We test the predictions of hadronic interaction models regarding the depth of maximum of air-shower profiles, X_{\max} , and ground-particle signals in water-Cherenkov detectors at 1000 m from the shower core, $S(1000)$, using the data from the fluorescence and surface detectors of the Pierre Auger Observatory. The test consists of fitting the measured two-dimensional ($S(1000)$, X_{\max}) distributions using templates for simulated air showers produced with hadronic interaction models Epos-LHC, QGSJet-II-04, SIBYLL 2.3d and leaving the scales of predicted X_{\max} and the signals from hadronic component at ground as free-fit parameters. The method relies on the assumption that the mass composition remains the same at all zenith angles, while the longitudinal shower development and attenuation of ground signal depend on the mass composition in a correlated way. The analysis was applied to 2239 events detected by both the fluorescence and surface detectors of the Pierre Auger Observatory with energies between $10^{18.5}$ eV to $10^{19.0}$ eV and zenith angles below 60° . We found, that within the assumptions of the method, the best description of the data is achieved if the predictions of the hadronic interaction models are shifted to deeper X_{\max} values and larger hadronic signals at all zenith angles. Given the magnitude of the shifts and the data sample size, the statistical significance of the improvement of data description using the modifications considered in the paper is larger than 5σ even for any linear combination of experimental systematic uncertainties.

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I. INTRODUCTION

The dominant contribution to uncertainties in the determination of the mass composition of ultrahigh-energy cosmic rays (UHECR, energy $E > 10^{18.0}$ eV) comes from the modeling of extensive air showers. Modern hadronic interaction models used for this purpose are based on

extrapolation of interaction parameters like cross sections, multiplicities, elasticities, etc., measured at accelerators at lower beam energies up to $\sqrt{s} = 13$ TeV for proton-proton (pp) collisions at the LHC and pseudorapidities $|\eta| \lesssim 5$ compared to energies $\sqrt{s} \gtrsim 50$ TeV and pseudorapidities¹ $\eta \approx 7$ to 11 driving the energy flow of the first interactions of UHECR in the atmosphere, where the target is different (mostly oxygen and nitrogen nuclei). Therefore, improvements in the description of the LHC data, implemented in the modern models do not necessarily lead to unambiguous, nearly hadronic model-independent predictions for the mass-sensitive air-shower observables. For instance, at $10^{18.7}$ eV the span in predictions for the mean depth of maximum of air shower profiles, $\langle X_{\max} \rangle$, between models used by the UHECR community (Epos-LHC [1], QGSJet-II-04 [2], SIBYLL 2.3d [3]) is ~ 25 g/cm², nearly independently of the primary particle mass and energy. Such a difference can be considered only a lower limit on the systematic uncertainty of the predicted X_{\max} scale. This is about one-quarter of the difference between $\langle X_{\max} \rangle$ values of the two astrophysical extremes, protons and iron nuclei. As a consequence, the mass composition of cosmic rays can be referred only with respect to X_{\max} scale predicted by a particular model. The largest differences in the predicted $\langle X_{\max} \rangle$ between the models, with a minimal impact on the elongation rate, come from the properties of the first hadronic interaction and production of nucleons-antinucleons in pion-air and kaon-air interactions that are

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¹The forward calorimeters at LHC can cover $\eta = 8.4$ to 15, but of neutral particles only.

not well-known in the relevant kinematic region (for more detailed discussion, see e.g., Ref. [4]). The general comparison of properties and different treatments of hadronic interactions by the three models used in this work is summarized in Ref. [5]. Note that although the models used in this work treat differently the properties of hadronic interactions, the range of air-shower properties predicted by these models does not need to include all the possibilities.

The difference in the standard deviation of X_{\max} distributions, $\sigma(X_{\max})$, between the models is within ~ 5 g/cm², whereas the difference between the X_{\max} fluctuations of protons and iron nuclei is ~ 40 g/cm². Therefore, the difference of $\sigma(X_{\max})$ in model predictions has a smaller effect on the mass composition inferences compared to the difference in predictions of $\langle X_{\max} \rangle$. Note, that there is no direct correspondence of the model scales of X_{\max} and $\sigma(X_{\max})$, i.e., the differences in $\sigma(X_{\max})$ are not a mere consequence of the differences in $\langle X_{\max} \rangle$.

In general, the signal produced by air-shower particles reaching the ground shows much lower sensitivity to the mass composition than in the case of X_{\max} . The model differences in predictions of the ground-particle signal, for instance, at 1000 m from the impact point of an air shower at $10^{18.7}$ eV detected at the Pierre Auger Observatory (Auger) [6] are at the level of ~ 3 VEM,² whereas the difference between protons and iron nuclei is about twice this value. The fluctuations of the ground signal are dominated by the detector resolution, suppressing any significant sensitivity to the model or primary mass [7].

A. Problems in the description of data with hadronic interaction models

The correctness of the model predictions can be tested using data from air-shower experiments. At the Pierre Auger Observatory, for instance, negative variance of the logarithm of primary masses [$\sigma^2(\ln A)$] and poor description of the measured X_{\max} distributions are obtained when simulations with QGSJet-II-04 are used for the interpretation of the measured X_{\max} moments in terms of the moments of $\ln A$ for $E \gtrsim 10^{18.5}$ eV [8–11]. The problem is that, due to relatively shallow $\langle X_{\max} \rangle$ predictions of QGSJet-II-04, the best possible description of the data is achieved with proton-helium mixes, but for these mixes the modeled X_{\max} distributions are broader than the observed ones. These findings are further supported by the observation of the negative correlation between X_{\max} and the signal in surface detector (SD) [11,12] in the Auger data near the “ankle” feature ($E \approx 10^{18.7}$ eV) of the UHECR spectrum. That can be achieved only for the mixed primary composition containing particles heavier than helium nuclei, which is a robust statement based on the general phenomenology of

²This unit is the signal produced by a muon traversing the station on a vertical trajectory.

air-shower development and, therefore, not sensitive to the properties of a particular hadronic model.

The deficiencies of the models are more evident for the SD observables, where, in some cases, the data are not even bracketed by the Monte Carlo (MC) predictions for protons and iron nuclei. The muon deficit in simulations, known as the “muon puzzle” [5], is the best-known example of this kind. In particular, this was observed by Auger for inclined showers (zenith angles $\theta = 62^\circ$ to 80°) dominated by the muon component, for Epos-LHC and QGSJet-II-04 at $\sim 10^{19.0}$ eV [13], and in direct measurements with underground muon detectors at $E = 10^{17.3}$ eV to $10^{18.3}$ eV and $\theta < 45^\circ$ [14]. At the same time, the fluctuations of the muon signal measured by Auger [15] are consistent with the MC predictions, indicating that the muon deficit might originate from the accumulation of small deviations from the model predictions during the development of a shower, rather than be caused by a strong deviation in the first interaction. The range of predictions for the muon production depth of protons and iron nuclei is outside of the measured values for Epos-LHC above $10^{19.3}$ eV [16].

Less directly, the muon deficit in simulations was observed as a deficit of the total signal at 1000 m from the shower core, $S(1000)$, in the Auger SD stations [17] for vertical ($\theta < 60^\circ$) showers with energies around 10^{19} eV. In this analysis, within the assumption that the electromagnetic (em) component, X_{\max} , and, correspondingly, the mass composition inferred from the X_{\max} measurements, are predicted correctly by a particular model, the deficit of $S(1000)$ was interpreted as the underestimation of the hadronic signal (dominated by muons) in simulations by $(33 \pm 16)\%$ for Epos-LHC and by $(61 \pm 21)\%$ for QGSJet-II-04, with a strong dependence on the energy scale. An indicative summary of all these tests for the three models used in this work is given in Table I.

The use of an incorrect MC X_{\max} scale would lead one to a biased inference on the mass composition and, through this, to a biased estimate of the muon deficit, since the muon content in a shower scales with the primary mass $\propto A^{1-\beta}$, $\beta \approx 0.9$ [18]. Therefore, in a more comprehensive approach a modification of the MC scales of both X_{\max} and SD signals, going along with the fitting of the primary mass composition accounting for these modifications, should be considered.

B. Progressive testing of hadronic interaction models

In this work, progressive testing of the model predictions is performed. First, we allow for a rescaling of the signal on the ground produced by the hadronic shower component at 1000 m with a factor R_{had} . Then we add a zenith-angle dependence of R_{had} defining two parameters $R_{\text{had}}(\theta_{\min})$ and $R_{\text{had}}(\theta_{\max})$ at the two extreme zenith-angle bins. We assume a linear dependence of R_{had} on the distance of

TABLE I. Indicative summary of the results of tests of models using Auger data (✓—no tension, ✗—tension). In the case of SIBYLL 2.3d, we also show estimations based on the previous version of the model Sibyll when available in the literature.

Test	Energy/EeV	$\theta/^\circ$	Epos-LHC	QGSJet-II-04	SIBYLL 2.3d
X_{\max} moments [8–11]	~3 to 50	0 to 80	✓	✗	✓ (2.3c)
X_{\max} : $S(1000)$ correlation [11,12]	3 to 10	0 to 60	✓	✗	✓ (2.3c)
Mean muon number [13,15]	~10	~67	✗	✗	✗
Mean muon number [14]	0.2 to 2	0 to 45	✗	✗	...
Fluctuation of muon number [15]	4 to 40	~67	✓	✓	✓
Muon production depth [16]	20 to 70	~60	✗	✓	...
$S(1000)$ [17]	~10	0 to 60	✗	✗	...

X_{\max} to the ground in atmospheric depth units to relate R_{had} to different zenith angles. Finally, we consider a shift in the predicted X_{\max} distributions (ΔX_{\max}) that is assumed to be independent of the primary mass and energy. In this way, we consider freedom not only in the scale of the simulated hadronic part of the ground signal but also in the simulated X_{\max} scale. Consequently, the main differences in X_{\max} and $S(1000)$ predictions of the models are reduced, and similar mass composition inferences for the Auger data are obtained. It is remarkable, that a consistent description of the Auger data with all three models can be achieved with the modification of only two scale parameters.

The analysis is performed for the energy region around the ankle ($E \approx 10^{18.7}$ eV) in the energy spectrum where the UHECR mass composition is mixed [9,11,12]. Specifically, we find the values of ΔX_{\max} , $R_{\text{had}}(\theta)$, and fractions of four primary particles (protons, and helium, oxygen, iron nuclei) for which the best-fit of the measured two-dimensional distributions of ($S(1000)$, X_{\max}) is achieved. The remaining differences between the predictions of models with a smaller effect on MC templates like the fluctuations of X_{\max} and hadronic signal, and the mass composition dependence of $R_{\text{had}}(\theta)$ and ΔX_{\max} are not considered in this work.

In Sec. II, we give a detailed description of the method. In Sec. III, the method is applied to the data of the Pierre Auger Observatory. The results of the data analysis are discussed in Sec. IV followed by a summary of our findings in the Conclusions.

II. METHOD

The method stems from Ref. [19] and it was first introduced in Ref. [20] followed by a slight modification in the approach to the ground-signal rescaling. A preliminary application of the method to the Auger data was presented in Ref. [21].

We perform a binned maximum-likelihood fit of the measured two-dimensional distributions (S , X) with MC templates for four primary species simultaneously in five zenith-angle bins. The observables are $S(1000)$ and X_{\max}

corrected for the energy evolution using the fluorescence detector (FD) energy E_{FD} ,

$$S = S(1000) \left(\frac{E^{\text{ref}}}{E_{\text{FD}}} \right)^{1/B}, \quad (1)$$

and

$$X = X_{\max} + D \lg \left(\frac{E^{\text{ref}}}{E_{\text{FD}}} \right), \quad (2)$$

where $B = 1.031 \pm 0.004$ is the SD energy calibration parameter [22] and the elongation rate of a single primary $D = 58$ g/cm²/decade is taken as the average value over the four primary particles and three models used in this work. The value of the elongation rate varies only within ± 2 g/cm² around the mean, in accordance with the universality with respect to the primary mass predicted within the phenomenological model in Ref. [23]. This is a consequence of energy dependencies of multiplicity, elasticity, and cross section assumed in this phenomenological model. We chose the reference energy $E^{\text{ref}} = 10^{18.7}$ eV for the analyzed energy range of $E_{\text{FD}} = 10^{18.5}$ eV to $10^{19.0}$ eV.

The signal $S(1000)$ is assumed to be composed of the hadronic (S_{had}) and electromagnetic (S_{em}) components. The signal S_{had} is produced by muons, em particles from muon decays and low-energy neutral pions as in [17] according to the four-component shower universality model [24,25]. The signal S_{em} is produced by em particles originating from high-energy neutral pions.

