

Charm multiplicity distribution in high energy pp collisions with PYTHIA

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With the growth of statistics in the future experiments at the LHC, the number of events with charm production will increase substantially. It may become possible to measure the multiplicity distribution of charm particles. Using PYTHIA-8, we generated charm multiplicity distributions in pp collisions for different pseudorapidity ranges ($|\eta| < 0.5, 1.0, 2.0, 3.0$) and center-of-mass energies ($\sqrt{s} = 0.9, 2.36, 2.76, 7.0, 8.0, 13.0$ TeV). We investigated the role played by multiple parton interactions and color reconnection. We compared the multiplicity distribution of D mesons with the charm quark multiplicity distribution. We observe that the “quark-hadron” duality hypothesis is satisfied. With the obtained distributions, we tested the validity of the Koba-Nielsen-Olesen scaling. We also parametrized the charm distributions considering the Poisson distribution and negative binomial distributions.

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I. INTRODUCTION

In recent years, a large amount of data on multiplicity distributions, especially of charged particles, has been collected and made available by various experimental collaborations [1–7]. Several phenomenological studies addressing these data are also available in the literature [8–18]. Particle multiplicity is a global observable that enables the characterization of events in colliding systems. The multiplicity distribution can provide information about the dynamics of hadronic interactions at high energies and the formation of new states of matter. Analyzing this observable, we can look for qualitative changes in the reaction dynamics.

One of the expected changes is a transition between the soft and hard regimes of quantum chromodynamics (QCD). Another one is the onset of parton saturation and the formation of the color glass condensate (CGC) [19]. Finally, in ultracentral collisions we may have the formation of quark-gluon plasma (QGP) [20]. In the absence of QGP, in high-energy proton-proton (pp) collisions,

particles can be produced mainly in the following ways: (i) in an early stage of the collision, a perturbative parton cascade process occurs, governed by QCD evolution equations [21], such as the BFKL and the DGLAP equations, which determine how the parton distribution evolves with increasing collision energy and with the squared four-momentum of the probe; (ii) during the collisions inelastic parton-parton collisions may produce new partons; (iii) in the late stage of the collision partons hadronize, and there is additional particle production. At increasing energies, we expect to observe the dominance of the first way and eventually, the emergence of saturation.

The production of heavy quark-antiquark pairs comes from hard parton-parton scatterings that occur at the early stages of high energy hadronic collisions. The production cross section can be calculated with perturbative QCD (pQCD). The production of multiple heavy quark pairs in the same event raises new questions concerning the nature of the emitting source. The charm multiplicity distribution can help in answering these questions and improve our understanding about the production mechanism.

The increased luminosity and detector upgrades achieved during the Run-3 of the LHC, particularly in the ALICE experiment, significantly improved the sensitivity to charm production in proton-proton collisions [22]. These advances allow detailed studies of charm yields and correlations as a function of event activity, as well as the extraction of moments of the charm multiplicity distribution.

In view of the forthcoming data, we would like to know what to expect. So far, to the best of our knowledge, there is

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no model for the multiplicity distribution of charmed particles formed in pp collisions. In this situation, a natural first step is to use the most successful model of particle production to obtain a baseline estimate. The most well known model is PYTHIA [23,24].

In this work, we use the PYTHIA-8 event simulator to make the first prediction of charm multiplicity distributions, computed at different center-of-mass energies and different pseudorapidity windows. We compare these distributions with the charged particle distributions. In addition, we investigate the Koba-Nielsen-Olesen (KNO) scaling properties [25] of the obtained distributions and fit them to Poisson distributions, to single negative binomial distribution (NBD), as well as to the weighted sum of two NBDs.

The text is organized as follows: in Sec. II, we briefly introduce the PYTHIA event generator; in Sec. III, we present the charm multiplicity distributions and compare them with the charged particle distributions; in Sec. IV, we discuss KNO scaling in the obtained distributions; in Sec. V, we present the parametrization of the distributions with Poisson and NBD fits; we conclude by summarizing the main results.

II. PYTHIA EVENT GENERATOR

PYTHIA is an event generator designed to simulate particle collisions at high energies. An event is the outcome of a complete simulation of a collision (from the initial instant of interaction to the final state with detectable particles). Each event yields a list of particles with their momenta, energies, masses, and generation history. PYTHIA simulates the interaction between two particles by considering a sequence of steps that model the main phenomena of high-energy particle physics: hard processes, parton showers from the initial and final states, multiple interactions of the partons, and hadronization and decays.

Proton-proton collisions involve multiple perturbative scattering processes between the incident partons, which are implemented within the multiparton interactions (MPI) framework [26,27].

The perturbative scattering processes are accompanied by initial-state radiation and final-state radiation. Finally, PYTHIA uses the Lund string fragmentation model [28] to implement hadronization, where the created partons and the beam remnants are connected by strings (color flux tubes). When the partons move away, the strings break generating light quark-antiquark pairs. When we consider color reconnection [29], the strings are reorganized, reducing their total length, allowing partons of different PIs to connect with each other. Because many particles are produced by string breaking, this reduction implies a reduction in the total multiplicity.

The results presented in this work are obtained from simulations using PYTHIA version 8.313. We generated 20 million events at different center-of-mass energies

($\sqrt{s} = 0.9, 2.36, 2.76, 7.0, 8.0, 13$ TeV) and in different pseudorapidity windows ($|\eta| < 0.5, 1.0, 2.0, 3.0$). For the charm simulations, we considered the individual quark and antiquark counts without the effects of hadronization. In other words, we count the number of charm (and anti-charm) quarks present in a stage immediately preceding the hadronization phase. For comparison, we also looked at the charm after the hadronization process, counting the number of D mesons that form at this stage. For the simulations of D mesons (stable and likely to reach the detector), we considered the sum of the production of well-established charmed D mesons ($D^+, D^0, D^{*+}, D^{*0}, D_2^{*+}, D_2^{*0}, D_s^+, D_s^{*+}, D_{s2}^{*+}$) and their counterparts, disregarding the count of those that could originate from decays.

We emphasize that, in spite of its successes, PYTHIA is a model and not a first-principles calculation. Before applying it to charm multiplicity distributions, we computed the charm production cross section, $\sigma_{c\bar{c}}$, as a function of the center of mass energy. Since PYTHIA uses leading order partonic cross sections, we would expect that $\sigma_{c\bar{c}}$ would need a correction factor. Indeed, as shown in Fig. 1, if a correction factor of 3.5 is used, we find a good agreement with the experimentally measured cross sections. More than the absolute value, what is important for us is the correct energy dependence, which seems to be captured by PYTHIA. This is crucial specially for the discussion of KNO scaling. As shown in [11,30], KNO scaling can be understood from perturbative QCD.

In PYTHIA, the bulk of charm production takes place in multiple parton-parton scatterings, typically $gg \rightarrow c\bar{c}$. Since these scatterings are independent from each other [27], the multiplicity distribution of charm pairs should, in principle, be approximately a Poisson distribution. However, in practice, PYTHIA introduces corrections which distort the

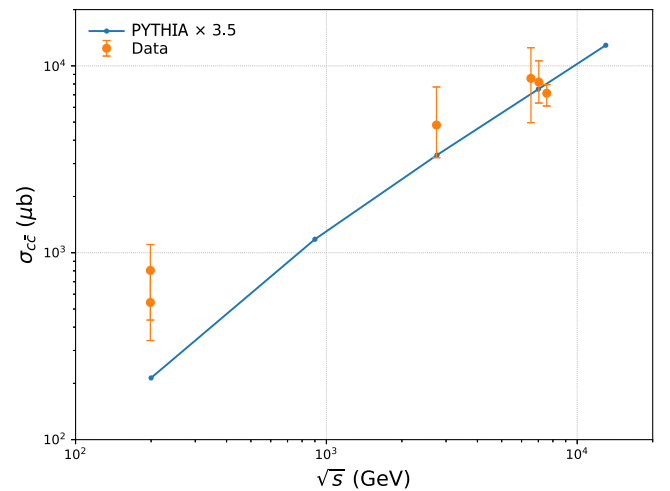


FIG. 1. Total inclusive charm production cross section as a function of the center-of-mass energy. The PYTHIA simulation is compared with data from different experimental collaborations [31–36].

Poisson distribution [37–39]. They are (i) energy-momentum conservation, which implies that later interactions have a reduced phase space. This reduces large n configurations; (ii) PDF rescaling: partons already used are removed from the PDFs, which are “depleted.” This alone, breaks the independence of different scatterings; (iii) impact parameter fluctuations: while for a fixed impact parameter, $P(n)$, might approach the Poisson limit, the final averaging over impact parameter will distort $P(n)$ making it closer to a negative binomial distribution (NBD); (iv) initial state radiation (ISR) and final state radiation (FSR) come together with MPI. These are parton showering processes which change the pure scattering picture and hence, distort the corresponding Poisson distribution; (v) color reconnection (CR): without CR each MPI contributes roughly independently to particle production, the multiplicity is roughly proportional to the number of MPIs and follows a distribution close to Poisson/NBD expectations. Introducing color reconnection, strings from different MPIs merge and the effective number of independent

particle sources is reduced. This leads to the suppression of the high-multiplicity tail.

III. CHARM MULTIPLICITY DISTRIBUTION

In Fig. 2, we present the D meson multiplicity distributions for pp collisions, where each panel shows results for different center-of-mass energies ($\sqrt{s} = 0.9, 2.76, 7.0, 13.0$ TeV) with a comparison between several pseudorapidity ranges ($|\eta| < 0.5, 1.0, 2.0, 3.0$). We can see that: the distributions reach a maximum at the beginning of the curve and then drop several orders of magnitude; the slope of the drop decreases slightly with increasing center-of-mass energy, and similarly, with increasing pseudorapidity window; at small values of N the curves approximately overlap; for large N , the difference between the curves becomes evident. As expected, the number of charm particles increases with increasing center-of-mass energy and with the pseudorapidity range considered. These observations are very similar to what one might find in

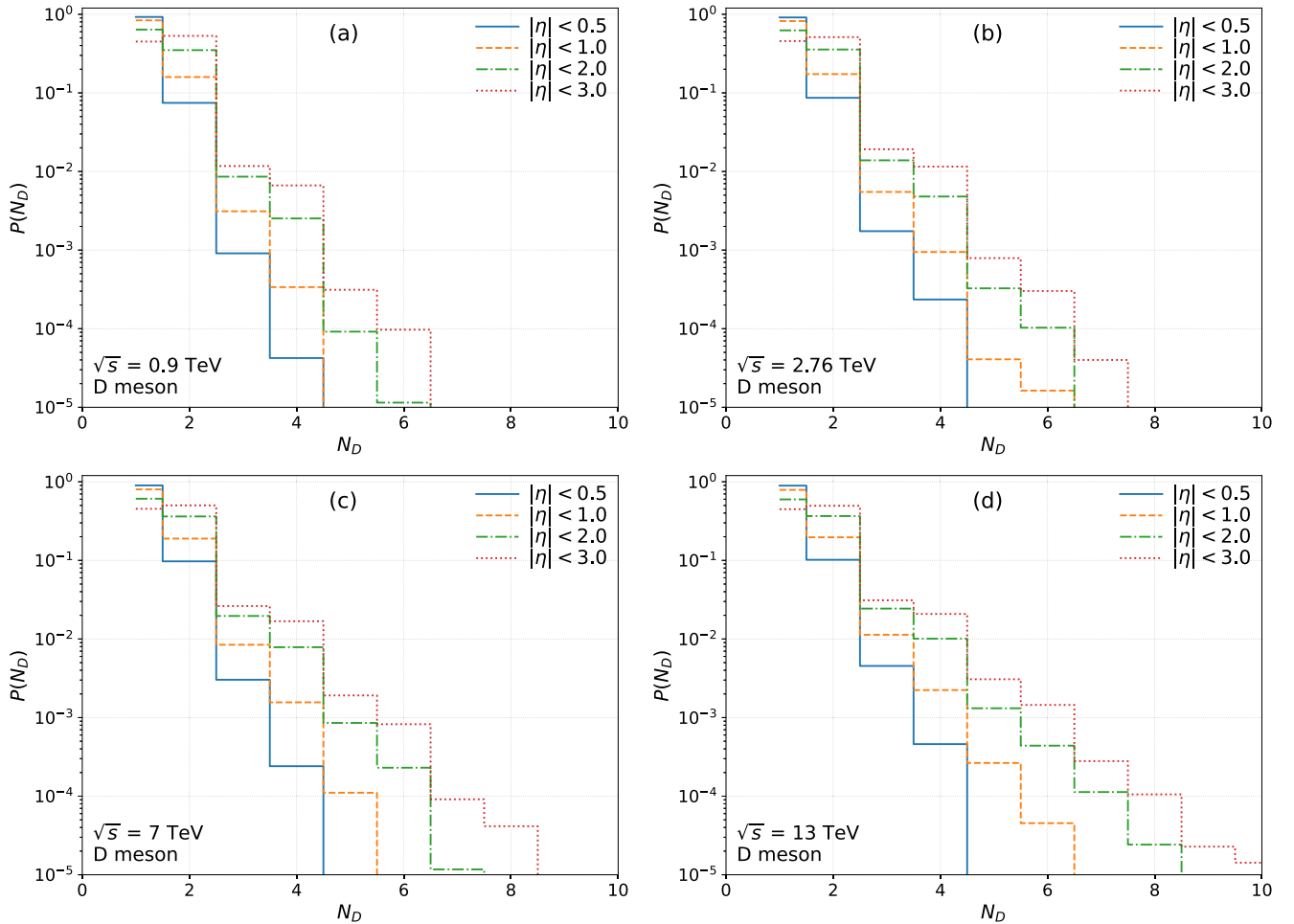


FIG. 2. D meson (hadronic level) multiplicity distribution: comparison of different pseudorapidity range ($|\eta| < 0.5, 1.0, 2.0, 3.0$). We show results for (a) $\sqrt{s} = 0.9$ TeV, (b) $\sqrt{s} = 2.76$ TeV, (c) $\sqrt{s} = 7$ TeV, and (d) $\sqrt{s} = 13$ TeV.