A. Monte Carlo templates

The MC templates were prepared using simulated showers from a library produced within the Pierre Auger Collaboration [26]. Air showers were generated with CORSIKA 7.7400 [27–29] with a flat zenith-angle distribution in $\sin^2 \theta$ [for $\theta \in (0^\circ, 65^\circ)$] and the energy distribution $\propto E^{-1}$. Subsequently, we reweight the events to match the measured energy spectrum [22]. Four different atmospheric profiles are considered to represent the typical variations of

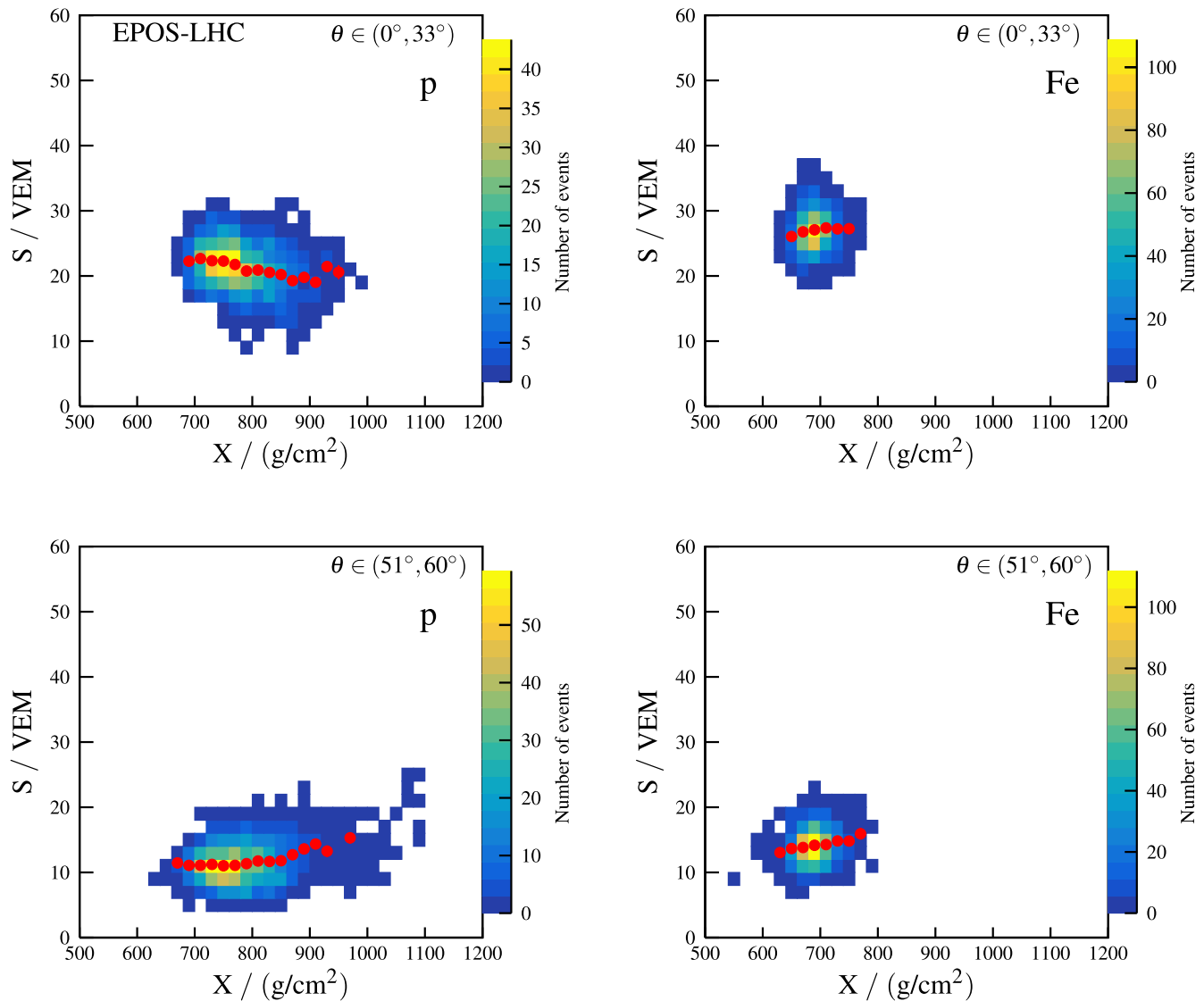


FIG. 1. Examples of two-dimensional distributions of S and X for protons (left) and iron nuclei (right) generated with Epos-LHC for zenith angles between 0° and 33° (top) and 51° and 60° (bottom). The red points indicate the mean values of S . $E = 10^{18.5}$ eV to $10^{19.0}$ eV.

atmospheric conditions at the location of the Pierre Auger Observatory. The simulation set includes three models (Epos-LHC, QGSJet-II-04, SIBYLL 2.3d) and four primary particles (p, He, O, Fe). In productions with Epos-LHC and SIBYLL 2.3d, the low-energy ($E_{\text{kin}} < 80$ GeV) interactions were simulated with URQMD [30], while QGSJet-II-04 was used in combination with FLUKA [31,32]. No significant dependency of the results on the choice of the low-energy model was found.

The detector simulations and event reconstruction were performed with the Auger Offline Framework [33]. In the standard event processing chain, not all effects related to the detector calibration, atmospheric conditions, long-term performances, etc., are included in the simulations and reconstruction. To account for them, for the FD part an

additional smearing of X_{max} distributions by ≈ 9 g/cm² is applied [9]. In the case of the SD part, the smearing of $S(1000)$ by 9%, corresponding to the maximal expected contribution from realistic operational conditions, was tested without finding any statistically significant effect on the results. The event selection is the same as applied to the data (see Sec. III). After the selection, the MC templates contain ≈ 15000 showers per primary species and model.

The analysis was carried out by splitting these simulated air-showers in five zenith-angle ranges containing nearly the same number of events, namely $(0^\circ, 33^\circ)$, $(33^\circ, 39^\circ)$, $(39^\circ, 45^\circ)$, $(45^\circ, 51^\circ)$, $(51^\circ, 60^\circ)$. Examples of the (S, X) distributions for protons and iron nuclei in the most vertical and most inclined angular ranges are shown in Fig. 1. Such two-dimensional distributions are then normalized and

fitted with the ansatz function Φ described in detail in Appendix A. This function is a convolution of the generalized Gumbel distribution of X and the Gaussian distribution of S with the mean value linearly changing with X , reflecting in this way their correlation indicated in Fig. 1. A set of these trial functions for each model, primary particle, and zenith-angle range is used as MC templates in the following fitting procedure.

B. Fitting procedure

For each model, we search for the most likely combination of the composition mix of the four primary species, the zenith-dependent rescaling parameter of the hadronic signal $R_{\text{had}}(\theta)$, and the constant shift of the depth of shower maximum ΔX_{max} in all the MC templates. The fitting method is a generalization of the fitting procedure used in Ref. [10] in the case of the X_{max} distribution and applied here to the two-dimensional (X, S) distributions in five zenith-angle ranges simultaneously.

The negative log-likelihood-ratio expression that is minimized for a given model is of the form,

$$\ln \mathcal{L} = \begin{cases} \sum_k \sum_j (C_{jk} - n_{jk} + n_{jk} \ln \frac{n_{jk}}{C_{jk}}), & n_{jk} > 0, \\ \sum_k \sum_j C_{jk}, & n_{jk} = 0, \end{cases} \quad (3)$$

with the sums running over the two-dimensional bins j in (X, S) for the five θ -bins k . The corresponding number of showers measured in bins j, k is denoted by n_{jk} and the predicted number of MC showers by C_{jk} . The latter number

is obtained using the total number of measured showers N_{data}^k as

$$C_{jk} = N_{\text{data}}^k \sum_i f_i \Phi_{i,k}(X'_{j,k}, S'_{j,k}), \quad (4)$$

where $\Phi_{i,k}$ denotes the template function Φ in θ -bin k for a given model and primary particle i with relative fraction f_i . The modified X prediction is of the form

$$X'_{j,k} = X_{j,k} + \Delta X_{\text{max}} \quad (5)$$

and the rescaled predicted ground signal is

$$S'_{j,k} = S_{j,k} f_{\text{SD}}^k(R_{\text{had}}(\theta), \Delta X_{\text{max}}), \quad (6)$$

where $X_{j,k}$ and $S_{j,k}$ are the center bin values of X and S , respectively, of the original MC distribution (X, S) .

The rescaling parameter f_{SD}^k of all signals $S_{j,k}$ is calculated as

$$f_{\text{SD}}^k = R_{\text{had}}(\theta) \frac{(E^{\text{ref}})^{\beta-1/B}}{\langle E_{\text{FD}}^{\beta-1/B} \rangle_k} g_{\text{had},k} f_{\text{had},k} + \frac{(E^{\text{ref}})^{1-1/B}}{\langle E_{\text{FD}}^{1-1/B} \rangle_k} g_{\text{em},k} (1 - f_{\text{had},k}), \quad (7)$$

where $S(1000) \propto E_{\text{FD}}^B$ is assumed to be composed only of $S_{\text{had}} \propto E_{\text{FD}}^\beta$ and $S_{\text{em}} \propto E_{\text{FD}}$, and $f_{\text{had}} = S_{\text{had}}/S(1000)$. The parameter $\beta = 0.92$ is chosen following Ref. [23]. The mean energy factors $\langle E_{\text{FD}}^{\beta-1/B} \rangle_k$ and $\langle E_{\text{FD}}^{1-1/B} \rangle_k$ are calculated

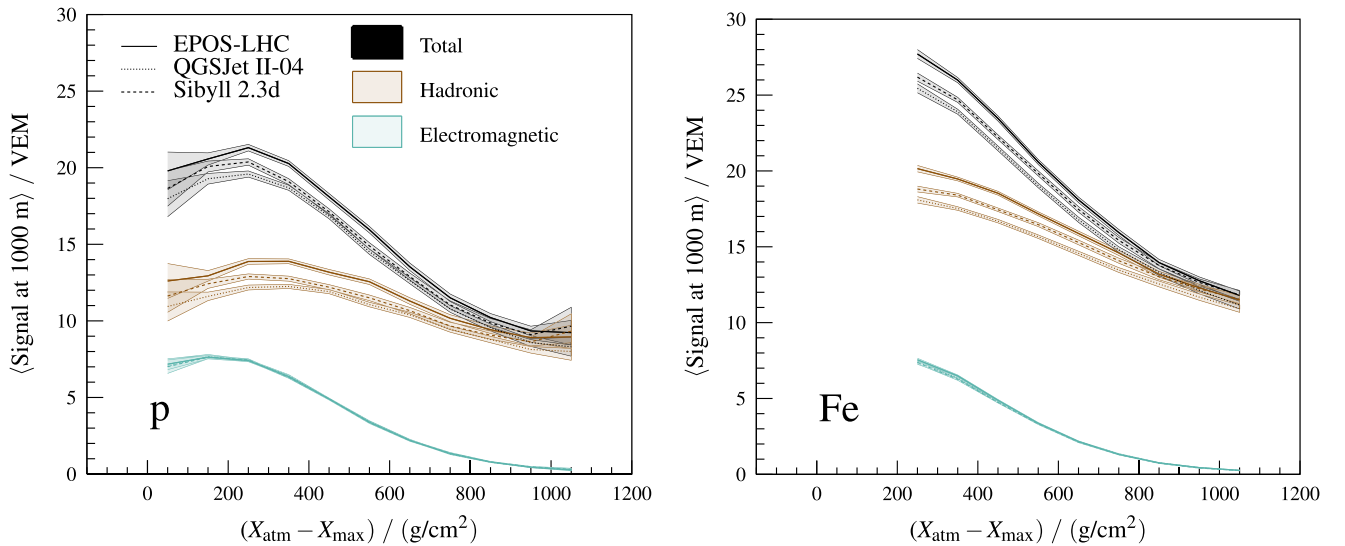


FIG. 2. The total ground signal at 1000 m from the shower core (black) and its hadronic (brown) and em (turquoise) components as a function of the distance from X_{max} to the ground in atmospheric depth units for protons (left) and iron nuclei (right) for different models. The bands contain the statistical uncertainty. $E = 10^{18.5}$ eV to $10^{19.0}$ eV, $\theta < 60^\circ$.

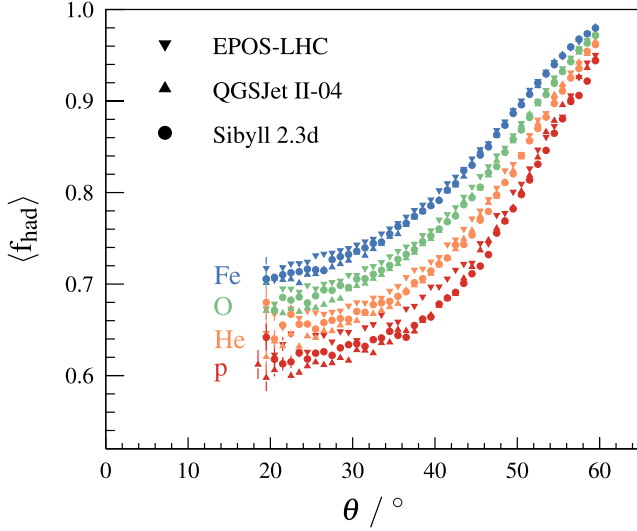


FIG. 3. The average fraction of hadronic signal at 1000 m from the shower core as a function of the reconstructed zenith angle for different models and primary masses. $E = 10^{18.5} \text{ eV}$ to $10^{19.0} \text{ eV}$.

from all measured showers in the energy range $10^{18.5} \text{ eV}$ to $10^{19.0} \text{ eV}$ and θ -bin k .³ The mean hadronic fraction, see also Fig. 3, in the θ -bin k , $f_{\text{had},k}$, is calculated using the average hadronic fractions $f_{\text{had},k,i}$ for simulated showers induced by a primary i and weighted over the relative primary fractions f_i as

$$f_{\text{had},k} = \sum_i f_i f_{\text{had},k,i}. \quad (8)$$

The average effect of the X_{max} change on the ground signal is incorporated through the separate effects on the em $g_{\text{em},k}$ and hadronic $g_{\text{had},k}$ signals, see Appendix B for details. We parametrized the evolution of the mean ground signal parts with the distance of X_{max} to the ground in atmospheric depth units, $X_{\text{atm}} - X_{\text{max}}$, where $X_{\text{atm}} = 880 \text{ g/cm}^2 / \cos \theta$, see the examples in Fig. 2. In this way, the total ground signal is estimated to be modified (via $g_{\text{em},k}$, $g_{\text{had},k}$) at most by about 7% for a change of X_{max} by 50 g/cm^2 . This is in accordance with the functional dependencies in Fig. 2 weighted over the relative contributions of hadronic and em signals (see Fig. 3) and over the primary fractions.

As a consequence of the four-component shower universality approach, the em signal is very similar in all three models, see Fig. 2. The differences in the total signal stem from the size of the hadronic signal at different zenith angles, corresponding to different $X_{\text{atm}} - X_{\text{max}}$ values. Therefore, the freedom in $R_{\text{had}}(\theta)$ and also

³Note that the choice of $E^{\text{ref}} \approx \langle E_{\text{FD}} \rangle$ minimizes the effect of the energy factors; $(E^{\text{ref}})^{\beta-1/B} / \langle E_{\text{FD}}^{\beta-1/B} \rangle_k \approx 1$ and $(E^{\text{ref}})^{1-1/B} / \langle E_{\text{FD}}^{1-1/B} \rangle_k \approx 1$.

ΔX_{max} (see Sec. I) removes the main differences in predictions of S and X for the three models. We assumed a linear dependence of $R_{\text{had}}(\theta)$ on $X_{\text{atm}} - X_{\text{max}}$ and defined rescaling parameters of the hadronic signal at two extreme zenith angles, $R_{\text{had}}(\theta_{\text{min}})$ and $R_{\text{had}}(\theta_{\text{max}})$, for $\sim 28^\circ$ and $\sim 55^\circ$, respectively (see Appendix B for the definition).

We have verified using MC-MC tests, see Appendix C, that the method is performing well and the observed biases were taken as sources of systematic uncertainty of the results.

III. DATA ANALYSIS

A. Data selection

The analysis is applied to hybrid events, i.e., events detected with both SD and FD of the Pierre Auger Observatory between 1 January 2004 and 31 December 2018. To select high-quality events, for the FD part we apply the selection criteria used for the X_{max} analysis [9,11], for the SD part the selection is the same as in the measurements of the SD energy spectrum [22], additionally removing events with saturated SD stations. In this way, we ensure an accurate estimation of the observables X_{max} , E_{FD} , θ , and $S(1000)$ used as the inputs to the method. The selection efficiency is similar for all four primary masses and all zenith-angle bins, therefore it does not introduce mass-composition biases. In total, 2239 hybrid events were selected in the FD energy range $10^{18.5} \text{ eV}$ to $10^{19.0} \text{ eV}$ ($\langle E_{\text{FD}} \rangle \approx 10^{18.7} \text{ eV}$) and zenith angles between 0° and 60° . The data were divided into five zenith-angle bins containing nearly the same ($N = 425\text{--}500$) and sufficiently large number of events, see Fig. 4.