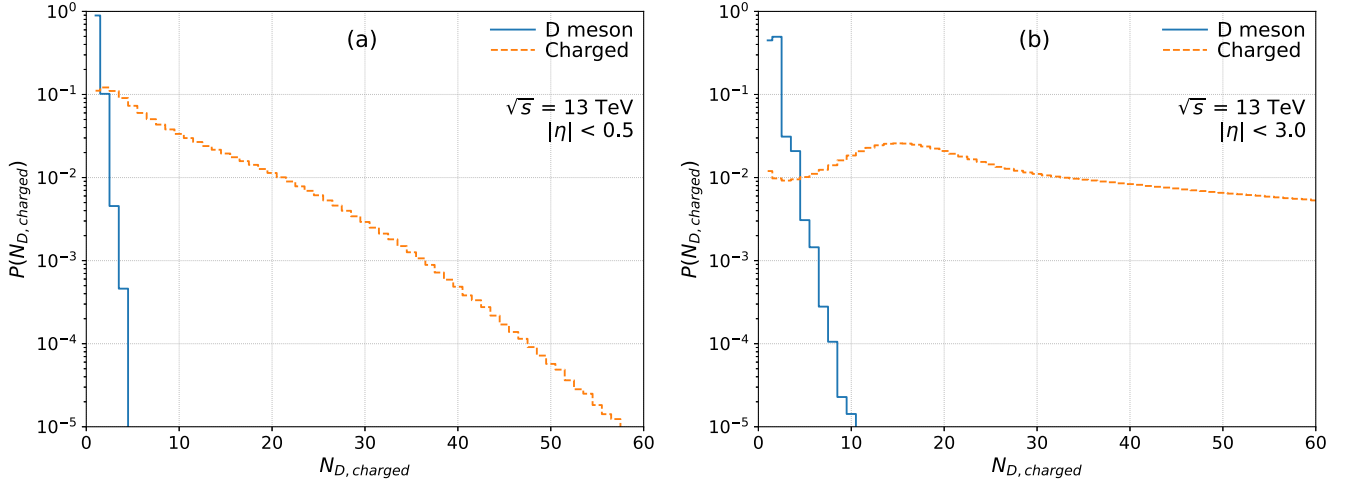


FIG. 3. Comparison between D meson and charged particle multiplicity distributions in pp collisions at 13 TeV. Panel (a) shows results for $|\eta| < 0.5$ and panel (b) for $|\eta| < 3.0$.

an analysis of the multiplicity of charged particles. The difference is in the magnitude since charged particles are produced more abundantly than charm quarks, as shown in Fig. 3.

In Fig. 3, we show the comparison between charm and charged particle distributions measured in pp collisions at 13 TeV. Panel (a) shows results for $|\eta| < 0.5$ and panel (b) for $|\eta| < 3.0$. As previously mentioned, charm quark multiplicities follow distributions that decrease sharply and are much narrower than those of charged particles. This happens because of the nature of the production process, i.e., the multiple independent parton-parton scatterings mentioned above. Besides, charged particles are produced in large numbers whereas charm production is relatively rare, and therefore, the charm multiplicity spectrum is much narrower than that of charged particles. We can also

see that the difference between the quantities increases as the pseudorapidity considered increases.

The partonic level charm distribution projects mostly onto D mesons. This implies that the shape of the partonic charm multiplicity distribution will be similar to that of D mesons, with an almost one-to-one conversion, as shown in Fig. 4. According to the so-called parton-hadron duality hypothesis, the partonic and hadronic multiplicity distributions should be approximately the same. In fact, this was shown [8] to be the case for charged particles measured in jets.

Using the charm multiplicity distribution, we can calculate the average multiplicity $\langle n_D \rangle$, which is shown in Fig. 5(a) as a function of the energy $\sqrt{s}$. An interesting feature of this figure is that $\langle n_D \rangle$ grows slowly with the energy and at the same rate for all the pseudorapidity

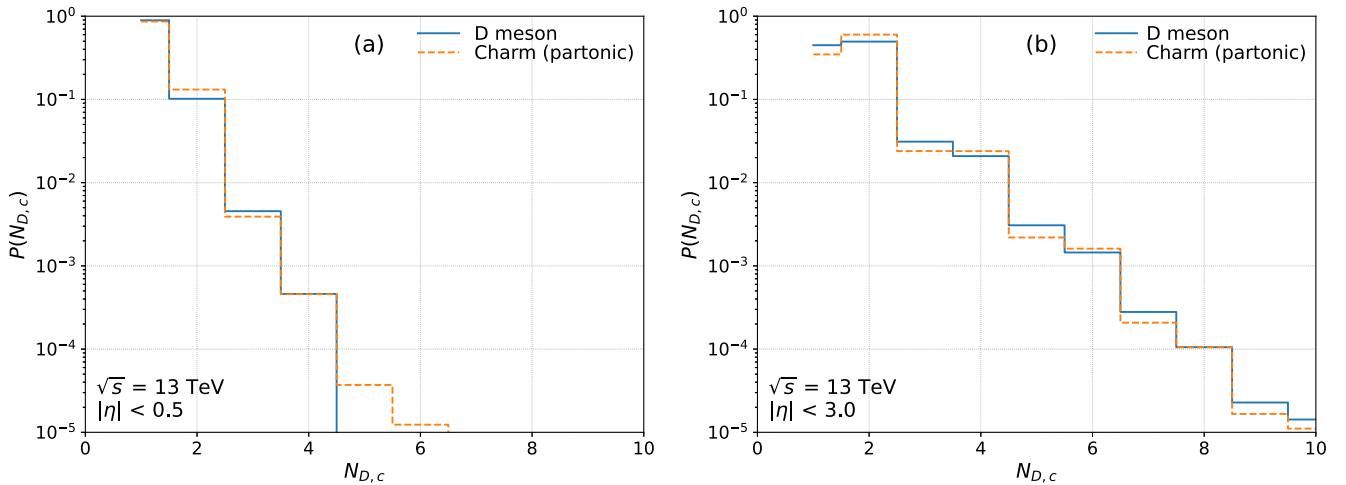


FIG. 4. Comparison between charm quark (parton level) and D meson (hadronic level) multiplicity distributions in pp collisions at 13 TeV for two pseudorapidity ranges (a) $|\eta| < 0.5$ and (b) $|\eta| < 3.0$.

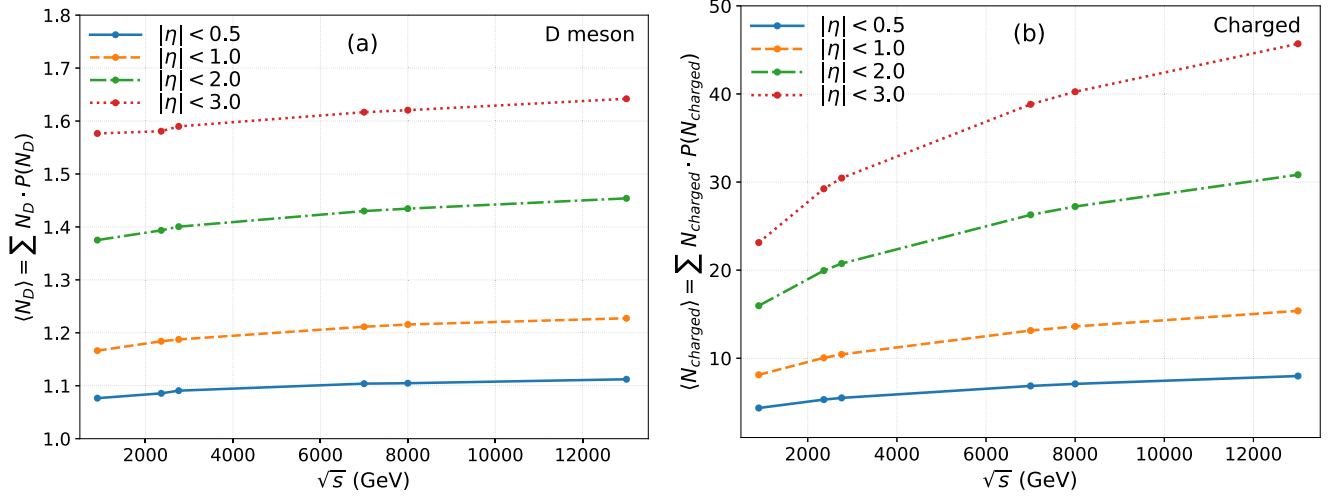


FIG. 5. (a) Average D meson multiplicity as a function of the center-of-mass energy. (b) Average charged particle multiplicity as a function of the center-of-mass energy.

intervals. In contrast, the multiplicity of charged particles shown in Fig. 5(b), grows faster with the energy. We note that the charm production cross section (see Fig. 1) grows faster than the total inelastic cross section. This means that, in PYTHIA, increasing the energy it rapidly becomes easier to produce *one* $c\bar{c}$ pair but the probability of producing two pairs (and also three and so on) does not grow so fast.

In Fig. 6, we show the effect of multiple parton interactions (MPI). As expected, switching MPI on leads to larger multiplicities. However, this effect is relatively small for $|\eta| < 0.5$ and is large for $|\eta| < 3$. This means that small and large pseudorapidity windows have a somewhat different physics. In Fig. 7, we show the effect of color reconnection (CR). We can see that this effect is very small for both cases $|\eta| < 0.5$ and $|\eta| < 3$.

IV. KNO SCALING IN CHARM MULTIPLICITY DISTRIBUTIONS

The Koba-Nielsen-Olesen (KNO) scaling [25], originally derived from the Feynman scaling, is a fundamental feature of multiplicity distributions, which suggests that at sufficiently high (asymptotic) energies the multiplicity exhibits universal scaling behavior. Thus, in a given collision, the probability $P(n)$ of producing n particles can be written as

$$P_n(s) = \frac{1}{\langle n(s) \rangle} \Psi\left(\frac{n}{\langle n(s) \rangle}\right), \quad (1)$$

where $\langle n(s) \rangle$ is the average particle multiplicity at a given center-of-mass value $\sqrt{s}$. From this, we expect the scaled distributions to become energy independent; i.e., the

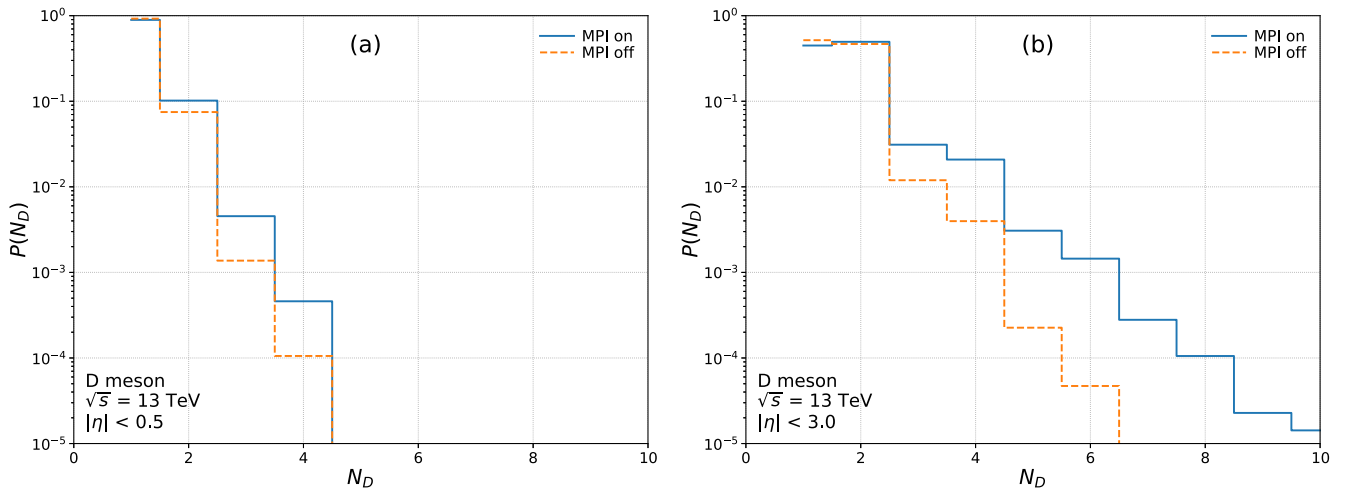


FIG. 6. Effect of including multiple parton interactions (MPI) in pp collisions at $\sqrt{s} = 13$ TeV. (a) $|\eta| < 0.5$. (b) $|\eta| < 3$.