To take into account long-term performance of the FD and SD [34], we applied a time-dependent correction to E_{FD} with a negligible systematic effect on the final results. The signal $S(1000)$ was corrected for seasonal atmospheric effects [35].

B. Results

The minimized values of the log-likelihood expression [see Eq. (3)] are summarized in Table II, progressively applying different modifications to the models. At all stages, the fits of the mass composition are performed with (p, He, O, Fe) fractions as the free-fit parameters. First, the model predictions without any modifications are used for fitting the data. Then we perform fits adding freedom in only one of the modifications ΔX_{max} , R_{had} (independent on zenith angle), $R_{\text{had}}(\theta)$ (zenith-angle dependent). Finally, the fits are performed using combinations of (R_{had} , ΔX_{max}) and ($R_{\text{had}}(\theta)$, ΔX_{max}). From the minimum values of the log-likelihood expression for these scenarios, and from the likelihood-ratio test for the nested model, one can see that the major improvements in the data description are achieved due R_{had} and then ΔX_{max} modifications.

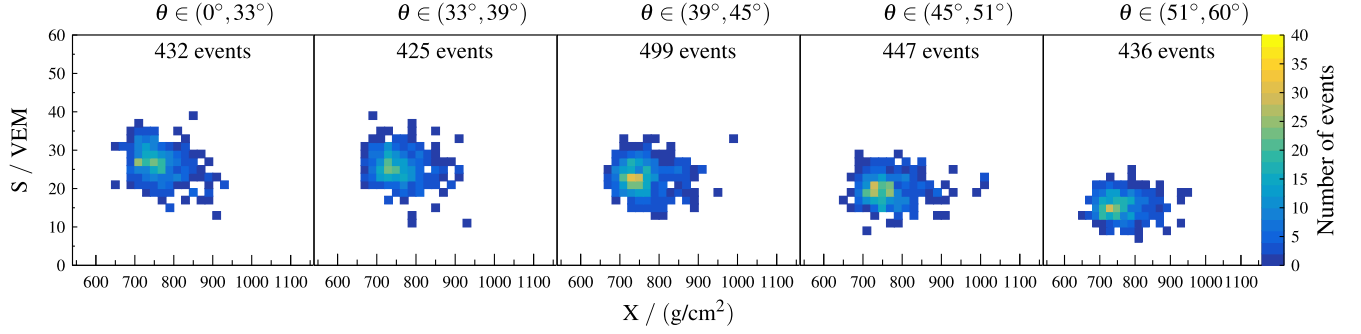


FIG. 4. Distributions of ground signal at 1000 m (S) and depth of shower maximum (X), see Eqs. (1) and (2), for the data of the Pierre Auger Observatory in the energy range $10^{18.5}$ eV to $10^{19.0}$ eV in five zenith-angle bins.

The improvement in the data description due to the introduction of the zenith-angle dependence in R_{had} is statistically significant for QGSJet-II-04, and less significant for SIBYLL 2.3d, with a negligible effect in the case of Epos-LHC.

The measured two-dimensional (S , X) distributions are described acceptably by MC templates modified by $R_{\text{had}}(\theta)$ and ΔX_{max} in all five zenith-angle bins with p -values estimated to be higher than 10% for all three models. These probabilities are obtained from MC-MC tests (see Appendix C) using distributions of values of log-likelihood expression from the fitting of 500 random samples consisting of 2239 simulated showers. Each MC sample had a mass composition and artificially modified X_{max} and $S_{\text{had}}(\theta)$ following the values obtained from the best fits to data. We plot in Fig. 5 projected distributions of X and S (together with plots in the logarithmic scale to stress the consistency also for the tails of distributions) and their zenith-angle dependent correlation using the Gideon-Hollister correlation coefficient [38] for the data and MC templates with the modifications of ($R_{\text{had}}(\theta)$, ΔX_{max}). In this way, we demonstrate that with the modified MC

TABLE II. Evolution of the minimum values of the log-likelihood expression [see Eq. (3)] fitting the data with different modifications of the model predictions. In all cases, except $R_{\text{had}} = \text{const}$ and ΔX_{max} , the significance of improvement of data description with the $R_{\text{had}}(\theta)$ and ΔX_{max} fit is above 5σ using the likelihood-ratio test applying the Wilks' theorem [36] for nested model [37]. In the case of $R_{\text{had}} = \text{const}$ and ΔX_{max} , the improvement of data description with $R_{\text{had}}(\theta)$ and ΔX_{max} fit is $\sim 0.1\sigma$, $\sim 4.4\sigma$, and $\sim 2.0\sigma$ for Epos-LHC, QGSJet-II-04, and SIBYLL 2.3d, respectively.

$\ln \mathcal{L}_{\text{min}}$	Epos-LHC	QGSJet-II-04	SIBYLL 2.3d
None	2022.9	4508.0	2496.5
ΔX_{max}	738.6	1674.8	1015.7
$R_{\text{had}} = \text{const}$	489.2	684.4	521.6
$R_{\text{had}}(\theta)$	489.2	673.9	517.6
$R_{\text{had}} = \text{const}$ and ΔX_{max}	452.2	486.7	454.2
$R_{\text{had}}(\theta)$ and ΔX_{max}	451.9	476.3	451.6

templates, we achieve a consistent simultaneous description of X_{max} , $S(1000)$ and their correlation for the data shown in Fig. 4. The models without modifications or only with the zenith-angle independent modification of R_{had} do not describe the data equivalently well (see Appendix D).

The resulting parameters of the data fits with ($R_{\text{had}}(\theta)$, ΔX_{max}) modifications are presented in Table III. For all three models, a deeper X_{max} scale is favored (see also left panels in Figs. 6 and 7) that would result in heavier primary mass composition derived from the X_{max} data compared to the inferences with nonmodified predictions of the models [10,39]. The modifications ΔX_{max} are such that they reduce the difference in X_{max} scales between the models (see Fig. 10 in Sec. IV) and, as a consequence, similar estimations of the fractions of the primary nuclei can be inferred from the data, see the right panel of Fig. 6.

Due to the shift of the X_{max} predictions deeper in the atmosphere, more shower particles reach the ground producing a few percent larger SD signals compared to the nonmodified models. Therefore, the total increase of S for the modified MC predictions consists of contributions from both ΔX_{max} (~ 0 to 7%) and $R_{\text{had}}(\theta)$ (~ 10 to 16%) as shown in the left panel of Fig. 8. The two effects from the modification of the X_{max} scale—heavier primary mass composition and a larger number of shower particles reaching the ground—lead to the values of $R_{\text{had}}(\theta)$ (Table III) that are smaller than the values previously found for Epos-LHC and QGSJet-II-04 in Ref. [17]. The modified and original S_{had} scales are shown for the three models in the right panel of Fig. 8.

C. Systematic uncertainties

There are four dominant sources of systematic uncertainties in the fitted parameters:

- (i) The uncertainty in the FD energy scale $\pm 14\%$ [22];
- (ii) The uncertainty in the X_{max} measurements $^{+8}_{-9}$ g/cm² [9];
- (iii) The uncertainty in the $S(1000)$ measurements $\pm 5\%$ [7];

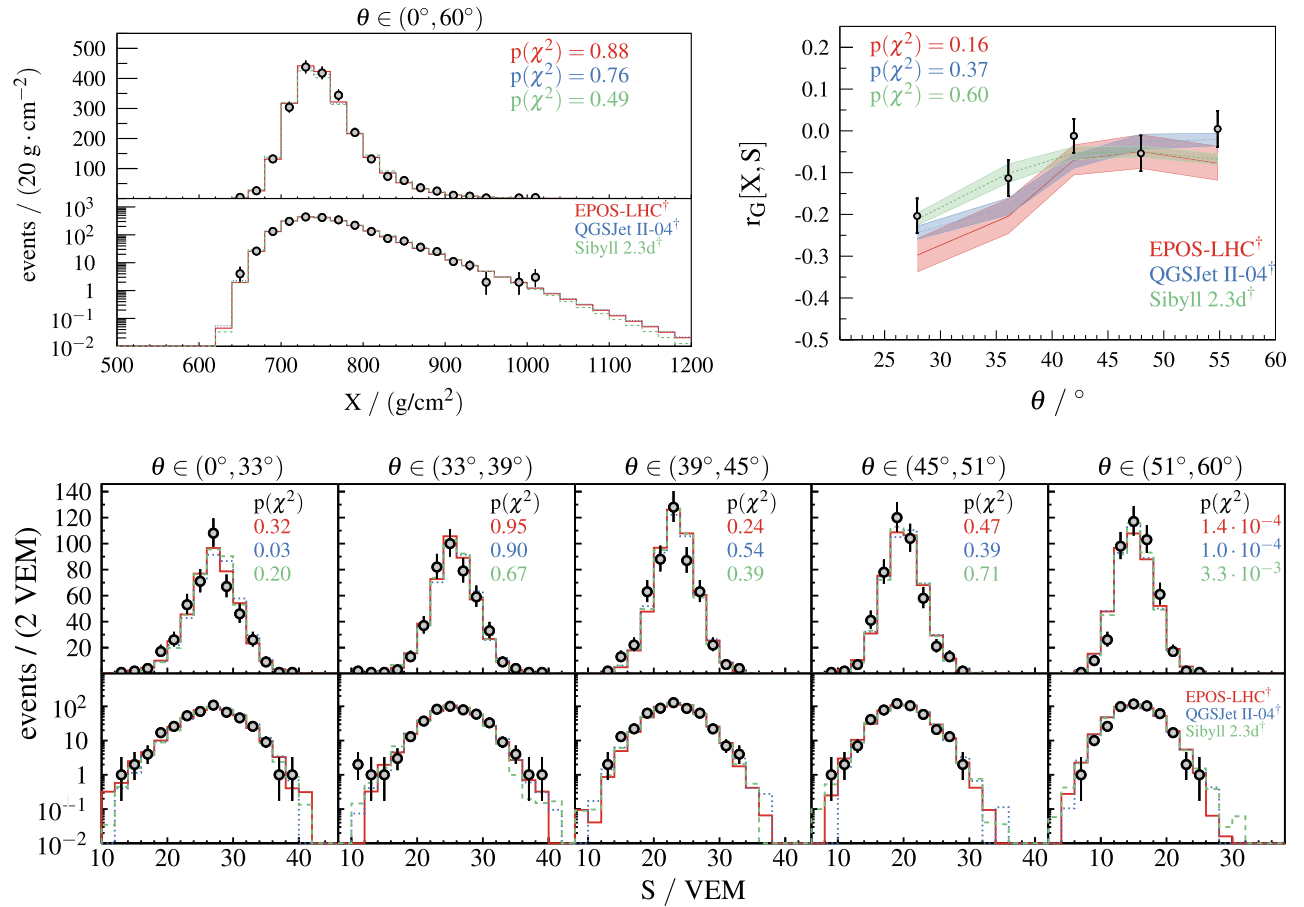


FIG. 5. Distributions of depth of shower maximum (X , top-left) and ground signal at 1000 m (S , bottom), see Eqs. (1) and (2), for the Auger data (points) and for the best fits of (S , X) distributions with $R_{\text{had}}(\theta)$ and ΔX_{max} modifications in predictions of three models (denoted by \dagger as templates were modified from original predictions). In the top-right panel, the dependence of the Gideon-Hollister coefficient of correlation [38] between S and X on the zenith angle is shown. The χ^2 probabilities characterize the compatibility between measurements and MC predictions in the individual plots.

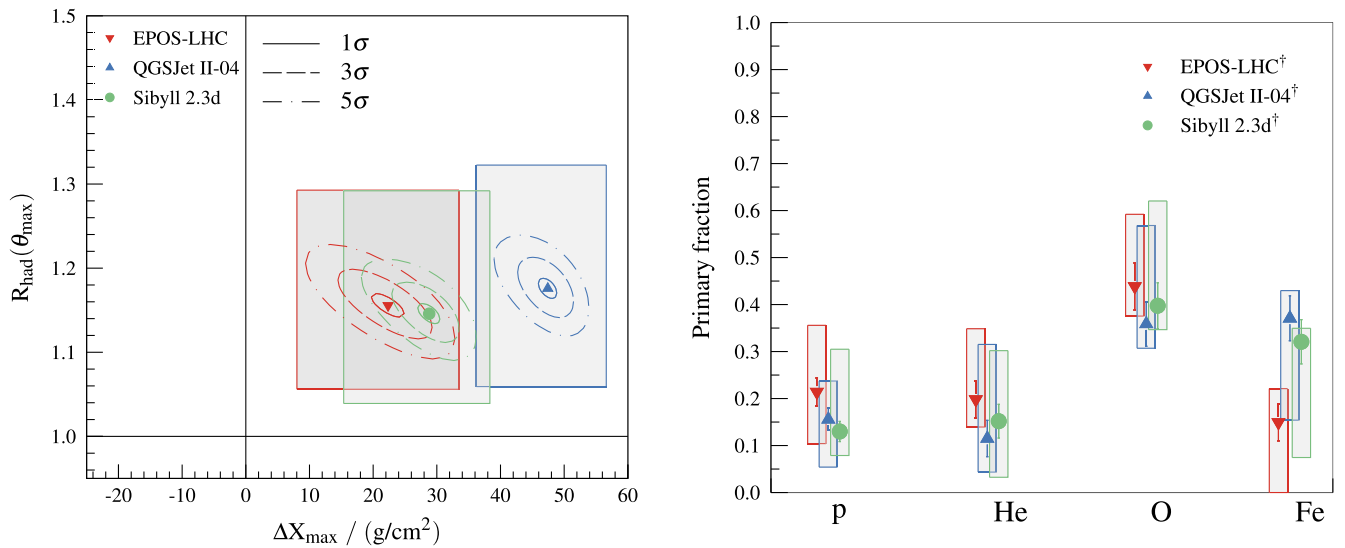


FIG. 6. *Left*: Correlations between ΔX_{max} and $R_{\text{had}}(\theta_{\text{max}} \approx 55^\circ)$ modifications of the model predictions obtained from the data fits. The contours correspond to 1σ , 3σ , and 5σ statistical uncertainties. The gray rectangles are the projections of the total systematic uncertainties. *Right*: The most likely primary fractions of the four components from the data fits using ΔX_{max} and $R_{\text{had}}(\theta)$. The height of the gray bands shows the size of projected total systematic uncertainties.