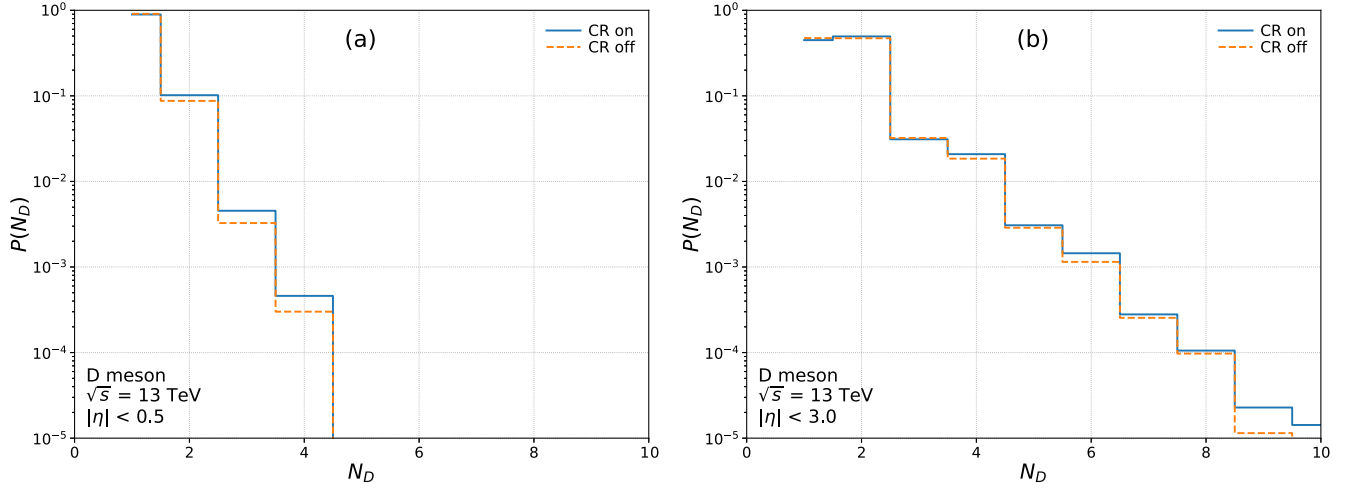


FIG. 7. Effect of including color reconnection (CR) in pp collisions at $\sqrt{s} = 13$ TeV. (a) $|\eta| < 0.5$. (b) $|\eta| < 3.0$.

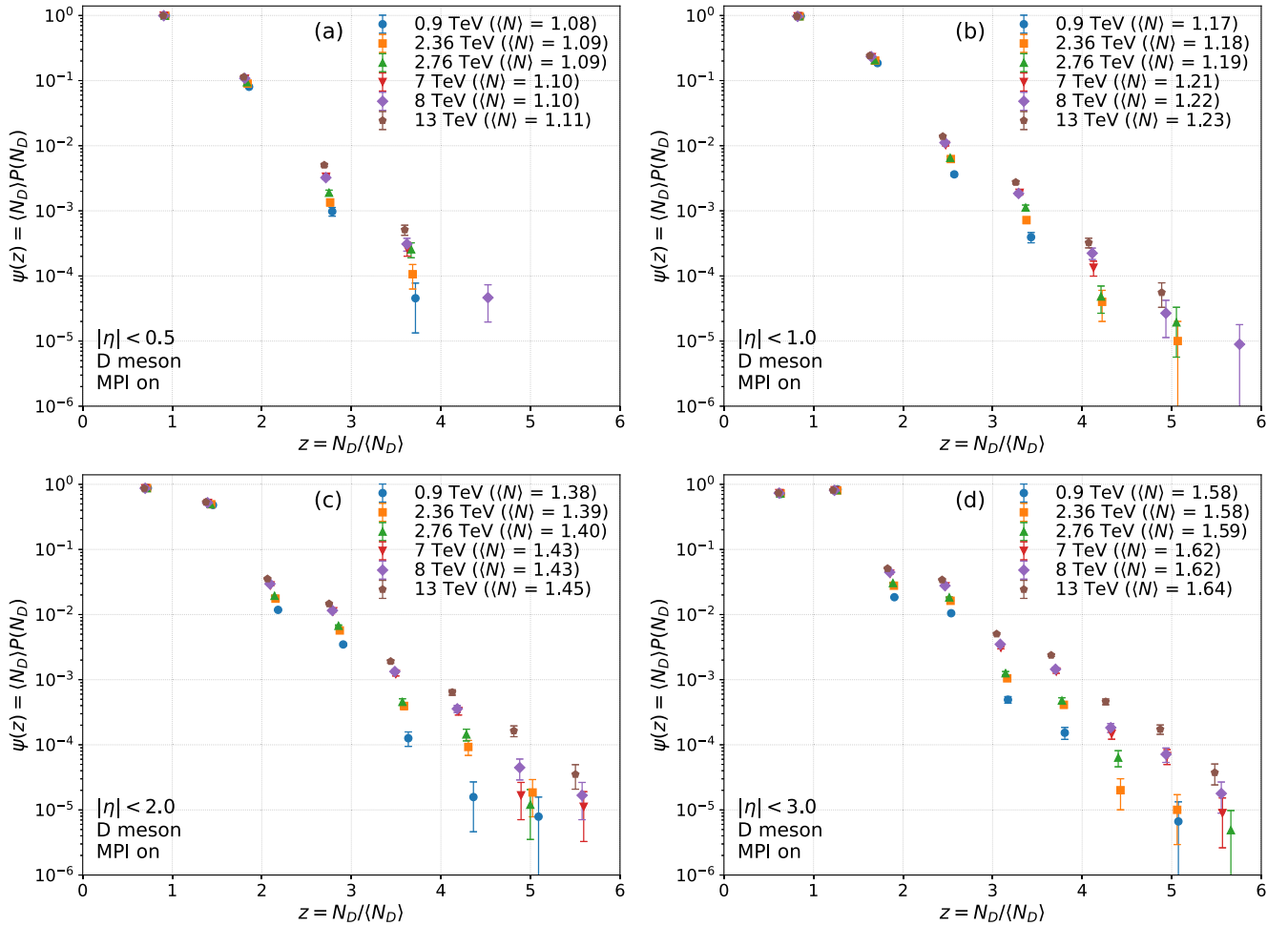


FIG. 8. D meson multiplicity distribution in the KNO form for pp collisions for different center-of-mass energies. (a) $|\eta| < 0.5$. (b) $|\eta| < 1.0$. (c) $|\eta| < 2.0$. (d) $|\eta| < 3.0$. Simulations performed with MPI on.

multiplicity distribution at different energies collapses into a universal curve.

There are theoretical and phenomenological studies available in the literature that provide important insights into the behavior of the KNO scaling in hadronic collisions. For example, in Refs. [40,41], the authors try to understand this phenomenon in terms of quark-gluon dynamics. They show that the KNO scaling appears when the theory describing the color charge fluctuations is approximately Gaussian, when the relevant coupling constant is running and when nonlinear saturation effects are present. Another example can be found in Ref. [42], where the authors systematically tested the KNO scaling in pp collisions using PYTHIA simulations at different center-of-mass energies and pseudorapidity ranges. The authors reported that the KNO scaling is valid approximately for $|\eta| < 0.5$, but significant violations appear as we consider larger pseudorapidity values, especially for large N , implying increasing fluctuations and the breakdown of universality in the particle production mechanism. More recently,

in Refs. [15,16], considering an explicit separation between soft and semihard processes in the k_T factorization approach, the authors observed that in pp collisions and within the central pseudorapidity region, the KNO scaling is valid. Studies on the multiplicity of charged particles measured in p -Pb can be found in Ref. [43], where the authors also address the existence of KNO scaling. They conclude that none of the considered models is able to satisfactorily describe the high multiplicity region of the data. However, a different conclusion was reached in [44].