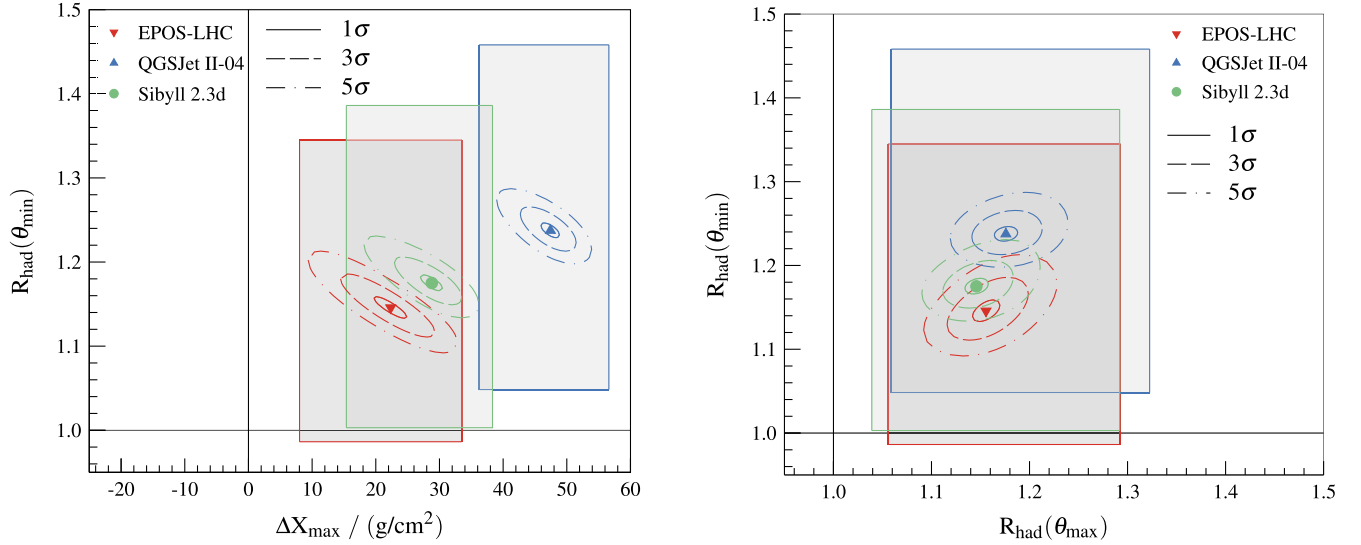


FIG. 7. *Left*: Correlations between ΔX_{\max} and $R_{\text{had}}(\theta_{\min} \approx 28^\circ)$ modifications of the model predictions obtained from the data fits. *Right*: Correlation between $R_{\text{had}}(\theta_{\max} \approx 55^\circ)$ and $R_{\text{had}}(\theta_{\min} \approx 28^\circ)$. The contours correspond to 1σ , 3σ , and 5σ statistical uncertainties. The gray rectangles are the projections of the total systematic uncertainties.

- (iv) The biases of the method estimated from the MC-MC tests (see Appendix B for the results of these tests).

Since the X_{\max} systematic uncertainty is strongly correlated with the modification ΔX_{\max} , its effect on the nuclei fractions is nearly cancelled out by the corresponding change of ΔX_{\max} . In general, the nuclei fractions, and therefore the inferences on the mass composition, are weakly sensitive to all experimental systematic errors due to the simultaneous fitting of ΔX_{\max} and R_{had} in the method. To explore the effect of those systematics, and as a simplifying ansatz, the total systematic uncertainties on the fit parameters are obtained by summing all four contributions in quadrature (see Appendix E for the size of individual contributions).

One can also note, that within systematic errors no significant dependence of R_{had} on the zenith angle was found. The difference between $R_{\text{had}}(\theta_{\min})$ and $R_{\text{had}}(\theta_{\max})$ shows a tight correlation with the uncertainty on the energy scale. However, given all the experimental uncertainties in the case of QGSJet-II-04, the measured data prefers within the method rather flatter attenuation of the hadronic signal at 1000 m than predicted by the model, indicating too hard spectra of muons predicted by this model.

The systematic uncertainties on the parameters B , D , β , used in Eqs. (1) and (2) for the energy correction of S , X , as well as corrections of the long-term performance and other effects related to the operation of the SD and FD, have a negligible contribution to the systematic uncertainties. We could not identify any significant dependencies of the results on the zenith angle or energy in the studied ranges.

D. Significance of improvement in data description

In Fig. 9, the results of our method for ΔX_{\max} and $R_{\text{had}}(\theta)$ applying also all possible combinations of the systematic uncertainties on E_{FD} , X_{\max} , and $S(1000)$ are shown with the full points. These points are located approximately in a plane, contour outlined with a dashed line, due to a correlation between the modification parameters through the mass composition describing the data (see the left panels of Figs. 6 and 7, e.g., increase of ΔX_{\max} leads to a heavier fitted mass composition and consequently to a decrease of R_{had}). The plane is tilted with respect to the $[R_{\text{had}}(\theta_{\min}), R_{\text{had}}(\theta_{\max})]$ plane. It is a consequence of the effect of ΔX_{\max} on the ground signal S at different zenith angles, see Eqs. (B1)–(B5) in Appendix B, and consequently on the fitted $R_{\text{had}}(\theta_{\min})$, $R_{\text{had}}(\theta_{\max})$. The color of

TABLE III. Modifications of the model predictions and primary fractions in the energy range $10^{18.5}$ eV to $10^{19.0}$ eV with statistical and systematic uncertainties for the best data fits and the p -values obtained using MC-MC tests.

	$R_{\text{had}}(\theta_{\min})$	$R_{\text{had}}(\theta_{\max})$	$\Delta X_{\max}/(\text{g}/\text{cm}^2)$	f_p (%)	f_{He} (%)	f_{O} (%)	f_{Fe} (%)	p -value (%)
Epos-LHC	$1.15 \pm 0.01^{+0.20}_{-0.16}$	$1.16 \pm 0.01^{+0.14}_{-0.10}$	$22 \pm 3^{+11}_{-14}$	$21 \pm 3^{+14}_{-11}$	$20 \pm 4^{+15}_{-6}$	$44 \pm 5^{+15}_{-6}$	$15 \pm 4^{+7}_{-15}$	10.6
QGSJet-II-04	$1.24 \pm 0.01^{+0.22}_{-0.19}$	$1.18 \pm 0.01^{+0.15}_{-0.12}$	$47^{+2}_{-1}{}^{+9}_{-11}$	$16 \pm 2^{+8}_{-10}$	$11 \pm 4^{+20}_{-7}$	$36 \pm 5^{+21}_{-5}$	$37 \pm 5^{+6}_{-22}$	19.8
SIBYLL 2.3d	$1.18 \pm 0.01^{+0.21}_{-0.17}$	$1.15 \pm 0.01^{+0.15}_{-0.11}$	$29 \pm 2^{+10}_{-13}$	$13 \pm 2^{+18}_{-5}$	$15 \pm 4^{+15}_{-12}$	$40 \pm 5^{+22}_{-5}$	$32 \pm 5^{+3}_{-25}$	32.6

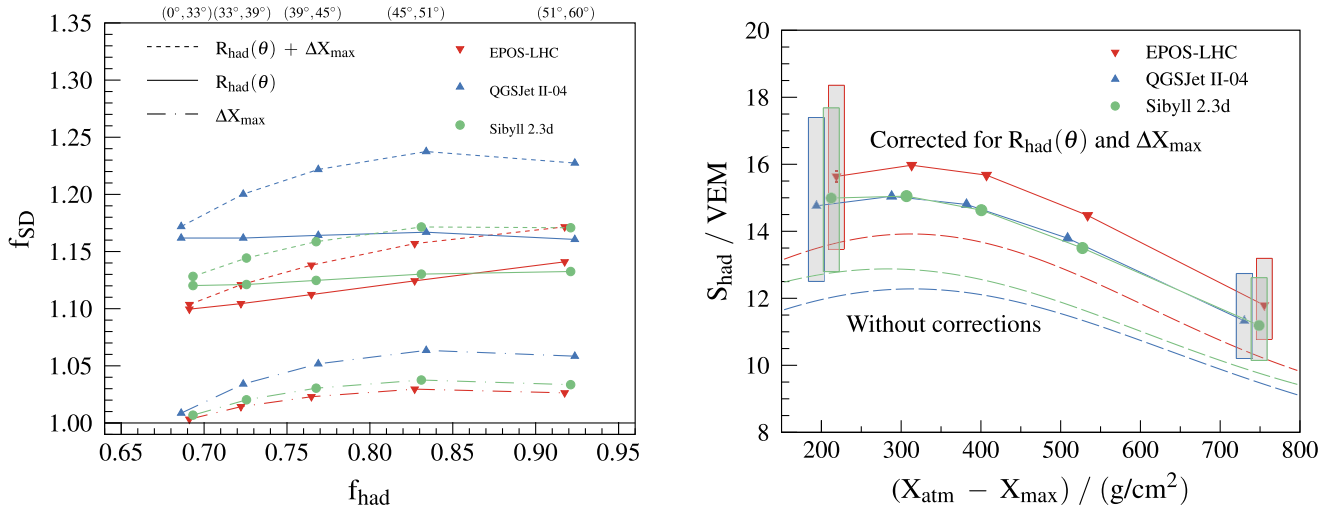


FIG. 8. *Left*: The total rescaling of S (dashed lines) broken down into the contributions from the rescaling of the hadronic signal $R_{had}(\theta)$ (solid lines) and the change of the predicted X_{max} scale (ΔX_{max}) (dash-dotted lines) for different models. *Right*: The dependence of the hadronic signal at 1000 m on the distance of X_{max} to the ground in atmospheric depth units as predicted for proton showers generated using nonmodified models (dashed lines) and accounting for the $R_{had}(\theta)$, ΔX_{max} modifications (solid lines). The height of the gray bands shows the size of projected total systematic uncertainties.

the points corresponds to the difference in fitted log-likelihood expressions ($\Delta \ln \mathcal{L}$) in case of no modifications and in case of the assumed template modifications. The closest approach to the point of no modification is estimated through a dense scan of linear combinations of experimental systematic uncertainties for the lowest values of $\Delta \ln \mathcal{L}$ that are, in some cases, even beyond the range of systematic uncertainties quoted by Auger (see Appendix F

for more details). For all three models, the closest approach of $\Delta \ln \mathcal{L}$ (indicated by a line in Fig. 9 connecting point $[1, 1, 0 \text{ g/cm}^2]$ with the plane) is >19 which is still higher than the value estimated using the Wilks' theorem in the likelihood-ratio test for nested model at the level of 5σ ($\Delta \ln \mathcal{L} \approx 16.62$). This confirms that the modifications of X_{max} and R_{had} scales are not an artifact of the systematic uncertainties of our measurements but a needed change in

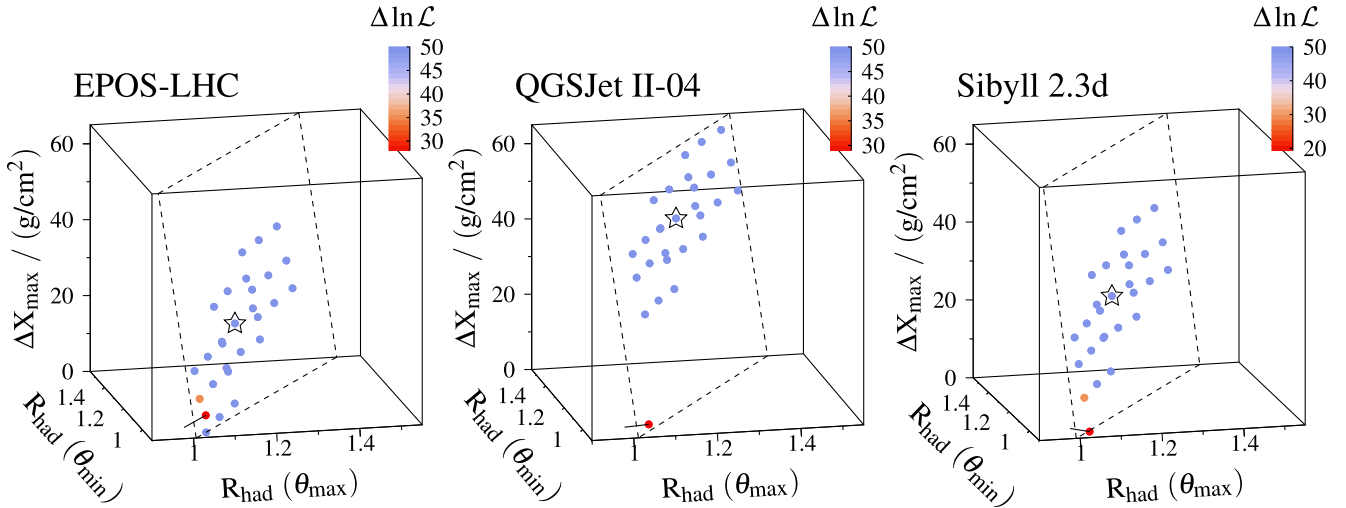


FIG. 9. Values of the modification parameters (points) for all possible combinations of experimental systematic uncertainties on the energy ($\pm 14\%$), X_{max} ($\pm_9^8 \text{ g/cm}^2$), and $S(1000)$ ($\pm 5\%$). The color of the points shows the difference in log-likelihood expressions ($\Delta \ln \mathcal{L}$) in the case of no modifications and in the case of the assumed template modifications, including the differences higher than 50 (note the slightly different scale between models). The results (see Table III) for no systematic shift of the data are highlighted by stars. Dashed lines outline the contour of the plane from the best-fit to the points. The closest approach to the nonmodified ($R_{had}(\theta) = 1$, $\Delta X_{max} = 0 \text{ g/cm}^2$) model predictions using a dense scan of linear combinations of experimental systematic uncertainties is connected with this point by a black line. The animated rotated views are available at [40].

the model descriptions. A correction of the results for the biases seen in the MC-MC tests leads to even larger significance values.

IV. DISCUSSION

A. Implications for inferences on mass composition

One straightforward consequence of the X_{\max} shift deeper in the atmosphere is the solution of the problem with the negative variance of the logarithmic mass $\sigma^2(\ln A)$ derived with QGSJet-II-04 from the measured $\langle X_{\max} \rangle$ and $\sigma(X_{\max})$ (as discussed in Sec. I). After application of the corresponding ΔX_{\max} shifts, one finds $\sigma^2(\ln A) \approx 0.5$ to 2.5 in the energy range $10^{18.5}$ eV to $10^{19.0}$ eV for all models used in this work. These values are consistent with the degree of mixing of the primary composition found in the analysis of the correlation between X_{\max} and $S(1000)$ with nonmodified models, since the correlation analysis relies on the general phenomenology of air showers and this way is weakly sensitive to the uncertainties in the description of hadronic interactions [11,12].