In Figs. 8 and 9, we present the scaled D -meson multiplicity distributions for pp collisions for different pseudorapidity ranges and calculated with MPI on and off, respectively. The propagation of statistical error was calculated using $\sigma_{P(n>0)} = \sqrt{N(n)}/N_{ev}$, where $N(n)$ is the number of events with multiplicity n and N_{ev} is the total number of valid events. We can see that, in all panels, the curves approximately overlap at small multiplicities but quickly begin to diverge. Furthermore, the tails increase with increasing energy. Strictly speaking, KNO scaling is

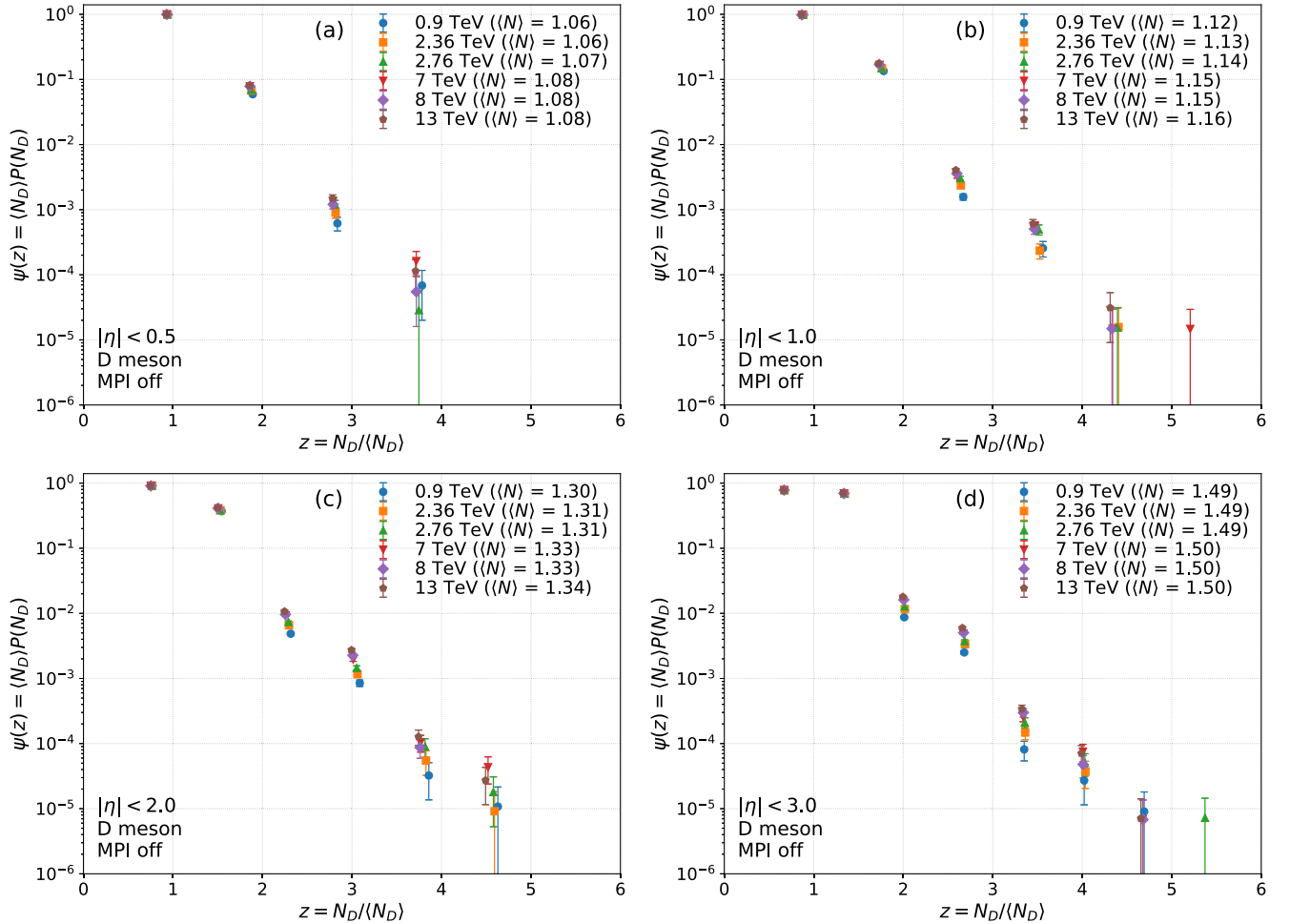


FIG. 9. D meson multiplicity distribution in the KNO form for pp collisions for different center-of-mass energies. (a) $|\eta| < 0.5$. (b) $|\eta| < 1$. (c) $|\eta| < 2$. (d) $|\eta| < 3$. Simulations performed with MPI off.

violated. However, we might argue that there is an approximate scaling in all pseudorapidity ranges when MPI is off. On the other hand, when MPI is on KNO scaling holds for narrower pseudorapidity windows and is violated for wider windows. Indeed, the comparison between these figures shows that Figs. 8(a) and 9(a) are quite similar whereas Figs. 8(d) and 9(d) are strikingly different.

V. PARAMETRIZATION WITH POISSON AND NBD

The Poisson distribution is a discrete probability distribution and works as a tool capable of modeling the probability of a number of events occurring, provided that these events occur at a constant average rate (λ) (and independently, of the time since the last event). Therefore, here the events are independent; i.e., the occurrence of one event does not influence or affect the probability of occurrence of the next event. The Poisson distribution is given by

$$P(N = n, \lambda) = \frac{\lambda^n e^{-\lambda}}{n!}, \quad (2)$$

where $n = 0, 1, 2, 3, \dots$ and λ is the average event rate. Since we cut $n = 0$ in the multiplicity results, for consistency, we also use the truncated form of the Poisson distribution,

$$P(N = n, \lambda | N \geq 1, \lambda) = \frac{\lambda^n e^{-\lambda}}{n!(1 - e^{-\lambda})}. \quad (3)$$

Another discrete probability distribution is the negative binomial distribution (NBD), which is used to describe the probability of observing a certain number of “successes” before a fixed number of “failures.” In the context of particle physics, it is widely used to model the multiplicity distributions of charged particles produced in high-energy collisions. NBD is known to describe multiplicity distributions up to the energies achievable at the LHC. The fact