Another outcome of the method can be foreseen by taking into account the quasiuniversal behavior of the X_{\max} elongation rate for all pure beams and models with values staying within 54 g/cm²/decade to 61 g/cm²/decade range. Changing the elongation rate within these limits introduces an energy-dependent uncertainty on the MC X_{\max} scale of about 4 g/cm²/decade at most. Under the assumption that the difference ΔX_{\max} between the models and data remains nearly independent of the primary energy, i.e., that there is no new physics that can significantly change the predictions for the X_{\max} elongation rate of single

primary species, one could speculate that at the highest energies ($E \gtrsim 10^{19.5}$ eV) the Auger X_{\max} measurements, see Fig. 10, can be described with a heavy mass composition having a low degree of mixing due to $\langle X_{\max} \rangle$ and $\sigma(X_{\max})$ staying between the extrapolated predictions of the modified models for oxygen and iron nuclei.

B. Primary species in the cosmic-ray beam

We checked if the shape of the data distribution of ground signal and X_{\max} and its zenith-angle evolution can be fitted better with an artificially reduced range of the masses in the MC templates and thus with different values of $R_{\text{had}}(\theta)$ and ΔX_{\max} . Due to the presence of deep events and $\sigma(X_{\max})$ values close to the predictions for protons in $10^{18.5}$ eV to $10^{19.0}$ eV range, we kept protons in the MC templates and used (p, He, O) and (p, He) mixes for the data fits. In both cases, the quality of data fits was found to be inferior compared to the fits with (p, He, O, Fe) nuclei (see Table IV). This was confirmed by the MC-MC tests and was observed using the fits to the measured data for all three models that the obtained X_{\max} scale decreases by about 5 g/cm² to 7 g/cm², 10 g/cm² to 17 g/cm², and 30 g/cm² to 40 g/cm² and the hadronic signal scale by about 2% to 5% , 4% to 9% , and 15% to 20% when the heaviest primary Fe is replaced by Si, O, and He in the fit, respectively.

For the five-component (p, He, O, Si, Fe) fits, the values of $R_{\text{had}}(\theta)$ and ΔX_{\max} remain well within statistical errors from the values obtained from the (p, He, O, Fe) fits. Though the fractions of silicon and iron nuclei are strongly anticorrelated in such fits, the silicon fraction remains low, $<5\%$.

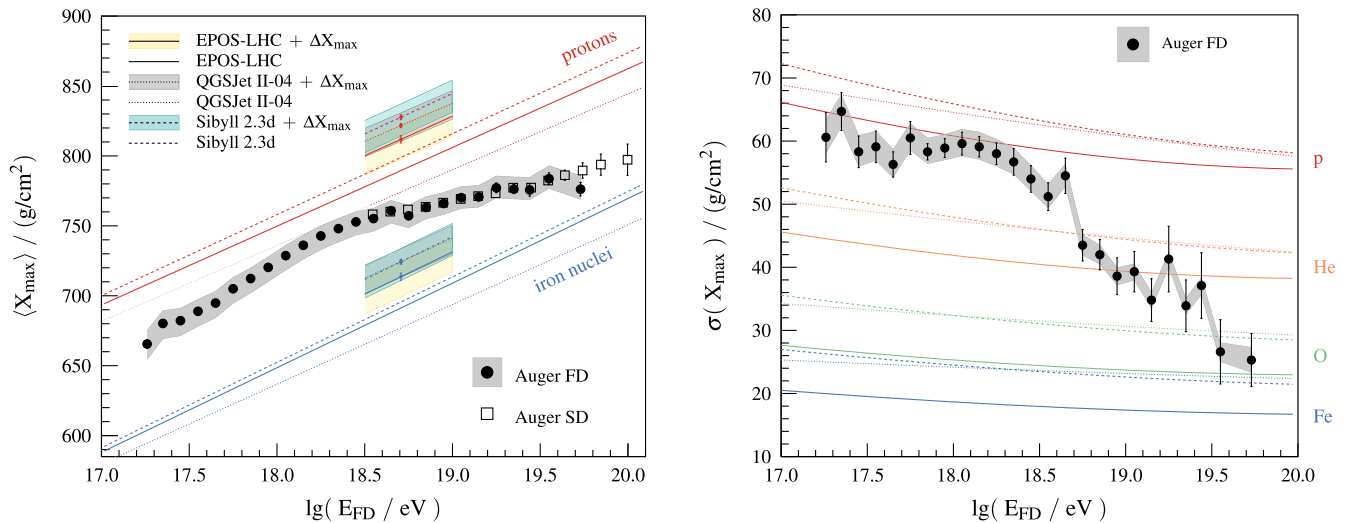


FIG. 10. The energy evolution of the mean (left) and the standard deviation (right) of the X_{\max} distributions measured by the Pierre Auger Observatory using FD [11] (solid circles) and SD [41] (open squares). The results of this paper for the modified X_{\max} scales (left panel) are shown with shaded bands with the heights corresponding to the systematic uncertainties. The original nonmodified model predictions for different primary species are shown with lines for the entire energy range.

TABLE IV. Minimum values of the log-likelihood expression [see Eq. (3)] for different number of primaries assumed to be present in the model predictions. In all cases, the significance of improvement of data description with the $R_{\text{had}}(\theta)$, ΔX_{max} , and p, He, O, Fe fit using the likelihood-ratio test applying the Wilks' theorem for nested model is above 5σ .

$\ln \mathcal{L}_{\text{min}}$	Epos-LHC	QGSJet-II-04	SIBYLL 2.3d
p He	518.3	633.5	563.5
p He O	467.5	523.3	486.6
p He O Fe	451.9	476.3	451.6

C. Modifications of hadronic interactions

Assuming the same modifications of hadronic interaction features as in Ref. [42], the observed increase of the X_{max} scale in MC predictions could be explained by an increase of the elasticity or a decrease of the multiplicity and cross section. A detailed study of the combinations of such modifications at the energy equivalent to this study is ongoing [43].

The elasticity is a very good candidate for a potential source of X_{max} modification because there are no precise data to constrain this in models at high energy. It could be precisely measured only in the region where no detector at the LHC experiments exists. Consequently, the different models have relatively different predictions with large uncertainties.

A reduction of the multiplicity can also increase X_{max} since the available energy is shared between fewer particles leading to higher π^0 energy at the first interaction. But at the same time, the same effect will reduce the energy available for muon production effectively increasing the tension in R_{had} .

The superposition model [44] makes an *ad hoc* modification of p - p cross section that would explain a single change of X_{max} scale for all primaries rather difficult. The change in the case of iron nuclei would correspond to a change of p -air cross section at the energy 56 times smaller, $\sim 9 \times 10^{16}$ eV, which starts to be in tension with the corresponding LHC measurements of p - p collisions [45]. Remarkably, the most recent cross section measurements by the ALFA experiment are lower and more precise [46] than the one used to tune the models, possibly indicating an overestimation of the current cross section of the air-shower simulations.

In the case of the multiplicity and elasticity, we can consider the model of shower development from Ref. [23] also assuming the energy increase of the total multiplicity as $N \propto N_0 E^\alpha$ and a decrease of the elasticity with energy $\kappa \propto \kappa_0 E^{-\omega}$. We see that an *ad hoc* change of the normalization of multiplicity (N_0) or elasticity (κ_0) would modify the X_{max} independently of the primary particle and energy,

$$\begin{aligned}
 X_{\text{max}}^A &= X_1^A + X_0 \ln \frac{\kappa E}{A 2N \xi_c^\pi} \\
 &= X_1^A + X_0 \left[(1 - \alpha - \omega) \ln \frac{E}{A \xi_c^\pi} + \ln \frac{\kappa_0}{N_0} \right], \quad (9)
 \end{aligned}$$

where ξ_c^π is the critical energy of pions at which their decay and interaction lengths are equal.

The hadronic signal can be increased by increasing the multiplicity or decreasing the ratio of neutral pions according to Ref. [42] but, as previously described, an increase in the multiplicity would decrease X_{max} increasing the tension there. A change in the ratios of different hadrons, in particular with more strange particles, is a more likely possible explanation according to recent LHC data [47,48].

The energy spectrum of muons naturally influences the dependence of S_{had} on $X_{\text{atm}} - X_{\text{max}}$. Though the systematic uncertainty of the energy scale limits a significant conclusion deduced from the method [see $R_{\text{had}}(\theta_{\text{min}}) - R_{\text{had}}(\theta_{\text{max}})$ in Appendix E], the QGSJet-II-04 model seems to predict too hard spectra of muons. For instance, a larger fraction of strange particles like kaons in the shower would lead to harder muon spectra because of the larger critical energy (smaller lifetime) of strange particles.

There are of course other possible modifications of hadronic interactions that could influence the observed differences between the predictions from the models and the measured data like cross sections of low-mass mesons, energy spectra of pions etc., (see e.g., Ref. [5]).

D. Limitations of the method

There are remaining differences between the models and, correspondingly, with the data due to various limitations of the method. Though our approach leads to a reduction of the differences between models in $\langle X_{\text{max}} \rangle$, the obtained modifications ΔX_{max} do not cancel out these differences completely. In particular, the modified X_{max} scale for Epos-LHC is shallower compared to QGSJet-II-04 and SIBYLL 2.3d (see the left panel of Fig. 10). We found, that a large part of this difference (~ 10 g/cm²) can be removed if an additional smearing of X_{max} is applied to Epos-LHC showers to compensate for the smaller X_{max} fluctuations predicted by this model in comparison to the other two (possibly partly due to strong defragmentation of nuclei in Epos-LHC [49], as recently confirmed by newer model EPOS-LHCR [50]). The remaining difference of about 5 g/cm² between the models might be due to the statistical errors on ΔX_{max} and differences between the models in the separation of the primary species in $\langle X_{\text{max}} \rangle$.

Possible dependencies of ΔX_{max} , $R_{\text{had}}(\theta)$, and fluctuations of X_{max} and $S(1000)$ on the primary mass are out of the scope of this paper. We checked that adding a linear mass dependence of ΔX_{max} into the method did not improve the fit significantly. The assumption of

a mass-independent ΔX_{\max} used in this paper was mainly motivated by the similar differences in predicted $\langle X_{\max} \rangle$ for different primaries [50]. Such a quasiuniversal difference is a consequence of the very similar energy dependencies of interaction features like multiplicity, elasticity, and cross section assumed in the models [51]. It means that an offset in these features would lead to an approximately mass-independent difference in the X_{\max} predictions. An *ad hoc* modification of the energy dependence of these features, like in [42,43], would lead to mass-dependent X_{\max} shift.

V. CONCLUSIONS

In this paper, we tested the predictions of the models QGSJet-II-04, SIBYLL 2.3d, Epos-LHC regarding the depths of maximum of air-shower profiles X_{\max} and the signal produced by air-shower particles in water-Cherenkov stations at 1000 m from the shower core, $S(1000)$, composed of electromagnetic and hadronic (S_{had}) parts. The test consisted of fitting with MC templates of two-dimensional distributions of $(S(1000), X_{\max})$ measured at the Pierre Auger Observatory and obtaining the scales of X_{\max} and $S_{\text{had}}(\theta)$ predicted by the models, as well as the fractions of four primary nuclei (p, He, O, Fe).

We found that for the best description of the data distributions in the energy range $10^{18.5}$ eV to $10^{19.0}$ eV for $\theta < 60^\circ$ the MC predictions of X_{\max} should be deeper in the atmosphere by about 20 g/cm^2 to 50 g/cm^2 , and the hadronic signal should be increased by about 15% to 25%. These modifications reduce the differences between the models in X_{\max} and $S(1000)$, and as a consequence, lead to smaller uncertainties on the estimated fractions of the primary nuclei. Due to the deeper MC X_{\max} scale and, correspondingly, a heavier mass composition inferred from the data compared with nonmodified models, the scaling factors for the hadronic signal are found to be smaller than in previous estimations not considering any modifications to the MC X_{\max} scales. The statistical significance of the improvement in the data description using the assumed modifications to the MC templates is above 5σ for all three models even accounting for all possible linear combinations of experimental systematic uncertainties. The difference in $R_{\text{had}}(\theta)$ at the two extreme zenith angles implies an indication that softer spectra of muons generated by QGSJet-II-04 in 1000 m from the shower core would describe the Auger data better.

The specific ways to produce the required changes in the models might consist in combinations of modifications of integral (cross section, multiplicity, elasticity, etc.) or differential (secondary particles energy spectra) characteristics of the hadronic interactions as discussed e.g., in Refs. [5,42,43]. Our method addresses only the first-order differences in the mean values of X_{\max} and hadronic signal without taking into account their possible dependencies on the primary mass or energy. These dependencies, as well as the investigation of a modification of fluctuations of

air-shower observables, need to be studied further to corroborate the scale adjustments found in this paper, supplemented also by future data with increased mass-sensitivity from AugerPrime [52], the upgrade of the Pierre Auger Observatory.