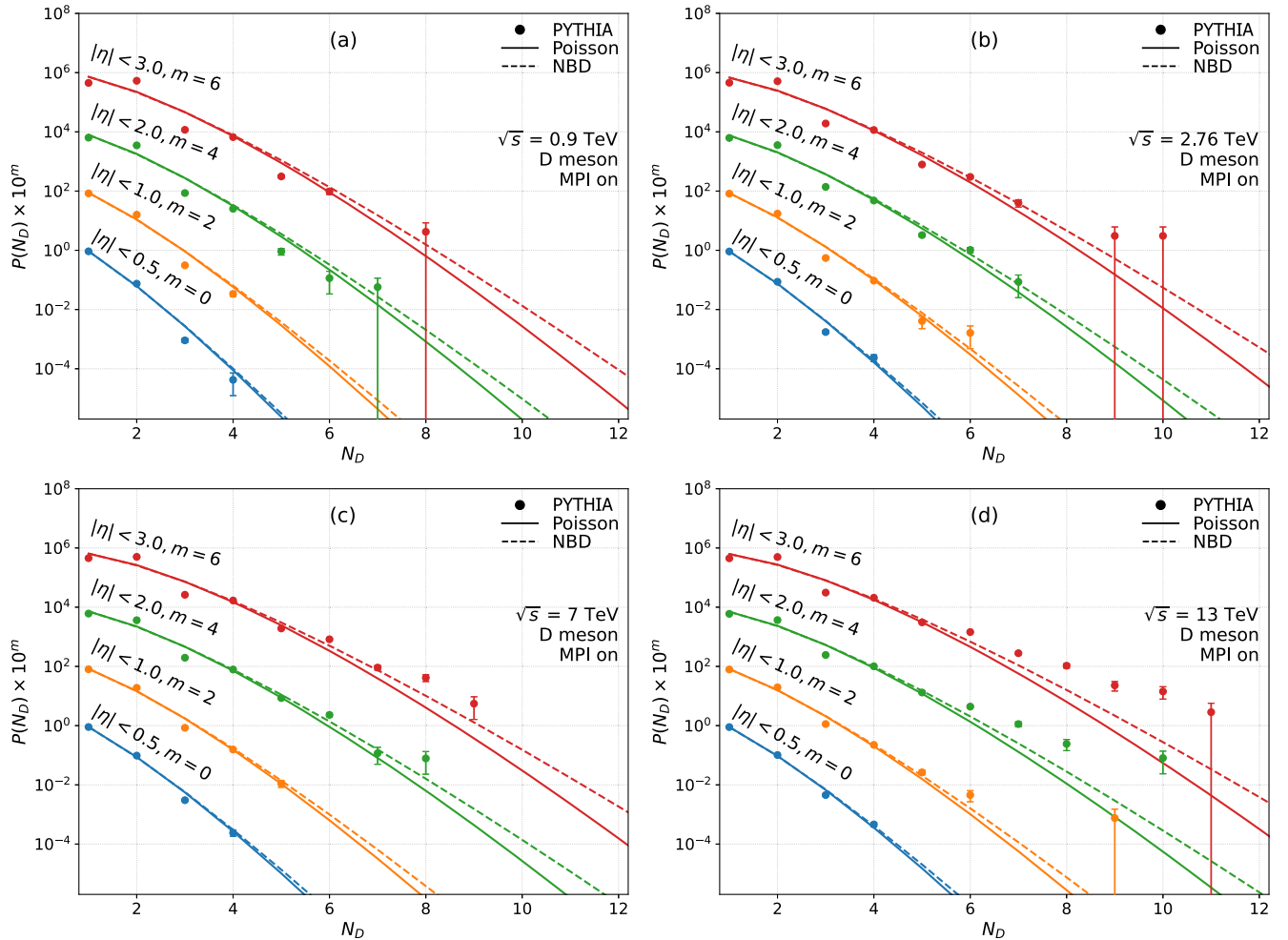


FIG. 10. Multiplicity distributions of D meson fitted to Poisson and NBD distributions. We show results for (a) $\sqrt{s} = 0.9$ TeV, (b) $\sqrt{s} = 2.76$ TeV, (c) $\sqrt{s} = 7$ TeV, and (d) $\sqrt{s} = 13$ TeV. Simulations performed with MPI on.

that the NBD is successful in describing data is a strong indication that particle production is not an independent process, pointing to the presence of correlations between the final particles. The NBD distribution can be expressed as

$$P(N = n; \langle n \rangle, k) = \frac{\Gamma(k+n)}{\Gamma(k)\Gamma(n+1)} \left(\frac{\langle n \rangle}{k + \langle n \rangle} \right)^n \left(\frac{k}{k + \langle n \rangle} \right)^k, \quad (4)$$

where $n = 0, 1, 2, 3, \dots$, $\langle n \rangle$ is the average of multiplicity and k is a grouping parameter. Since we cut $n = 0$ in the multiplicity results, for consistency, we also use the truncated form of the NBD distribution,

$$P(N = n | N \geq 1; \langle n \rangle, k) = \frac{\frac{\Gamma(k+n)}{\Gamma(k)\Gamma(n+1)} \left(\frac{\langle n \rangle}{k + \langle n \rangle} \right)^n \left(\frac{k}{k + \langle n \rangle} \right)^k}{1 - \left(\frac{k}{k + \langle n \rangle} \right)^k}. \quad (5)$$

The Poisson distribution is a particular case of NBD, when the parameter k tends to infinity. Many experimental and theoretical studies show that in many cases, for high energies, it is necessary to consider the combination of two NBDs [45], where each NBD corresponds to a different class of events: “soft” and “semihard” processes. This classification is based on different types of events and not on different particle production mechanisms within a single event. As a result, no interference term appears between the two components, and the multiplicity distribution can be written in the form,

$$P(n) = \lambda [\alpha_{\text{soft}} P_{\text{NBD}}(n, \langle n \rangle, k_1) + (1 - \alpha_{\text{soft}}) P_{\text{NBD}}(n, \langle m \rangle, k_2)]. \quad (6)$$

However, unlike the case of charged particle production, the charm quark is produced in a small quantity, resulting in a narrow multiplicity distribution, as seen in the previous figures. Therefore, a double NBD is not expected to adequately describe the charm multiplicity distribution.