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Appendix A: PARAMETRIZATION OF MC TEMPLATES

The MC templates of the two-dimensional distributions of (S, X) normalized by the total number of simulated showers N_{MC} and weighted to correspond to the measured energy spectrum are fitted using the following function:

$$\begin{aligned} \Phi &= \frac{dN}{N_{MC}dXdS} \\ &= A_{Gauss}A_{Gumbel}f_{Gumbel}(X)f_{Gauss}(X, S). \end{aligned} \quad (A1)$$

The X_{max} part is described by the generalized Gumbel distribution [53],

$$f_{Gumbel}(X) = \exp[-\lambda(x - \exp x)], \quad (A2)$$

where $x = (X - m)/s$ and the ground-signal part is assumed to follow the Gaussian distribution with the mean value linearly dependent on X

TABLE V. Parameters of MC templates for air showers generated with model Epos-LHC and initiated by a primary particle i , see Eq. (A1).

i	θ	f_{had}	$m/(g/cm^2)$	$s/(g/cm^2)$	λ	$p/(VEM/(g/cm^2))$	q/VEM	r/VEM
p	(0°, 33°)	0.64	757	49	1.2	-1.6×10^{-2}	3.10	34.3
p	(33°, 39°)	0.67	755	44	1.1	-3×10^{-3}	2.85	22.9
p	(39°, 45°)	0.71	755	43	8.9×10^{-1}	6.7×10^{-3}	2.88	13.8
p	(45°, 51°)	0.77	754	47	9.8×10^{-1}	1.2×10^{-2}	2.83	6.3
p	(51°, 60°)	0.88	757	53	1.3	1.1×10^{-2}	2.68	3.0
He	(0°, 33°)	0.67	741	51	2.1	-2.7×10^{-3}	2.78	25.3
He	(33°, 39°)	0.70	739	49	2.0	7.7×10^{-3}	2.60	16.1
He	(39°, 45°)	0.75	742	61	2.6	1.7×10^{-2}	2.47	7.2
He	(45°, 51°)	0.81	741	57	2.5	1.7×10^{-2}	2.55	3.5
He	(51°, 60°)	0.91	739	64	2.7	1.3×10^{-2}	2.50	2.6
O	(0°, 33°)	0.71	714	63	5.7	-1.6×10^{-3}	2.61	26.2
O	(33°, 39°)	0.74	714	65	5.4	8.8×10^{-3}	2.45	16.9
O	(39°, 45°)	0.78	714	66	5.5	1.9×10^{-2}	2.41	6.8
O	(45°, 51°)	0.84	711	48	2.9	2.2×10^{-2}	2.37	1.8
O	(51°, 60°)	0.93	714	82	7.5	1.7×10^{-2}	2.33	1.0
Fe	(0°, 33°)	0.74	688	76	13.2	1.4×10^{-2}	2.65	17.4
Fe	(33°, 39°)	0.77	688	100	19.4	1.3×10^{-2}	2.62	15.7
Fe	(39°, 45°)	0.81	687	81	13.4	1.4×10^{-2}	2.51	11.9
Fe	(45°, 51°)	0.87	688	134	32.7	1.8×10^{-2}	2.41	6.2
Fe	(51°, 60°)	0.94	687	176	48.1	1.3×10^{-2}	2.34	4.9

TABLE VI. Same as in Table V, but for model QGSJet-II-04.

i	θ	f_{had}	$m/(\text{g}/\text{cm}^2)$	$s/(\text{g}/\text{cm}^2)$	λ	$p/(\text{VEM}/(\text{g}/\text{cm}^2))$	q/VEM	r/VEM
p	(0°, 33°)	0.62	741	49	1.1	-1×10^{-2}	2.67	27.6
p	(33°, 39°)	0.65	748	70	1.9	1.1×10^{-3}	2.53	18.0
p	(39°, 45°)	0.69	743	56	1.3	1.2×10^{-2}	2.54	8.0
p	(45°, 51°)	0.76	739	47	9.5×10^{-1}	1.6×10^{-2}	2.51	2.2
p	(51°, 60°)	0.88	737	50	1.0	1×10^{-2}	2.35	2.7
He	(0°, 33°)	0.65	727	68	2.7	3.3×10^{-3}	2.49	19.0
He	(33°, 39°)	0.69	729	88	4.7	1.2×10^{-2}	2.35	11.0
He	(39°, 45°)	0.74	727	74	3.1	1.8×10^{-2}	2.38	4.5
He	(45°, 51°)	0.80	725	60	2.3	2×10^{-2}	2.20	4.6×10^{-1}
He	(51°, 60°)	0.91	724	74	3.0	1.1×10^{-2}	2.21	3.2
O	(0°, 33°)	0.69	700	99	9.5	1.1×10^{-2}	2.40	15.1
O	(33°, 39°)	0.73	702	87	6.6	1.5×10^{-2}	2.38	10.9
O	(39°, 45°)	0.77	702	91	7.5	2.1×10^{-2}	2.27	4.0
O	(45°, 51°)	0.84	704	102	8.0	2.1×10^{-2}	2.22	8.4×10^{-1}
O	(51°, 60°)	0.93	701	84	5.6	1.5×10^{-2}	2.15	1.8
Fe	(0°, 33°)	0.72	675	68	6.7	1.6×10^{-2}	2.41	13.9
Fe	(33°, 39°)	0.76	676	77	8.2	2.1×10^{-2}	2.37	8.2
Fe	(39°, 45°)	0.81	676	91	11.9	2.2×10^{-2}	2.37	4.7
Fe	(45°, 51°)	0.87	675	87	10.7	1.6×10^{-2}	2.24	6.4
Fe	(51°, 60°)	0.94	675	162	31.6	1.1×10^{-2}	2.19	5.6

$$f_{\text{Gauss}}(X, S) = \exp\left[-\frac{y^2}{2r^2}\right], \quad (\text{A3})$$

$$A_{\text{Gauss}} = \frac{1}{\sqrt{2\pi}r} \quad \text{and} \quad A_{\text{Gumbel}} = \frac{\lambda^\lambda}{s\Gamma(\lambda)}, \quad (\text{A4})$$

where $y = S - pX - q$. The normalization terms are given by

where Γ is the gamma function. The six free parameters in each of the MC template fits are m , s , λ of the generalized

TABLE VII. Same as in Table V, but for model SIBYLL 2.3d.

i	θ	f_{had}	$m/(\text{g}/\text{cm}^2)$	$s/(\text{g}/\text{cm}^2)$	λ	$p/(\text{VEM}/(\text{g}/\text{cm}^2))$	q/VEM	r/VEM
p	0°–33°	0.63	769	70	2.1	-9×10^{-3}	2.97	27.7
p	33°–39°	0.65	771	68	1.8	7.8×10^{-4}	2.96	19.0
p	39°–45°	0.69	772	71	2.0	1.1×10^{-2}	2.84	9.0
p	45°–51°	0.76	766	62	1.5	1.4×10^{-2}	2.73	4.4
p	51°–60°	0.87	766	52	1.1	9.2×10^{-3}	2.77	4.0
He	0°–33°	0.66	747	56	2.2	-1.3×10^{-3}	2.68	23.3
He	33°–39°	0.69	745	50	1.8	1×10^{-2}	2.55	13.1
He	39°–45°	0.73	742	54	1.8	1.6×10^{-2}	2.51	6.8
He	45°–51°	0.80	744	58	2.1	2×10^{-2}	2.41	7.7×10^{-1}
He	51°–60°	0.90	743	58	2.1	1.5×10^{-2}	2.41	6×10^{-1}
O	0°–33°	0.70	715	48 2.3	8.2×10^{-3}	2.44	18.1	
O	33°–39°	0.73	716	65	4.3	1.6×10^{-2}	2.41	10.8
O	39°–45°	0.77	716	62	3.6	2.1×10^{-2}	2.36	4.9
O	45°–51°	0.84	717	57	3.0	1.8×10^{-2}	2.26	3.8
O	51°–60°	0.93	717	67	3.9	1.5×10^{-2}	2.25	1.8
Fe	0°–33°	0.73	688	60	5.6	1.4×10^{-2}	2.61	16.2
Fe	33°–39°	0.77	690	62	5.8	2.2×10^{-2}	2.40	8.6
Fe	39°–45°	0.81	690	60	5.5	2.3×10^{-2}	2.40	5.5
Fe	45°–51°	0.87	690	97	12.1	2×10^{-2}	2.35	3.8
Fe	51°–60°	0.94	690	96	11.8	1.9×10^{-2}	2.24	8.7×10^{-1}

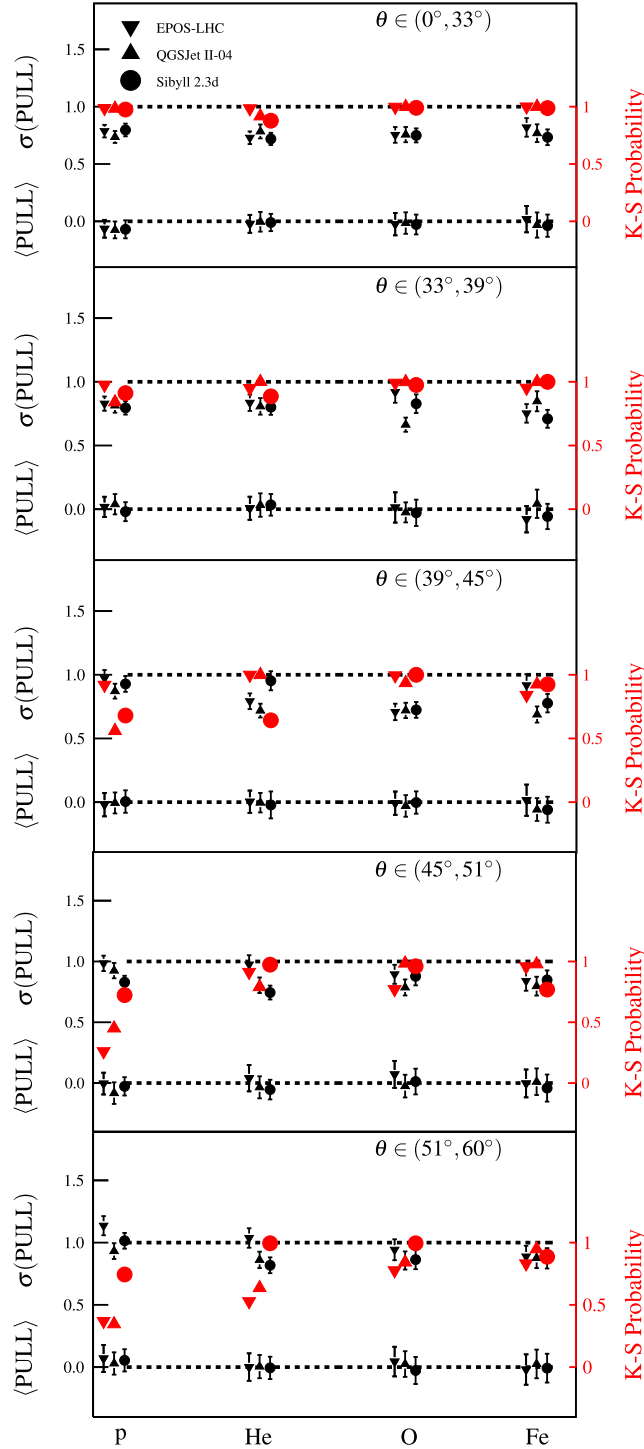


FIG. 11. The mean and the standard deviation of the MC distribution of $\text{PULL} = (N_{\text{fit}} - N_{\text{mc}}) / \sqrt{N_{\text{mc}}}$ where N_{fit} is the value of the fitted function Eq. (A1) and N_{mc} is the value for each bin of the two-dimensional MC distribution (S, X) . The probability of consistency between the parametrized function and MC distribution (red) is tested with the two-dimensional Kolmogorov-Smirnov (K-S) test. $E = 10^{18.5}$ eV to $10^{19.0}$ eV.

Gumbel distribution, and p, q, r of the Gaussian part. These fitted parameters for the three models used in this work are listed in Tables V–VII.

In Fig. 11, we show the mean and the standard deviation of the pull distribution for the description of each bin of the two-dimensional distribution (S, X) , see examples in Fig. 1, by the fits with a function Eq. (A1). The goodness of the description of the MC templates with these fits is also tested with the two-dimensional Kolmogorov-Smirnov test [54] demonstrating very good consistency between the MC templates and MC distributions of (S, X) .

Appendix B: PARAMETRIZATION OF ATTENUATION OF GROUND SIGNALS

The electromagnetic and hadronic signals at 1000 m were corrected for the energy evolution as $S_{\text{em}}^{\text{ref}} = S_{\text{em}}(E^{\text{ref}}/E_{\text{FD}})$ and $S_{\text{had}}^{\text{ref}} = S_{\text{had}}(E^{\text{ref}}/E_{\text{FD}})^{1/\beta}$. The dependence of these average signals on the distance of X_{max} to the ground in atmospheric depth units, $t = X_{\text{atm}}(\theta) - X_{\text{max}}$, see Fig. 2, was parametrized with the Gaisser-Hillas function [55] allowing its vertical offset,

$$\langle S_{\alpha}^{\text{ref}} \rangle(t) = S_{\alpha}^0 \left(\frac{t - t_{\alpha}}{u_{\alpha} - t_{\alpha}} \right)^{Z(t_{\alpha})} \exp(Z(t)) + w_{\alpha}, \quad (\text{B1})$$

where $\alpha = \text{had}$ or em , and normalization scaling $Z(x) = (u_{\alpha} - x)/v_{\alpha}$. t_{α} is the value of $X_{\text{atm}}(\theta) - X_{\text{max}}$ where the function reaches its maximum, u_{α} and v_{α} are parameters without a straightforward physics interpretation, and S_{α}^0, w_{α} are the rescale and offset parameters, respectively. The fitted parameters are listed in Tables VIII and IX for em and hadronic signal, respectively.

The factor $g_{\text{em},k}$ reflecting the average change of em signal due to the change of X_{max} scale for a mix of primary species i with relative fractions f_i in zenith-angle bin k is calculated as

$$g_{\text{em},k} = \sum_i f_i \frac{S_{\text{em}}(\langle t \rangle_k - \Delta X_{\text{max}})}{S_{\text{em}}(\langle t \rangle_k)}, \quad (\text{B2})$$

where $\langle t \rangle_k$ is the average measured $X_{\text{atm}}(\theta) - X_{\text{max}}$ in a zenith-angle bin k : ~ 241.2 g/cm², ~ 335.5 g/cm², ~ 429.4 g/cm², ~ 556.1 g/cm², ~ 777.6 g/cm², for respective increasing average values of the zenith angle. The factor g_{had} for the hadronic signal is obtained as

$$g_{\text{had},k} = \sum_i f_i \frac{S_{\text{had}}(\langle t \rangle_k - \Delta X_{\text{max}}) R_{\text{had}}(\langle t \rangle_k - \Delta X_{\text{max}})}{S_{\text{had}}(\langle t \rangle_k) R_{\text{had}}(\langle t \rangle_k)}, \quad (\text{B3})$$

where

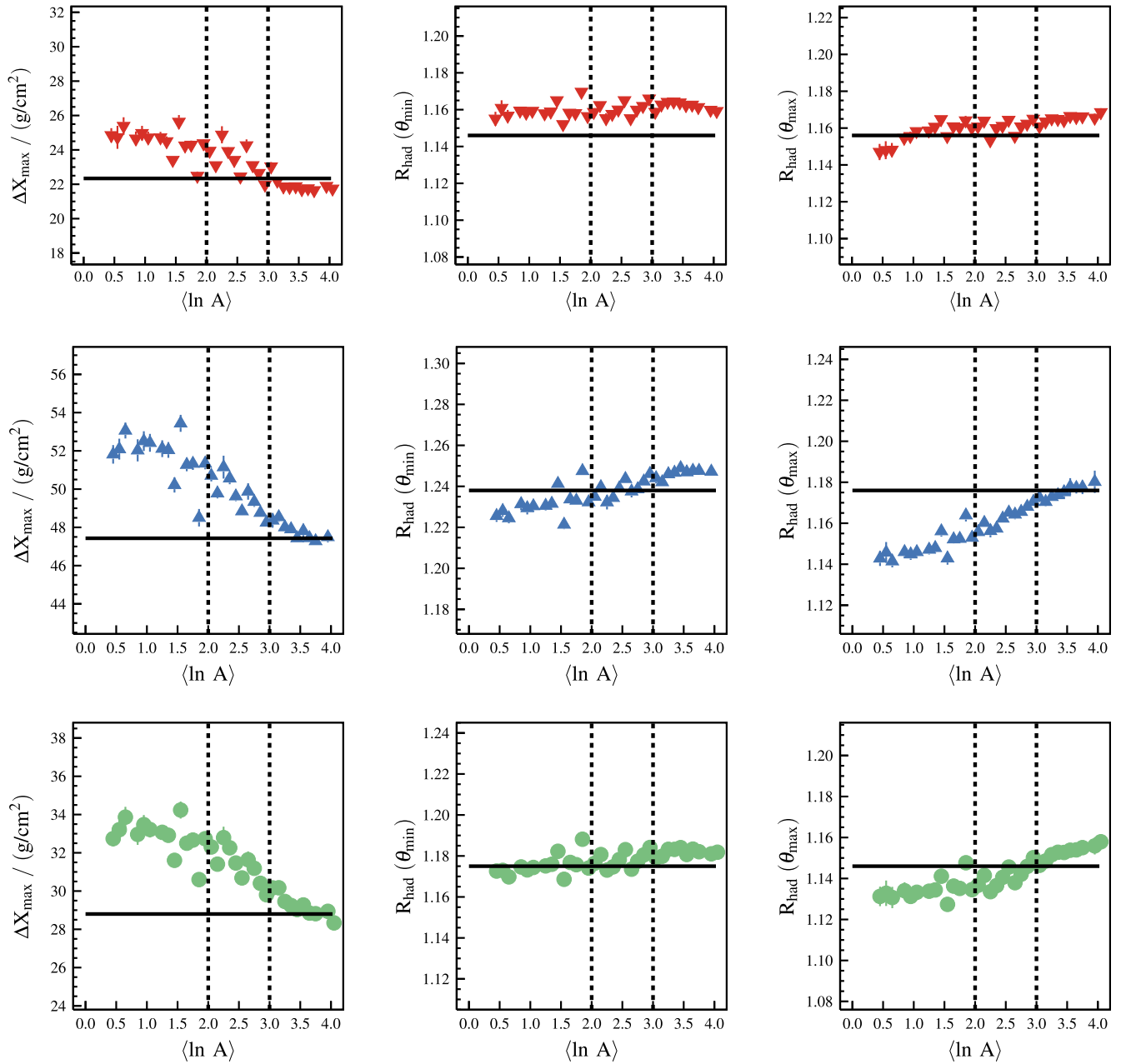


FIG. 12. The values of modification parameters found by the method (points) in the MC samples with artificially modified ΔX_{\max} and $R_{\text{had}}(\theta)$. The values of artificial modifications, shown with solid horizontal lines, are applied to each simulated shower individually. The MC samples contain all possible combinations of primary nuclei with 0.1 steps in relative fractions, iron nuclei are present in all samples (relative fraction ≥ 0.1), and the mean logarithmic masses of the samples are marked on horizontal axis. Hadronic interaction models used in the tests: Epos-LHC (top row, red), QGSJet-II-04 (middle row, blue), SIBYLL 2.3d (bottom row, green). The systematic uncertainties are taken as the maximum biases within the $\langle \ln A \rangle = 2$ to 3 range indicated with dashed lines.

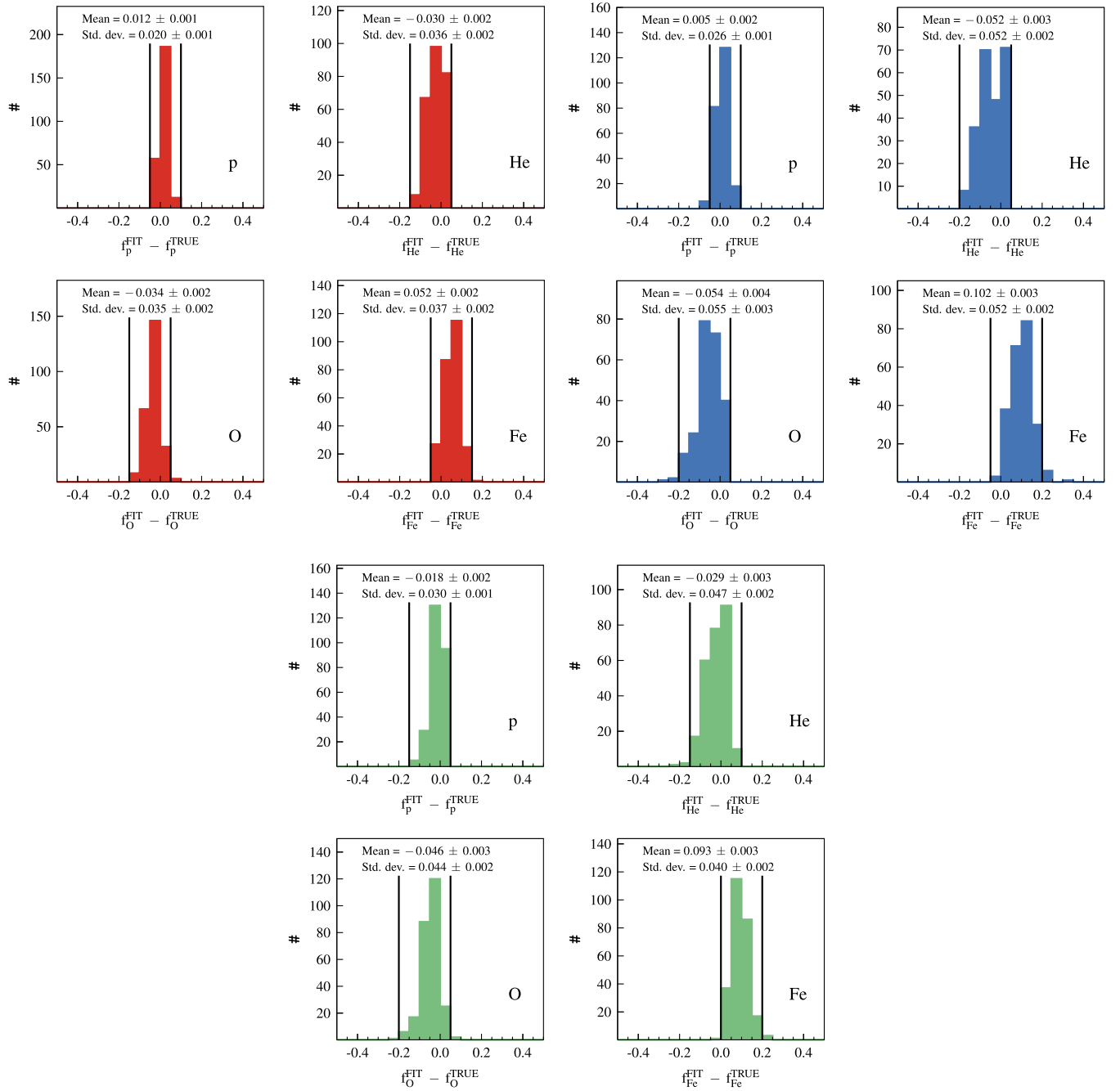


FIG. 13. Biases of the method on the (p, He, O, Fe) fractions for the MC samples with artificially modified ΔX_{\max} and $R_{\text{had}}(\theta)$ as described in Fig. 12. Additionally, we select the fitted relative fractions with $0.0 \leq f_p^{\text{FIT}} \leq 0.4$, $0.0 \leq f_{\text{He}}^{\text{FIT}} \leq 0.3$, $0.2 \leq f_{\text{O}}^{\text{FIT}} \leq 0.6$, and $0.0 \leq f_{\text{Fe}}^{\text{FIT}} \leq 0.5$ which correspond to the ranges obtained by the data fits. The range considered as a contribution to the systematic uncertainty is indicated by vertical lines. Hadronic interaction models used in the tests; Epos-LHC (top left, red), QGSJet-II-04 (top-right, blue), SIBYLL 2.3d (bottom, green).

$$R_{\text{had}}(\theta) \equiv R_{\text{had}}(\langle t \rangle_k) = R_{\text{had}}(\theta_{\text{min}}) + \quad (\text{B4})$$

$$+ (R_{\text{had}}(\theta_{\text{max}}) - R_{\text{had}}(\theta_{\text{min}})) \frac{\langle t \rangle_k - \langle t \rangle_{\text{min}}}{\langle t \rangle_{\text{max}} - \langle t \rangle_{\text{min}}}, \quad (\text{B5})$$

for $\langle t \rangle_{\text{min}}$ and $\langle t \rangle_{\text{max}}$ corresponding to minimum and maximum zenith-angle bins, respectively.

Appendix C: MC-MC TESTS OF THE METHOD

To evaluate the precision and reliability of the method, we performed tests on the MC simulations with artificially modified predictions on the event-by-event basis using the shift ΔX_{max} and the factors $R_{\text{had}}(\theta_{\text{min}})$, $R_{\text{had}}(\theta_{\text{max}})$ obtained from the fits to the measured data, see Table III.

For each model, all possible mixes of (p, He, O, Fe) with relative fractions changing in 0.1 steps are used to estimate the biases on modification parameters as a function of

mean logarithmic mass of the primary beam $\langle \ln A \rangle$. In the tests, we use only the composition mixes containing primary iron nuclei, as there can be additional biases stemming from the assumption on the presence of different species in the primary beam, see discussion in Sec. IV B. For each composition mix, five different samples of simulated showers are randomly selected with the same number of events as in the data ($N = 2239$) and following the shape of the measured energy spectrum. The biases of the method for each composition mix are calculated as an average over the biases for these five random sets. The results of the MC-MC tests are summarized in Fig. 12. We find that for $2 < \langle \ln A \rangle < 3$, the range of the masses inferred from the data analysis (Sec. III B), the maximum overestimation of the fitted X_{max} scale with the method is 5 g/cm^2 , and biases on the fitted $\langle S_{\text{had}} \rangle$ scale are within 3%. These resulting values of these MC–MC tests are considered as systematic uncertainties of the method on the modification parameters, see Fig. 16. The systematic

TABLE VIII. Fitted parameters of functional dependence of the average em signal part of $S(1000)$ vs distance of X_{max} to the ground in atmospheric depth units for air showers initiated by a primary particle i , see Eq. (B1).

	i	$S_{\text{em}}^0/\text{VEM}$	$t_{\text{em}}/(\text{g/cm}^2)$	$u_{\text{em}}/(\text{g/cm}^2)$	$v_{\text{em}}/(\text{g/cm}^2)$	w_{em}/VEM
Epos-LHC	p	7.58	−1,638	172	42	1×10^{-1}
Epos-LHC	He	7.76	−580	179	81	6×10^{-2}
Epos-LHC	O	7.83	−1,412	161	48	9×10^{-2}
Epos-LHC	Fe	7.64	−407	204	86	7×10^{-2}
QGSJet-II-04	p	7.56	−2,006	175	35	1×10^{-1}
QGSJet-II-04	He	7.71	−495	183	87	3×10^{-2}
QGSJet-II-04	O	7.77	−763	167	72	7×10^{-2}
QGSJet-II-04	Fe	7.52	−278	206	103	2×10^{-3}
SIBYLL 2.3d	p	7.57	−1,152	176	53	1×10^{-1}
SIBYLL 2.3d	He	7.62	−490	185	88	3×10^{-2}
SIBYLL 2.3d	O	7.54	−665	187	73	6×10^{-2}
SIBYLL 2.3d	Fe	7.74	−1,892	152	39	9×10^{-2}

TABLE IX. Same as in Table VIII, but for the average hadronic-signal part of $S(1000)$.

	i	$S_{\text{had}}^0/\text{VEM}$	$t_{\text{had}}/(\text{g/cm}^2)$	$u_{\text{had}}/(\text{g/cm}^2)$	$v_{\text{had}}/(\text{g/cm}^2)$	$w_{\text{had}}/\text{VEM}$
Epos-LHC	p	5.6	−9,999	312	9	8.3
Epos-LHC	He	7.2	−9,419	232	16	8.4
Epos-LHC	O	9.0	−1,298	228	98	8.7
Epos-LHC	Fe	10.7	−8,304	171	24	9.6
QGSJet-II-04	p	5.1	−1,880	314	47	7.2
QGSJet-II-04	He	7.2	−300	255	222	6.8
QGSJet-II-04	O	7.2	−4,934	205	34	8.7
QGSJet-II-04	Fe	9.6	−1,614	166	115	8.7
SIBYLL 2.3d	p	4.8	−8,519	283	11	8.1
SIBYLL 2.3d	He	6.7	−3,557	225	44	8.0
SIBYLL 2.3d	O	8.4	−1,521	207	100	8.4
SIBYLL 2.3d	Fe	8.9	−5,078	194	35	10.1

uncertainties of the method on the primary fractions are within $\pm 20\%$, which corresponds to the maximum bias of the method on the fractions inferred from $\sim 90\%$ of the studied MC samples, see Fig. 13.

The performance of the method [20] is compatible with these estimations of systematic uncertainties also for a test when one of the models is used for the analysis of the MC samples prepared with other models. This is in agreement with the expectations that the main differences in MC templates between the models are due to the differences in X_{\max} and S_{had} scales. Finally, we checked that the number of zenith-angle bins does not affect the

results unless it is too small (2 bins are not enough to disentangle the hadronic and em parts of the ground signal) or too large (> 10) when the event statistics per zenith-angle bin becomes too low.

Appendix D: DATA DESCRIPTION USING FITS WITH LESS FREEDOM IN MC TEMPLATES

The description of Auger data using fits without any modification to MC templates and with zenith-angle independent R_{had} are shown in Figs. 14 and 15, respectively.