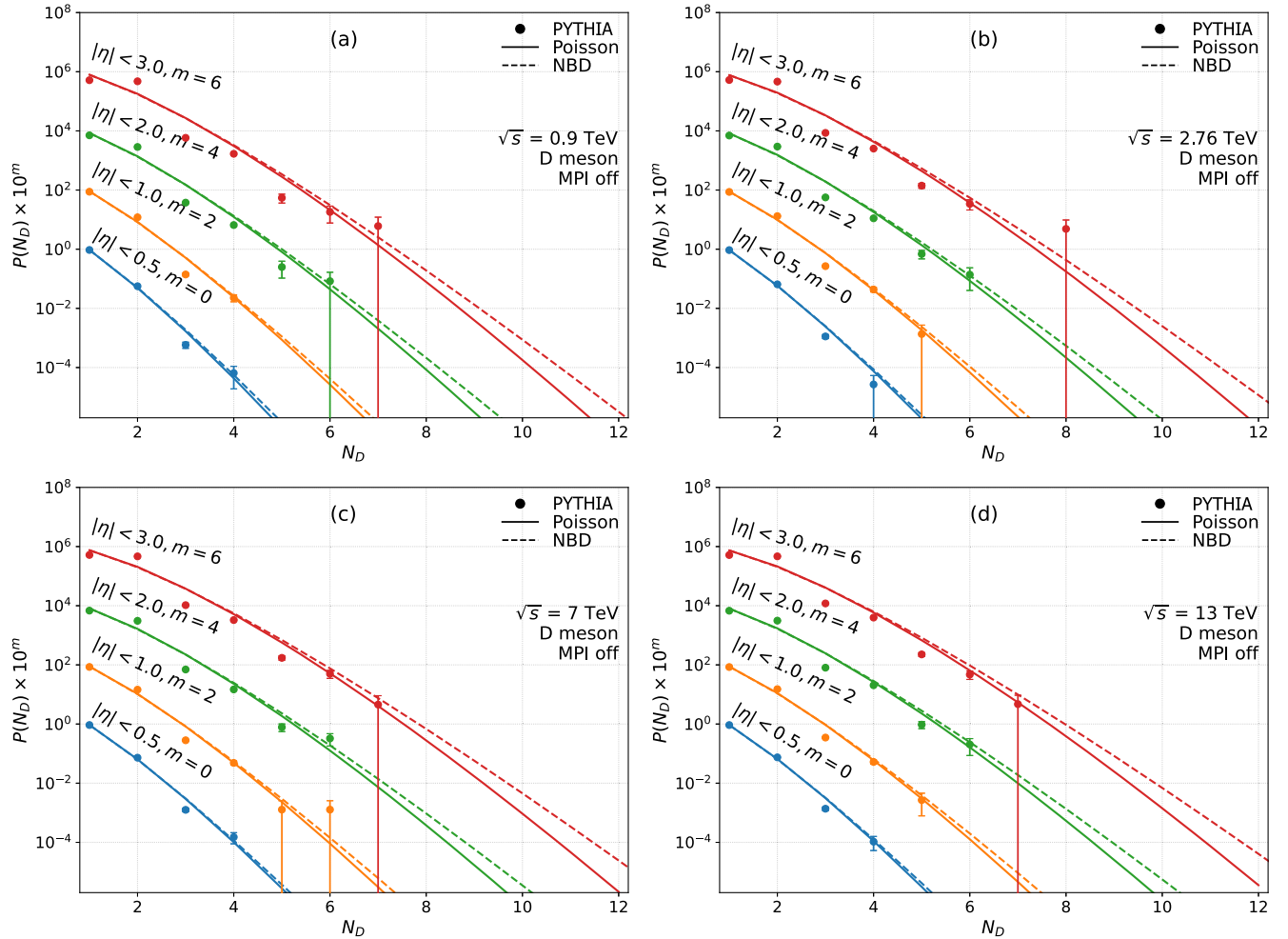


FIG. 11. Multiplicity distributions of D meson fitted to Poisson and NBD distributions. We show results for (a) $\sqrt{s} = 0.9$ TeV, (b) $\sqrt{s} = 2.76$ TeV, (c) $\sqrt{s} = 7$ TeV, and (d) $\sqrt{s} = 13$ TeV. Simulations performed with MPI off.

The narrow shape of this distribution suggests a simple NBD distribution or even a Poisson form. In fact, when we try to fit the PYTHIA points with (6), we find that $\alpha_{\text{soft}} = 0$.

In Fig. 10, the charm meson multiplicity distributions, simulated with PYTHIA (MPI on) are compared with Poisson and NBD fits for different pseudorapidity ranges ($|\eta| < 0.5, 1.0, 2.0, 3.0$). Each panel refers to a different center-of-mass energy ($\sqrt{s} = 0.9, 2.76, 7.0, 13.0$ TeV). The propagation of statistical error was calculated using $\sigma_{P(n>0)} = \sqrt{N(n)}/N_{ev}$. We multiply all points by the factor 10^m , where $m = 0, 2, 4, 6$, to make it easier to visualize. In Fig. 11, we show the charm meson multiplicity distributions calculated with same settings used in Fig. 10 but now with MPI off. We can see a similar behavior of the results with MPI on (Fig. 10) and with MPI off, with a small difference in the tail of the higher pseudorapidity windows.

We can see that, in both figures and in all panels, the Poisson and NBD fits are close to each other. As expected, the NBDs are wider and give a better description of the simulation points. This seems to suggest that, in spite of all the distorting effects mentioned in Sec. II, the charm multiplicity distributions generated by PYTHIA remain, to a large extent, close to Poisson distributions. The exceptions are the curves for larger pseudorapidity windows ($|\eta| < 2$ and $|\eta| < 3$) at the largest energy $\sqrt{s} = 13$ TeV and with MPI on, shown in Fig. 10(d). This is another manifestation of the effect seen in Fig. 6.

VI. CONCLUSION

In this work, we have used the PYTHIA Monte Carlo event generator to study open charm production at the LHC. We focused on the multiplicity distribution (MD) of charm quarks and charm mesons. Our main conclusions are

- (i) The MD of charm is much narrower than the MD of charged particles and is close to a Poisson distribution. This is not surprising since multiple charm production in PYTHIA comes from independent multiple parton-parton scattering.
- (ii) The charm MD is not very different from the charm meson MD, showing that hadronization does not distort the charm quark MD. This finding gives support to the “quark-hadron duality” hypothesis.
- (iii) Going from smaller to larger rapidity windows the MD becomes broader allowing for larger average multiplicities. However, for all the windows, $\langle n_D \rangle$ grows with $\sqrt{s}$ in the same way.

- (iv) Multiple parton interactions are not relevant at narrow pseudorapidity intervals but play a significant role for large pseudorapidity intervals. Color reconnection effects are irrelevant.
- (v) Strictly speaking, we never observe KNO scaling. However, it is possible to argue that we observe some scaling for $|\eta| < 0.5$ and scaling violation for $|\eta| > 1.0$. Moreover, we have shown that KNO scaling holds for MPI off and is violated (in the larger η windows) for MPI on.
- (vi) An attempt to fit the points with the double negative binomial (DNBD) leads to the conclusion that the fraction of semihard events is very large, and the fraction of soft events is negligible. This brings us back to the single NBD fit which is reasonable, just as the Poisson fit.

As mentioned in the introduction, the improvements achieved during the Run-3 of the LHC allow detailed studies of charm yields. Nevertheless, a direct measurement of the full event-by-event charm multiplicity distribution remains challenging in Run-3 due to reconstruction efficiencies and large corrections. In this context, the results presented in this work provide a necessary baseline, establishing expectations for the shape, width, and scaling properties of charm multiplicity distributions. Looking ahead, the proposed ALICE 3 [22] at the HL-LHC is expected to enable a qualitative step forward, making direct measurements of charm multiplicity distributions at the hadronic level feasible. Such measurements will allow a direct confrontation between experimental data and the baseline predictions discussed here, including tests of Poisson-like behavior, negative binomial parametrizations, and KNO scaling in charm production.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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