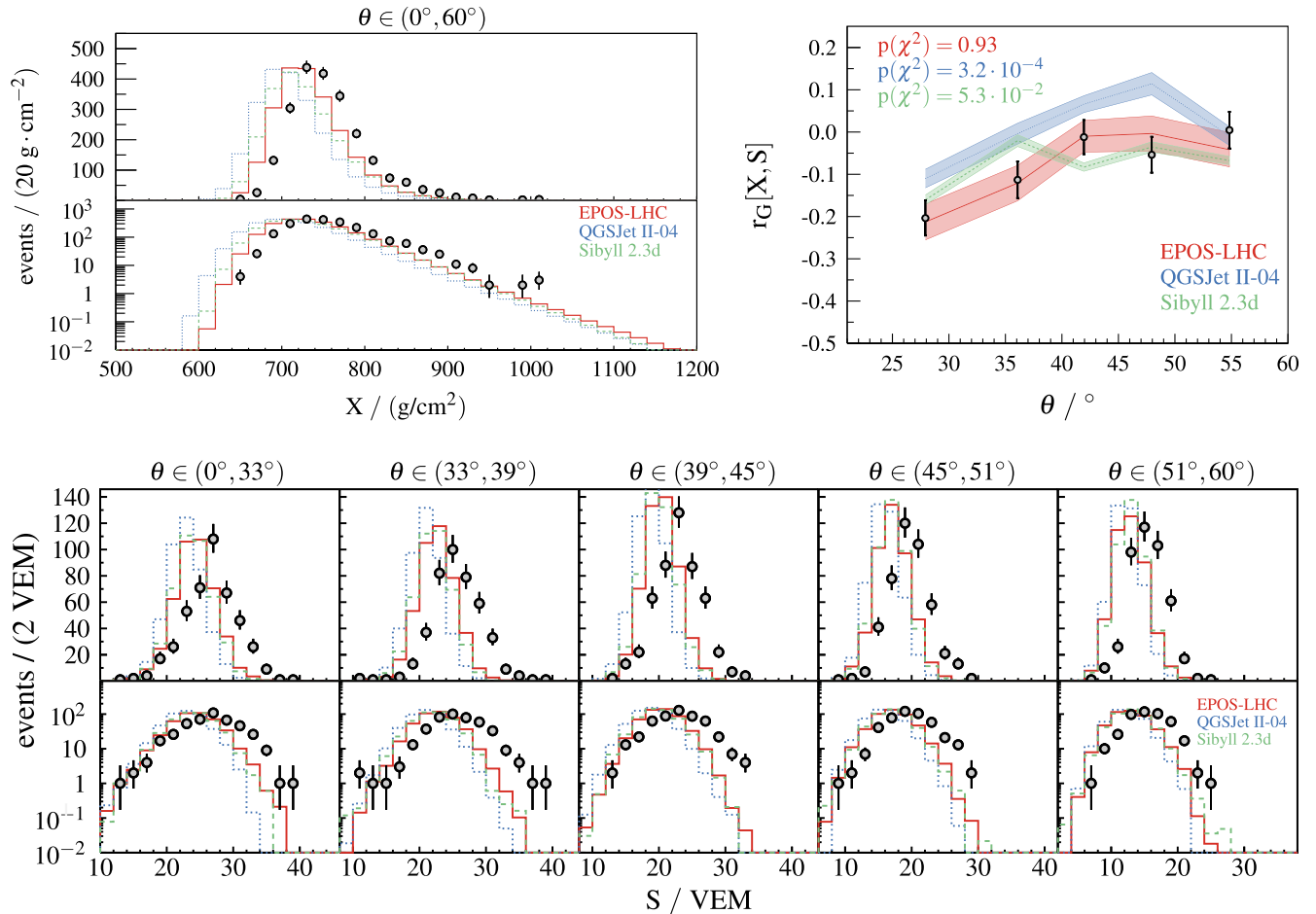


FIG. 14. Same as in Fig. 5, but for the data fits performed without any modification of the predictions of models.

Appendix E: SYSTEMATIC UNCERTAINTIES

The individual contributions to the total systematic uncertainties are plotted in Fig. 16.

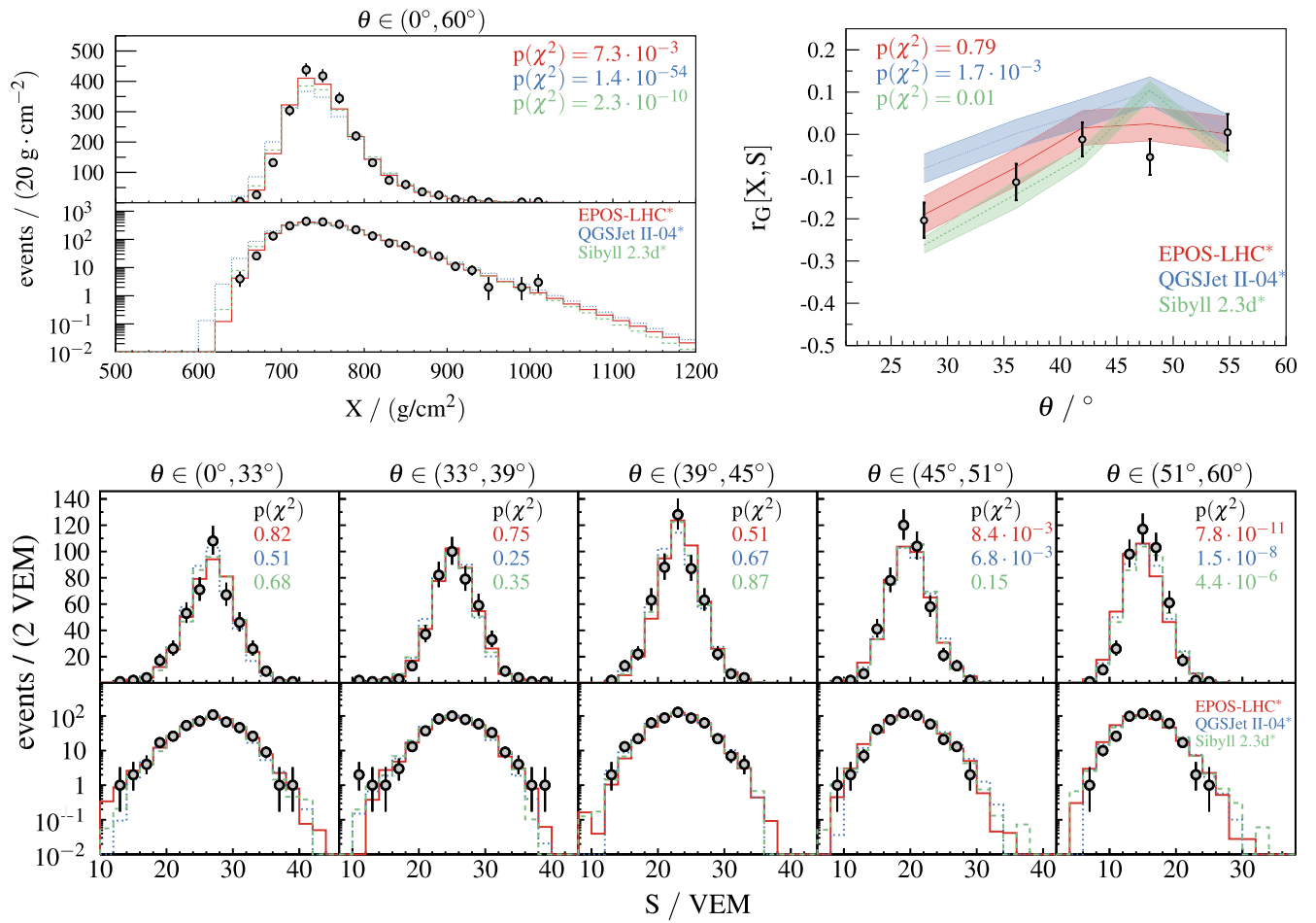


FIG. 15. Same as in Fig. 5, but for the data fits performed with only zenith-angle independent modification R_{had} of the predictions of models (denoted by * as templates were modified from the original predictions).

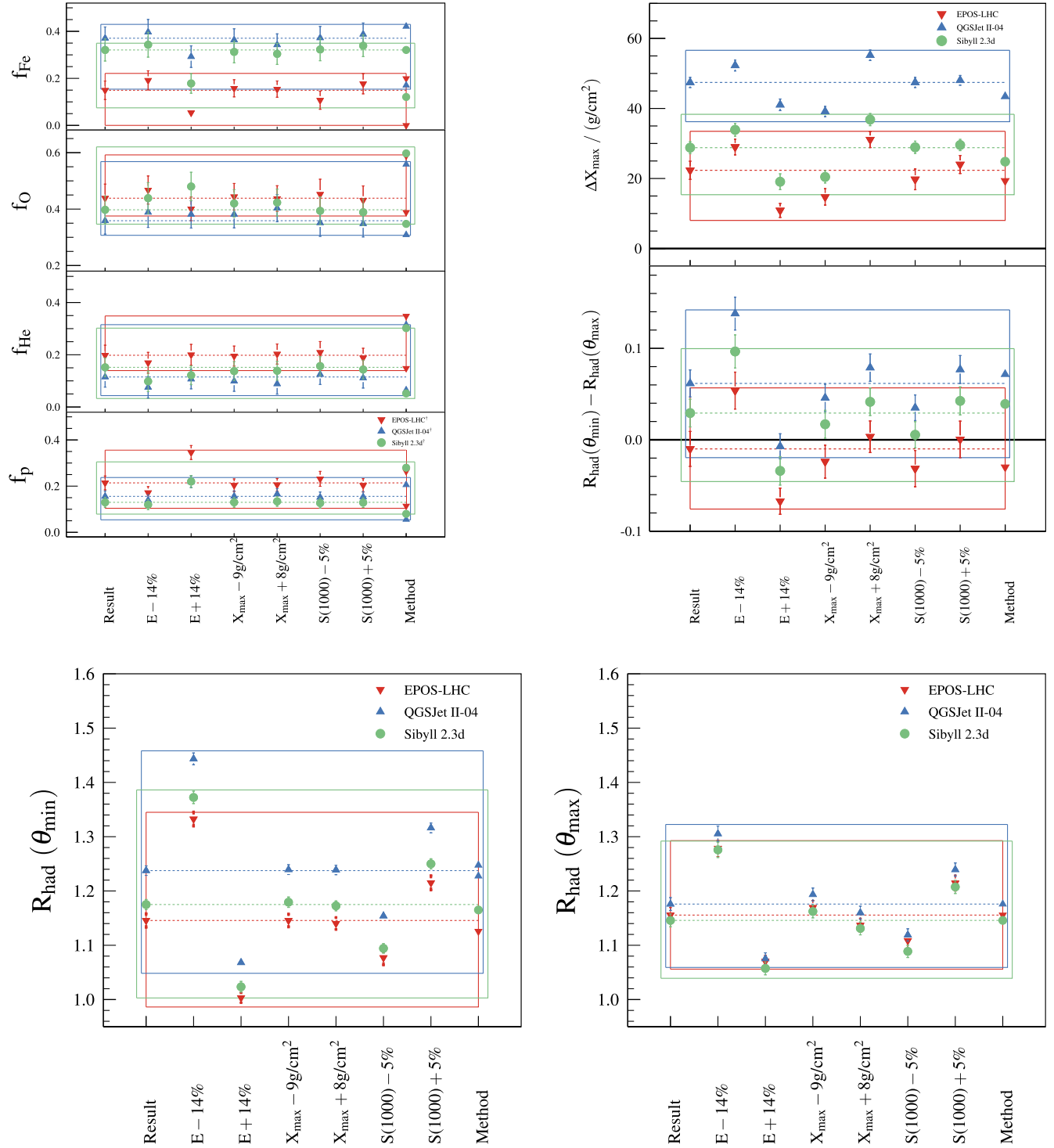


FIG. 16. Contributions of individual experimental systematic uncertainties on energy, X_{max} , $S(1000)$ and of the method biases inferred from the MC–MC tests (see Appendix B) to the total systematic uncertainties on fractions of primary nuclei (top left), ΔX_{max} (top right), $R_{had}(\theta)$ (bottom) and zenith-angle difference of R_{had} (top right). Colored bands are the total systematic uncertainties obtained by summing individual contributions in quadrature with the best-fit results indicated by dashed horizontal lines.

Appendix F: SCAN FOR THE LINEAR COMBINATIONS OF EXPERIMENTAL SYSTEMATIC UNCERTAINTIES MOST FAVORABLE FOR THE MODELS

In Fig. 17, the histogram of difference in log-likelihood expressions ($\Delta \ln \mathcal{L}$) for fits using nonmodified and ΔX_{\max} , $R_{\text{had}}(\theta)$ modifications is shown for dense scans in linear combinations of experimental systematic uncertainties.

The ranges of these uncertainties were selected in a way to estimate the closest approach to the nonmodified value ($R_{\text{had}}(\theta) = 1$, $\Delta X_{\max} = 0 \text{ g/cm}^2$) even for cases when the uncertainties were out of the range of uncertainties quoted by Auger. It was not possible to find such a linear combination of experimental systematic uncertainties that would decrease the significance of improvement in data description below 5σ .

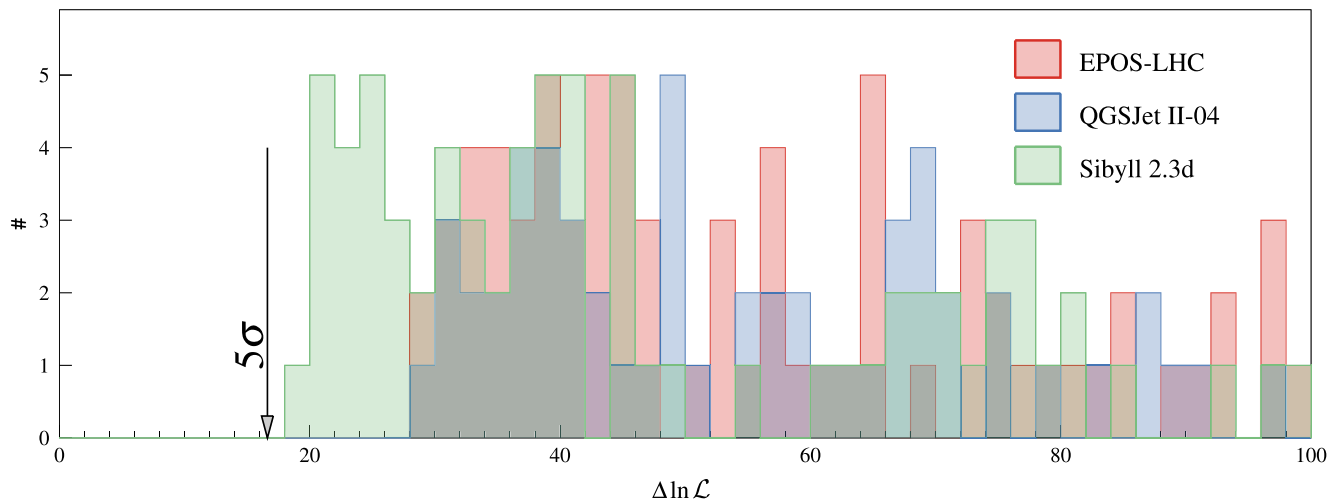


FIG. 17. Number of scans in linear combinations of experimental systematic uncertainties for fits using modifications ΔX_{\max} and $R_{\text{had}}(\theta)$ to estimate the closest approach to the point ($R_{\text{had}}(\theta) = 1$, $\Delta X_{\max} = 0 \text{ g/cm}^2$) from fits with nonmodified MC templates in the difference of log-likelihood $\Delta \ln \mathcal{L}$. The value estimated using Wilks' theorem in the likelihood-ratio test for the nested model at the level of 5σ ($\Delta \ln \mathcal{L} \approx 16.62$) is indicated by the arrow.

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